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Geochemistry Database Audit: historical modifications and conditioning applied to First Series geochemical atlas data

Information Management Programme

Internal Report IR/06/087

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Geochemistry Database Audit: historical modifications and conditioning applied to First Series geochemical atlas data

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The author gratefully acknowledges the use of A. Mackenzie's "Gridder" software that was used to produce geochemical images utilised as part of the data analysis required for the production of this report.

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Summary

This report describes work undertaken as part of the BGS Information Management Programme, with the aim of improving the quality, metadata attribution and utility of historical regional geochemical data stored in the Geochemistry Database. The particular focus of this report is the status of the earliest geochemical data generated by the ongoing Geochemical Baseline Survey of the Environment (G-BASE) project. Analysis of stream sediment samples collected in northern Scotland between 1969 and 1972 formed the basis of the first four published geochemical atlases covering Shetland, Orkney, Caithness and Sutherland. These four areas form a discrete unit in terms of utilising common sampling and analytical methodologies and are described hereafter as the "First Series" geochemical atlases.

The data held in the Geochemistry Database for these areas has until recently been regarded as of unknown quality, with no known documentation regarding quality issues, intra- or inter-atlas modifications to data. The recent commencement of a systematic database audit, also undertaken as part of the Information Management Programme, has allowed these data to be examined in detail, which, in turn, has led to the production of this report, giving information on historical quality issues and modifications made to data in an attempt to provide a contiguous geochemical baseline for the British land area.

The first part of the report introduces the project while subsequent sections describe the historical approaches taken to error control in G-BASE, and an element by element analysis of the status and quality of data with a record, where possible, of what modifications have been made in the past. The report appendices show historical documents that record modifications made to data that are relevant to the First Series atlases. The provision of the information presented in this report should lead to improved integrity of the database, and in turn increase the confidence of data users and enable informed treatment/manipulation of data to be undertaken during preparation of key products such as national geochemical maps.

1 Introduction

The "First Series" geochemical atlas publications are those based on the first analytical suite utilised by the BGS's ongoing geochemical survey of the UK (Figure 1), and represent the first areas sampled as part of the survey. Atlases published for Shetland (IGS,1978), Orkney (IGS, 1978), Caithness and South Orkney (IGS, 1979), and Sutherland (IGS, 1982) utilised three analytical methods for stream sediments: Optical Emission Spectroscopy (OES) for Ag, B, Be, Ba, Co, Cu, Cr, Fe, Mn, Mo, Ni, Pb, U, V, Zn, Zr; Atomic Absorption Spectroscopy (AAS) for Cu, Pb, Zn and, thirdly, Delayed Neutron Activation (DNA) for U. DNA was also utilised for U analysis of stream waters. With the exception of the atlases themselves, no documentation exists regarding these areas and no original hard copy data has been located. The status of the data held on the Geochemistry Database is thus uncertain with only the atlases as hardcopy references to the pre-database results. Until now, the view has been that this data is "beyond redemption" in terms of understanding modifications that may have been made to it, reasons why such changes may have been made, and what implications these changes may have had for overall data quality and database integrity.

Argyll (8)	Orkney (2)
East Anglia (17)	Shetland (1)
East Grampians (7)	Shetland Follow-up
East Midlands (16)	S Orkney & Caithness (3)
Great Glen (6)	SE England (18)
Hebrides (5)	S Scotland (9)
Humber-Trent (13)	SW England (19)
Lake District (10)	Sutherland (4)
NE England (11)	Wales & W Midlands (soil, sediment) (14)
Northern Ireland (W) (20)	Wales & W Midlands (water) (15)
NW England & N Wales (12)	
	[Atlases listed in blue are to be completed, the Humber-Trent Atlas is awaiting publication. Yellow-shaded areas on map have been sampled]

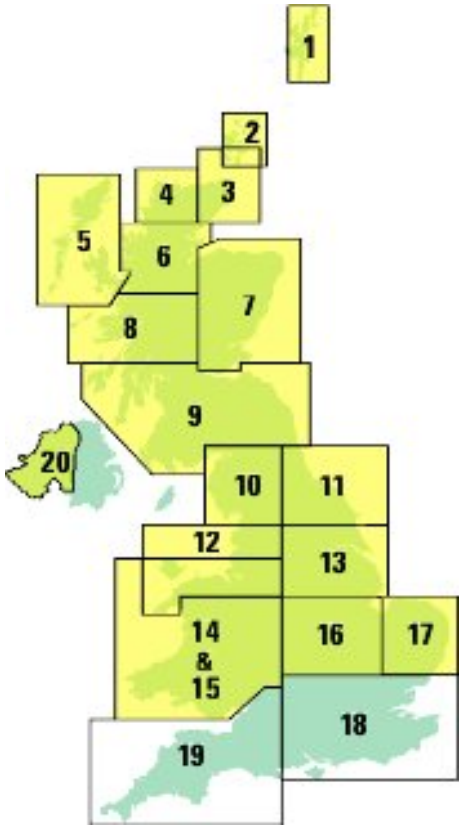


Figure 1: Summary of G-BASE atlas areas

During the ongoing audit of the Geochemistry Database (reports in prep), comparison of Northern Scottish data with published atlas data has confirmed the anecdotal evidence that for some elements, substantial changes to data have taken place. However, in the light of detailed statistical analysis, utilisation of GIS and scrutiny of records of modifications to other atlas areas it is now possible to elucidate most of the changes made. This report aims to: appraise and record, where possible, the nature of the modifications undertaken and the reasons why; note any implications these modifications may have on either the integrity of the Geochemistry Database or on the quality of any national geochemical maps that incorporate the "first series" data; where

appropriate, recommend further modifications recommend to improve, augment or correct previous changes.

1.1 BACKGROUND TO THE "FIRST SERIES" ATLAS AREAS

Orientation work to determine the most appropriate sampling methodologies for a regional geochemical mapping programme was undertaken in Caithness in 1968 (Plant, 1971). Following this, the survey commenced with sampling undertaken in Caithness and Sutherland in 1969, and Orkney and Shetland in 1970. Sampling continued in Sutherland until 1972. The sampling of these areas was not organised on the atlas schedule that we recognise now, but on the basis of alphabetic codes, representing discrete areas sometimes defined by catchments or road accessibility and determined by an individual team leader in a particular sampling season. In some cases groups of samples identified by a common 2-digit alphabetic code crossed atlas boundaries, for example, samples coded FN (05) lie in Caithness, Sutherland, and Great Glen atlas areas. The decision to publish the regional geochemical data as the existing series of atlases defined by the 1:250,000 solid geology sheet boundaries was taken sometime after the sampling of these areas was initiated.

The Shetland, Orkney, Caithness and Sutherland atlas areas are classified as the First Series atlases because they utilised a common stream sediment sampling methodology (Wet sieving at site to 2 mm followed by dry sieving in a field lab to 150 microns) and common analytical methodologies (OES, AAS and DNA). Thus they gave rise to a standardised element suite (described previously) for geochemical map production. Subsequent atlases, from Hebrides and Great Glen onwards, utilised direct-reading emission spectrometry to give a wider range of elements, and there was thus no routine requirement for AAS. Also, sampling methodologies evolved to utilise wet sieving of stream sediment at site to recover the minus 150 micron fraction of stream sediment.

The use of the same analytical methodologies over the four atlas areas gave rise to data with uniform detection limits and similar data quality issues across the first series atlases. The individual atlas publications give details of the analytical conditions and some quality issues.

When the Geochemistry Database was created in the early 1990s (Harris and Coats,1992) data for these areas was loaded from files held in Oracle tables on the Vax/VMS and managed by GBASE project staff.

1.2 AN OUTLINE OF G-BASE ERROR CONTROL AND DATA CONDITIONING

Maintaining data quality has always been a key part of the G-BASE project. There are numerous aspects of sample collection and data generation that require systems to monitor quality and deal with identifiable problems. Historically this work was termed "error control" by the project and some aspects, such as monitoring of accuracy and precision are briefly described in the introductory sections of the geochemical atlases. One aspect of the error control work that has received little attention in published form is what has recently been termed "data conditioning". This refers to modifications which may be made to element data in order to produce comparable data from samples analysed under differing analytical conditions, i.e. to try and correct for systematic analytical error which may prevent the production of a contiguous geochemical baseline for a given element/parameter. Such errors may be attributable to differing calibrations or use of different instruments/methodologies to determine the concentration of an element.

Data conditioning often results in modifications to raw data received from the analysts and it is such modified data that has been stored in the ANALYTE_DETERMINATIONS table in the Geochemistry Database in order that users may create "seamless" geochemical maps of the UK land surface.

Current G-BASE data conditioning procedures dealing with XRF data have recently been described in detail (Lister and Johnson, 2005). Briefly, these procedures typically use results of analysis of a range of G-BASE reference standards (i.e. secondary reference materials) of known concentration to identify and correct for analytical error. The usual method of correction is to create a regression line plot from the results of secondary reference materials included in normal and problem batches, and to apply the appropriate correction to the problem batch.

A similar method of monitoring and correcting for systematic analytical error based on the same reference materials has been in place for many years in G-BASE. However, the standard of documentation and reporting of corrections/changes applied to data under different phases of error control/data conditioning work has been somewhat variable. In recent years, changes applied as a response to variable analytical conditions have been documented clearly e.g. see Appendix 1. However, for data generated in the earlier parts of the project the situation is not so clear, although this partly reflects the difficulty of processing vast amounts of numerical data without the aid of modern computational methods. The error control tasks were undertaken on an atlas-by-atlas basis for Great Glen onwards, and there are numerous un-indexed, unsorted files containing information stored in offices of G-BASE staff. Generally they contain details of corrections made to deal with within-atlas problems and then, variably, to deal with inter-atlas issues. Additionally, further files/information deal specifically with inter-atlas issues and action taken to deal with them.

It is of some importance that users of the G-BASE data held in the Geochemistry Database are able to determine if data has been modified, why it has been modified and how it has been modified, as these criteria may limit the way in which it can be used, presented and manipulated in the future.

1.3 ERROR CONTROL AND CONDITIONING OF FIRST-SERIES ATLAS AREAS

With the exception of the atlases themselves, no files or documentation relating specifically to the error control of any of the "First-Series" geochemical atlas datasets have been located. Information presented in the atlases covers accuracy and presents international reference material data, but also indicates that G-BASE internal control standards were analysed to check for inter-batch analytical variations. There is no suggestion however that inter-batch variations were serious enough to warrant any correction of data. There is no evidence to suggest that any substantive work concerning data modifications that might be required because of inter-atlas analytical errors was undertaken prior to preparation of Great Glen Atlas. It is anticipated that this was not considered a major issue at the time for of a number of reasons: firstly, it was difficult to look at the data for the combined areas because of the limited processing and presentational methods available; secondly because the organisation of sampling and analytical batches was not strictly based on atlas boundaries as described in Section 1.2 and thirdly, because the absence of land boundaries between Shetland, Orkney and Caithness would serve to minimise any evidence of inter-atlas analytical variations or errors.

The only clear record of modifications made to the first-series data relate to work undertaken by Bob Lister in 2003 to allow XRF data for southern Britain to be presented alongside AAS/OES/DR data for northern Britain to produce seamless maps. This resulted in application of a series of conditioning factors to all non-XRF G-BASE stream sediment data in the Geochemistry Database (Appendix 1). Hereafter these factors are referred to as TRL 2003.

The oldest Error Control files that can be located are those relating to Great Glen atlas area, which contain a complex and confusing series of suggested corrections to data. These files are highly relevant because it was during the preparation of Glen, whilst utilising the I^2S image processing facility at the Experimental Cartography Unit (ECU) at NERC, Swindon, that the concept of inter-atlas correction was first dealt with. The files for Glen dealt with the issue of levelling AAS/OES geochemical data with that generated by Direct-Reading Emission

Spectroscopy (DC-OES). Also addressed was the variation introduced by changes in sampling method although that is not considered further here.

A document prepared at the end of April 1982 (Appendix 2) gives the first traceable project strategy for dealing with intra- and inter-atlas analytical errors. In summary it was agreed that each atlas area should be corrected internally for short-term variations, by using control standards, before inter atlas variations were addressed using the I^2S to look at differences in mean/median values over background levels on same lithologies over map boundaries. It was determined that controls would not be used for inter-atlas corrections and that background differences between sheets would only be adjusted "at levels > 0.5 times the lower limit of detection (LLD)" i.e. only data greater than half detection would be modified. This document indicates clearly that the method of establishing an inter-atlas correction is quite different and much less refined than that undertaken now. The procedure established in the document was to adjust for differences in median/means over similar lithologies by simple addition/subtraction of values on problem regions. All areas were to be corrected to the most precise/accurate areas. This would have provided a fairly crude correction that assumed that the error was similar over the whole concentration range. Further evidence provided in other files relating to Great Glen error control indicates that these guidelines were not strictly adhered to and the types of corrections utilised evolved to try and account for different parts of the concentration range, but were still based on an empirical approach utilising the I^2S.

1.4 GREAT GLEN ERROR CONTROL FILES

The Great Glen files comprise three main categories of information/documents that are relevant to the first series atlases.

i) A series of typed element-by-element summaries describing the problems within Great Glen relating to variations in analytical and sampling methodologies and what was undertaken to deal with them. In many instances the wider implications for and necessary modifications to other First series datasets were also covered. These were prepared by Rod Smith (RTS).

ii) A carefully recorded and dated log of corrections made to Great Glen and N. Scottish datasets on the basis of I^2S work was prepared by Alan Stephenson (AGS) and Phil Green (PMG) (Appendix 3).

iii) A random collection of hand-written documents by RTS which deal with issues and recommend corrections to Glen and other N. Scottish datasets (often undated) which may precede or supersede either of the above.

All of the three types of records described above include recommendations for corrections to be carried out to OES and northern Scottish data. In the first instance, often the corrections are recommended for project codes 04/05/06 (those which cross into Great Glen) but scrutiny of the database indicates that these have been extrapolated to the other First Series projects and thus form a good starting point in attempting to unravel the data history. These files will be stored in the National Geoscience Records Centre (NGRC), and indexed in the GBASE-NGRC records index.

2 Discussion of individual elements

In the following section, each element that was analysed in the AAS/OES/DNA suite is discussed individually. Any known documentation that may be relevant is summarised and then data and atlases are compared and analysed in the context of any such relevant documentation.

For each of the four "first series" atlas areas, element statistics and distributions have been examined to try and determine what, if any, modifications were made to the data in the past. In order to do this, the first step involved reversing the only properly documented modification to the data (i.e. the TRL 2003 correction), and then comparing datasets with data, summary statistics and histograms presented in the atlases. Where earlier modifications appear to have been made, the data have been analysed in the light of records of possible changes, and have been compared using GIS on a point by point basis with atlas data. No original hard copy data is available for these areas and the point source presentation format of the data in the atlases proved invaluable as a record of apparently unmodified data.

2.1 BORON

No records have been found that indicate any problems, recommended changes or executed changes. Statistics presented in atlases are identical to those generated from data held in database.

Shetland: Unmodified

Orkney data*:* Unmodified

Caithness: Unmodified

Sutherland: Unmodified

2.2 BARIUM

Trying to establish what modifications may have been made to Barium has proved to be complex and confusing. There was believed, at the time of analysis, to be a problem with underestimation at lower values by OES (pers. comm. N. Breward), and Ba was not presented in Sutherland Atlas, presumably because of concerns with data quality.

Records held in the Great Glen error control files show that numerous "corrections", mis-corrections and re-corrections were made to northern Scottish OES data sets and that there appears to have been confusion about the process of correcting the data. This leads to low confidence in the status and quality of data as currently exists on the database. It should be noted however that when plotted as a gridded geochemical map (Figure 2), there are no evident boundaries between individual areas in northern Scotland, and while most values plot in mid-range categories and there is a marked absence of low values, areas indicated as high concentrations are probably meaningful. Thus the results may still be useful when used at a regional level, but may not stand up to rigorous local level interpretation or statistical analysis.

It is evident that a three-stage correction appears to have been made to northern Scottish OES data sets, with different corrections applied to different sections of the data distributions, the biggest constant having been added to low values to try and correct for underestimation. As a result of the three-stage correction all low values have been lost from the N. Scottish data whether real or not because of the magnitude of the values that were added uniformly to the lower end of data distribution. Histograms of the barium data held in the Geochemistry Database for First Series atlases are very different to those presented in the atlases with all data tending towards a compressed mid-range section (e.g Figure 4). The Shetland data has been analysed in

detail to try and elucidate what was done and it appears that processes applied to the other datasets have been very similar.

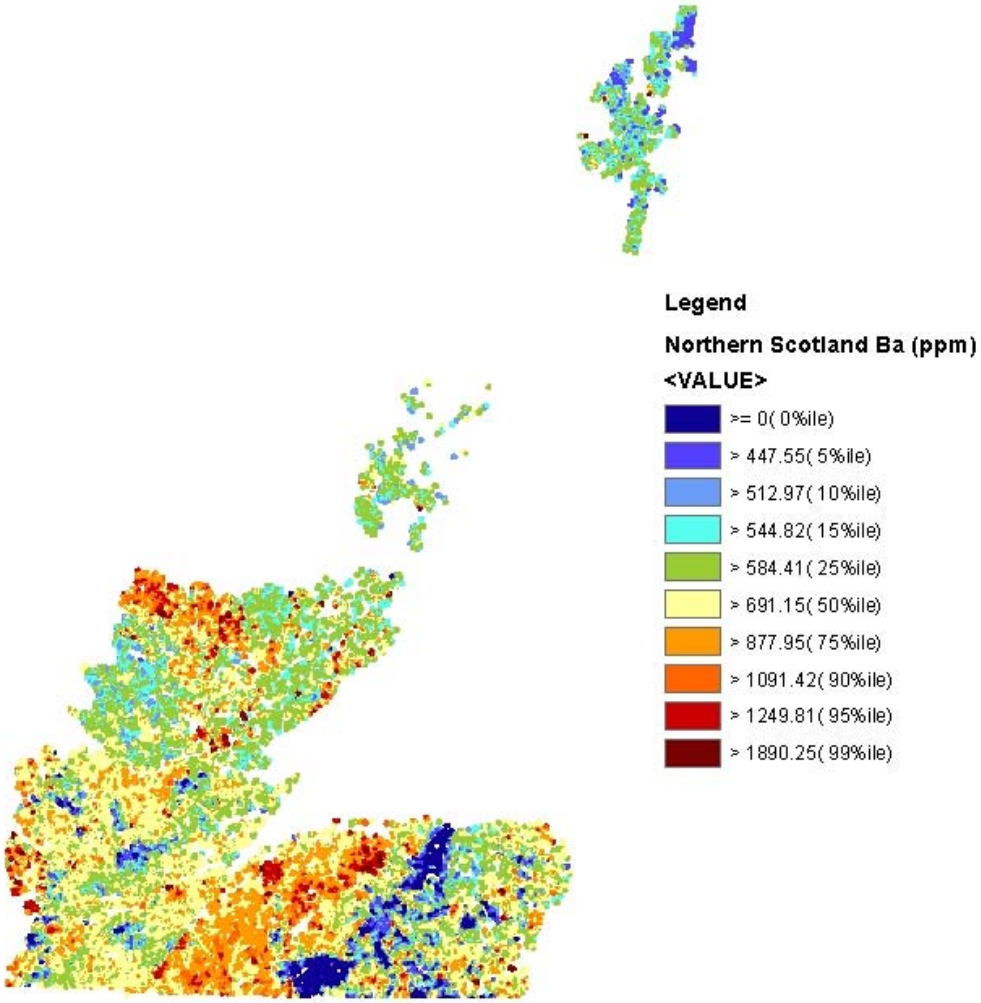


Figure 2: Ba in stream sediments, northern Scotland.

Shetland:

Comparison of individual values presented in the atlas with data from the database (but with TRL 2003 unapplied) indicates that the data is substantially modified and comparison of the atlas histogram (Figure 3) with database values (Pre-TRL 2003)(Figure 4) shows that the overall distribution has been much changed with more data pushed into a compressed mid-range.

Two different records were located in the Great Glen Files for corrections to Shetland data.

a) For Orkney/Shetland

Ba = Ba + 500 for Ba<=300

Ba = Ba +300 for Ba >=301 and Ba<=810

b) To adjust Ba on OES to DR for project codes 01/02/03/04/05/06.

Values <= 300 add 550

Values >=301 and <=560 add 250 (though as the handwriting is unclear this may be 350)

The data held in the database reflect the type of corrections seen in the above records but does not precisely match with either of the recorded sequence of possible corrections.

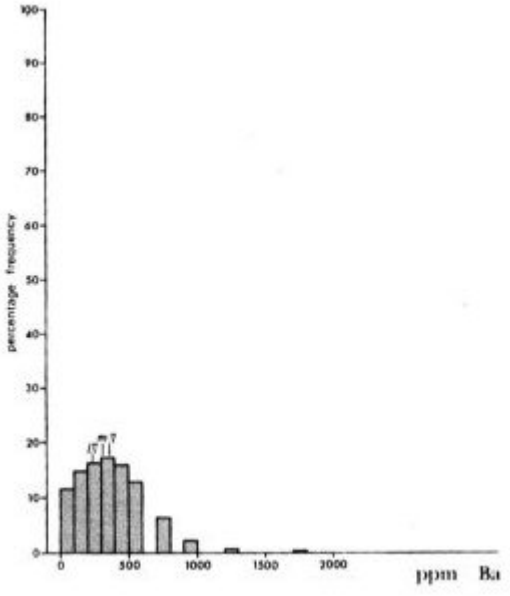


Figure 3: Shetland regional geochemical data: Frequency distribution of Ba as shown in geochemical atlas (scanned copy)

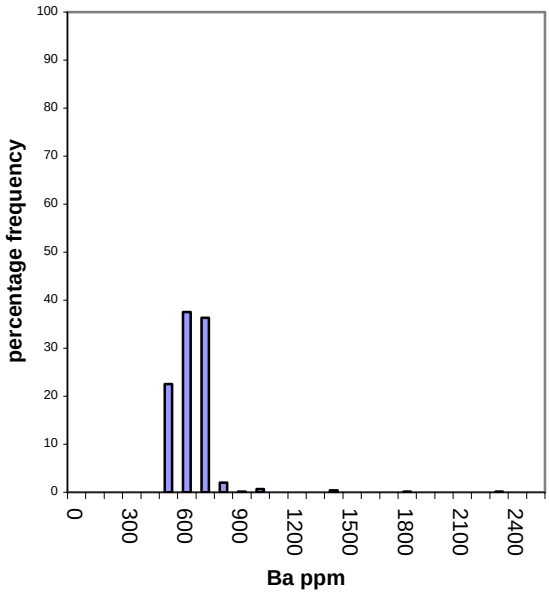


Figure 4: Shetland regional geochemical data: Frequency distribution of Ba data stored in Geochemistry database

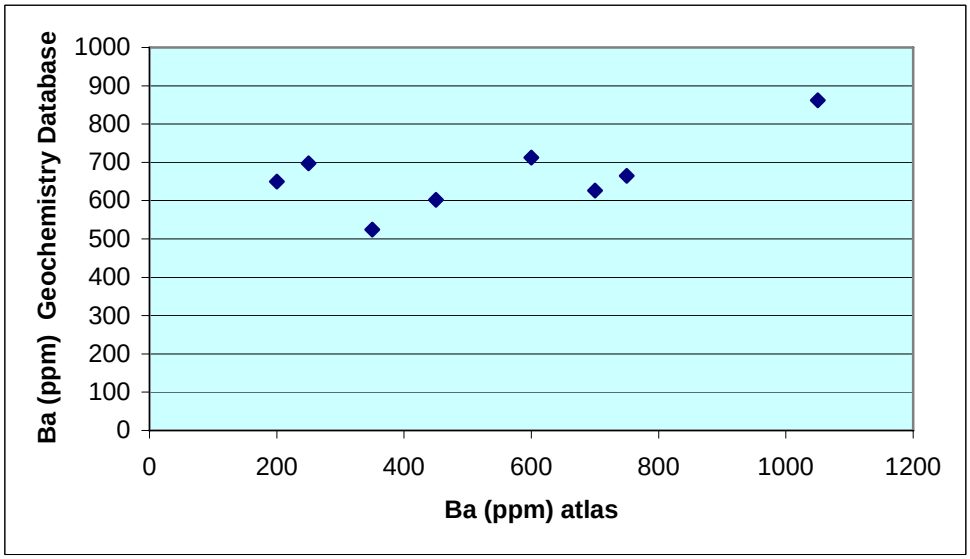


Figure 5: Comparison of Ba data held on Geochemistry Database and that presented in regional geochemical atlas of Shetland

Analysis of data (on which the TRL 2003 corrections have been undone) shows that there are three populations, each of which has different relationships between the atlas and database values. There are three steps on the x-y plot of atlas v database values (Figure 5), consistent with different modifications over three parts of the concentration range. The original OES data was

apparently reported in 50 ppm intervals, which makes comparison simple. 300 ppm appears to be the cut-off for first correction and values <300 (atlas) have had approx 450 ppm added, while the second cut-off appears to be c. 650 ppm. The values between 400 and 650 have been increased by a smaller margin, but not with a constant value, while values of 700 and over have been reduced. The end result is such that an original value of 250 ppm now has a higher value (697) than an original value of 750 ppm (now 665).

In none of the three data steps does the modified data represent simple addition of a constant figure, thereby suggesting that a further slight modification involving a multiplier has also taken place. As yet this is an unknown factor. Overall, the nature of the correction is suspect and the resulting data must be classed as being of dubious quality.

Orkney: Similar corrections appear to have been applied to the Orkney results, with high values reduced and low values increased substantially, suggesting a three-stage correction that used multipliers and constants. The corrections cannot be precisely unravelled and on the basis of the distributions, the data quality appears to have been seriously compromised.

Caithness: Appears to have similar modifications with low values increased and high values reduced. Because of the scale of presentation in atlas it is impossible to compare values in detail and the history of modifications cannot be unravelled. The nature of correction appears a little dubious, although a contiguous boundary between areas exists. The minimum database value of 413 compared with <32 in the atlas shows the magnitude of modifications.

Sutherland: Probably as per Shetland (data are not presented in Atlas so difficult to establish) but a geochemical map of northern Scotland shows contiguous background between Caithness and Sutherland and the absence of values below 507 in pre-TRL dataset suggesting low values have been increased. It is impossible to unravel this corrections but it gives the impression of having compromised the data quality, which must be regarded as dubious.

2.3 BERYLLIUM

Records contained in the Great Glen file show that northern Scotland OES data had 2.5 added pre-Jan 1983 but then subsequently were lowered by 1.2 during I^2S work in early 1983; However this must have been subsequently modified, with no record, and had 0.1 added such that all northern Scotland OES data have had a net addition of 1.4 ppm relative to original data. This is confirmed by comparison of Atlas stats with database stats. So as at March 2006 all northern Scotland Be = original Be +1.4. All corrections were apparently made on basis of I^2S regional comparisons.

Shetland: Be = Be + 1.4

Orkney data: Be = Be + 1.4

Caithness: Be = Be + 1.4

Sutherland: Be = Be + 1.4

2.4 CHROMIUM

There are no written records indicating any major cross-boundary issues for Cr in northern Scotland. The I^2S log (Appendix 3) shows that a correction was recommended for the samples with project code 05 and 06: Cr = Cr+20 for Cr>=10 and Cr<=40; Cr = Cr+10 for Cr>=41. There is no evidence that this has been applied to data in the four atlases considered here.

Shetland: After undoing the conditioning factors applied by TRL 2003 the database and atlas statistics are identical. Only TRL 2003 has been applied.

Orkney: As for Shetland. Only TRL 2003 has been applied.

Sutherland: As for Shetland. Only TRL 2003 has been applied.

Caithness: As for Shetland. Only TRL 2003 has been applied.

2.5 COBALT

The only information regarding cobalt is taken from a handwritten sheet dated 1982 which states (re: Great Glen) "No observable boundary with Sutherland OES or between other map sheets."

Shetland: After undoing the conditioning factors applied by TRL 2003 the database and atlas statistics are identical, therefore it is assumed that only TRL 2003 has been applied.

Orkney: As for Shetland. Only TRL 2003 has been applied.

Sutherland: As or Shetland. Only TRL 2003 has been applied.

Caithness: As or Shetland. Only TRL 2003 has been applied.

2.6 COPPER

No typed notes or handwritten sheet were found for copper. The only record of possible changes to northern Scotland copper data relates to the I^2S log (Appendix 3), which contains two separate episodes of modification to copper for OES datasets collected under project codes 04/05/06:

23/11/82

Cu = Cu + 6 for Cu<=20

Cu = Cu + 15 for Cu>=21

Then Cu = Cu+6 for samples 68395-69336

25/5/83

Cu = Cu-5 for Cu>=36

Cu = Cu – 3 for Cu<=35

Shetland: By undoing these two episodes of copper corrections as well as TRL 2003, and using GIS to compare individual sample values with that presented in the Atlas, it can be confirmed that they have been applied to the data held in the Geochemistry Database. The nature of the Cu correction is fairly crude, breaking the distribution into two sections and treating those two sections differently. The result in this case is to introduce a break into the distribution in the mid concentration range. This is demonstrated in the following series of histograms (Figure 6 to Figure 9) showing the frequency distribution of the Shetland copper data after each stage of correction.

Caithness: As for Shetland.

Sutherland: As for Shetland.

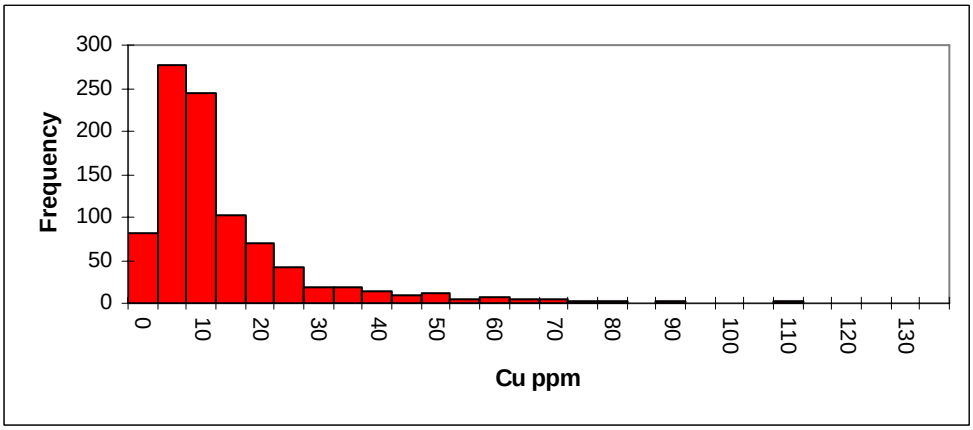


Figure 6: Frequency distribution of Shetland copper data pre-modification

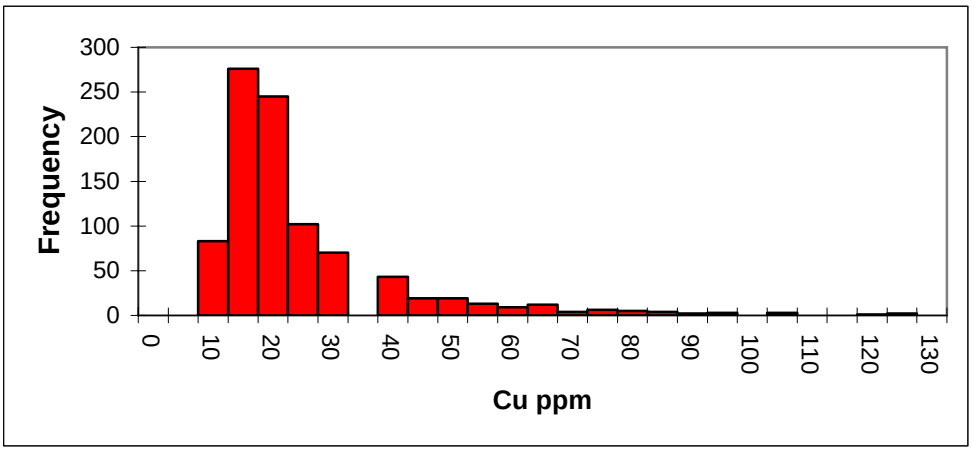


Figure 7: Frequency distribution of Shetland copper data after first modification (1982)

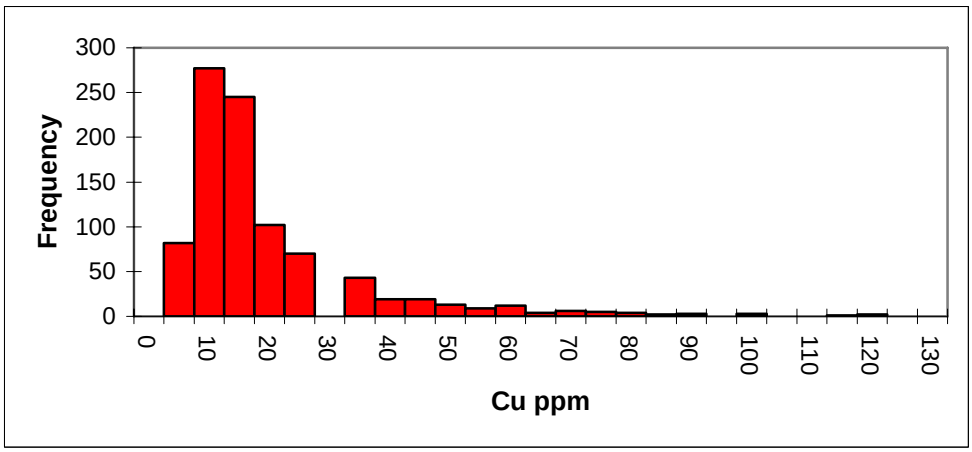


Figure 8: Frequency distribution of Shetland copper data after second modification (1983)

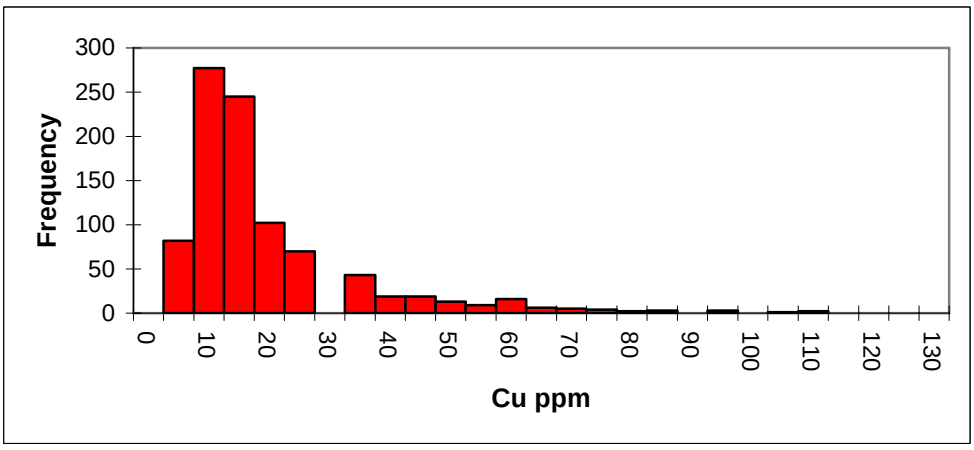


Figure 9: Frequency distribution of Shetland copper data after 3rd modification (TRL 2003)

Orkney: After undoing TRL 2003 it can be seen that lower values appear to be elevated by 6 ppm and higher values by 15 ppm, which would indicate that the corrections of 23/11/82 were made. However, closer inspection of data using GIS to compare individual values with the data presented in atlas showed that in fact the correction was made in three stages, assumed to be by way of an error introduced by transposition of cut-offs and constants. So, what was done in 11/82 was in fact:

1) Cu= Cu + 6 for Cu<15

2) Cu = Cu+ 21 for Cu>=15

3) Cu = Cu +15 for Cu>=21.

It is recommended that this should be unravelled and corrected. As the data was originally reported in 5 ppm intervals this should be possible.

2.7 IRON

No typed sheet or hand-written notes were found. The I^2S correction log lists one correction for Fe:

1/3/83

Fe = Fe + 1.3 project codes 04/05/06/10/12/13/14/15/16/17

Shetland: The data (pre-TRL 2003) are markedly different between atlas and database, indicating that the data held on database has been substantially modified. The modifications do not reflect the above noted modification of 1/3/83. Lower values have certainly been increased but higher values have been reduced giving a different histogram distribution. The precise nature of modification cannot be determined.

Orkney: The data (pre TRL 2003) are very different in the atlas and database with the values in database having a lower median and mean. The correction of 1/3/83 has not been applied and a similar correction to that for Shetland1 has not been applied. It is too complex to work out exact corrections that were applied.

Sutherland: After undoing TRL 2003, it can be seen that data is modified from atlas. The minimum is higher and maximum is lower than the atlas and the median is different. It cannot be determined precisely what modification has been made. Comparison of actual values from the database shows that low values have been increased, mid range are apparently identical and higher values have been lowered.

Caithness: After undoing TRL 2003, it can be seen that data is modified from atlas. It cannot de determined accurately what modification has been made. Comparison of actual values using GIS shows that low values have been increased, mid range are apparently identical and higher values have been lowered but exact corrections are unknown.

Overall the data have been substantially modified in a fairly crude way and the data quality may have been compromised. At a regional scale the data may still have value, but at a point source level, they should be used with caution.

2.8 LEAD

There are no typed or hand-written notes relevant to First Series atlas areas, however, a very useful piece of information held in I^2S correction log:

9/2/83

Pb = Pb+10 for Pb=0 projects 04/05/06/07/20

Pb = Pb + 15 for Pb = 10

Pb = Pb + 20 for Pb>=20 and Pb <=50

Pb = Pb + 15 for Pb>=60

This correction was for AAS data (i.e. all First Series atlases) and indicates that it was thought that the AAS data was abnormally low relative to subsequent data generated by DC-OES. It has been suggested (Neil Breward, pers. comm.) that over-correction by analysts may have occurred leading to unrealistically low baseline values. Importantly, an unusual comment on the update log states that this correction was for production of a smoothed map of northern Scotland and not for publication of individual atlases. This would suggest some confusion at the time over whether data in the database should be modified and is consistent with the current observation that data in the database for northern Scotland looks unrealistically low (Figure 10). The low lead values for northern Scotland should now be reconsidered and a new attempt to correct the data made, preferably on the basis of regression based on percentiles from consistent lithologies either side of an AAS/DR boundary.

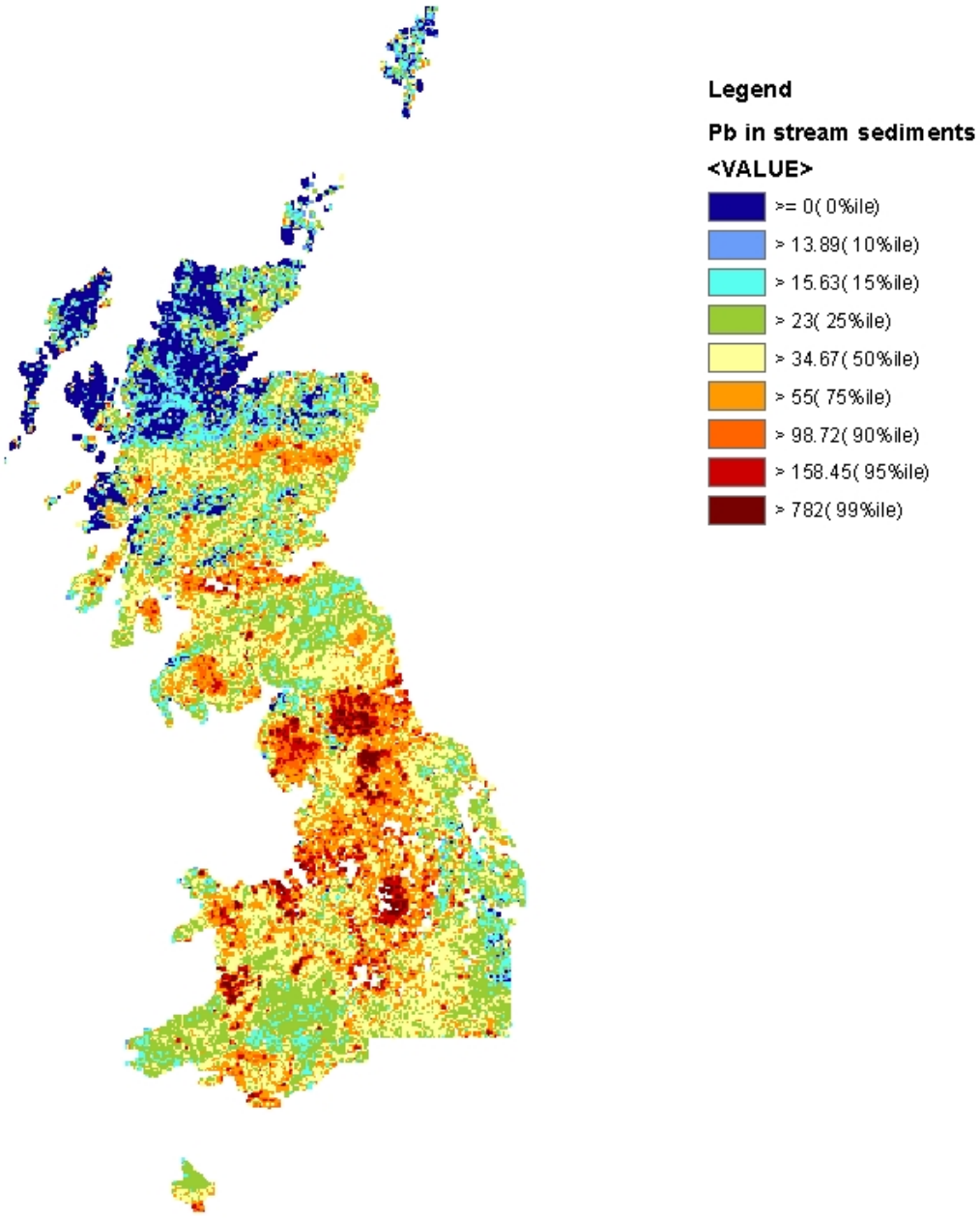


Figure 10: Geochemical map of lead in stream sediments (concentrations in ppm)

Shetland: data is unmodified from atlas, apart from TRL 2003.

Orkney: data is unmodified from atlas, apart from TRL 2003.

Sutherland: data is unmodified from atlas, apart from TRL 2003

Caithness: data is unmodified from atlas, apart from TRL 2003

2.9 MANGANESE

Typed notes indicate no concerns with OES data in N. Scotland; No relevant hand-written notes; no relevant information entered on I^2S log, therefore no reason to believe that anyone saw the need for any changes to be made.

Shetland: data is unmodified from atlas. Needs TRL 2003 to be applied imminently as part of detailed atlas audit

Orkney: data is unmodified from atlas, apart from TRL 2003.

Sutherland: data is unmodified from atlas, apart from TRL 2003.

Caithness: data is unmodified from atlas. Needs TRL 2003 to be applied imminently as part of atlas audit

2.10 MOLYBDENUM

No typed or hand-written notes found; one I^2S log recommendation:

October 1982: Mo=0.1 where Mo is 0, OES data, project codes 04/05/06.

This does not appear to have been applied to any of the atlas areas under consideration.

Shetland: Atlas statistics are identical to database so assume no modifications made.

Orkney: Atlas statistics are identical to database so assume no modifications made.

Caithness: Atlas values are identical to database so assume no modifications made.

Sutherland: Atlas statisticss are identical to database so assume no modifications made.

2.11 NICKEL

Typed notes do not refer specifically to OES areas/data. Hand-written sheet was found in the Great Glen file recommending Ni*1.5 for all OES areas.

Shetland: After undoing TRL 2003, the summary statistics and data values show increase by factor of 1.5 compared with the atlas results.

Orkney: After undoing TRL 2003, the summary statistics show increase by factor of 1.5 compared with the atlas results.

Sutherland: After undoing TRL 2003, the summary statistics show increase by factor of 1.5 compared with the atlas results.

Caithness: After undoing TRL 2003, the data show increase by factor of 1.5 compared with the atlas results.

2.12 SILVER

Shetland: data is unmodified (not presented in atlas).

Orkney: data is unmodified (not presented in atlas).

Sutherland: data is unmodified (not presented in atlas).

Caithness: data is unmodified (not presented in atlas).

2.13 TIN

Shetland: All values <= 24 have been set to 0.1(not presented in atlas).

Orkney: data is unmodified (not presented in atlas).

Sutherland: All values <= 24 have been set to 0.1(not presented in atlas).

Caithness: All values of 0 have been set to 0.1 (not presented in atlas).

Record in I^2S log shows that for projects 4, 5, 6 were set to 0.1 where Sn <= 24. This has also been applied to Shetland but not to Caithness or Orkney. Probably all four areas should have been treated consistently.

2.14 URANIUM

No typed or hand-written notes; not mentioned on I^2S log; no evidence to suggest any indication of problems. Same method of analysis used for whole of Scotland so no boundaries would have been expected.

Shetland: data is unmodified from atlas

Orkney: data is unmodified from atlas

Sutherland: data is unmodified from atlas

Caithness: data is unmodified from atlas

2.15 VANADIUM

No typed notes; there is mention on a hand-written note of a boundary between Great Glen DR and Sutherland OES data where background is lower on Sutherland. No mention of V on I^2S log.

Shetland: data is unmodified other than TRL 2003

Orkney: data is unmodified other than TRL 2003

Sutherland: data is unmodified other than TRL 2003

Caithness: data is unmodified other than TRL 2003

2.16 ZINC

No typed sheet, no hand-written notes. One reference in I^2S log:

23/11/82

Zn = (Zn+8) *1.17 project codes 04/05/06

Shetland: data has been modified as per 23/11/82 and as per TRL 2003. After undoing TRL2003 the data and statistics are exactly consistent with data modification as indicated.

Orkney: data has been modified as per 23/11/82 and as per TRL 2003. After undoing TRL2003 the data and stats are exactly consistent with data modification as indicated.

Sutherland: data has been modified as per 23/11/82 and as per TRL 2003. After undoing TRL2003 the data and stats are exactly consistent with data modification as indicated.

Caithness: data has been modified as per 23/11/82 and as per TRL 2003. After undoing TRL2003 the data and stats are exactly consistent with data modification as indicated.

2.17 ZIRCONIUM

Zirconium seems to have been very problematical and there are many notes in Great Glen file that refer to both Great Glen and other northern Scotland areas. Problems have been made worse by incorrectly applied corrections and attempts to undo them.

Typed notes indicate that efforts were made to correct for differences between DR and OES areas in northern Scotland by adjusting OES data. However, various attempts were made to correct datasets, some of which were made wrongly, or made twice (in error). As some sheets are not dated it is difficult to see what has actually taken place and in which order. The following corrections that are relevant to northern Scotland have been recorded on hand-written sheets:

1) change Ork & Shet where Zr<=1700 Zr = Zr + 400, then where Zr>=750 and <=3000 Zr = Zr*1.65 (5/11/82)

2) for Suth, Ork, Cath, Suth: go back to original data and then: where Zr<=1700; Zr = Zr + 600 then where 950<=Zr<=4000; Zr = Zr * 1.4 *this correction should have been implemented rather than the previous one. (approx December1982)*

3) all OES files: where Zr>=750 Zr = Zr – 150

Shetland: Once TRL 2003 has been undone, the data has had some type of staged correction, broadly similar to above, applied with 400 added to low range values, but impossible to unravel the other parts of correction which do not relate exactly to any of the above records but are similar. Figure 11 and Figure 12 below show that the distribution has been substantially affected; low values have been removed and breaks in the distribution introduced.

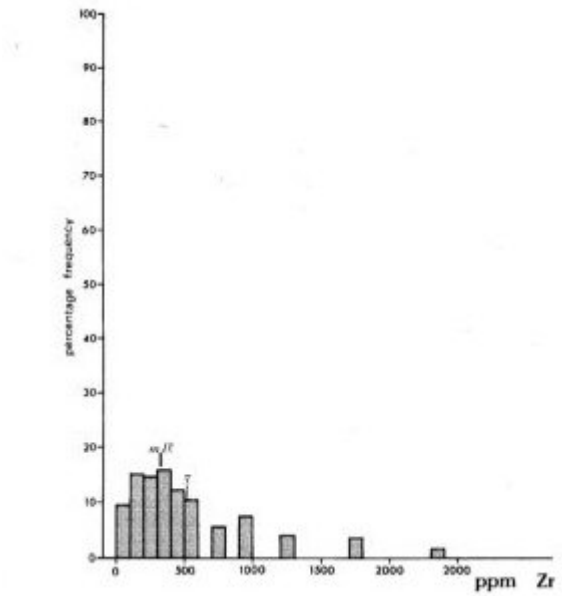


Figure 11: Shetland Zr histogram (scanned from the Shetland atlas)

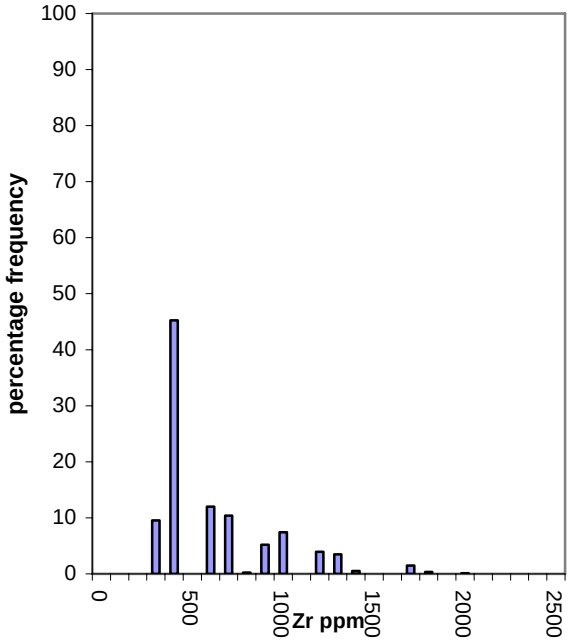


Figure 12: Shetland Zr histogram plotted with results from the Geochemistry database

Orkney: Has not been modified according to the above corrections, or in any similar fashion. The minimum and median are only slightly higher (c. 10 ppm) than the atlas while the mean and maximum values are lower than the atlas. It's not known what has been done but the recommendations of Great Glen file appear to have been totally ignored in the case of Orkney.

Sutherland: After undoing TRL 2003 it can be seen that the database has been modified; low values are higher and high values are lower. Corrections appear to have been applied, as per handwritten note of 1/12/82 prepared by RTS, in three stages: 1) Zr = Zr + 600 where Zr<=1700; 2) Zr = Zr*1.4 where 950<=Zr<= 4000; and 3) Zr= Zr-150 for Zr>=750. It can readily be established that lower values have had 600 ppm added and higher values have had 150 deducted. Attempts to work back through this correction give a similar end result to the original data although not identical but because of the staged nature of the correction it is impossible to confirm that 1.4 has been used as a multiplier. It is assumed here, however, that the modification has been made as per the recorded correction.

Caithness: low values have had 600 added and high values appear to have had 150 deducted. The scale of presentation of the data points in the atlas makes it difficult to compare accurately, and additionally there are no very high values on Caithness. It is assumed that modification is the same as for Sutherland.

The crude and staged nature of these corrections has affected the integrity of the data, which should only be used with caution.

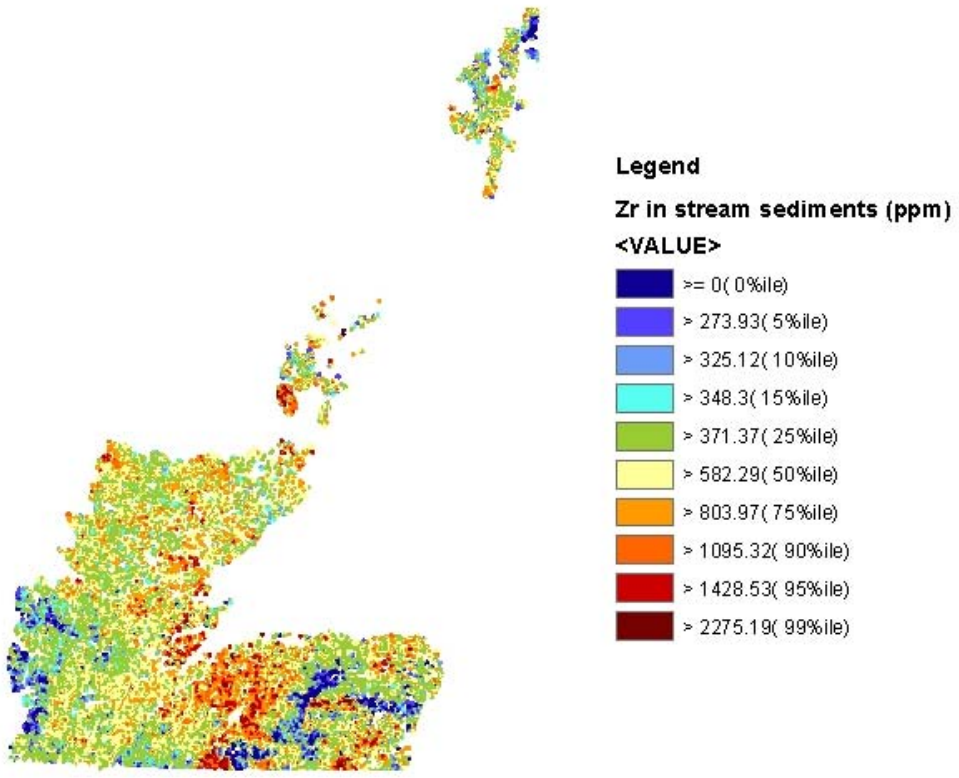


Figure 13: Zircon map for the First Series atlases

3 Conclusions and Recommendations

3.1 CONCLUSIONS

1. No dedicated paper or digital record set exists that describes error control or data conditioning undertaken on the First series atlases. A variety of hand-written/typed notes held in the Great Glen error control files refer to earlier OES datasets covering the First Series atlases. However this is an incomplete and poorly ordered record of changes that *may* have taken place.

2. The First Series atlas data held in the Geochemistry database appear to be unmodified for some elements and reflect the original raw data. (Table 1)

Element
Boron
Molybdenum
Silver
Uranium

Table 1: Unmodified element concentrations

3. For many elements modifications **have** been made to the First Series atlas datasets and in some instances we can deduce what corrections have been made.

It can be inferred that two main phases of modifications were undertaken: during Great Glen atlas error control, in 1982/83 when using the I^2S, inter-atlas problems in N. Scotland were first addressed; secondly in 2003 when a major conditioning exercise was undertaken to level OES/AAS/DR data for N. Scotland with XRF data for S. Britain. The second set of modifications are fully documented (Appendix 2) but have been improperly applied to the Geochemistry Database (see section 3.2). Some elements have only been modified by TRL 2003 (Table 2).

Element	Modification
Chromium	(Cr*0.8853) + 1.3894
Cobalt	(Co*0.8439) + 12.041
Lead	(Pb*0.8658) – 1.6866
Manganese	Mn*0.9059 -165
Vanadium	(V*1.2928) – 11.962 Apply where V >=15

Table 2: Elements modified only by TRL 2003 (see Appendix 2)

Beryllium and tin have only been modified once, at the time of the Great Glen error control work (1982/83). (Table 3)

Element	Modification
Be	Be + 1.4
Sn*	Sn = 0.1 for Sn <=24
Sn**	Sn = 0.1 for Sn = 0

Table 3: Elements modified only in 1982/83; *Shetland and Sutherland, **Caithness

4. Six elements appear to have undergone two episodes of modification. (Table 4).

Element	Modification 1(1982/83)	Modification 2 (TRL 2003)
Barium	uncertain	(Ba * 0.8608) + 30.058
Copper*	Cu + 6 for Cu<=20 Cu + 15 for Cu>=21, then, Cu+6 for samples 68395-69336, then, Cu-5 for Cu>=36 Cu – 3 for Cu<=35	(Cu*0.8905) + 1.9691
Iron	uncertain	(Fe*0.8098) + 3990
Nickel	Ni *1.5	(Ni* 0.6888) + 3.0522
Zinc	(Zn+8) *1.17	(Zn*0.5248) + 20.912
Zirconium	uncertain	(Zr*0.4128) +85.694

Table 4 Elements that have undergone two episodes of modification.

* For Orkney, modification 1 was wrongly applied to Orkney, resulting in a different modification to the other First Series Atlases.

5. It has been established that the modifications applied in 1982/83 were derived using an empirical approach: the I^2S was utilised to look at mean/median values over consistent lithologies crossing atlas boundaries. A strategy was prepared at the time to correct by simple addition/subtraction of mean/median value on problem atlas. This procedure appeared to evolve into a more complex method for some elements where different corrections were made to different parts of the concentration range for certain elements (rather than addition/subtraction of median across entire concentration range). As a result, the corrections applied to the First Series atlas data were crude and in some cases (e.g. Ba, Zr, Cu, and Be) inappropriate, and have resulted in breaks in the distribution of the elements and destroyed the integrity of the data. These data still have some value when plotted at a regional level but are not considered good enough quality to stand rigourous detailed use or meaningful statistical analysis at a local level.

6. For most elements, the four atlas datasets that comprise the First Series have been treated consistently. Therefore it is assumed that no major differences between these atlas areas were observed at the time of the I^2S investigations. Only in the case of Cu, Ba, Sn and Zr is there evidence to suggest that individual atlas datasets were treated differently, and for Cu that was because of a mistake.

7. There is no evidence to suggest that modifications were made to any of the individual datasets to correct for internal analytical errors.

8. Lead should have been modified but was forgotten – see note on I^2S log. This is evident on Scottish map of Pb where low values are seen over the First Series atlases.

3.2 RECOMMENDATIONS

1. The copper correction for Orkney appears to have been wrongly applied and should, if possible, be investigated and modified as part of the Orkney audit.

2. The nature of the copper correction introduces a break in the distribution and should be re-evaluated in the context of the national dataset for Scotland following completion of the atlas-by-atlas audit. The qualifier "*" defined in the Geochemistry Database domain table BGS_MTA_DOM_ANALYSIS_QUALIFIER to indicate data of dubious quality should be applied to the first series copper data because of this.

3. The correction for Be (add 1.4 to all data) is very crude and removes all low values. This should be re-evaluated in the context of the national dataset for Scotland, following completion of the atlas-by-atlas audit.

4. All Ba and Zr data for First Series atlas areas should be qualified with "*" (dubious quality) because of the inappropriate modifications applied to them.

5. The modification to Mn recommended in TRL 2003 has not been applied. Sutherland and Orkney have been updated to include this during the atlas-by-atlas database audit, but Shetland and Caithness are outstanding and should be attended to as part of the audit process.

6. Re-address Pb correction. Suggest using regression of percentiles over contiguous geological units across atlas boundaries.

Appendix 1 : DC-OES vs. XRF normalisation procedures and regression calculations for G-BASE data (TRL 2003 correction).

Data held on the corporate Geochemistry Database comprises a mixture of determinations derived from a number of different analytical techniques. Prior to the introduction of XRF at the outset of the Wales analytical campaign as the routine method for GBASE analysis, DCOES was utilised, preceded by AAS. An extensive QC task had previously been carried out to normalise all non XRF data, in order to compile combined, 'seamless' geochemical images of North England and Scotland. With the exception of a very limited number of elements, this initial QC has proved successful.

At present, no factors have been applied to non XRF data in order to normalise these to XRF. As a result, 'seamless' images of all GBASE data held on the Geochemical Database cannot be generated.

During the analysis of samples for the Wales Geochemical Atlas, approximately 3300 samples previously analysed by DCOES, were reanalysed by XRF. The comparative study of these data provided the information necessary to undertake the task of DCOES data normalisation.

Three different forms of regression calculation were adopted.

1. Based on GBASE internal reference standards analysed throughout both methods of analysis.
2. Calculations using direct comparison of all samples.
3. Calculations using comparative cumulative percentile distributions.

Strictly speaking, the calculation using GBASE standards should be implemented, however the nature of STD S3B is such that, for several elements, unacceptable levels of interference are generated by the XRF analytical method. Bearing this in mind, the most appropriate regression equation , relative to each individual element, was selected.

Colour enhanced images of 'raw' data (as stored on the Geochemistry Database) were generated for each element in order to identify any discordance between the analytical methods.

Using update queries in Access, DCOES data for individual elements were normalised, according to the appropriate regression, and new colour enhanced images generated. Visual inspection of the new images determined the success of the respective normalisation equations applied.

As a result of this exercise, satisfactory normalisation of the following elements may be carried out.

The regression calculations for each element are:

Barium	(DCOES x 0.8608) + 30.058
Calcium	(DCOES x 0.6489) + 1607
Cobalt	(DCOES x 0.8439) + 12.041
Chromium	(DCOES x 0.8853) + 1.3894
Copper	(DCOES x 0.8905) + 1.9691
Iron	(DCOES x 0.8098) + 3990
Gallium	(DCOES x 0.7262) + 1.6013
Potassium	(DCOES x 0.8414) + 4249
Magnesium	(DCOES x 0.848) +767
Manganese	(DCOES x 0.9059) – 165
Nickel	(DCOES x 0.6888) + 3.0522
Lead	(DCOES x 0.8656) – 1.6866
Rubidium	(DCOES x 0.6411) + 18.058
Titanium	(DCOES x 0.9313) – 153
Strontium	(DCOES x 0.7653) – 1.0335
Vanadium	(DCOES x 1.2928) – 11.962 Apply where DCOES V >=15
Yttrium	(DCOES x 0.8783) + 3.2308
Zinc	(DCOES x 0.5248) + 20.912
Zirconium	(DCOES x 0.4128) +85.694

In view of the increasing demand for G-BASE data on a large-scale, it is as a matter of high priority that the data populating the Geochemistry Database are updated without delay.

A comprehensive report detailing the above procedures will be prepared in due course.

Bob Lister

March 6th 2003

Appendix 2 : Scanned copy of procedure for conditioning of Northern Scotland data file, 1982

Stored in GBASE Box 29 in NGRC

R.T.S. - 81a

AGREED PROCEDURE FOR CORRECTION OF NORTHERN SCOTLAND DATA FILE

The following criteria for correction of the N Scotland Geochemical Data Base was agreed after examination of beryllium on the I^2S at ECU (29 April - Dr Plant, P.M. Green, K. Holmes, R. Smith):

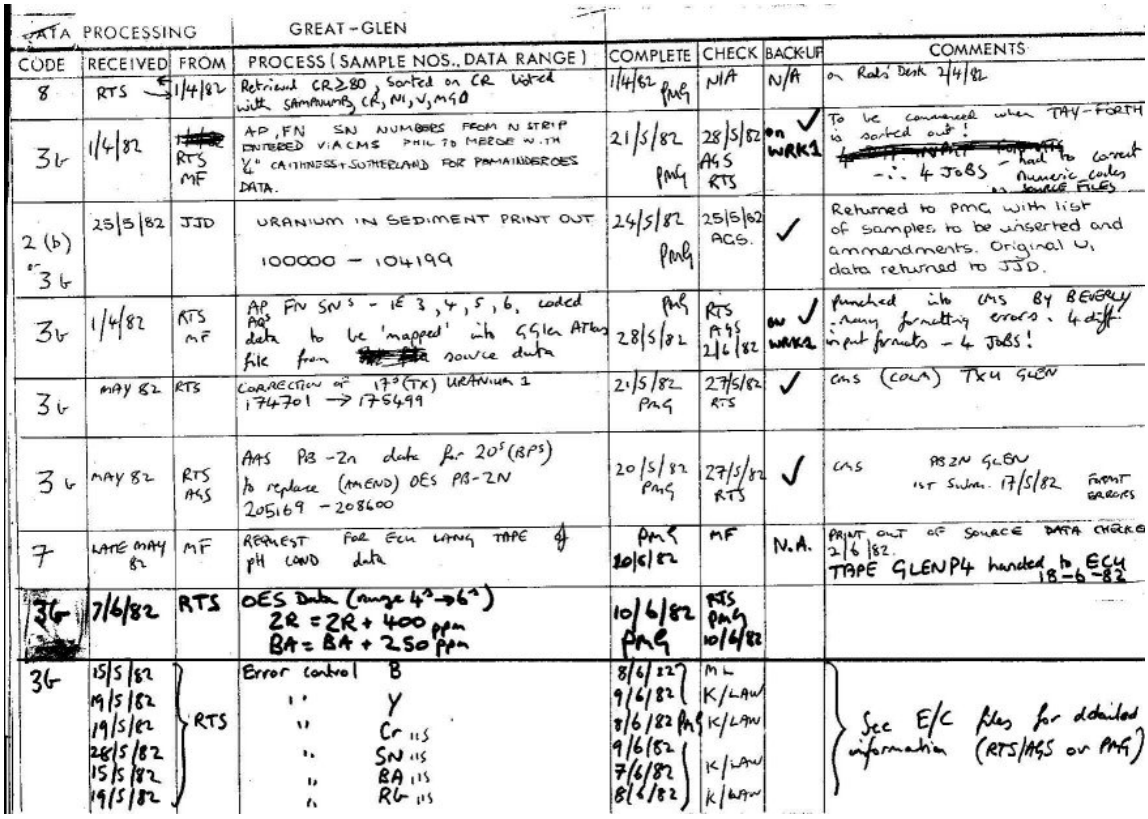
1. Each map area should be corrected for short-term variations in precision before proceeding with the correction for background differences between map sheets.
2. Short-term corrections will be based on changes in the mean values for S1 - S4 over minimum analytical periods of one week. Variations in the weekly mean which exceed the average value for the map sheet by more than 0.5 x limit of detection, will be corrected for. In the absence of S1-S4, the RMHS control will be used for corrections to the Great Glen file.
3. The adjustments will, in most instances, involve addition or subtraction of a constant, except where there is good evidence of bias affecting the entire concentration range. Linear regression may, for example, be used to correct some elements on Great Glen where reanalysis during the Moray-Buchan period provides evidence of constant bias.
4. There will be no attempt to use control data for adjusting levels between map sheets.
5. Unless Keith advises otherwise, backgrounds between map sheets will be adjusted at levels greater than 0.5 x limit of detection.
6. The I^2S system will be used to establish the difference in mean (or median?) value between similar lithologies of naturally low element concentration occurring on two adjacent map areas. Selection of the size and location of the "Blotch" areas will be based on geologically and geochemically uniform areas (principally Moinian). Finally, the data sets will be adjusted by addition or subtraction of the difference between the mean values. All data will be normalised to the mean background level of the most precise and accurate analytical data i.e. either Tay-Forth or Moray-Buchan.

R. T. Smith.

R.T.S.

Appendix 3 : Scanned log of Great Glen and northern Scotland data modifications made on basis of I^2S work

Note the original file is located in NGRC Box GBASE 29



DATA PROCESSING — GREAT-GLEN

CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACK-UP	COMMENTS
8	RTS	1/4/82	Retrieval CR≥80, sorted on CR listed with SAMPNUMB, CR, Ni, V, MgO	1/4/82 PMG	N/A	N/A	on Rob's Desk 2/4/82
3b	1/4/82	RTS MF	AP, FN SN NUMBERS FROM N STRIP ENTERED VIA CMS PHIL TO MERGE WITH V.[illegible] CAITHNESS-SUTHERLAND FOR REMAINDER OF DATA.	21/5/82 PMG	28/5/82 AGS RTS	on ✓ WRK1	To be commenced when TAY-FORTH is sorted out! [illegible] – had to correct numeric codes in SOURCE FILES – ∴ 4 JOBS
2(b) or 3b	25/5/82	JJD	URANIUM IN SEDIMENT PRINT OUT 100000 – 104199	24/5/82 PMG	25/5/82 AGS.	✓	Returned to PMG with list of samples to be inserted and ammendments. Original U, data returned to JJD.
3b	1/4/82	RTS MF	AP FN SN's – IE 3, 4, 5, 6, coded AGS data to be 'mapped' into GGlen ATlas file from [illegible] source data	PMG 28/5/82	RTS AGS 2/6/82	on ✓ WRK2	punched into CMS BY BEVERLY – many formatting errors. 4 diff. input formats – 4 JOBS!
3b	MAY 82	RTS	CORRECTION of 17°(TX) URANIUM 1 174701 → 175499	21/5/82 PMG	27/5/82 RTS	✓	CMS (COLA) TX4 GLEN
3b	MAY 82	RTS AGS	AAS PB-Zn data for 205(BPS) to replace (AMEND) OES PB-ZN 205169 – 208600	20/5/82 PMG	27/5/82 RTS	✓	CMS PBZN GLEN 1ST Subm. 17/5/82 FRONT GRAVES
7	LATE MAY 82	MF	REQUEST FOR ECH LANG TAPE of pH COND data	PMG 10/6/82	MF	N.A.	PRINT OUT OF SOURCE DATA CHECKED 2/6/82. TAPE GLENP4 handed to ECH 18-6-82
3b	7/6/82	RTS	OES Data (range 4³→6³) ZR = ZR + 400 ppm BA = BA + 250 ppm	10/6/82 PMG	RTS PMG 10/6/82		
3b	15/5/82	RTS	Error control B	8/6/82	ML		See E/C files for detailed information (RTS/AGS or PMG)
	19/5/82		" Y	9/6/82	K/LAW		
	19/5/82		" Cr ppm	8/6/82 PMG	K/LAW		
	28/5/82		" SN ppm	9/6/82	K/LAW		
	15/5/82		" BA ppm	7/6/82	K/LAW		
	19/5/82		" RB ppm	8/6/82	K/LAW		

DATA PROCESSING — GREAT-GLEN

CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACK-UP	COMMENTS
3b	4/6/82	RTS	Error control Mn ppm	8/6/82	K/LAW PMG		See error control file RTS, AGS / PMG for detailed information.
	"	"	" " Ti	"			
	"	"	" " Ni ppm	" PMG	K/LAW		
	16/2/82	RTS	" " Sr	March 82	AGS ✓	✓	
	March'82	[illegible] RTS	" " Zr ppm	March'82	AGS ✓	✓	
	21/6/82	RTS	" " K_2O				
3	October'82 AGS	RTS	1) Set Mo values of ≤ 7 to 0·1 ppm for projects 10, 12, 13, 14, 15, 16, 17.	23rd Sept 1982	AGS	✓	All remaining values of 8 and above listed and entered on CMS 13th October '82. (values ≥ 8 which remained on file after substitution of colorometric reanalyses). New values substituted on 14th October '82. Job complete at 19/10/82
			2) Substitute colorimetric reanalyses	1st Oct. 82	AGS	✓	
			3) Set all remaining Mo values of zero to 0·1 ppm for projects 4, 5, 6, 20.				
3	5/4/82	RTS	further amends to ZR – see E/C file for details. OES –400 then: ≥750 ≤3000 × 1·65	9/11/82 PMG	JG	✓	Fluid Correction for ZR? No.
3	16/11/82 AGS	RTS	Further amendments to Zr. AGS 208154 – 208600 × 1·33 Job ran 16/11/82 VQC7Ø150 Amending statement entered on ZR2 GLEN	18/11/82	RTS ✓		See Argyll Data Processing for explanation.
3	17/11/82 AGS	RTS	Amendment to Barium 208154 – 209449 Add 150 ppm 210001 – 210545 Add 150 ppm Amending file BA ARGL Job ran 18/11/82 : VQC7Ø164	18/11/82	AGS ✓		

DATA PROCESSING — GREAT-GLEN

CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACK-UP	COMMENTS
3b	19/11/82 ACS	RTS	Amendment to Chromium 206235 - 206864 ≥50 Subtract 10 ppm 207549 - 208153 ≤49 Subtract 5 ppm Job ran 19/11/82 : VQC70189	19/11/82	ACS ✓		Further amendment : replace all 04 OES values of zero by DR value.
3b	23/11/82 ACS	RTS	Amendment to Copper Projects 04, 05, and 06. For values ≤20 Add 6ppm " ≥21 Add 15ppm Job ran 23/11/82 VQC70256.	29/11/82	ACS ✓		Further amendment : 68345 - 69336 add 6ppm to all values.
3b	23/11/82 ACS	RTS	Amendment to Zinc : Projects 4, 5, 6, 7 and 20 For all samples add 8ppm then multiply by 1.17. Job ran 23/11/82 VQC70257	1/12/82	ACS ✓		Completed.
3b	23/11/82 ACS	RTS	Amendment to Boron 102650 - 3266 ≥10 subtract 5 ppm 208154 - 8600 =6 subtract 4 ppm Job ran 23/11/82 VQC70236.	1/12/82	ACS ✓		
3b	1/12/82 ACS	RTS	Amendment to Beryllium Projects 04, 05, 06 add 2.5 ppm ① All DR Projects (07-17) add 1.5 ppm ②	10/12/82	ACS ✓		This amendment adjusts all OES DR data on Glen to a common DR background (NB 2.5 added to all OES Data). To adjust to a common OES background, subtract 2.5 ppm from all (OES + DR) data in N. Scotland data file.
3b	22/11/82 PMG	RTS	Amendment to Yttrium All samples on Great Glen except 07, 20, 05, 06, 09 Add 50 ppm to Y values ≥250 ppm Add 6 ppm to Y values ≤249 ppm	1/12/82	ACS ✓		
3b	26/11/82 PMG	RTS	Amendment to Rubidium : Projects 04, 05, 06 Rb values ≥220 (×1.0 - 200) Rb " ≤150 (×1.3) then for all samples in project 06 multiply by 0.78.	1/12/82	ACS ✓		

DATA PROCESSING — GREAT-GLEN

CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACK-UP	COMMENTS
3b	29/11/82 ACS	RTS	Amendment to Barium. Projects 04, 05, 06 Subtract 250 ppm from all values then ≤550 add 300 ≥551 and ≤810 Add 50 ppm	ACS 10/12/82	ACS ✓		Amendment was necessary due to detection of data processing error (250 ppm was added twice to the file)
3	1/12/82 PMG	RTS	Amendment to Zr 4 → 6 prefix ≥2501 subt 800 ≤2500 subt 200 Then when resultant values ≥950 ≤4000 × 1.4	PMG 14/12/82	✓ ACS		
3	1/12/82 PMG	RTS					
3b	17/1/83 ACS	RTS	Amendment to Molybdenum Samples in project 20 : Set all values ≤8 to 0.1. (leaving colorimetric re-analyses on file. i.e. values ≤8 are still present on file.) in 20.... samples.	3/2/83	ACS ✓		
3b	PMG	RTS	6° Rb = Rb ×1.3 4° – 7° all 0.0 Rbs = −1.0	PMG 19/1/83	PMG →		further corrections to -1.3 values underway - VQC 70219
3b	PMC 27/1/83 VQC70311	RTS 26/1/83	Amendment to Zinc (based on I²S visit) 1. Projects 04, 05 Samples 40125, 40129, 40199, 54207 Set Zn to -1. ✓ Projects 10, 12, 13, 14, 15, 16, 17 values of 0 set to -1 values of 1 set to 0 2. Projects 10, 12, 13, 14, 15, 16, 17 Adjust AAS to DR by (a) (AAS values + 8) × 1.17, (b) then correct for sampling differences by addition of 10 ppm combining 2 (a) and (b) final correction is : [AAS × 1.17] + 20				Awaiting second correction to amend values of 18.83 to 0.00 - 1 and 21.17 to 20.00. VQC70283 1st March 1983. ACS. 14th MARCH VALUES OF 21.17 HAVE BEEN SET TO 20.00 Ammendment to values of 18.83 in progress.

DATA PROCESSING — GREAT-GLEN

CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACK-UP	COMMENTS
3b	PmC 24/1/83 VQC70249	RTS	Amendment to Strontium Samples coded 07 : Values ≥ 150 multiply by 0·87 Samples coded 04,05,06,10,12,13,14,15,16,17 Values ≥ 150 . Subtract 20	14/2/83	AGS ✓		Further amendment required Projects 4,5,6 all values have had ~~50~~ ppm subtracted values < 130 add 20 ppm. Commenced 28/2/83 VQC70284 ✓
3b	PmC 26/1/83	RTS	Amendment to Titanium All samples All values Add 0·13%	14/2/83	AGS ✓		-1 values have been amended. Re-set to -1. Completed 28/2/83 and checked AGS/RTS.
3b	AGS 25/1/83	RTS	Amendment to ~~Manganese~~ Chromium Project 04 Set all 0 values to −1 " 05,06 Values ≥ 10 and ≤ 40 +20 ≥ 41 +10	14/2/83	AGS ✓		
3b	PmC 24/1/83	RTS	Amendment to Beryllium Subtract 0·3 from all values. Projects 04,05,06 Subtract 0·5 ppm	14/2/83	AGS ✓		Projects 04,05,06 have had compounded amendment i.e. 0·8 has been subtracted.
3b	PmC 9/2/83	RTS	Amendment to Lead. Projects 04,05,06,07,20 Values of 0 Add 10ppm 10 Add 15ppm 20-50 Add 20ppm ≥ 60 Add 15 ppm	9/2/83	AGS PmC. ✓		Amendment for production of N. Scotland Smoothed map and not for publication of individual map area. These cells based on AAS data for Great Glen & map sheets already published. Held on worksite 1.
3b	AGS 1/3/83	RTS	Amendment to MgO ~~P~~ Projects 04,05,06 All samples add 0·3% VQC7~~0~~~~0~~9	14/3/83	✓ AGS		Correction based on I²S visit February 1983.

DATA PROCESSING — GREAT-GLEN

CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACK-UP	COMMENTS
3b	AGS 1/3/83	RTS	Amendment to Titanium Project 20 Subtract 0·13%	14/3/83	AGS ✓	✓	Based on I²S visit Feb '83.
3b	AGS 1/3/83	RTS	Amendment to Copper Projects 10,12,13,14,15,16,17 All values ≤ 10 ppm, subtract 3 ≥ 11 ppm, subtract 5.	14/3/83	✓ AGS	✓	Based on I²S visit Feb '83
3b	AGS 1/3/83	RTS	Amendment to Lanthanum 130035 - 130087 140001 - 140027 165501 - 165620 4~~0~~~~0~~1 - 40362 51764 - 58611 68405 - 69335 when La ≥ 1·0 Add 8 ppm	14/3/83	✓ AGS	✓	Based on I²S visit Feb '83.
3b	7/3/83 AGS	RTS	Amendment to Tin Projects 4,5,6 all values ≤ 24 set to 0·1 re-instate 52337 to 5.00 ppm 52352 to 5.00 ppm	14/3/83	✓ AGS	✓	Values not yet re-instated 14/3/83 AGS.
3b	7/3/83 AGS	RTS	Amendment to Molybdenum Projects 10,12,17. Subtract 2 ppm from values ≤ 4.			✓	
3b	16/5/83 PmG	RTS	Fe_2O_3 SnO_2 06 amended 68064 - 69336.	16/5/83	✓ PmG JO		

DATA PROCESSING			GREAT-GLEN				
CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACKUP	COMMENTS
3b	ACS 1/3/83	RTS	Ammendment to Calcium Projects 04,05,06 (Values ≤ 1.0%) Add 0.8% VQC70010	✓ 14/3/83	ACS ✓		Ammendment based on I²S visit February 1983.
3b	ACS 1/3/83	RTS	Ammendment to Iron Projects 04,05,06,10,12,13,14,15,16,17 All values ; Add 1.3% VQC70011	14/3/83	ACS ✓		Based on I²S visit Feb '83.
3b	ACS 1/3/83	RTS	Ammendment to Nickel. Projects 04,05,06,10,12,13,14,15,16,17 All values : Add 8 ppm VQC70016	14/3/83	ACS ✓		Based on I²S visit Feb'83
3b	ACS 1/3/83	RTS	Ammendment to Beryllium Projects 10 → 17 Subtract 0.25 ppm Projects 04 → 06 Subtract 0.4 ppm Set all – values to 0.1 ppm VQC70017	14/3/83	ACS ✓		Based on I²S visit Feb'83
3b	PMC 1/3/83	RTS	Ammendment to Lead Projects 10 → 17 Values of 0 ; Add 10 ppm Values of 10 ; Add 15 ppm Values ≥ 20 and ≤ 50 ; Add 20 ppm Values ≥ 60 ; Add 15 ppm	~~14/3/83~~	~~ACS~~		Based on I²S visit Feb'83 Ammendment to Workfile 1.
3b	ACS 1/3/83	RTS	Ammendment to Yttrium VQC70023 Projects 4 → 6 ; Add 15 ppm Projects 10 → 17 ; Subtract 6 ppm Sample number 100699 – 396 ppm " " 102666 – 248 ppm	14/3/83	ACS ✓		Based on I²S visit Feb'83
3b	ACS 1/3/83	RTS	Ammendment to Barium All samples ~~add~~ or multiply by 0.787 Then add 75 ppm	14/3/83	ACS ✓		Based on I²S visit Feb'83 First stage commenced 1/3/83
3b	ACS 1/3/83	RTS	Ammendment to Zirconium All samples ≥ 750, subtract 150 ppm VQC70264	14/3/83	ACS ✓		Based on I²S visit Feb'83

DATA PROCESSING			GREAT-GLEN				
CODE	RECEIVED	FROM	PROCESS (SAMPLE NOS., DATA RANGE)	COMPLETE	CHECK	BACKUP	COMMENTS
3b.	6/6/83 ACS	RTS	Ammendment to Lanthanum 68064 - 68404 all values × 0.38 + 8 ppm	6th June 1983	✓ ACS		
3b	25/5/83 ACS	RTS	Amendment to Copper Values ≥ 36 Subtract 5 ppm ≤ 35 Subtract 3 ppm For projects 4, 5, and 6 only	25th May 1983	✓ ACS		
3b	19/5/83 ACS	RTS	Amendment to Copper Projects 10 → 17 Add 1 ppm to all values.	19th May 1983	✓ ACS		
3b	11th May 1983	RTS	Amendment to Zirconium 207512 - 208151 values ≥ 700 Add 150 × 1.28 Same range values ≤ 699 × 1.28	11th May 1983	✓ ACS		
3b	5th May 1983	RTS	Amendment to Barium 205615 - 208101 : All values × 1.27 then subtract 45 ppm 208102 - 208600 values ≥ 980 No change 208102 - 208600 values ≤ 980 × 1.27 then subtract 45	5th May 1983	✓ ACS		
3b	5th May 1983	RTS	Amendment to Yttrium Projects 04, 05, 06 Subtract 6 ppm from all values	5th May 1983	✓ ACS		

References

Most of the references listed below are held in the Library of the British Geological Survey at Keyworth, Nottingham. Copies of the references may be purchased from the Library subject to the current copyright legislation.

HARRIS, J R, and COATS, J S. 1992. Geochemistry databse: data analysis and proposed design. *British Geological Survey Technical Report*, WF/92/5.

INSTITUTE OF GEOLOGICAL SCIENCES. 1978a. *Regional Geochemical Atlas: Shetland*. (London: Institute of Geological Sciences.) ISBN 0 85272 061 0

INSTITUTE OF GEOLOGICAL SCIENCES. 1978b. *Regional Geochemical Atlas: Orkney*. (London: Institute of Geological Sciences.) ISBN 0 85272 060 2

INSTITUTE OF GEOLOGICAL SCIENCES. 1979. *Regional Geochemical Atlas: South Orkney and Caithness*. (London: Institute of Geological Sciences.) ISBN 0 85272 064 5

INSTITUTE OF GEOLOGICAL SCIENCES. 1982. *Regional Geochemical Atlas: Sutherland*. (London: Institute of Geological Sciences.) ISBN 0 85272 068 8

LISTER, T R, and JOHNSON, C C. 2005. G-BASE data conditioning procedures for stream sediment and soil chemical analyses. *British Geological Survey*, BGS Internal Report Number IR/05/150.

PLANT, J A. 1971. Orientation studies on stream sediment sampling for a regional geochemical survey in northern Scotland. *Transactions of the Institute Mining & Metallurgy*, Vol. 80, 323-346.