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Geochemical data as a standard reference data set for the SIGMA project

Digital Geoscience Spatial Model

Internal Report IR/04/026

BRITISH GEOLOGICAL SURVEY

INTERNAL REPORT IR/04/026

Geochemical data as a standard reference data set for the SIGMA project

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BRITISH GEOLOGICAL SURVEY

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Summary

Geochemical data are considered to be a standard reference data set identified by the SIGMA project that could be used before and after fieldwork and which should be available within a project GIS. The currently active Geochemical Baseline Survey of the Environment (G-BASE) project and the former Mineral Reconnaissance Programme are the main contributors of data to the corporate Geochemistry Database. These data and their application are described, as are the methods for accessing and retrieving the data from the Geochemistry Database. This report is not a course in geochemical data interpretation but informs geoscientists on how the geochemical data can be presented and the geological problems to which different elements and their associations can be applied. It also describes the limitations on the use of the geochemical data highlighting the issues of data quality and suitability. The appendices list summary references to fields and codes in the Geochemistry Database and summarises the progress of geochemical baseline mapping to-date by atlas sheet area.

1 Introduction

The BGS SIGMA (System for Integrated Geospatial Mapping) Project has identified geochemical data as being one of the standard reference data sets available to geologists within a project GIS that could be used both before and after fieldwork (Howard and others, In Preparation). This report looks at the sources of geochemical data in BGS, the principal source being the corporate Geochemistry Database. Methods of accessing data in the Geochemistry Database are described as are the main data sets generated by the Mineral Reconnaissance Programme (MRP) and Geochemical Baseline Survey of the Environment (G-BASE) Project.

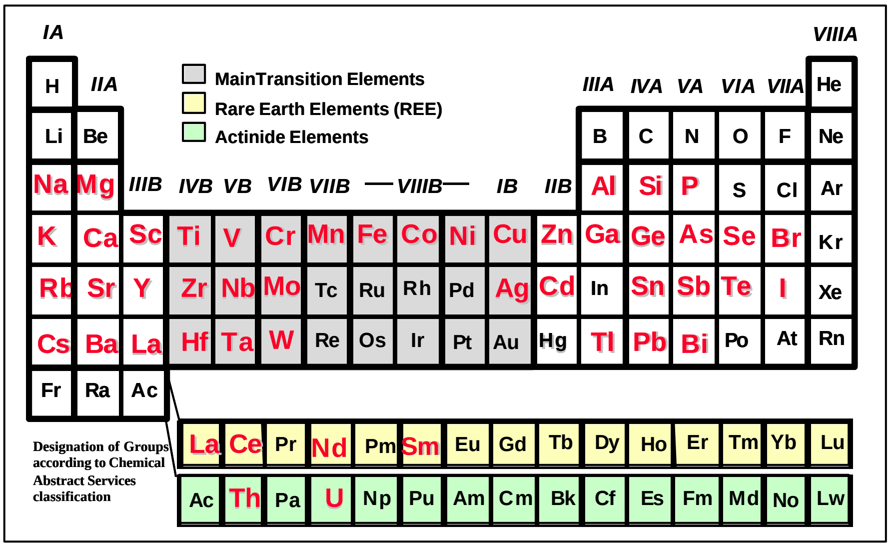
The term "geochemistry" was first used by C F Schönbein (the discoverer of ozone) in 1838, some three years after the establishment of the British Geological Survey (BGS). Geochemistry is the study of the distribution and movement of chemical elements within the earth and at its surface and can be considered as a sub-discipline of earth science. In recent years it has also become an important sub-discipline of environmental sciences and as such it is an area of work that is very relevant to the stated mission and objectives of both the British Geological Survey and its parent body, the Natural Environment Research Council (NERC).

Geochemistry is a very broad topic, in fact it is so broad geochemists will invariably specialise in a specific field ranging from isotopic dating to medical geology, exploration geochemistry to mineralogy and petrology. Applications in geochemistry range from the atomic scale in mineral structures to a global overview of element distributions on a continental scale. It is a sub-discipline within the earth sciences to which we can have a quantitative approach. Modern automated analytical techniques will generate results for a many elements of the Periodic Table - Figure 1 shows the elements currently determined for the BGS G-BASE project.

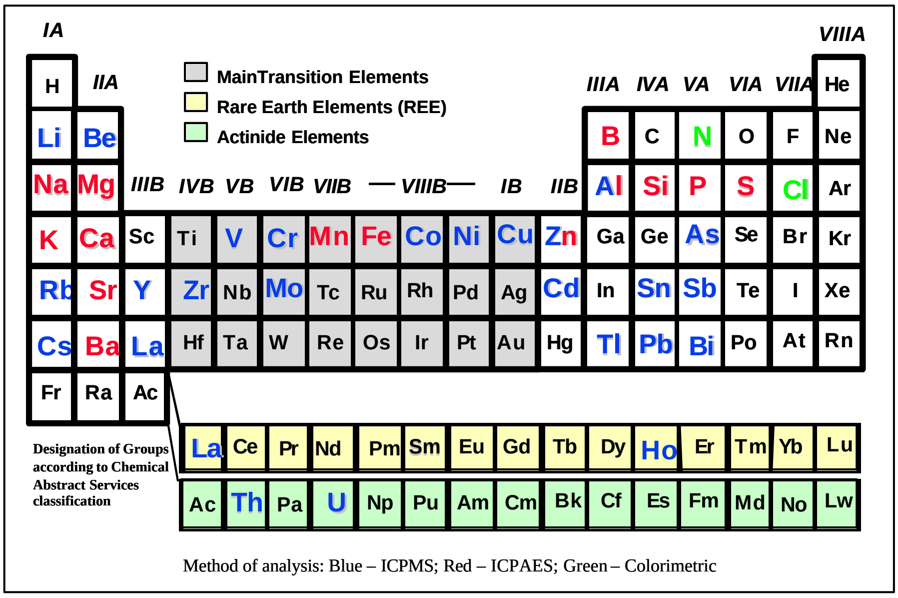
A geochemical project will generate a database of geochemical results that are readily transferable and usable in a GIS, and ideal fodder for statistical manipulation and colourful map production. Therein lies a significant problem in the use and interpretation of geochemical data. The results alone are meaningless without supplementary information such as: the method of collection; sample preparation procedures; method of analysis; detection limits; spatial resolution of sample site location; site information at the time of collection. It is also important that control sample information is available, that is, results for duplicate, replicate and standard reference samples. These can be used to assess the accuracy and precision of the results so that data sets generated by different projects over a period of time can be joined to form seamless geochemical maps. These are all factors that determine the "fit for purpose" use of geochemical data.

Using geochemical data requires knowledge and experience of the statistical techniques that can be applied to geochemical data and an understanding of the different methods for presenting the data graphically. It also requires knowledge of the distribution and behaviour of the chemical elements in our environment. Geochemical sampling will usually involve collecting a sample (whether it be water, soil, rock, sediment, vegetation or gas) from a specific site and that sample, or a set of samples collected using a predetermined sampling plan, will be taken to represent a much larger area. The results must be used with an understanding of the errors involved and how representative a single site is when extrapolated over a larger area. Misuse of geochemical data can blight large areas with the associated legal consequences. The identification of soil sites in urban areas with high levels of potentially harmful elements such as lead, cadmium or arsenic would be an example of this. Failure to correctly interpret the geochemical data from a mineral exploration project could result in the difference between a failed prospect or the development of a multi-million dollar mine. The knowledge, experience and understanding to use and interpret geochemical data are the specialist skills of the geochemist.

This report is not a course on how to interpret geochemical data or a substitute for a geochemistry handbook. It seeks to inform earth scientists, environmentalists, project managers and information managers about the geochemical data available in the BGS Geochemistry Database and provide the supplementary information essential to use it. However, warnings concerning the limitation on how the data can be used and the requirement for specialist skills are not unique to geochemistry and should not be used as an excuse to restrict the use of geochemical data to only geochemists. As a standard data reference set for the SIGMA project a greater use of geochemical data throughout BGS and NERC is to be encouraged.



(a) Elements determined in surface soils and stream sediments (highlighted in red). Loss-on-ignition and pH are also routinely measured on soils.



(b) Elements determined in surface waters (highlighted in red, blue and green). Conductivity, pH, bicarbonate and non-purgeable organic carbon (NPOC) are also routinely measured.

Figure 1. Figure showing the elements routinely determined on G-BASE samples

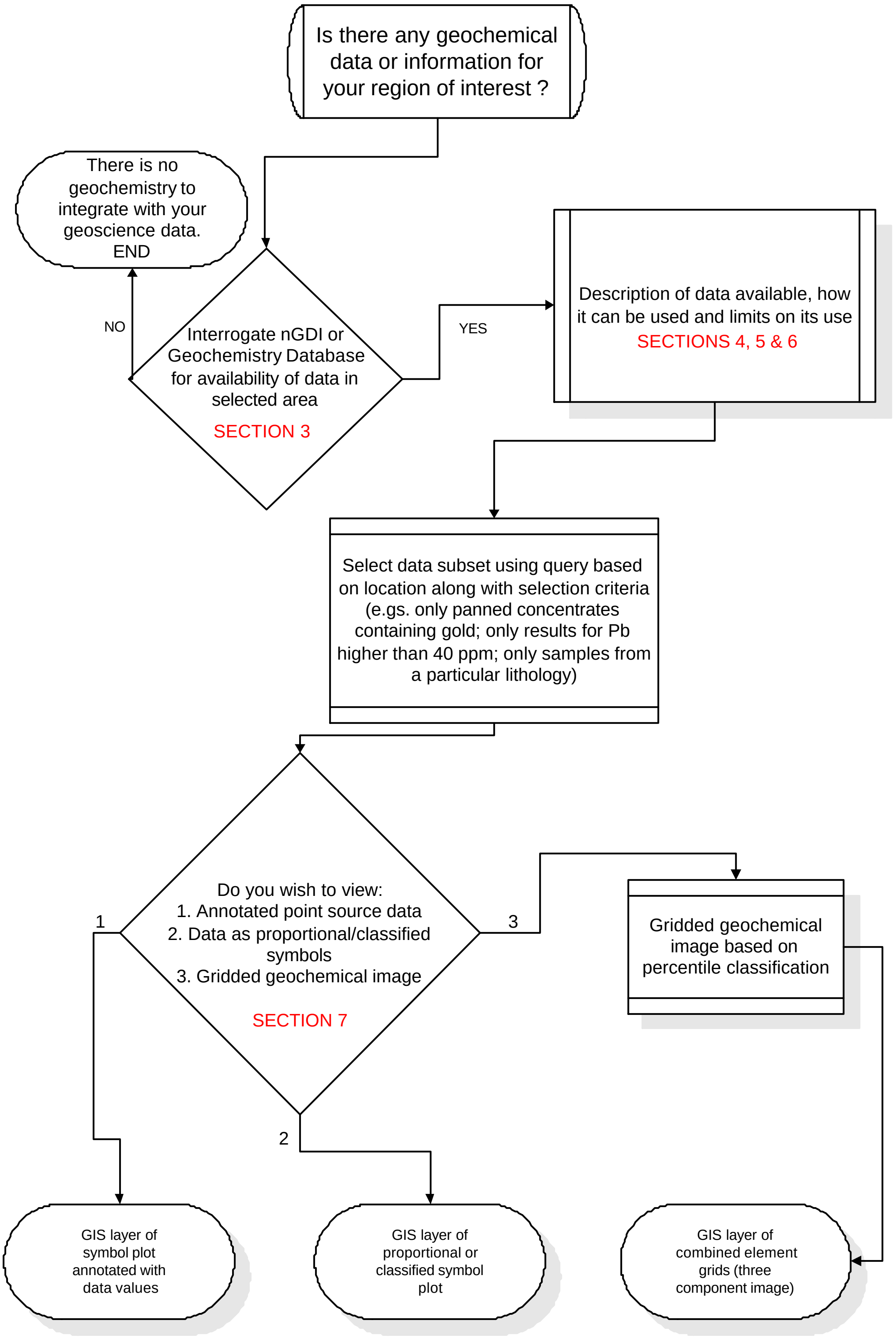


Figure 2. Steps in the use of data from the Geochemistry database

(Section references refer to this report)

The use of geochemical data from the Geochemistry Database will follow the steps shown in the Figure 2. A brief summary of the sources of geochemical data within BGS is given in Section 2 and ways of accessing data in the Geochemistry Database are discussed in Section 3. The main geochemical data sets (G-BASE and Mineral Reconnaissance Programme (MRP)) are described in Section 4 and the applications of geochemical data in Section 5. Section 6 discusses some of the factors that need to be considered when using geochemical data and different ways of presenting the data are given in Section 7.

2 Sources of Geochemical Data in BGS

The principal source of geochemical data in BGS is the corporate Geochemistry Database, designed in 1992 (Harris and Coats, 1992 and Coats and Harris, 1995) and implemented as an Oracle database accessible to all BGS staff. The Geochemistry Database is described in Section 3 and is the source of geochemical data from BGS's two major geochemical programmes, namely the Geochemical Baseline Survey of the Environment (G-BASE) and the Minerals and Mineral Reconnaissance Programmes (MRP). Whilst G-BASE continues to be an active project with twenty percent of Great Britain still to be sampled, the Minerals Programme will cease in 2004. A third component of the Geochemistry Database is the lithogeochemical results from rock and borehole analyses generated by Land Survey projects. Whilst this report is predominantly concerned with the use of the Geochemistry Database as a source of geochemical data there are additional sources of geochemical data that are described below.

2.1 G-BASE REGIONAL GEOCHEMICAL DATA

In 1968 the Institute of Geological Sciences (IGS) (now BGS) began a regional geochemical sampling programme in the northern Highlands of Scotland. This work was aimed at producing maps to show the distribution of trace elements in stream sediments and waters. Prior to this, earlier geochemical studies were mainly involved with uranium reconnaissance work, a programme supported by the UK Atomic Energy Authority (1967 –1972). The earliest samples are from the Sutherland atlas area and were collected in the summer of 1968 as part of the uranium reconnaissance work. The first systematic sampling for the regional geochemistry started in Orkney and Shetland in the summer of 1970 following a comprehensive orientation study (Plant, 1971). The work has progressed southwards from northern Scotland ever since. The first geochemical data from the regional survey of northern Scotland was placed on open file in 1972 for the Caithness quarter inch geological map sheet area.

Work on the Orkney and Shetland geochemical atlases commenced in 1974 and the Shetland atlas was the first to be published in 1978 (IGS, 1978). Between 1975 and 1990 the work was funded by the UK Department for Trade and Industry (DTI). After 1990 funding for the work came from the Department of Education and Science and subsequently, the Office of Science and Technology. The Regional Geochemistry Research Programme (RGRP) was renamed the Geochemical Survey Programme (GSP) in 1988 and again in 1994 to the Geochemical Baseline Survey of the Environment Project (G-BASE).

Analytical, statistical and data processing techniques have evolved substantially during the lifetime of this long project. Initially stream sediments were analysed for 16 elements using optical emission spectroscopy, atomic absorption spectrophotometry and delayed neutron activation (U). A direct-reading emission spectrometer was used to determine some 25 elements for the Hebrides and subsequent atlas areas. The current analytical method is x-ray fluorescence spectrometry (XRFS), which commenced on the Welsh stream sediments and determines 48 elements. Major changes in the analytical methodology have meant there has been a need to standardise results produced by different analytical methods over a long period of time. The strict analytical controls and use of standard, duplicate and replicate samples initiated at the start of the work should make it possible to maintain a high quality and seamless geochemical database.

Improved analytical techniques for natural waters (using inductively coupled plasma (ICP) optical emission spectroscopy (OES) and mass spectroscopy (MS)) has enabled the project to complete a greater range of determinants on the water samples which were originally just analysed for pH, bicarbonate, conductivity, F and U. The collection of soil samples has also increased as a consequence of moving into lowland areas dominated by intensive agriculture and more mature drainage systems. In particular, the demand for geochemical baseline data in urban areas has been significant enough to justify sampling soils in major urban centres.

2.2 MINERAL RECONNAISANCE PROGRAMME

During the Mineral Reconnaissance Programme (1972-1997) samples of stream sediments, panned concentrates, soils, tills, rocks and drill core have been collected and analysed for a wide range of elements. A summary of the MRP up to 1990 is given by Haslam and others (1990) and of the geochemical data by Hobbs and others (2000). This multidisciplinary programme involved targeted mineral exploration and so the associated geochemical results are more site specific than for the G-BASE project. Initially the MRP was concerned with base metals but later effort focused on strategic metals such as manganese and tungsten and on other commodities such as barite, gold and the platinum-group metals. The MRP was followed in 1997 by the Minerals Programme which only carried out limited fieldwork and geochemical analysis, mainly for gold. However, one of its main aims was to use new techniques of data integration and modelling to provide mineral prospectivity analysis of specific regions with a potential for economic mineral deposits. The DTI Minerals Programme will finish in April 2004.

2.3 LITHOGEOCHEMISTRY

In addition to the rock samples collected by the Minerals and Mineral Reconnaissance Programmes a number of other BGS projects have carried out systematic studies of lithogeochemistry. In particular the multidisciplinary mapping projects of Snowdonia, the Lake District and East Grampians collected a large number of rock samples and their analyses have been incorporated in the Geochemistry Database. Recently, a number of high purity limestone analyses from the Peak District and Mendips have been added. In total the Geochemistry Database contains analyses of 13 000 rock and 18 000 drill core samples and their distribution is illustrated as Figure 10 in Hobbs and others (2000).

2.4 INTERNATIONAL GEOCHEMISTRY DATA SETS

The BGS Geochemistry Database is exclusively for data from the UK landmass and so excludes the substantial amount of regional geochemical data that BGS holds for countries outside the UK. The international data holdings up to 1992 are reported by Jones and Coats (1993) and this report covers the large residential Overseas Development Administration (ODA) projects which were responsible for regional geochemical surveys. The Jones and Coats report was updated by Peter Pitfield in 2002 but the revised information remains as an unpublished report. As a result of a BGS Innovation Funding, results from the major international regional geochemical surveys have been collated onto CD-ROMs and made available under licence. These are described on the BGS web site at http://www.bgs.ac.uk/geochemcd. Subsequent work in Ecuador, Morocco, Zambia and Mauritania has been funded from other sources and BGS is not responsible for the sale or licensing of the geochemical data.

2.5 OFF-SHORE GEOCHEMICAL DATA

More than thirty elements were analysed in sea-bed sediments from the North Sea and UK Continental Shelf to the west of Scotland. This work was funded by the Department of Energy (which later merged with the Department of Trade and Industry) and is documented by Stevenson and others (1995). Digital data from this project is available as a restricted access corporate database and is described by the OGEOCHEM discovery metadata.

The sea area around the United Kingdom is used for a wide range of human activities, all of which have a significant impact on the marine environment. The naturally-occurring concentrations of chemical elements in sea-bed sediments may be enhanced by contaminants introduced by input from rivers and the atmosphere and by more localised sources arising from shipping operations, exploitation of oil and gas, and by direct discharges from drainage systems, sewage outfalls, effluents from industry and waste disposal at sea. It is therefore important to identify components of sea-floor sediments that are due to the rocks or older sediments from which they are derived, and those that are introduced into the environment. BGS offshore geochemical data, consisting of 38 elements, are available from sea-bed samples collected from a variety of sediment types occurring in a wide range of environments. Samples have been collected offshore of the eastern coast of the UK where major river systems which drain heavily populated and industrialised catchment areas, such as the Thames, Humber and Tyne, flow into the North Sea. In contrast, samples are also available from the shelf west of Scotland where man's activities have had much less impact. The data provide a baseline for chemical element concentrations in sea-bed sediments against which future work may be assessed. It should therefore be of significance to a diverse range of interests including pollution control, fishing, natural resources, nature conservation, shipping, tourism, recreation, and waste disposal management. In addition the information derived from the data will be of use to geologists in identifying the source of sea-bed sediments and the underlying glacial deposits.

Geochemical data for estuarine sediments (for example, Mersey, Clyde and Humber estuaries) have been produced in recent years but have not yet been captured into any corporate database. Such data can be obtained from the "Estuarine Contamination" project manager (Dave Jones).

2.6 WATER CHEMISTRY

The G-BASE project collects stream water from 1st and 2nd order streams for chemical analyses the results of which are found in the Geochemistry Database and published in the geochemical atlases (e.g. BGS, 1999). However, the majority of BGS hydrogeochemistry (e.g. Baseline Quality in UK aquifers) is carried out at BGS Wallingford and data is held there. Such hydrogeochemical data can be obtained from the hydrogeochemical database which is currently being updated (contact Chris Milne or Andrew McKenzie, BGS Wallingford).

2.7 OTHER MISCELLANEOUS SOURCES

The Department of International Development (DFID) and its predecessor the ODA have sponsored a number of research projects involving the environment and health that have involved sample collection and geochemical analysis. The geochemical results are generally available in BGS technical reports such as the work by Williams (1997); Fordyce and others, (1998); and Johnson and others (2003b).

Another source of geochemical data that is available to BGS staff are site investigation (SI) reports usually produced for a site specific, applied geological investigation and containing a limited amount of geochemical data. The data is usually of limited use because of: its site specific application; commercial in confidence nature; non-standard methodologies and procedures; and non-total element analyses for a small range of specific elements.

Natural radioactive elements such as K, U and Th can be determined radiometrically by measuring their γ-ray spectra. However, this method is indirect because the sample may not be in equilibrium and some of the daughter products may have been gained or lost by the sample. Because elevated concentrations of these elements can have health implications, BGS has a separate natural radioactivity project. Soil gas radon and soil field γ spectrometric data are recorded in Excel files and are available from the project manager (Dave Jones).

Isotopic geochemical data are generated by the NERC Isotope Geosciences Laboratory (NIGL) at Keyworth and results from this work are generally found in published papers or university theses. Records and reports relating to the NIREX project are held by BGS and some of these contain geochemical data (see NIREX discovery metadata).

3 The Geochemistry Database

The history, design and current usage of the BGS Geochemistry Database is discussed in a recent BGS internal report written by Dr Stan Coats (Coats, 2004) who, apart from being the principal instigator and manager of the database, was involved in the early analytical work and the MRP projects. The Geochemistry Database has its origins in the early 1970s when field cards were in use by geochemists collecting samples. Subsequent projects, active in collecting a large number of samples, led to the creation of large data files in the BGS G-EXEC data system and in simple Oracle databases. This data was incorporated into a unified Geochemistry Database, the design of which was proposed in 1992. Information systems have changed markedly over the last ten years and the current client-server model used for interrogating the database has been made possible by the development of desktop computing.

3.1 ACCESSING THE GEOCHEMICAL DATABASE

3.1.1 Oracle

All applications to look at or retrieve data from the database involve Oracle in some way as the database is stored as Oracle data tables. The most direct way is using SQL*PLUS where SQL commands are typed into a command line interface and data is retrieved to a screen or file. However, the majority of users would not have the SQL skills to do this and there are a number of alternatives described below.

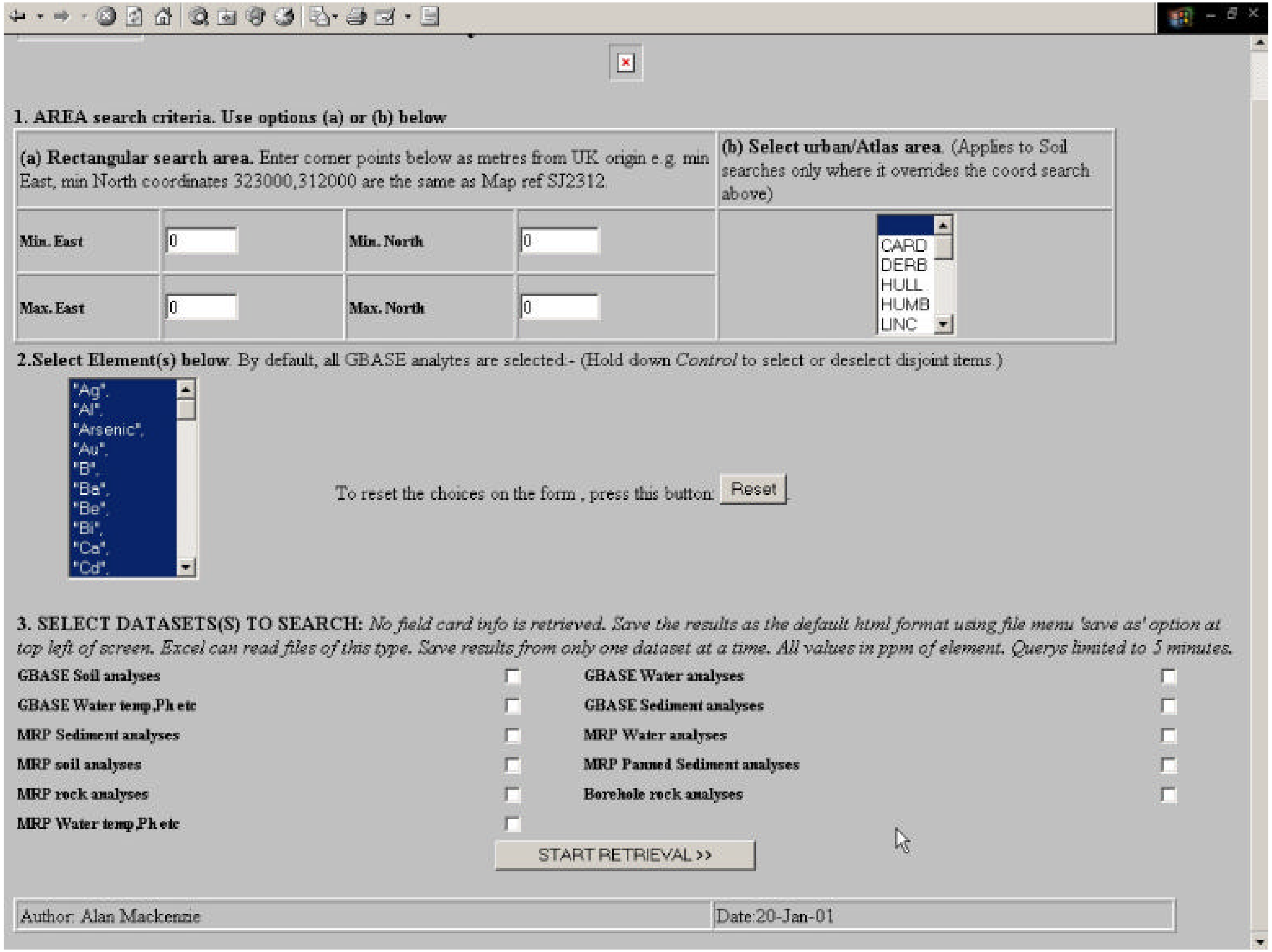
3.1.2 Intranet Data Access (IDA)

The IDA[1] system provides BGS staff with a method of searching BGS data held in Oracle tables. At present this Coldfusion application does not include geochemical data but there is no reason why it could not be extended to data held in the Geochemistry Database. A Coldfusion application[2] has been written for G-BASE staff to download data for licencing and the form for this is shown in Figure 3.

---

[1] http://intranet/resources/data/ida/idamain.htm

[2] http://kwnts99:82/scripts/ida/geog/geog2_combformb.cfm



1. AREA search criteria. Use options (a) or (b) below

(a) Rectangular search area. Enter corner points below as metres from UK origin e.g. min East, min North coordinates 323000,312000 are the same as Map ref SJ2312.

(b) Select urban/Atlas area. (Applies to Soil searches only where it overrides the coord search above)

Min. East	0	**Min. North**	0
Max. East	0	**Max. North**	0

2.Select Element(s) below. By default, all GBASE analytes are selected:- (Hold down *Control* to select or deselect disjoint items.)

To reset the choices on the form , press this button:

3. SELECT DATASETS(S) TO SEARCH: *No field card info is retrieved. Save the results as the default html format using file menu 'save as' option at top left of screen. Excel can read files of this type. Save results from only one dataset at a time. All values in ppm of element. Querys limited to 5 minutes.*

GBASE Soil analyses	☐	**GBASE Water analyses**	☐
GBASE Water temp,Ph etc	☐	**GBASE Sediment analyses**	☐
MRP Sediment analyses	☐	**MRP Water analyses**	☐
MRP soil analyses	☐	**MRP Panned Sediment analyses**	☐
MRP rock analyses	☐	**Borehole rock analyses**	☐
MRP Water temp,Ph etc	☐		

Author: Alan Mackenzie

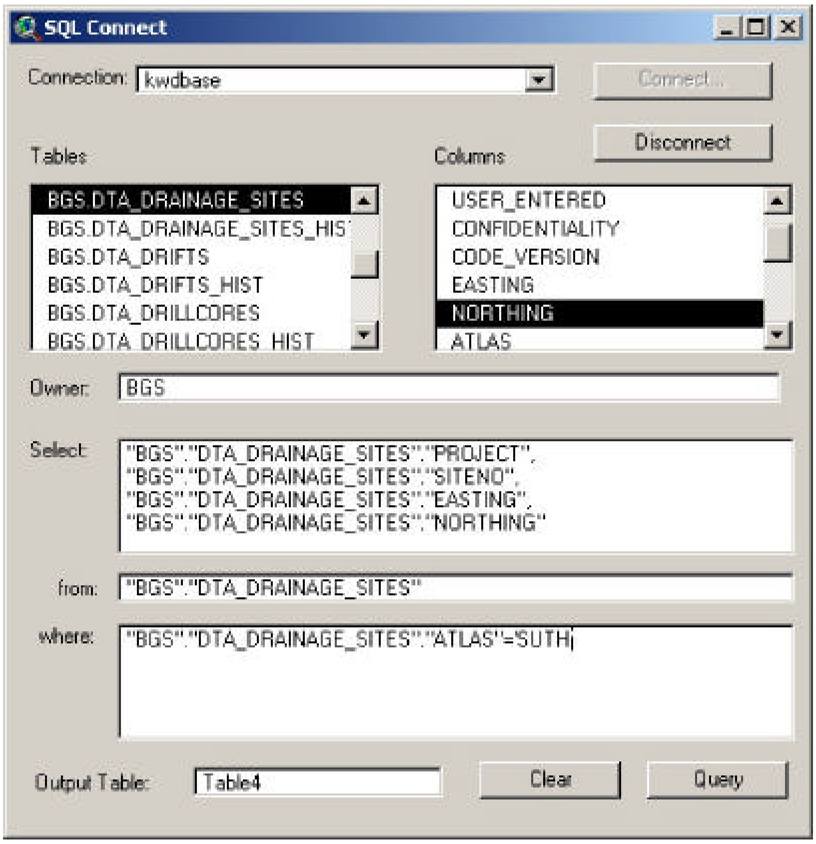
Date:20-Jan-01

Figure 3. Intranet data access form for accessing the Geochemistry Database

3.1.3 ArcView 3.*

ArcView can be used to connect to the BGS Oracle Databases if a user has a valid Oracle id and password. A step-by-step guide to linking ArcView to an Oracle database is given by Hobbs (2004). The important steps are:

1. Open a new or existing project in ArcView
2. On the main ArcView Menu Select "Project" then "SQL Connect"
3. Select kwdbase from the drop down "Connection" list and click "Connect"
4. Enter Oracle id and password when asked by the Oracle ODBC Driver Connect
5. When connected to kwdbase a blank version of Figure 4 appears
6. In the owner column enter BGS and press return. All the database tables will appear (these tables are discussed in more detail in the next subsection)
7. Select and click on the table you wish to use, for example, BGS.DTA_DRAINAGE_SITES. The fields in this table will appear in the columns box (see Figure 4).
8. Select the columns you wish to use by double clicking on them
9. In order to create a query enter the table you wish to use in the "from" box and construct a query as shown in Figure 4. The example shown here selects all the samples from the Sutherland (SUTH) atlas area.
10. A new table of results is added to the ArcView project.



Connection: kwdbase

Owner: BGS

Select:
"BGS"."DTA_DRAINAGE_SITES"."PROJECT",
"BGS"."DTA_DRAINAGE_SITES"."SITENO",
"BGS"."DTA_DRAINAGE_SITES"."EASTING",
"BGS"."DTA_DRAINAGE_SITES"."NORTHING"

from: "BGS"."DTA_DRAINAGE_SITES"

where: "BGS"."DTA_DRAINAGE_SITES"."ATLAS"='SUTH

Output Table: Table4

Figure 4. Example of Arc View query of the Geochemistry database

3.1.4 Arc GIS 8.*

Accessing the Geochemistry Database using Arc GIS 8.* is different to ArcView 3.* and not as satisfactory. In Arc GIS the whole database table is accessed before a SQL query can be performed. It is therefore recommended that MS Access is used first to create a data table using the "make table" option. The developing GDI 8 will include script that will enable SQL queries.

3.1.5 GeoScience Data Index (GDI)

ArcView can also be used to access geochemistry data via the BGS internal iGDI[3]. Some geochemistry themes are loaded when the GDI is opened, others can be loaded from the "GIS Layers" menu option. The public have access to the external eGDI via the BGS web site though the public version has no data and lists only site locations.

3.1.6 MS ACCESS

1. Firstly, ensure that you have Oracle and the ODBC software correctly installed on your PC (this can be done by your local computer support)
2. Create a new database or open an existing database to which you want to add tables from the Geochemistry Database.
3. Select the tables you wish to link from the Oracle database by carrying out the following:
    a) Select File/Get external Data/Link Tables from the main menu
    b) From the Links menu select ODBC Database ()

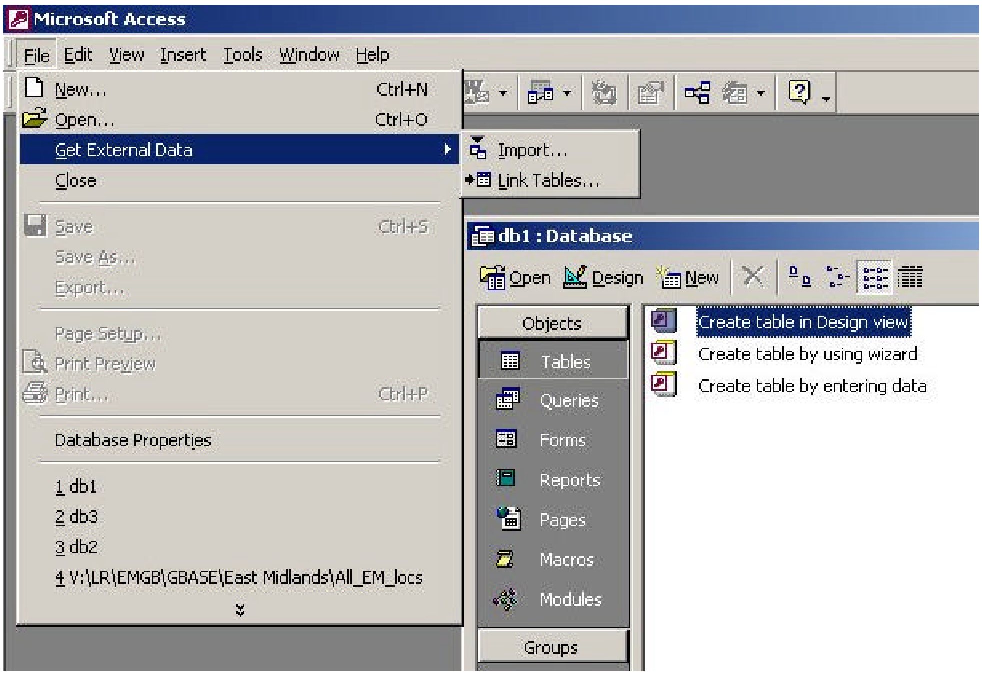


Figure 5. Screen capture illustrating the "Get External Data" option in MS Access

---

[3] Q:\Gdi\gdi31.apr where Q: is kwnts1 BGS corporate data server at Keyworth

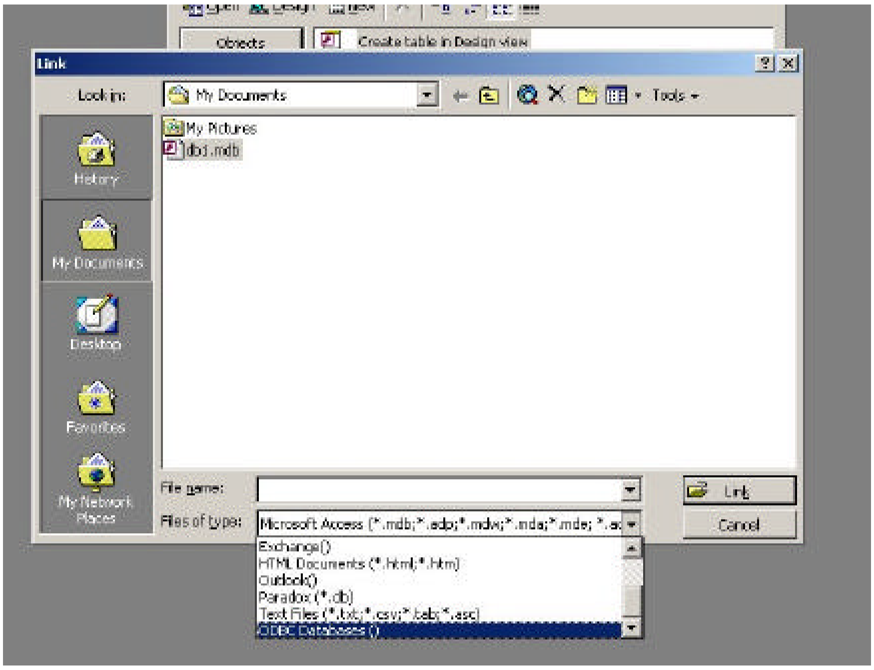
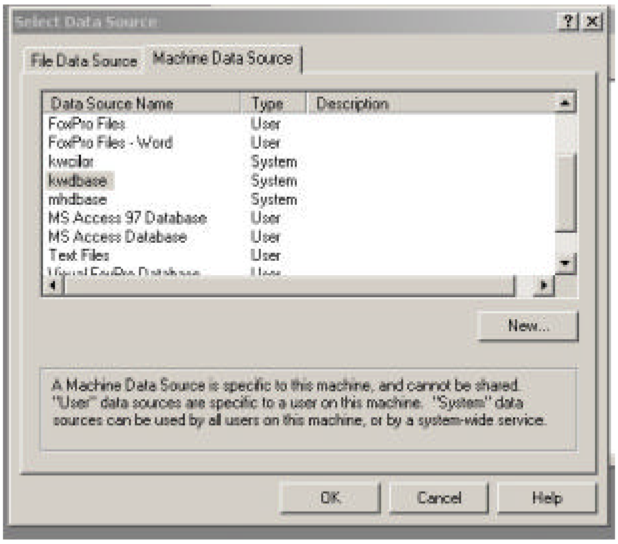


Figure 6. Screen capture illustrating selecting the ODBC option in MS Access

c) Select the Machine Data Source tab and select kwdbase



Data Source Name	Type	Description
FoxPro Files	User	
FoxPro Files - Word	User	
kwcilor	System	
kwdbase	System	
mhdbase	System	
MS Access 97 Database	User	
MS Access Database	User	
Text Files	User	

A Machine Data Source is specific to this machine, and cannot be shared. "User" data sources are specific to a user on this machine. "System" data sources can be used by all users on this machine, or by a system-wide service.

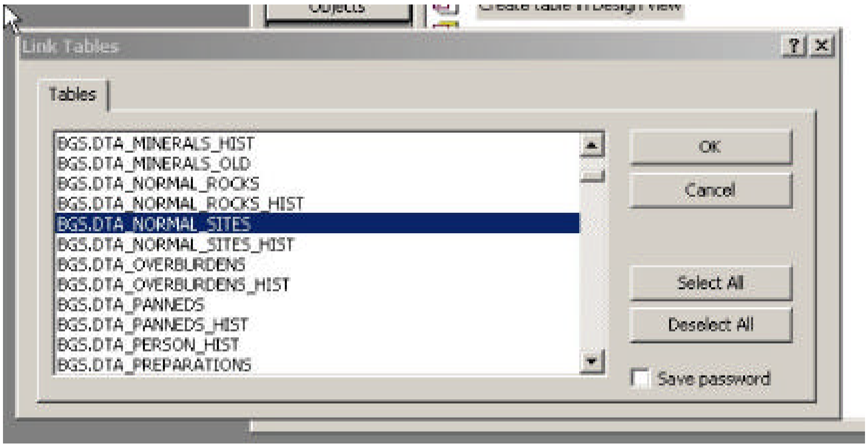
Figure 7. Screen capture illustrating the selection of the BGS database server in MS Access

d) Enter Oracle user id and password

e) Select the tables you wish to link.. Geochemistry Database tables commence with BGS.DTA and BGS.MTA_DOM

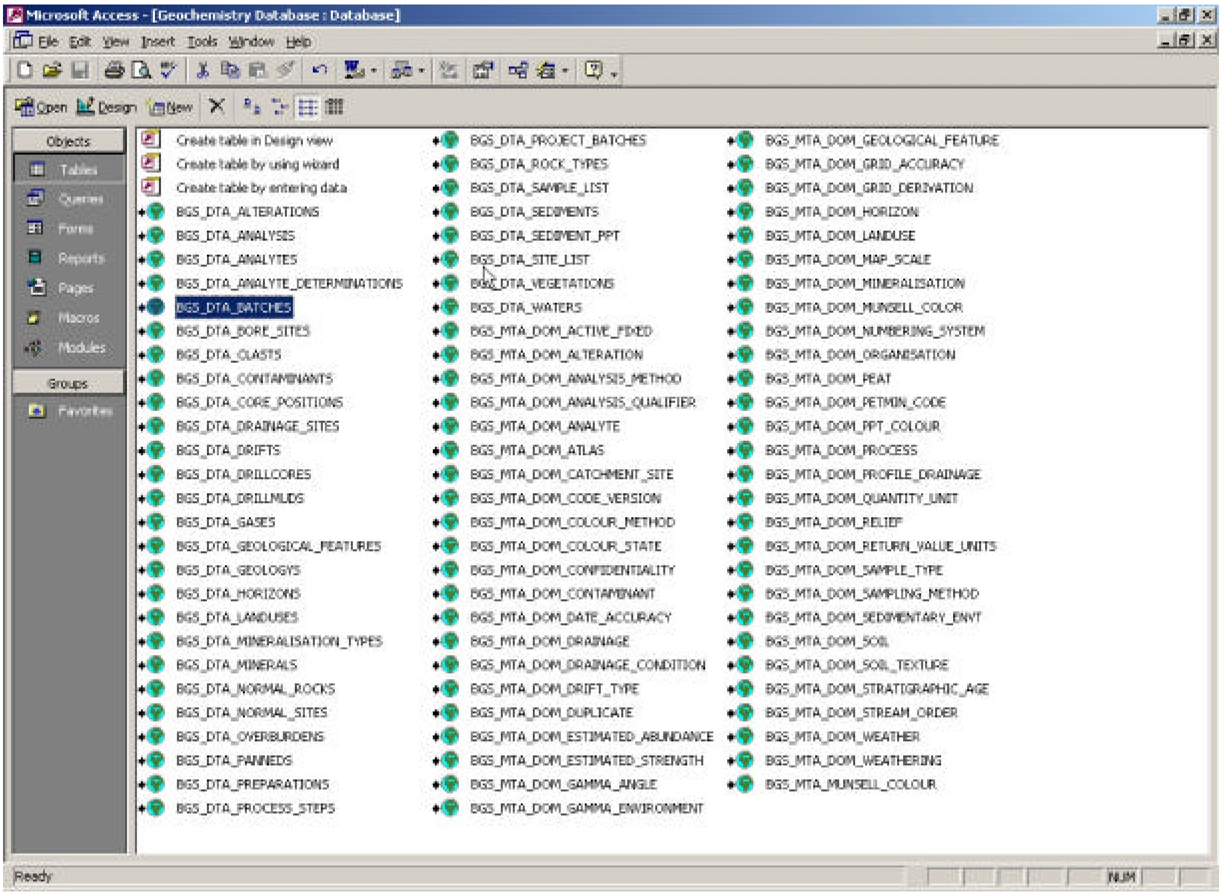
You are now ready to start using the tables of the Geochemistry Database employing Access as the front-end. It is important that you have an understanding of what can be found in each of the tables, the more important fields are discussed in Appendix 1. Some of the codes used in the database fields are described in Appendix 2, a more detailed description of which is found in Harris and Coats (1992) in the chapter on 'Detailed Domain Definitions'. The database manager can determine who has access to the tables by setting security permissions for each table. The current setting is that all BGS staff with Oracle ids have read access to all the Geochemistry Database tables. A list of all the tables associated with the Geochemistry Database is given in

Figure 9. Worked examples of downloading G-BASE data from the Geochemistry Database are given in Appendix 3.



BGS.DTA_MINERALS_HIST
BGS.DTA_MINERALS_OLD
BGS.DTA_NORMAL_ROCKS
BGS.DTA_NORMAL_ROCKS_HIST
BGS.DTA_NORMAL_SITES
BGS.DTA_NORMAL_SITES_HIST
BGS.DTA_OVERBURDENS
BGS.DTA_OVERBURDENS_HIST
BGS.DTA_PANNEDS
BGS.DTA_PANNEDS_HIST
BGS.DTA_PERSON_HIST
BGS.DTA_PREPARATIONS

Figure 8. Screen capture illustrating some of the Geochemistry Database Oracle tables



BGS_DTA_ALTERATIONS
BGS_DTA_ANALYSIS
BGS_DTA_ANALYTES
BGS_DTA_ANALYTE_DETERMINATIONS
BGS_DTA_BATCHES
BGS_DTA_BORE_SITES
BGS_DTA_CLASTS
BGS_DTA_CONTAMINANTS
BGS_DTA_CORE_POSITIONS
BGS_DTA_DRAINAGE_SITES
BGS_DTA_DRIFTS
BGS_DTA_DRILLCORES
BGS_DTA_DRILLMUDS
BGS_DTA_GASES
BGS_DTA_GEOLOGICAL_FEATURES
BGS_DTA_GEOLOGYS
BGS_DTA_HORIZONS
BGS_DTA_LANDUSES
BGS_DTA_MINERALISATION_TYPES
BGS_DTA_MINERALS
BGS_DTA_NORMAL_ROCKS
BGS_DTA_NORMAL_SITES
BGS_DTA_OVERBURDENS
BGS_DTA_PANNEDS
BGS_DTA_PREPARATIONS
BGS_DTA_PROCESS_STEPS
BGS_DTA_PROJECT_BATCHES
BGS_DTA_ROCK_TYPES
BGS_DTA_SAMPLE_LIST
BGS_DTA_SEDIMENTS
BGS_DTA_SEDIMENT_PPT
BGS_DTA_SITE_LIST
BGS_DTA_VEGETATIONS
BGS_DTA_WATERS
BGS_MTA_DOM_ACTIVE_FIXED
BGS_MTA_DOM_ALTERATION
BGS_MTA_DOM_ANALYSIS_METHOD
BGS_MTA_DOM_ANALYSIS_QUALIFIER
BGS_MTA_DOM_ANALYTE
BGS_MTA_DOM_ATLAS
BGS_MTA_DOM_CATCHMENT_SITE
BGS_MTA_DOM_CODE_VERSION
BGS_MTA_DOM_COLOUR_METHOD
BGS_MTA_DOM_COLOUR_STATE
BGS_MTA_DOM_CONFIDENTIALITY
BGS_MTA_DOM_CONTAMINANT
BGS_MTA_DOM_DATE_ACCURACY
BGS_MTA_DOM_DRAINAGE
BGS_MTA_DOM_DRAINAGE_CONDITION
BGS_MTA_DOM_DRIFT_TYPE
BGS_MTA_DOM_DUPLICATE
BGS_MTA_DOM_ESTIMATED_ABUNDANCE
BGS_MTA_DOM_ESTIMATED_STRENGTH
BGS_MTA_DOM_GAMMA_ANGLE
BGS_MTA_DOM_GAMMA_ENVIRONMENT
BGS_MTA_DOM_GEOLOGICAL_FEATURE
BGS_MTA_DOM_GRID_ACCURACY
BGS_MTA_DOM_GRID_DERIVATION
BGS_MTA_DOM_HORIZON
BGS_MTA_DOM_LANDUSE
BGS_MTA_DOM_MAP_SCALE
BGS_MTA_DOM_MINERALISATION
BGS_MTA_DOM_MUNSELL_COLOR
BGS_MTA_DOM_NUMBERING_SYSTEM
BGS_MTA_DOM_ORGANISATION
BGS_MTA_DOM_PEAT
BGS_MTA_DOM_PETMIN_CODE
BGS_MTA_DOM_PPT_COLOUR
BGS_MTA_DOM_PROCESS
BGS_MTA_DOM_PROFILE_DRAINAGE
BGS_MTA_DOM_QUANTITY_UNIT
BGS_MTA_DOM_RELIEF
BGS_MTA_DOM_RETURN_VALUE_UNITS
BGS_MTA_DOM_SAMPLE_TYPE
BGS_MTA_DOM_SAMPLING_METHOD
BGS_MTA_DOM_SEDIMENTARY_ENVT
BGS_MTA_DOM_SOIL
BGS_MTA_DOM_SOIL_TEXTURE
BGS_MTA_DOM_STRATIGRAPHIC_AGE
BGS_MTA_DOM_STREAM_ORDER
BGS_MTA_DOM_WEATHER
BGS_MTA_DOM_WEATHERING
BGS_MTA_MUNSELL_COLOUR

Figure 9. A screen capture from MS ACCESS showing all the Oracle tables associated with the Geochemistry Database

4 Description and extent of the main data sets

The two main geochemical data sets that are available in the Geochemistry Database are described below, namely the MRP and G-BASE data. When retrieving data from the Geochemistry Database the "Numbering System" field can be used to distinguish between MRP (code 3) and G-BASE (code 4) data.

4.1 FIELD DATA

Both the MRP and G-BASE data in the Geochemistry Database are derived from two sources - field data and analytical results. Field data is taken from field cards completed at the time the sample was collected. Figure 10 illustrates a stream sediment field card currently in use by the G-BASE project and described in Johnson and others (2003a).

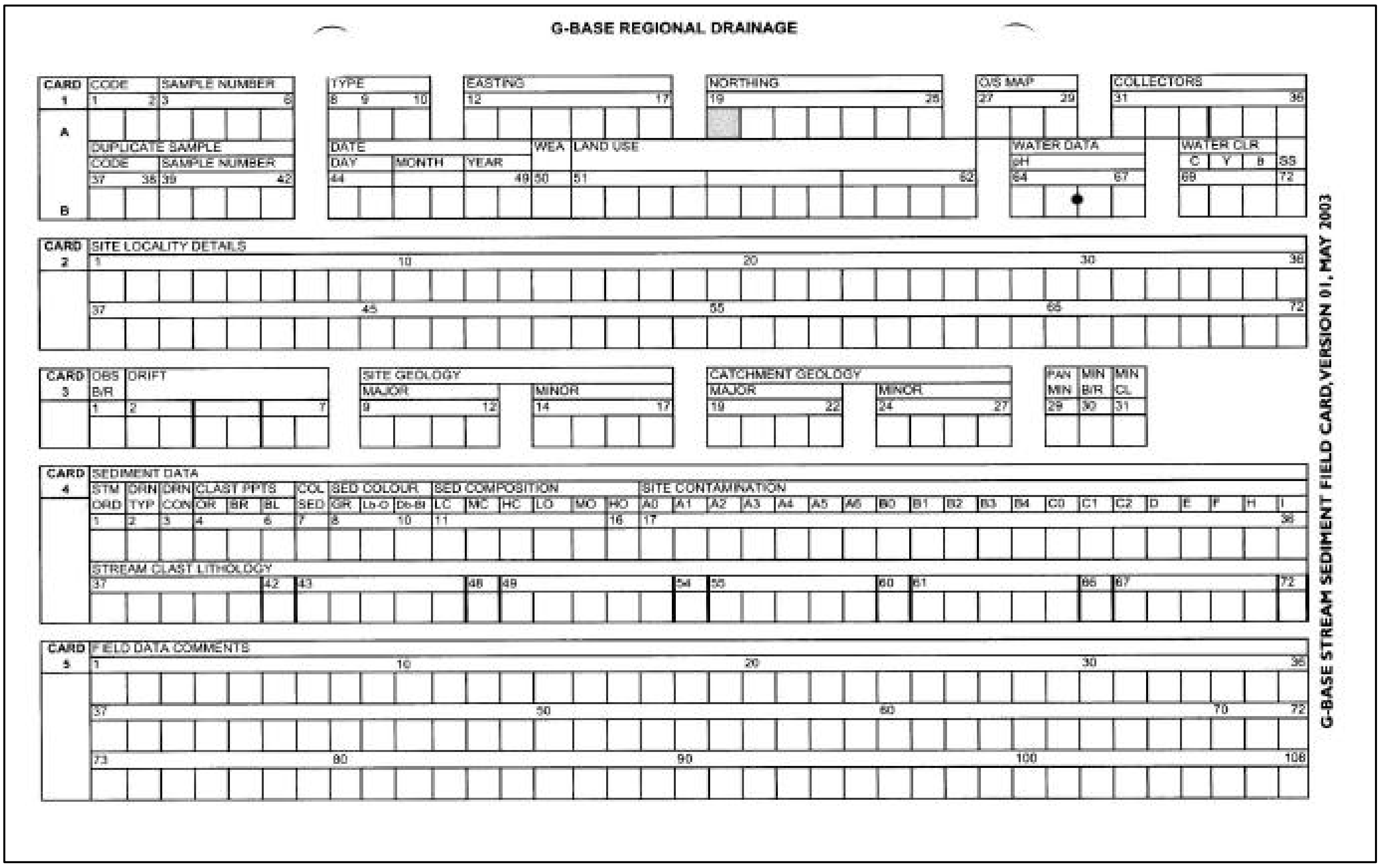


Figure 10. **Example of a G-BASE field card for stream sediments**

Field cards for the MRP and G-BASE have generally been of a similar format and the version of the field card used can be identified in the Geochemistry Database by the "Code version" field. The field codes used to complete field cards are shown in Figure 11. Original field cards are stored in National Geoscience Data Centre (NGDC) and G-BASE field data is now routinely entered on a daily basis during the field campaign into a MS Access field database. At the end of the field season, after the field database has been validated by the team leader, the field data will be loaded into the Geochemistry Database. For samples collected before the advent of desktop computing only essential fields (e.g. grid reference and site number) have been entered into the

Geochemistry Database and the hardcopy field form remains the definitive record of the site and sample description. The amount of information collected and entered into the database is quite variable between different MRP projects.

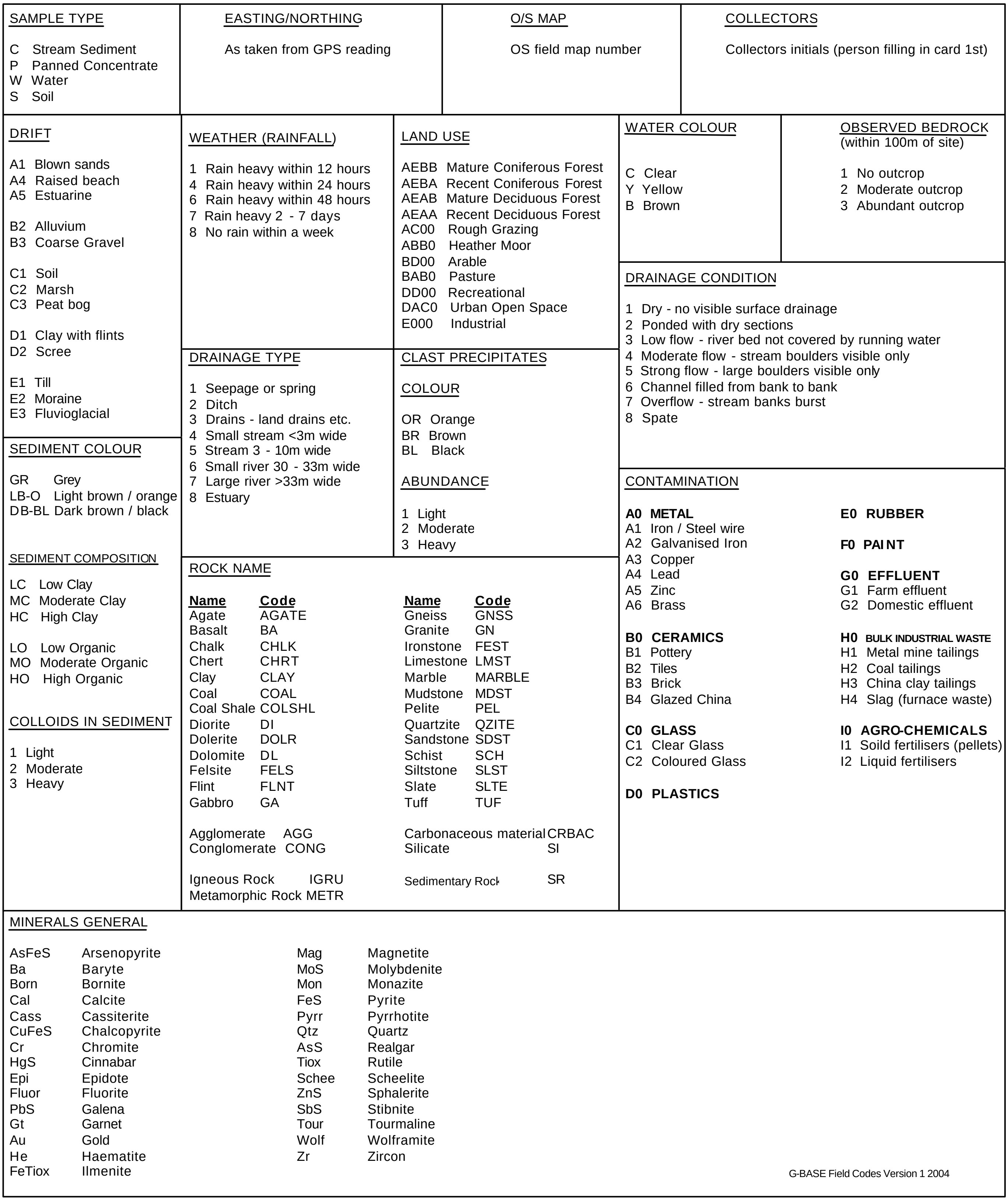
4.2 ANALYTICAL RESULTS

The vast majority of chemical analyses on G-BASE samples have been done by BGS laboratories but MRP results are derived from a mixture of internal and external laboratories. The organisation responsible for carrying out the analyses is identified by the "Lab" field of the analyte determination table in the Geochemistry Database. Original raw data (as received from the laboratories) for the oldest samples in the database exist only as hardcopy lists stored in the NGDC. From the 1980's onwards, when digital data was more readily available, original batch files from the laboratories generally exist in digital form though not in any corporate database and are poorly documented. Data received from laboratories needs to go through a series of data conditioning procedures before it is fit for use. These procedures for the G-BASE stream sediment and soils data are described by Lister and others (In Prep).

It is a deficiency of the Geochemistry Database that the extent to which data has been conditioned is not described, and within the database there is great variability in the amount of conditioning that has been done. All results are subjected to basic error checking before being passed as suitable for loading to the Geochemistry Database. The G-BASE data also undergoes standardisation and levelling so there is a consistency between field campaign boundaries and so that seamless regional geochemical maps can be produced. G-BASE data in the database is therefore processed data in which some elements will have been added to or multiplied by a series of correction factors to give a standardised data set. Data is first standardised within atlas boundaries then to a national standard. This is an ongoing process and the regional data for sediments and soils is currently being standardised against the Welsh stream sediment results. Original data for the MRP has been entered into the Geochemistry Database and many paper records are stored in NGDC.

The combination of different data sets, with different element detection limits, can be problematical and is discussed in Section 6. The problem of lower detection limits is not such a problem for MRP exploration data sets as their use is usually to define anomalously high values. However, when used for environmental purposes the full range of elemental results are of interest, for example, studies of trace element deficiencies need to delineate areas of low results.

Discovery metadata is available for subsets of data within the database (see Appendix 4). It is proposed that a certain level of index metadata will be attached to the Geochemistry Database utilising the information provided here in Appendix 5.



SAMPLE TYPE

C Stream Sediment
P Panned Concentrate
W Water
S Soil

EASTING/NORTHING

As taken from GPS reading

O/S MAP

OS field map number

COLLECTORS

Collectors initials (person filling in card 1st)

DRIFT

A1 Blown sands
A4 Raised beach
A5 Estuarine

B2 Alluvium
B3 Coarse Gravel

C1 Soil
C2 Marsh
C3 Peat bog

D1 Clay with flints
D2 Scree

E1 Till
E2 Moraine
E3 Fluvioglacial

WEATHER (RAINFALL)

1 Rain heavy within 12 hours
4 Rain heavy within 24 hours
6 Rain heavy within 48 hours
7 Rain heavy 2 - 7 days
8 No rain within a week

LAND USE

AEBB Mature Coniferous Forest
AEBA Recent Coniferous Forest
AEAB Mature Deciduous Forest
AEAA Recent Deciduous Forest
AC00 Rough Grazing
ABB0 Heather Moor
BD00 Arable
BAB0 Pasture
DD00 Recreational
DAC0 Urban Open Space
E000 Industrial

WATER COLOUR

C Clear
Y Yellow
B Brown

OBSERVED BEDROCK
(within 100m of site)

1 No outcrop
2 Moderate outcrop
3 Abundant outcrop

DRAINAGE CONDITION

1 Dry - no visible surface drainage
2 Ponded with dry sections
3 Low flow - river bed not covered by running water
4 Moderate flow - stream boulders visible only
5 Strong flow - large boulders visible only
6 Channel filled from bank to bank
7 Overflow - stream banks burst
8 Spate

DRAINAGE TYPE

1 Seepage or spring
2 Ditch
3 Drains - land drains etc.
4 Small stream <3m wide
5 Stream 3 - 10m wide
6 Small river 30 - 33m wide
7 Large river >33m wide
8 Estuary

CLAST PRECIPITATES

COLOUR

OR Orange
BR Brown
BL Black

ABUNDANCE

1 Light
2 Moderate
3 Heavy

SEDIMENT COLOUR

GR Grey
LB-O Light brown / orange
DB-BL Dark brown / black

SEDIMENT COMPOSITION

LC Low Clay
MC Moderate Clay
HC High Clay

LO Low Organic
MO Moderate Organic
HO High Organic

COLLOIDS IN SEDIMENT

1 Light
2 Moderate
3 Heavy

ROCK NAME

Name	Code	Name	Code
Agate	AGATE	Gneiss	GNSS
Basalt	BA	Granite	GN
Chalk	CHLK	Ironstone	FEST
Chert	CHRT	Limestone	LMST
Clay	CLAY	Marble	MARBLE
Coal	COAL	Mudstone	MDST
Coal Shale	COLSHL	Pelite	PEL
Diorite	DI	Quartzite	QZITE
Dolerite	DOLR	Sandstone	SDST
Dolomite	DL	Schist	SCH
Felsite	FELS	Siltstone	SLST
Flint	FLNT	Slate	SLTE
Gabbro	GA	Tuff	TUF
Agglomerate	AGG	Carbonaceous material	CRBAC
Conglomerate	CONG	Silicate	SI
Igneous Rock	IGRU	Sedimentary Rock	SR
Metamorphic Rock	METR		

CONTAMINATION

A0 METAL
A1 Iron / Steel wire
A2 Galvanised Iron
A3 Copper
A4 Lead
A5 Zinc
A6 Brass

B0 CERAMICS
B1 Pottery
B2 Tiles
B3 Brick
B4 Glazed China

C0 GLASS
C1 Clear Glass
C2 Coloured Glass

D0 PLASTICS

E0 RUBBER

F0 PAINT

G0 EFFLUENT
G1 Farm effluent
G2 Domestic effluent

H0 BULK INDUSTRIAL WASTE
H1 Metal mine tailings
H2 Coal tailings
H3 China clay tailings
H4 Slag (furnace waste)

I0 AGRO-CHEMICALS
I1 Soild fertilisers (pellets)
I2 Liquid fertilisers

MINERALS GENERAL

AsFeS	Arsenopyrite	Mag	Magnetite
Ba	Baryte	MoS	Molybdenite
Born	Bornite	Mon	Monazite
Cal	Calcite	FeS	Pyrite
Cass	Cassiterite	Pyrr	Pyrrhotite
CuFeS	Chalcopyrite	Qtz	Quartz
Cr	Chromite	AsS	Realgar
HgS	Cinnabar	Tiox	Rutile
Epi	Epidote	Schee	Scheelite
Fluor	Fluorite	ZnS	Sphalerite
PbS	Galena	SbS	Stibnite
Gt	Garnet	Tour	Tourmaline
Au	Gold	Wolf	Wolframite
He	Haematite	Zr	Zircon
FeTiox	Ilmenite		

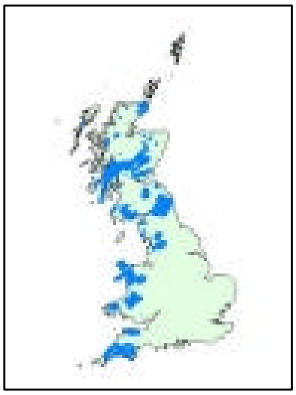
G-BASE Field Codes Version 1 2004

Figure 11. Field codes used to complete a G-BASE stream sediment field card

The field data is linked to analytical data by a key field which is a unique number created by a combination of the "Project" and "Siteno" fields in the Geochemistry Database. In order to avoid confusion with MRP codes the original G-BASE character project codes assigned during sampling prior to the implementation of the Geochemistry Database have been translated and these are included in the information in Appendix 5. A further complication in site numbering arises from the fact that G-BASE now assigns the same site number to soil samples collected at the surface and at depth so the database manager has added 50 000 to the original site number of the deeper soils, but see Coats (2004) for the alternative re-numbering system employed in the Minerals Programme.

4.3 MINERAL RECONNAISSANCE PROGRAMME EXPLORATION DATA

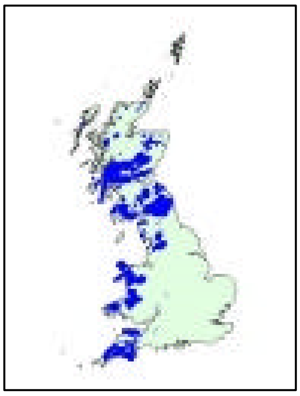
4.3.1 Stream sediment samples



The database holds information on about 26 700 samples of stream sediment collected from small streams and rivers in the UK during the Mineral Reconnaissance Programme.

Figure 12. An index map showing location of MRP stream sediment sites

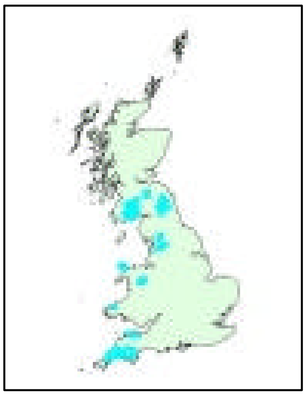
4.3.2 Panned concentrate samples



The Mineral Reconnaissance Programme normally collected a heavy mineral concentrate sample from most drainage sites and these have been analysed for a variety of base and precious metals. The analytical data is stored in the Geochemistry database along with field observations by the collector of the heavy mineral content. In total over 29 000 panned concentrate samples have been collected.

Figure 13. An index map showing location of MRP panned concentrate sites

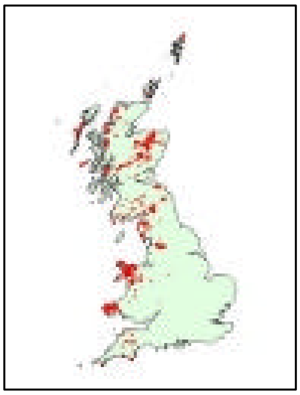
4.3.3 Waters



There were approximately 9 000 waters (stream and some well waters) collected and analysed for the Mineral Reconnaissance Programme.

Figure 14. An index map showing location of MRP water sites

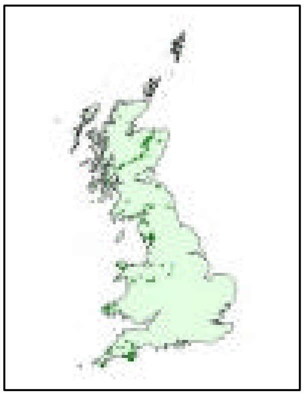
4.3.4 Rock samples



The BGS Geochemistry Database holds information on about 13 000 rock samples collected from surface outcrops and shallow auger holes throughout the UK. The majority have been collected during the Mineral Reconnaissance Programme but various field mapping and lithogeochemical studies have collected data on rocks collected from natural exposures and quarries. Data on the mineralogical and petrological character of these and other rock samples is held in the BGS BritRocks database.

Figure 15. An index map showing location of MRP rock sample sites

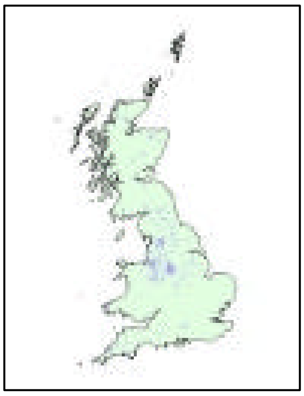
4.3.5 Soil and till samples



The BGS Geochemistry Database holds data on about 65 000 samples of soil and till collected using hand augers, shallow auger or percussion drills, and from pits. These have been collected by the Mineral Reconnaissance Programme in mineralised areas and by the G-BASE in areas of low drainage density and in urban areas in England. Data on the horizons collected, depth, textures and clasts are recorded in the database.

Figure 16. An index map showing location of MRP soil and till sites

4.3.6 Borehole samples

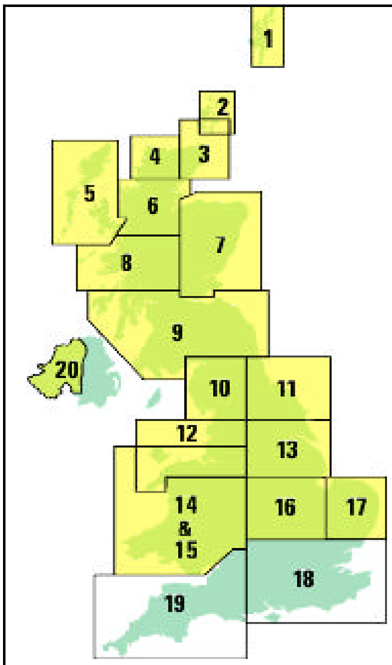


BGS holds locational data on over half a million boreholes from the UK which have been were drilled for a wide variety of purposes including site investigations, coal, water etc. Data on the locations and depths can be accessed from a CD-ROM (British Borehole Catalogue) and detailed logs for most boreholes are available from the National Geoscience Data Centre at BGS. The MRP drilled a number of boreholes, generally less than 150m depth, in the course of its exploration activities and the logs of these are available in the MRP reports. Analyses of the borehole samples together with locational and geological information are held in the Geochemistry Database.

Figure 17. An index map showing location of MRP borehole sample sites

4.4 GEOCHEMICAL BASELINE DATA

The current coverage of baseline data is summarised in Figure 18. The main product of the G-BASE project is a series of geochemical atlases and these are also listed in this figure. The current atlas area under survey (East Anglia) was started in 2000 and sampling will be finished in 2004. Although most geochemical results for the existing samples from East Anglia are available, it has been G-BASE practice not to load data to the Geochemistry Database until all the quality control for data over a complete atlas area is finished. The data conditioning (see Section 6.4) is done on the complete atlas data set. From 2005 onwards G-BASE will adopt a drainage catchment approach to sampling and the time between sample collection and loading results to the Geochemistry Database will be reduced to an annual cycle.



Twenty-one urban areas have been sampled: Cardiff, Corby, Coventry, Derby, Doncaster, Glasgow, Kingston-upon-Hull, Leicester, Lincoln, Manchester, Mansfield, Northampton, Nottingham, Peterborough, Scunthorpe, Sheffield, Swansea, Stoke-on-Trent, Telford, Wolverhampton and York

1. Shetland	11. NE England
2. Orkney	12. NW England and N Wales
3. South Orkney and Caithness	13. Humber-Trent
4. Sutherland	14. Wales & W Midlands (soil and sediment)
5. Hebrides	15. Wales & W Midlands (surface water)
6. Great Glen	16. East Midlands
7. East Grampian	17. East Anglia
8. Argyll	18. SE England
9. Southern Scotland	19. SW England
10. Lake District	20. Northern Ireland

An index map of atlas sheet areas showing areas sampled. Shaded areas have been sampled (area 17 due for completion in 2004). Areas 1 - 15 have been reported as geochemical atlases (Area 13 Humber-Trent due for publication in 2004). Areas 18 and 19 remain to be sampled though part of the Tamar drainage catchment was sampled and reported in 2003. Surveying in N Ireland has been done as commissioned work, a complete geochemical survey of this region is due to start in 2004 as part of the RESI project (Resource & Environmental Survey of Ireland).

Figure 18. A figure showing the G-BASE atlas areas and summary of sampling progress and information

	Sampling	***Sample Preparation and Analyses***
 Stream sediment	Sediment is collected from the active drainage channel of 1st or 2nd order streams. The sediment is wet sieved firstly through a 2 mm nylon screen then a 150 µm nylon sieve. The fine stream sediment is collected in a Kraft™ paper bag. Sampling density varies according to land use and drainage pattern but averages at one sample every one to two square kilometres.	Sediments are dried initially by air drying then freeze drying before being pulverised in agate ball mills. Samples are pelletised ready for XRFS analyses at the BGS laboratories in Keyworth. A combination of wave and energy dispersive techniques gives a range of 48 elements (Ag, Al, As, Ba, Bi, Br, Ca, Cd, Ce, Co, Cr, Cs, Cu, Fe, Ga, Ge, Hf, I, K, La, Mg, Mn, Mo, Na, Nb, Nd, Ni, P, Pb, Rb, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Te, Th, Ti, Tl, U, V, W, Y, Zn and Zr)
 Panned concentrate	The =150 and =2000 µm fraction from the sieving of the sediment is panned on site in a wooden Malaysian-style "dulang" pan. A full pan is panned down to give a constant volume in the centre of the pan. The heavy minerals are scanned for evidence of mineralisation or pollution.	Panned concentrates are not routinely analysed or examined in detail. They are stored for future reference and follow-up as required. Minerals observed in the pan are recorded in the Geochemistry Database
 Stream water	Filtered (0.45 µm cellulose filter) and unfiltered waters are collected from the same site as the drainage sediment. Samples are stored in Nalgene™ bottles and acidified as required by the analytical method.	Alkalinity (by colorimetric titration), pH and conductivity determined on location. Samples analysed at BGS. **ICP-MS**: Ag, Al, As, Ba, Be, Bi, Cd, Ce, Co, Cr, Cs, Cu, Ho, La, Li, Mo, Mn, Nd, Ni, Pb, Rb, Sb, Se, Sn, Th, Tl, U, V, Y, Zn & Zr [31 elements]. **ICP-AES**: Al, B, Ba, Ca, Fe, K, Mg, Mn, Na, P, Si, S (reported as SO_4), Sr & Zn [14 elements]. **Ion Chromatography**: Br, Cl, F, NO_2, NO_3, SO_4, PO_4 [7 ions]. **TIC/TOC analyser** for Non-purgeable organic carbon (NPOC)
 Soil	Soils are collected using a one metre Dutch auger taking five sub-samples at the corners and centre of a 20 m square. A surface sample (0 - 15 cm) and a deeper sample (30 - 45 cm) are taken at each site. Samples are collected from alternate 1 km grid squares apart from urban areas where sampling density is four samples every 1 km^2. Samples are collected in Kraft™ paper bags	The deeper soil samples are dried then sieved to -2 mm. Samples are only routinely analysed in areas where drainage is absent. The surface samples are dried and sieved to -2 mm and pulverised in agate ball mills, then palletised for XRFS analyses as per stream sediment samples. Loss-on-ignition (450 °C) and pH is also routinely measured for soils.

Table 1. A table summarising G-BASE sampling and analytical methods

G-BASE provides baseline geochemical data for onshore Great Britain and N Ireland using stream sediments, stream water and soils at a sampling density of 1 sample per 1 - 2 km^2. The sampling and analytical methods are summarised in Table 1. Data is used to identify regional trends rather than site specific characteristics. In urban areas, the Geochemical Survey of the Urban Environment (GSUE) project collects soil samples at a sampling density 4 samples per 1 km^2. A combination of rural and urban baseline data can be used to assess the extent of anthropogenic modification to the environment. Demand for this data is legislatively driven resulting from recent environmental laws and directives such as the Water Framework Directive (CEC, 2000) and the Environmental Protection Act Part IIa (DETR, 2000).

Information about the G-BASE data in the Geochemistry Database is summarised in Appendix 5 by atlas areas.

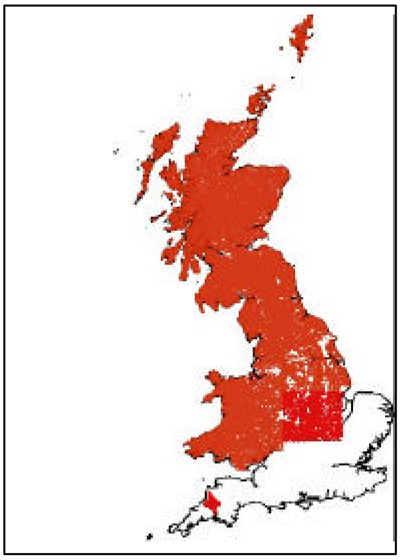


Figure 19: An index map showing location of G-BASE drainage sites (for stream sediment, stream water and panned concentrates). Not including samples from ongoing East Anglia sampling or Northern Ireland

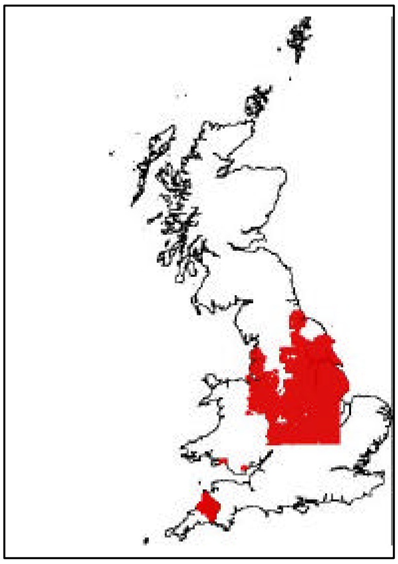


Figure 20: An index map showing location of G-BASE soil sites. Not including samples from ongoing East Anglia sampling

5 Application of geochemical data

5.1 APPLICATION FOR INTEGRATED GEOSCIENCE SURVEYS

5.1.1 Solving geological problems

Geochemical maps are usually interpreted with respect to the known geology, mineralisation and other factors such as land-use and man-made contamination to explain an element's distribution. However, high-quality regional geochemical maps can be used to help in the mapping and interpretation of the geology (Stone and others, 1991; 2003). An example of where this is especially useful is where the field geologist is faced with a large area of fairly monotonous lithology and poor exposure, but the geochemistry shows clear variations which can be attributed to changes in the bedrock. In the Southern Uplands of Scotland, for example, the regional geochemical maps for many elements, irrespective of their overall abundance, produce a marked strike-parallel, NE-SW linearity. The steepest gradients are coincident with tract-bounding faults, but different elements show different distribution patterns. The regional geochemical data thus provides a means of tracking the variation in greywacke provenance through time, and interpreting that variation in terms of tectonic events involved in closure of the Iapetus Ocean.

A bibliographic review of regional geochemical mapping for Quaternary studies has recently been completed by Fordyce (2003). This review covers both BGS and other international work, much of the latter originating from Canada. The preliminary work carried out by the BGS in the Vale of York using the G-BASE soil data suggests an encouraging association between soil chemistry, textural inferences and Quaternary Deposit type (Cooper and others, 2004).

5.1.2 Element Associations

Mineralisation

In the BGS the application of geochemistry to locate mineral deposits in Great Britain and Northern Ireland has been done principally through the now discontinued Minerals and Mineral Reconnaissance Programmes in which regional geochemical data generated by the G-BASE project were used to identify targets for further follow-up work. Geochemistry, combined with geophysics, detailed geological mapping and drilling has successfully identified new mineral deposits in many areas of Great Britain. Notable successes, which have attracted significant commercial investment, include discoveries of gold in Devon and the Ochil Hills, barytes near Aberfeldy, and base-metals and platinum in Shetland.

The G-BASE project produces regional overviews of the geochemistry in the form of its geochemical atlas series, and geochemical anomalies that may be of interest for more detailed exploration are high-lighted. In the past, follow-up investigations of anomalies were carried out as part of the MRP but this is now left to private companies and consultants who use the BGS data under licence. Examination of the regional geochemistry will provide information on the association, and type, of any mineralisation found during the survey. There are many different types of mineralisation, and a few examples of the more common types are shown in

Table 2. Vein-type sulphides such as those of Pb, Cu, Zn and Cd are common, and are often associated with barytes, $BaSO_4$ and fluorite CaF_2. Lesser amounts of trace elements such as Sb, Bi and Ag may be present, depending on the source of the mineralising fluids and the host rock. Red-bed mineralisation is usually characterised by high Ba and Cu values, perhaps with Bi, Ag and even V enrichment, while porphyry-type mineralisation always shows Mo, Cu and Sb enrichment. Gold mineralisation is rare, but the use of pathfinder elements such as elevated As, Sb and Bi levels can be used to focus on likely areas or to characterise a known gold deposit as primary, secondary or derived (such as a placer deposit).

Lithological

Some element associations that are found in the G-BASE data are summarised in

Table 2 and are discussed below. Unsurprisingly calcareous carbonate rocks such as limestones and dolomites, and their metamorphic equivalents, are high in calcium (CaO). Magnesium levels are also high over dolomitised limestones, and the Mg/Ca ratio can be used with caution to estimate the degree of dolomitisation. However, limestone sequences can contain basaltic volcanic horizons in which high Mg levels are normally associated with elevated Cu and Ni values, so these should be readily identified. Strontium is almost always high in limestones and calcareous mudstones, though it is much less abundant than Ca and Mg.

Argillaceous rocks are dominated by clay minerals, hydrous micas and chlorite which are all high in aluminium. However, Al is ubiquitous and therefore a poor discriminant. The trace elements lithium (Li), boron (B) and gallium (Ga) are much more effective indicators of argillites. Gallium is such a close analogue of aluminium that it can be used as a normalising element, for example to compensate for grain-size variation in sediments. Unfortunately Li and B cannot be readily determined by X-ray Fluorescence analysis. Gallium is useful alone, but cannot be used in areas of Zn mineralisation as it is enriched in sphalerite (ZnS).

Argillaceous Red Beds, of which the Mercia Mudstone in the English Midlands is a prime example, show the high levels of elements normally associated with argillites, with high levels of K_2O and MgO, plus Ca, Sr, SO_4 (when determined) and Se especially when gypsum and other evaporites are present. Levels of up to 5% K_2O and 4.5% MgO are typical in sediments over the Mercia Mudstone in the Humber-Trent area, for example.

Black shales and their metamorphic equivalents, graphitic schists, are a highly distinctive lithology produced by slow sedimentation in restricted, anoxic basins, often with a low input of terrigenous material plus high organic matter and sulphide levels, and sometimes associated with submarine exhalative volcanism. Their occurrence tends to be limited both spatially and in time, generally forming thin horizons individually rarely than a metre thick. However, their geochemistry may also be highly unusual and characteristic, with high levels of barium (Ba), molybdenum (Mo), vanadium (V) and uranium (U) being typical. Elevated levels of other elements such as Cu, Ni, Ag, Cd, S, As and Se may also be present, but these are more variable components. Three-component maps using those elements in the above list which have a low natural background level (especially Mo and U) are very useful for delineating Black Shale outcrops.

Sedimentary ironstones fall into two main groups: the sideritic ironstones containing mostly iron carbonate $FeCO_3$ and the goethitic FeO.OH or hydrous oxide group. The former are products of anoxic deposition in swamps and are fairly common in Coal Measures in Britain, the latter are oxic marine deposits often associated with oolites and sandstones and are most common in the Jurassic and Lower Cretaceous in Britain. The sideritic ores rarely give a distinctive geochemical signature from the rest of the Coal Measures, but may also show higher Ca and Mg levels as the mixed carbonate ankerite $(Fe,Ca,Mg)CO_3$ may be locally common. Phosphorus may also be elevated if the mineral vivianite (an iron(II) phosphate) forms, but this is rare. The goethitic ores are geochemically more interesting as the iron (III) oxides react strongly with several other elements to form stable sorbtion products. Principal amongst these is phosphate, which forms a basic $FeO.OH\text{-}FePO_4$ mixture of variable composition. Associated with this is arsenic, which as the arsenate ion AsO_4^{3-} is chemically very similar to phosphate PO_4^{3-} and likewise reacts to give a stable sorption compound like an impure scorodite, $FeAsO_4$. Uranium is also strongly bound to phosphates, and relatively high levels of As and U are often found in association with such ironstones.

Basic igneous rocks such as basalt, dolerite and gabbro usually show high levels of MgO, TiO_2, Ni, Cu and a high V/Cr ratio, whereas in ultrabasic rocks and sediments derived from them, high Cr is most characteristic element, with high MgO and Ni as with basic rocks, but a high Cr/V ratio. A high MgO/TiO_2 ratio is typical of ultrabasic rocks, while conversely a high TiO_2/MgO ratio is more indicative of basic igneous rocks, especially basalts.

Evolved granites and pegmatites are notable for their high content of light, 'misfit' and volatile elements and usually show high Be, Li, U, Sn levels and a high Rb/K_2O value. Boron and other rarer elements such as niobium (Nb) may also be high in pegmatites, while Y and La levels are also higher than in most 'normal' granites. Beryllium is also common in normal granites along with high K_2O, Rb, U and Li levels, but with a lower Rb/K_2O ratio than in evolved granites. Strontium may be high, but this is more abundant in, and characteristic of, granodiorites and syenites which may also show higher Ca levels than in 'true' granites. Beryllium (Be) and K_2O are also present at high levels, but unfortunately Be cannot be determined by XRF analysis.

The 'resistate' elements are those which form, or occur in, minerals which are highly resistant to chemical and physical weathering, and are mainly those which are also high field strength (HFE) elements. As the minerals are persistent in sedimentary environments, but may be derived from different source terrains, they are very useful for provenance studies. Those elements listed in

Table 2 are the most commonly used, and ratios and combinations of these can be very effective discriminants in otherwise monotonous mudstone and greywacke dominated sedimentary sequences, especially when used in conjunction with mineralogical studies.

Quaternary Deposits

The geochemistry of Quaternary deposits will depend largely on the parent material from which they have been derived as described above. The erosion/dispersion/deposition path of the more exotic lithologies with strong geochemical characterisation (e.g. pegmatites) should be discernable from the analysis of stream sediments and soils. However, the origins of glacial deposits can be very complex and the links between surface sediment geochemistry and provenance are difficult to determine using geochemistry alone. A useful way of differentiating between drift deposits is on the basis of their texture (see Figure 21). Sand deposits will have a different geochemical signature to clay deposits and these can be distinguished by doing factor analysis and plotting the factor scores for the different factors attributable to textural differences.

Urban contamination

Urban-industrial contamination is widespread in Britain, especially - but not exclusively - in the coalfield conurbations. Indeed, such is the degree of historical contamination in the coalfields that it is difficult to establish a pre-industrial geochemical baseline for the Coal Measures in many areas. Many elements, especially heavy metals such as Pb, Cu and Zn, give an 'urban' signature, but the most distinctive are those which have a low natural abundance (excluding mineralisation) such as tin (Sn), antimony (Sb) and cadmium (Cd). Where coal mining has been accompanied by related heavy industries such as iron and steel making and engineering, the range of metal contaminants is wider and includes Cr, Ni, V and Mn, which are widely used as alloys in tool steels etc. In Britain, many coalfields show a natural elevation of Ni values, so this must be considered. Coal-burning, both domestic and industrial, appears to be the main source of several metals, and petrol lead can also be detected by its isotopic signature. Coal ash and other industrial wastes such as furnace slag are often a major component of 'made ground' in urban areas, and these may also be high in metals.

Germanium data, available from the East Midlands atlas area onwards, is also likely to be a good indicator of industrial/coal waste contamination as it is often enriched in coal waste.

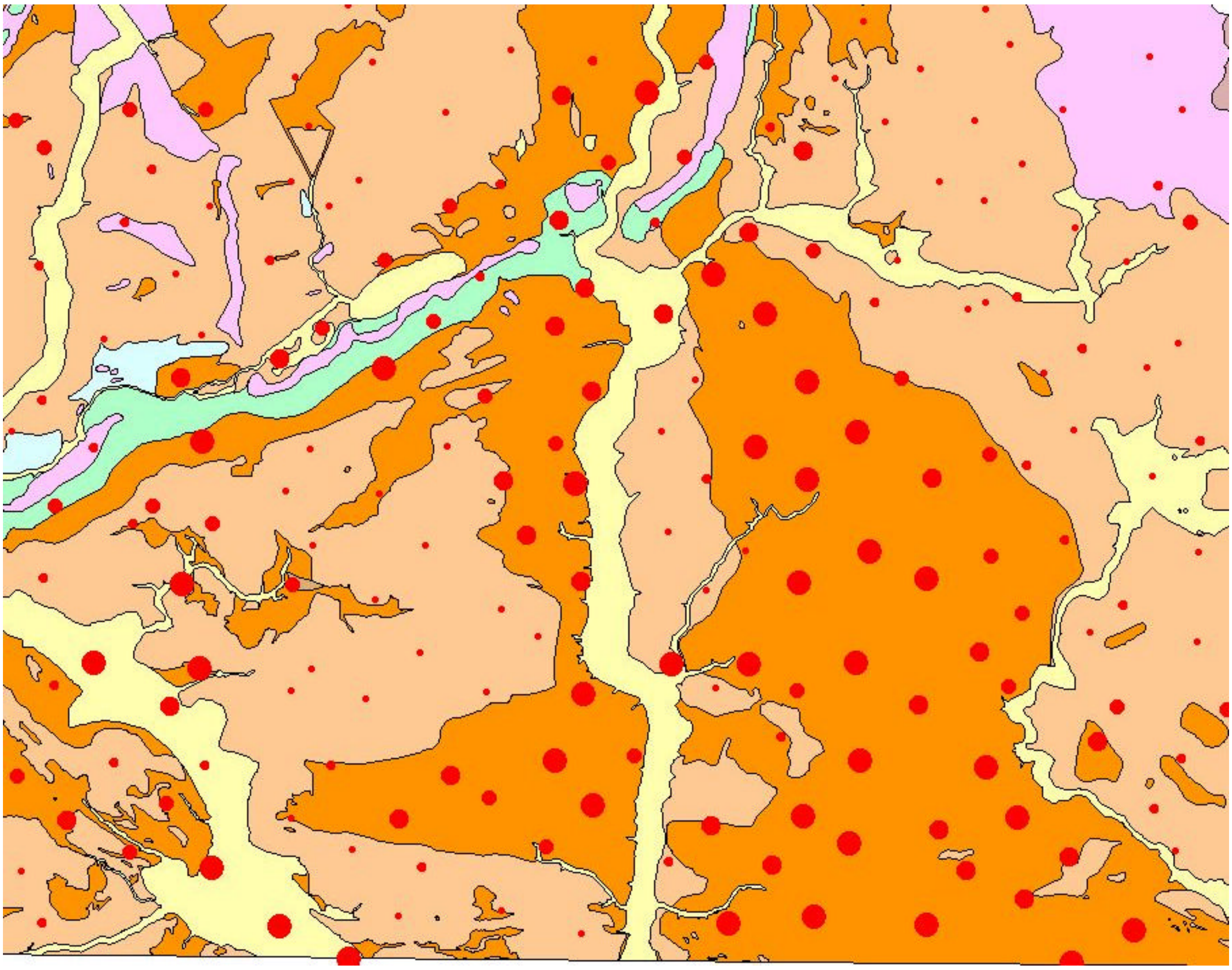


Figure 21. Geochemistry of the near surface, determined in soils to differentiate geological lithologies. The large red dots indicate high levels of titanium oxide in the soil and correspond to the clay lithologies. The sands have small dots and are depleted in titanium oxide. This type of analysis has helped to determine areas where mapping needed revision (after Cooper and others, 2004)

Secondary precipitations

In stream sediments and soils, secondary geochemical processes may, under certain conditions, be sufficiently influential to alter the concentrations of certain elements, such that a primary source control may be overwritten. Most prominent of these is the formation of secondary hydrous oxides of iron and manganese, which occurs when Fe and Mn, transported in reduced form as M^{2+} ions or as organic complexes in shallow groundwater, are oxidised in contact with oxygenated water in surface streams to form Fe(III) and Mn(III) and (IV) hydrous oxides or 'ochres'. The process is most common in waterlogged, acid, upland peaty catchments; and such streams are often marked by prominent yellow to orange precipitates and black-coated pebbles. These hydrous oxide coatings and precipitates are effective sorbants for certain other elements, notably cobalt (Co) and arsenic (As). Cobalt is very strongly and selectively absorbed by Mn oxides in which may be a coupled oxidation-reduction reaction which As is bound to hydrous iron oxides as AsO_4^{3-}, along with PO_4^{3-}, as with sedimentary ironstones discussed above. Lead is also bound strongly to secondary oxides, other elements much less so. Copper, for example, is much more likely to bind to organic material such as humic acids.

Geological or environmental features	**Principal associated elements and ratios**
Carbonate rocks (limestones, dolomites, calc-schist)	CaO Sr MgO
Argillaceous and pelitic source rocks	Li B Ga
Argillaceous Red Beds (eg Mercia Mudstone) with evaporites	K_2O MgO Sr *Se*
Black shales and graphitic schists	Ba Mo V U *Cu Ni Ag Se Cd*
Sedimentary ironstones	Fe_2O_3 As P_2O_5 U
Basic igneous rocks in unmineralised areas	MgO TiO_2 Ni Cu V/Cr
Ultrabasic rocks and derived sediments	Cr MgO Ni Cr/V
Evolved granites	Be Li U Sn Rb/K_2O *Y La*
'Normal' Granites	Be K_2O Rb U Li *Sr*
Granodiorites and some intermediate igneous rocks	Be Sr Ca K_2O
Resistate elements for sediment provenance variation, especially in greywackes and arenites	La Y Zr TiO_2 Th Ce Nb - and ratios of these.
Generalised Urban – industrial contamination	Sn Pb Cu Sb Cd Zn
Industrial contamination – heavy engineering	Sn Pb Cu Sb Cd Zn Cr Ni V Mn
Secondary hydrous oxide formation in stream sediments	Mn Co As Fe_2O_3
Mineralisation (vein type sulphide)	Pb Zn Ba Cu Cd *Sb Bi*
Mineralisation (Red-bed type)	Ba Cu *Bi Ag*
Mineralisation (porphyry type)	Mo Cu Sb
Gold mineralisation ('pathfinder' elements)	As Sb Bi

Table 2: Summary of some element associations and their application (*elements in italics are not of primary importance in associations)*

5.1.3 Graphical representation of element associations

Single element distributions and patterns can be used to solve geological problems, and identify areas of mineralisation or anthropogenic contamination. A combination of different elements or "element associations" can be used like a fingerprint to characterise a particular geological setting, identify a style of mineralisation or determine the origin of contamination.

In its simplest form this may be a non-parametric ranked approach where samples that have the higher values of a particular elements are assigned a high score. For example, samples containing the highest levels of Mo, Cu, and Sb could be indicative of porphyry type mineralisation. However, element associations determined by statistical analysis of sites could miss spatial patterns that are best seen by plotting maps and using a GIS. The study of element associations must be a combination of graphical representation and statistical analysis.

Statistical analysis has many limitations and techniques have to be used with caution. Howarth (1983) and Davis (1986) are texts that describe methods that can be used in geochemical data analysis. It is best practice to use several statistical techniques to identify element associations and look for a consensus of associations shown between them. Correlation, cluster and factor analysis are the three main methods used for identifying site specific element associations. These methods give tables of results from which element associations can be determined, results that are best presented graphically as illustrated in Figure 22 and Figure 23. Factor analysis applied to regional geochemical data is discussed by Reimann and others, 2002.

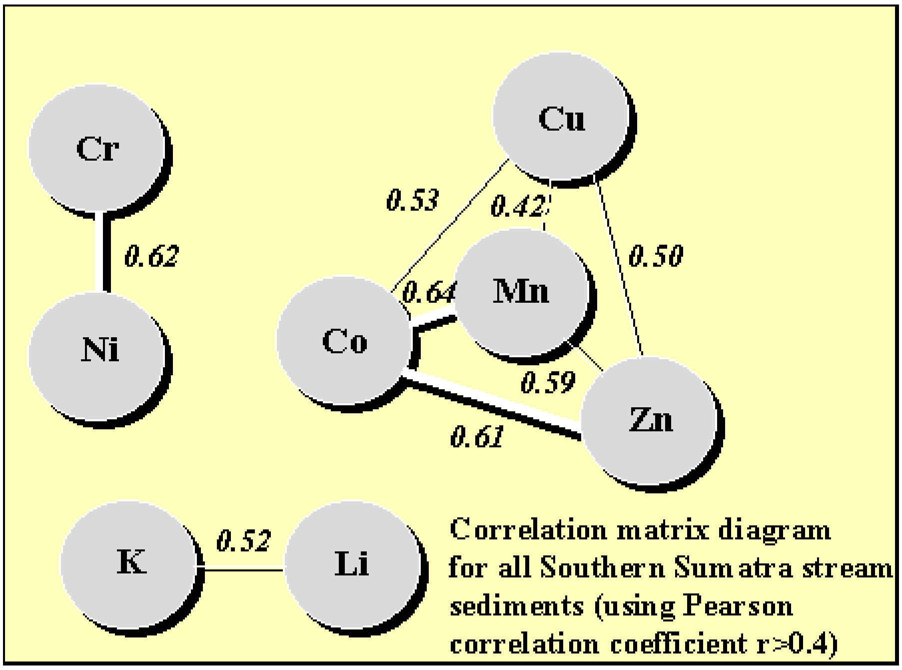


Figure 22: A correlation matrix diagram showing the three principle element associations of the Sumatra regional geochemistry data (after Machali and others, 1997)

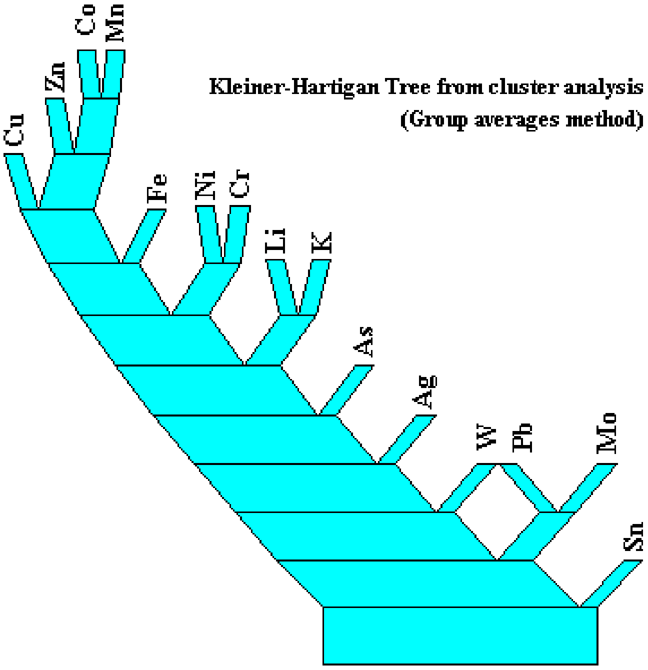


Figure 23: Example of a Kleiner-Hartigan tree - a graphical representation of cluster analysis (from Machili and others, 1997). This show the three element association determined by correlation analysis shown in Figure 22.

In factor analysis of geochemical data the different factors represent different element associations. The different factor scores can be plotted to indicate which areas of the map are dominated by a modelled element association (Figure 21). A further way of presenting element associations as three component maps is discussed in Section 7.3.

5.2 ENVIRONMENTAL AND WIDER APPLICATIONS

5.2.1 Environmental applications

It is estimated by the Environment Agency that some 300,000 hectares of land in the UK are affected by contamination resulting from industrial activity. Local Authorities are required by legislation introduced in 2000 to identify and deal with such contamination. Part IIA of the Environmental Protection Act (1990) (DETR, 2000) provides a framework for the regulation of contaminated land and has been introduced progressively throughout Great Britain since April 2000.

G-BASE baseline geochemistry, particularly that for urban areas, can be used in the context of the Contaminated Land Exposure Assessment (CLEA) model, an ongoing programme of work supported by DEFRA, the Environment Agency and Scottish Environmental Protection Agency. Soil Guideline Values (SGV) produced by the model are given on the right as a function of land use and indicate a concentration below which a site can be considered safe.

The EU Water Framework Directive (CEC, 2000) came into force in December 2000, a framework for the integrated protection of the water environment. G-BASE provides information about surface water geochemistry that is used in support of this Directive (Ander, 2004).

Pollutant	Residential with plant uptake#	Residential without plant uptake*	Allotments@	Commercial/ Industrial~
As	20	20	20	500
Cd	1 (pH 6) 2 (pH 7) 8 (pH 8)	30	1 (pH 6) 2 (pH 7) 8 (pH 8)	1400
Cr	130	200	130	5000
Hg	8	15	8	480
Ni	50	75	50	5000
Pb	450	450	450	750
Se	35	260	35	8000

(all concentrations in mg/kg dry weight soil)

\# House with a garden and therefore the possibility of ingestion of home-grown vegetables

* House or apartment with no private garden area

@ Open space, often made available by the local authority, for people to grow fruit and vegetables for their own consumption

~ Assumes that work takes place in a single-storey building, factory or warehouse where employees spend most time indoors involved in office-based or light physical work. Does not apply to sites with 100% hard cover, such as car parks

Table 3: CLEA soil guideline values (DEFRA and EA, 2002)

G-BASE baseline data can be used to delineate areas of pollution and contamination. Whilst sampling aims to collect samples representing the natural baseline it is not possible to collect samples that have not in some way been affected by human activity. Examples include, heavy metal contaminated soils associated with drained fenland in Lancashire (Breward, 2003) and the Capper Pass Tin Smelter anomaly near Hull (O'Donnell and Rawlins, 2003 and Figure 24). The report on the Stoke-on-Trent urban soil geochemistry is a comprehensive account how the geochemical data can be applied in an urban environment (Fordyce and Ander, 2003).

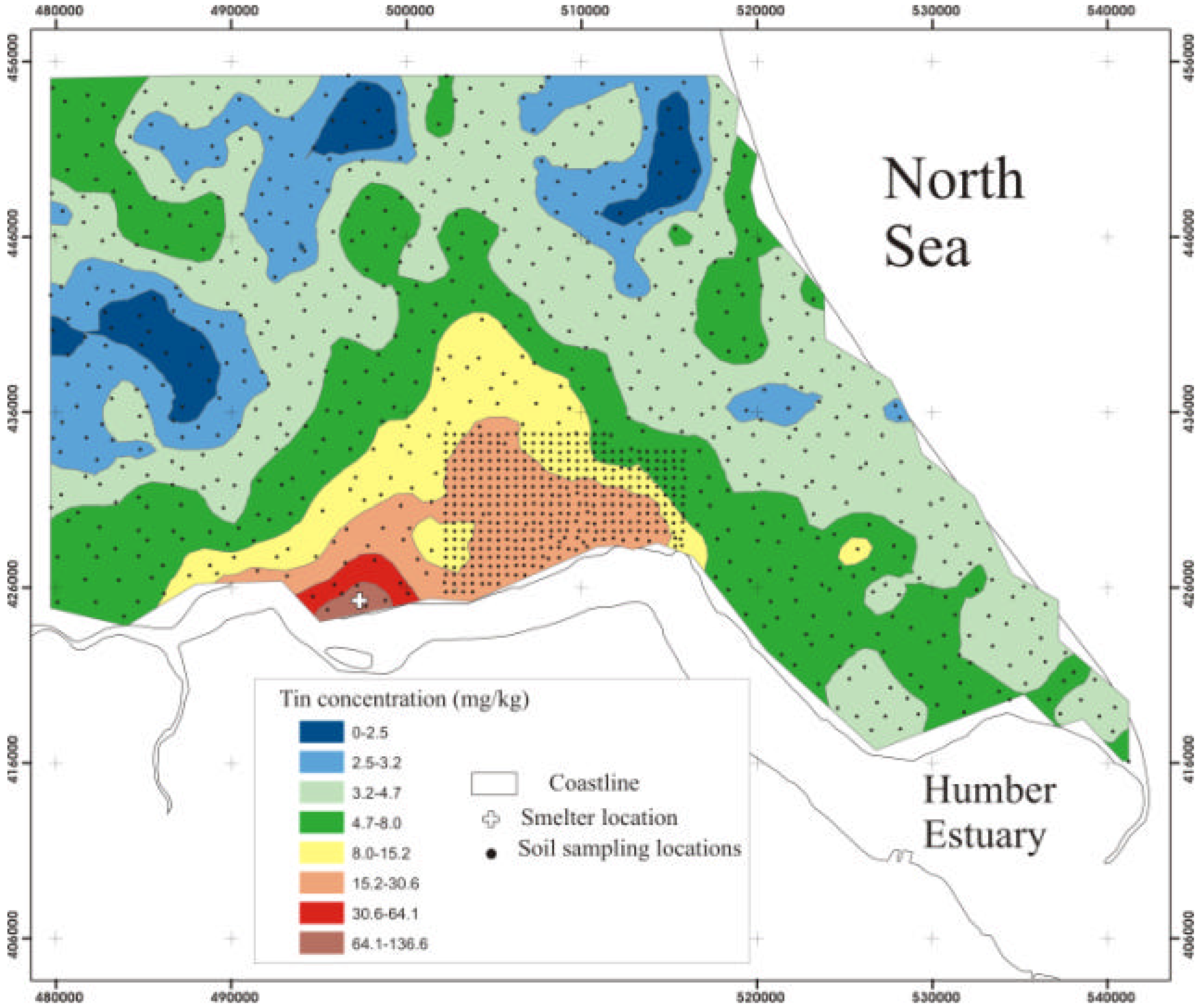


Figure 24: Plume of tin (Sn) in soil surrounding the Capper Pass smelter delineated by the integration of G-BASE rural and urban (Hull) soil geochemical baseline data (after O'Donnell and Rawlins, 2003)

Geochemistry and Health

The application of regional geochemistry to problems in medical geology was pioneered in the 1960s by Professor John Webb (Imperial College) in the UK. This work demonstrated numerous relationships between geochemistry and animal and plant health such as: incidences of cobalt deficiency in sheep; selenium toxicity and molybdenum-induced copper deficiency in cattle; arsenic and lead toxicity in animals; copper and manganese deficiency in seedling spruce; and manganese deficiency in cereals. Early G-BASE involvement in this field is described by Thornton and Plant (1980).

Historically we depended on the local environment for our food and water supply. Local environmental deficiencies in essential trace elements such as iodine and selenium can result in endemic diseases caused by insufficient quantities of such elements in the daily diet. Lack of iodine, for example, causes a host of medical conditions grouped together as iodine deficiency disorders ranging from the manifestly obvious goitres (swollen necks) to mental retardation and cretinism. Our current diet of food from a diversity of areas and non-localised water supplies have made such endemic diseases a thing of the past in the UK, but they still persist in many of the developing countries of the world. However, such trace element deficiencies also afflict livestock and measures have to be taken to supplement their diet of predominantly home-grown fodder. Geochemical maps of the UK can help us to predict where such deficiencies occur and such areas can be targeted with trace element supplements.

Two main groups of chemical elements are important for health:

Essential to Animal Life	Potentially Harmful Elements (PHEs)
Fe, Mn, Ni, Cu, V, Zn, Co, Cr, Mo, Sn, Se and I	As, Cd, Pb, Hg

Some elements that are essential can also be toxic. Selenium and molybdenum are examples of elements which show a relatively narrow concentration range between toxicity and deficiency. The potentially harmful inorganic elements are considered to be part of the PBT chemicals, that is, persistent, bioaccumulative and toxic pollutants. These are long-lasting and highly toxic substances that can build up in the food chain to levels that are harmful to ecosystem health.

Elementary detectives

G-BASE samples have been used to help determine where materials may have originated as the geochemical data can be used as geochemical fingerprints. For example, this has been done to help archaeologists determine the origins of some Scottish redware pottery using some forty-five trace and minor elements. Isotopic studies in particular have utilised G-BASE samples to distinguish between natural and anthropogenic sources of Pb and U. It is possible to distinguish between lead anomalies in the environment derived from ore deposits and the lead derived from petrol engines. High levels of natural uranium can be distinguish from that associated with the nuclear industry.

Dissolved sulphate can cause damage to concrete structures due to reaction with the calcium aluminate phases in Portland cement. This is recognised as a engineering problem in the UK and such damage has been recognised on the M5 motorway in the Worcestershire Basin in the southern Midlands of England. The use of combined sulphur and strontium isotopes in G-BASE water samples can be used to identify sources of certain solutes and distinguish between natural and anthropogenic sources (e.g. fertilisers).

G-BASE has both a vast store of soil samples and soil geochemical data. With other techniques such as mineralogical analysis, geochemical finger printing may have an increasingly important role in forensic geoscience. This is currently being studied as a "development of capabilities" project within BGS.

6 Limitations on the use of geochemical data

The Geochemistry Database contains a field that indicates the confidentiality level of the data (see Appendix 1, Question 2). This must be considered as the first factor that might limit the use of the data. All regional G-BASE data loaded to the Geochemistry Database is available for BGS and other NERC researchers to use for non-commercial research. For users outside NERC the data are available under licence where specific terms apply according to use. The following sections consider the technical limitations that may constrain the use of the data.

6.1 SPATIAL RESOLUTION AND LOCATIONAL ACCURACY

Regional baseline geochemical samples are collected using 1:50 000 OS topographic base maps but the earliest work would have used the old 1" OS maps. Urban baseline data is collected using 1:25 000 OS maps. MRP samples would have been collected using maps at a variety of scales but as some of the results represent detailed follow-up of mineralisation, maps of 1:10 000 scale or less will have been utilised. With the 1:50 000 scale maps it is estimated sites could be plotted to the nearest 50 m and with 1:25 000 maps to the nearest 25 m. Since 2000 the G-BASE project has used GPS systems to determine the grid reference at location and this is estimated to give an accuracy of ± 10 m. Full British National Grid references are used that cite locations to the nearest metre though in view of the accuracy possible for map plotting the last metre digit holds little meaning. The 100 km two-letter map codes are not utilised, for example, the correct database grid reference for the location of BGS Keyworth would be [462160 331720] and not [SK 62160 31720]. **Grid_accuracy** is a field that is available in the site tables of the database. It is a field that has not been fully utilised and it recommended that data added from now onwards should have a value in this field and that the field is populated for the G-BASE data already in the database.

A knowledge of the accuracy to which samples have been collected is now much more important as desktop GIS users of the database can zoom in and out to display the results at inappropriate scales. The suggested cut off scales below which data should not be displayed in a GIS are:

- G-BASE and MRP drainage sample data - 1:25 000
- G-BASE regional soil data - 1:25 000
- G-BASE urban data - 1:20 000
- MRP soils and tills - 1:10 000
- MRP rock and drill core 1:10 000

It is important to emphasise that regional geochemical mapping is done to identify regional trends rather than site specific anomalies. This is particularly important for the display of urban data where a single anomalous soil site could blight an area if the data is not displayed appropriately.

6.2 SITE INFORMATION

Site information is recorded on standard field cards such as that shown in Figure 10. The version of the field card and codes is another under-used field in the Geochemistry Database site tables called Code_Version. Field card version codes are listed in the domain table **BGS_MTA_DOM_CODE_VERSION**.

Much of the information recorded for the site is from a restricted list of codes say for example, land use, contamination at site, soil/sediment colour. Free text comments qualifying coded information is entered on the field card but not necessarily loaded into the Geochemistry

Database. When following up anomalous data from a specific site it is standard practice to refer back to the original field card (see Section 4.1).

6.3 ERROR, ACCURACY AND PRECISION OF ANALYTICAL RESULTS

Quantifying error and defining analytical accuracy and precision is part of the "data conditioning" process (see next sub-section). Errors will occur throughout the sampling, analytical and interpretative procedures. Human error is a major contributor but the sampling or analytical equipment will contribute to the total error. It is essential to have procedures in place that minimise error yet at the same time steps are taken so that the error can be quantified. If the error contribution in a result is greater than the natural variability then the sampling and/or analytical strategies may need to be revised. Error can be quantified by the use of control samples that go through all the steps in the geochemical sampling and analysis procedures. These blank, duplicate, replicate and standard control samples are generally "blind" to the operators and can be used as estimates of error, accuracy and precision. These estimates will let a geochemist understand how "fit for purpose" geochemical results are.

Methods for determining accuracy and precision will not be described here (see Lister and others, In Prep) but it is worthwhile to define what these terms mean. **Accuracy** is a measurement of how closely a result is to the true value. In reality we will never know the true concentration but we can produce a consensus value from repeated analyses, preferably using a variety of methods and being cognisant that some techniques give only the partial concentration of some elements. We use an **accepted value** rather than the true value. **Bias** is the difference between the actual result and the accepted value and different analytical methods will be associated with a particular bias. **Precision** is a way of expressing how repeatable and comparable a result is. Good precision does not necessarily mean high accuracy. The **sensitivity** of a method is the degree to which small changes in analyte concentrations can be determined and generally if the method can distinguish between small changes, a good lower **detection limit** (the lowest concentration that can be estimated from a single determination) can be achieved. If the sensitivity of a method is poor then the results will be reported in steps, say for example, every 10 mg kg^{-1}. Such data is referred to as **censored** data.

Unfortunately the Geochemistry Database has not been used to store control sample data or information about precision and accuracy. This must be taken from accompanying documentation such as a geochemical atlas or MRP report. It is now part of the G-BASE procedure to produce a quality control report (in the BGS Internal report series) for data before it is loaded into the Geochemistry Database (e.g. Lister, 2002). An ANOVA analysis from such a report is given in Table 4. This shows the percentage variance associated with: the natural variation between sites; the variability between samples collected at the same site (i.e. duplicates); and the analytical variance from splits of the same sample (replicates). The table shows there are analytical issues to be considered for U, Cd and Sb and these need to be borne in mind when interpreting the data.

Element	Between Site (%)	Between Sample (%)	Within Sample (%)
MnO	96.03	3.92	0.05
Fe_2O_3	96.62	3.36	0.01
V	97.85	2.09	0.06
Cr	93.46	5.55	0.99
Co	94.00	5.62	0.38
Ba	97.39	2.56	0.05
Ni	95.96	3.83	0.21
Cu	98.87	1.08	0.06
Zn	92.64	7.34	0.02
Mo	93.59	3.23	3.17
Pb	96.51	3.43	0.06
As	97.87	1.82	0.31
U	76.92	10.99	12.09
Cd	65.44	3.95	30.61
Sn	95.77	2.42	1.81
Sb	87.68	3.05	9.27

Table 4: Results from the ANOVA analysis of some G-BASE urban control samples (after Lister, 2002)

Geochemical data published in journals need to be accompanied by results for international reference standards so readers and users of the results can assess their accuracy and compatibility.

When using geochemical data remember to:

- consider whether the results are accurate, i.e. could the high or low levels be an artefact created by inaccurate analysis. Accuracy is not so important if you are just considering relative amounts of an element within a specific area
- question whether the data you are using represents total or partial concentrations
- look at the precision for the element your are interpreting. It is no use discussing variations of 1 mg kg^{-1} levels of an element if the precision of the method is such that result reproducibility is ± 5 mg kg^{-1}
- use the appropriate number of significant figures for the precision of the data
- convert elements that are usually reported as percentage oxides from the elemental ppm results recorded in the database. The Geochemistry Database stores all data in ppm. Conversion factors are given in Appendix 3.

6.4 DATA CONDITIONING

The term conditioning is used in the sense of "*to render fit for work or use*" and is discussed by Lister and others (In Prep). The process of data conditioning includes a number of steps that the data undergoes before it should be loaded to the Geochemistry Database. Data quality control (QC) using established quality assurance (QA) procedures includes error checking, determination of accuracy and precision and standardisation of the data within a field campaign, within atlas boundaries and in the context of the national data set.

The time spent preparing data for use is always an under-estimated part of any geochemical project yet vital to its success. The Geochemistry Database provides good quality controlled and assured results that can be applied to a variety of uses. The main failing of the Geochemistry Database is that, because of a lack of staff resources since its creation, the domain field codes have not been kept up-to-date and useful fields that provide information about the data (such as grid accuracy or map sheet scale) have not been populated.

One issue that has been addressed is standardisation of the regional G-BASE results (sediments and soils) so that seamless geochemical maps and images can be plotted. This takes into account the different analytical methods used and removes any analytical drift between field campaigns. The G-BASE data in the Geochemistry Database is not the raw data as received from the laboratories but data to which a standardisation factor has been applied. Data standardisation can be done by a variety of methods (Lister and others, In Prep) and the G-BASE data is currently standardised with respect to the Welsh atlas area analyses. G-BASE water data has not been standardised because full data conditioning has only been completed on the Welsh stream waters though it is in progress for the Humber-Trent and East Midlands areas.

Previous to the Welsh atlas (in which soils and sediments were analysed by XRFS), direct reader optical emission spectroscopy was used. This has meant significant data standardisation has been required to make the two analytical subsets compatible because of the inevitable bias between the two analytical methods (Section 6.3). This has been done for the following twenty elements:

barium, calcium, cobalt, chromium, copper, iron, gallium, potassium, magnesium, manganese, nickel, lanthanum, lead, rubidium, titanium, strontium, vanadium, yttrium, zinc and zirconium. For other elements standardisation is in progress.

6.5 DETECTION LIMIT ISSUE

One of the more problematical issues in using geochemical data is how to deal with data that is reported as being below (or above) the reporting limit for the analyte in question. Over the past thirty five years:

- the range of trace elements determined has increased
- detection limits for analytes have generally improved
- the way in which below (or above) detection limit data is reported from the laboratories has changed and is variable. Some analytical techniques now report a different detection limit for each sample depending on the sample matrix
- below detection limit data has been loaded into the Geochemistry Database and includes '0' for some of the Scottish G-BASE data.

The Geochemistry Database does have adequate provision for presenting the user with detection limit information. For each laboratory batch analysed there is a table into which analyte detection limits can be entered (**BGS_DTA_ANALYTES**) but generally this table has not been populated so this information is not readily available. Furthermore, the table **BGS_DTA_ANALTYE_DETERMINATIONS** has a qualifier field to indicate whether the data is below (<) or above (>) detection. Unfortunately, this field has been neglected in both the loading and retrieval of data from the database so generally information about results outside the detection limit is difficult to recognise. For many purposes, mineral exploration for example, low results are of little interest so knowledge of the lower detection limit is of little consequence. However, for environmental baseline data regional trends on all the results are important to interpret and if no measures are taken to deal with below detection data, artificial trends will appear on the maps. Figure 25 showing thorium in stream waters from the Humber-Trent atlas area illustrates this point well. Thorium levels are generally low and close to the detection limit currently cited at 0.01 µg l^{-1}. Stream waters were collected over three field seasons, firstly to the north of the Humber in estuary 1994, then in 1995 in an east-west area across the middle of the region, finishing in the south in 1996. Each year the water samples were analysed and the detection limit for 1994 is cited at 0.098 µg l^{-1} compared with 0.01 µg l^{-1} for 1995 and 1996. Because most of the results are near or below detection the patterns shown on the geochemical image can vary enormously depending how the below detection results are handled. In particular, the distinctive detection limits means that yearly campaign boundaries are well defined if each year's limits are applied to the respective data sub-sets (Figure 23(b)). However, without doing anything about detection limits, real data values reported below detection may show meaningful trends (Figure 23(a)). Applying a single common detection limit to all the data produces completely different images according to whether the highest or lowest value is employed (Figures 23(c) and (d)). The "safest" representation is probably that of Figure 23(d) in which all the data has been degraded to accommodate the worst detection limit. This gives good distinction of highs and lows but loses all the detail and trends seen when other detection limits are used. Generally, in geochemical atlases G-BASE has used this conservative "safe" approach which is unfortunate in that it degrades meaningful data but it does eliminate campaign boundaries. Such detection limit contrasts are also to be expected between atlas areas, for sediments as well as soils.

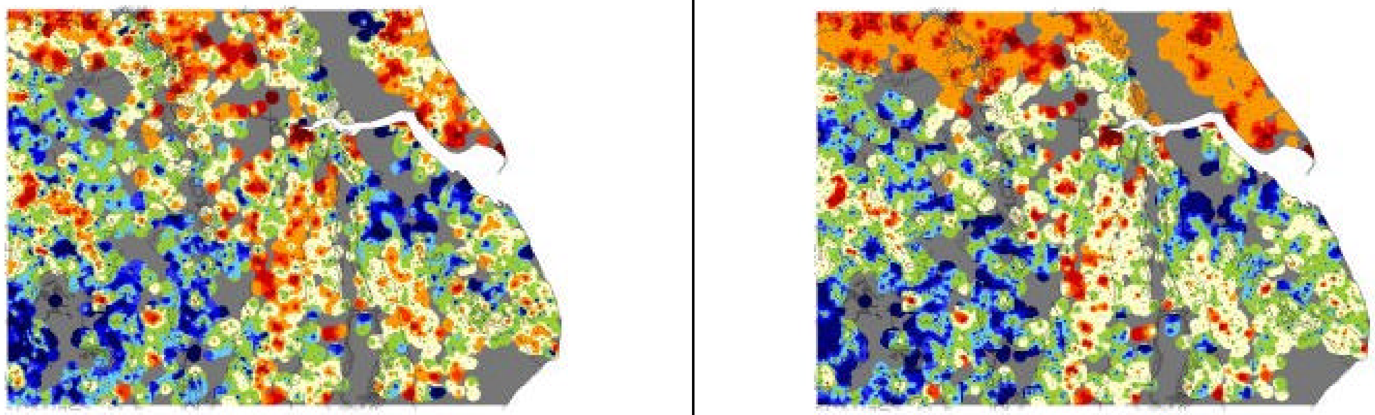
A recent review of below detection data in the Geochemistry Database has suggested that loading results that are actually below an analytical method's cited detection limit is useful but it is very important that the qualifier field and detection limit information is also loaded. In this way it is up to the user of the results to deal with the detection limit issue in the manner appropriate to the purpose for which the data is being used.

Non-geochemists using data from the database should be aware of this detection limit issue and if they are using data that is predominantly below or near the lower detection limit they should seek advice from a geochemist on how to deal with it.

6.6 COMBINING DIFFERENT SUB-SETS OF GEOCHEMICAL DATA

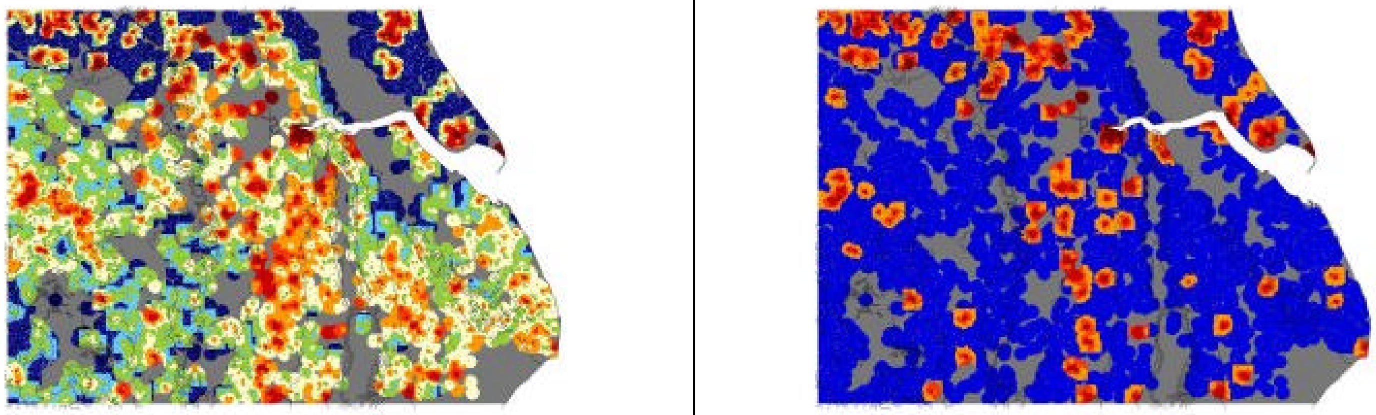
The Geochemistry Database provides the means of drawing together for a single area all the geochemical data generated by BGS projects, particularly a combination of MRP and G-BASE data. Because there is a degree of standardisation between methods and procedures used, combining the data from different BGS projects is generally not problematical. However, there are certain rules to observe:

1. Never interpret different sample types as a single data set (i.e. do not mix sediments and soils or panned concentrates with stream sediments). Be careful to check that similar sample types have been processed in a similar way. For example, a -2 mm soil fraction should not be mixed with analyses of a -150 µm soil fraction
2. Never mix results generated by total and partial extraction without doing data standardisation first
3. Be aware that data within your data set may have been analysed by different analytical methods or laboratories. Always check that the data has been standardised first
4. Be aware that data generated by different projects will have been generated for different purposes. This may mean that different techniques may have been applied, for example partial extraction during chemical analyses
5. Sampling techniques may have changed with time, particularly for panned concentrates, which formerly were panned to a 'heavy mineral concentrate" but latterly panned to a constant volume. This information may not have been recorded in the database but is normally available in the associated MRP report or atlas description of the sampling methodology.



(a) Raw data as reported from laboratory

(b) Data with different detections limits applied for three different annual sampling campaigns



(c) Detection limit correction applied using best detection limit (i.e. lowest) to data from the three different annual sampling campaigns

(d) Detection limit correction applied using worst detection limit (i.e. highest) to data from the three different annual sampling campaigns

Figure 25: A figure showing the effect of using different detection limits on a geochemical image of thorium in stream waters from the Humber-Trent collected over a period of three years (i.e. three summer field campaigns). See text for explanations.

7 Using Geochemical Data in a GIS layer

This section is a brief description of how geochemical data can be presented. Before preparing maps it is worth thinking about what you want to show on the map and who is the map for, remembering the important equation:

DATA + KNOWLEDGE => INFORMATION => DECISIONS

What needs to be shown on the map should be clearly seen and not obscured by information that is not required. The map user must clearly understand what the map shows with a visual impact that is more informative than the tables of raw data.

7.1 ANNOTATED POINT MAPS

Annotated point maps (sometimes called posted data point maps) are the simplest way of representing geochemical data. The element concentration (or concentrations if a list of analytes is being displayed) is printed next to the sample location on the map usually represented by a cross or dot (Figure 26). This is a simple way of listing results with no interpretation and can be multi-element if more than one element is listed. Two problems with such maps are that the annotations inevitably overlap, particularly for high density sampling, and the user's attention is not drawn to significant results. The latter can be remedied by doing some simple interpretation and plotting, say for example, the highest 5% of results with red text annotation.

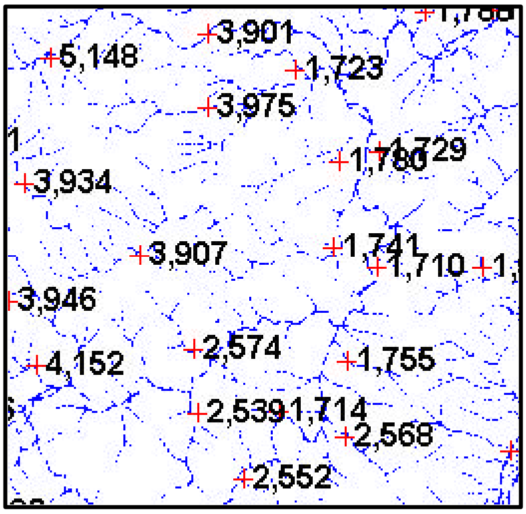


Figure 26: Example of annotated point map. This example is from the Morocco geochemical project showing a map generated in MapInfo and displaying sample number.

7.2 SYMBOL POINT MAPS

These are the commonest form of map used in geochemistry and they can be "univariate" (i.e. showing just one element) or multivariate (showing many elements). The sample site is usually represented by a symbol whose size and/or colour is related to the element concentration. Hexagons and circles are the most commonly used symbols, preferably with an indication of where the symbol centre is. The colouring can be used to give an immediate visual impression of element levels and can either be monochrome with varying levels of intensity (e.g. very deep red to very pale red) or use two or more colours usually with red/brown colours indicating highs and blue lows. The symbol size can be directly proportional to a function of the element concentration (e.g. $\log_{10}x$) with a necessary upper truncation to avoid oversized symbols. Such maps are referred to as proportional symbol plots. The symbol size can be graduated with a fixed size of symbol representing a particular class or range of element concentrations. A graduated classified symbol plot is the preferred way of representing BGS urban baseline geochemical data (Figure 27).

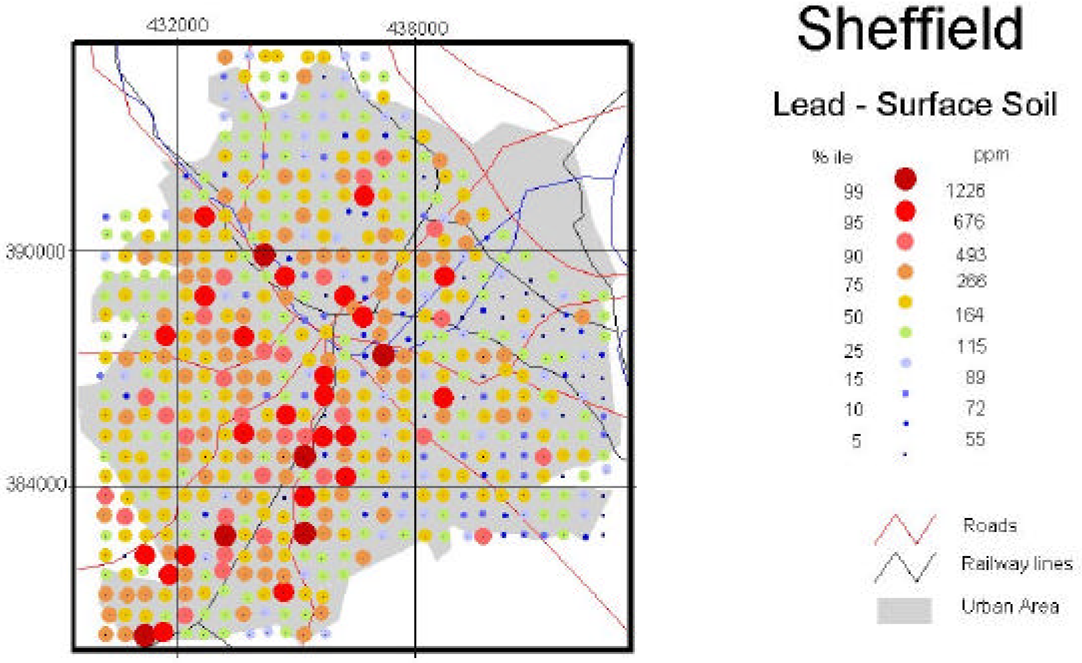


Figure 27: Example of a classified symbol plot. This example is taken from the report on the Sheffield baseline geochemical mapping (Freestone and others, 2002)

7.3 GRIDDED IMAGES AND THREE COMPONENT MAPS

The preferred method for presenting regional geochemical results is coloured gridded images (Figure 28). Such maps require greater computing skills than required for the point maps and tend to represent a highly interpretative way of displaying geochemical data that is very subjective to parameters chosen in the gridding software. The gridding needs to take into account the size of each grid cell, the number of samples contributing to each cell value, the radius of search, search direction and the weighting factor for more distant samples. It is very important that the gridding parameters used to produce the image are documented so those using the image can understand its derivation. This method of map production is ideal for soils collected on a regular grid but has to be used carefully for something like drainage samples where extrapolation across drainage catchment boundaries is not desirable. When gridding stream sediments it is best to use small cell sizes and small search radii. The standard method for the production of G-BASE gridded images is as follows:

The geochemical and locational data are retrieved from the BGS Geochemistry Database using one of the methods described in Section 3.1. In order to generate, process and edit the geochemical images for single elements, the concentration data need to be interpolated. This can be done either by a proprietary gridding software module developed at BGS (Breward and Herd, 1998) as an add-on to the widely-available public-domain NIH-Image™ vs. 1.62 programme running on a Macintosh G3 computer, or by the ArcView extension called GRIDDER (see Lister and others, In Prep, for documentation). The GRIDDER extension is currently being updated to run with ARC GIS 8 (contact Alan Mackenzie). Previously, a gridding package developed in BGS ran as an add-on to Arc-Info software running on a Sun Sparc workstation, but this system (G-Map) is now obsolete. In both the Image system and GRIDDER, the gridding algorithms used are broadly similar and produce a nearly identical output to other commercial gridding packages such as Northwood's Vertical Mapper for MapInfo. Various gridding parameters, such as search radius and weighting power, may be adjusted prior to gridding to suit the data and map required. The current software produces grids for each chemical element by interpolation of the data using the method of 'Inverse Distance Weighting', where each grid cell (pixel) represents a chosen size on the ground, e.g. 250 x 250m for regional maps. In this technique, each grid cell is given a calculated value derived from data for nearby sample sites (eight 'neighbour' sites are currently used). The calculation uses data from all sample sites within 3000 m, weighted in accordance with distance (r) following an inverse square law such that the weighting is proportional to r^{-2}.

In areas of low sampling density, a gridded image can give misleading results. Accordingly gridded areas which fall more than (e.g.) 2000 m from a sample point are zone-blanked, i.e. set to null (no value) after interpolation and prior to classification. This has the additional desirable effect of removing over-extrapolated data from the percentile classification, allowing a more accurate 'fit' with the data distribution of the real data.

The gridded data are used to produce percentile-based colour-classified images. Most of the images used in the BGS geochemical atlases have standard class interval boundaries set at the 5, 10, 15, 25, 50, 75, 90, 95 and 99 percentile levels. An appropriate colour scheme is then applied to the resolved classes (see Figure 28). Other percentile ranges can be used for more specialist maps, such as Hazard Quotients or ranges based on Soil Guidance Values.

The raster maps produced by these methods are imported into a GIS environment using MapInfo™, ArcView™, and GRIDDER and geo-registered so that other spatial information such as geology and topographical features can be accurately mapped with the geochemical data. The gridding packages also generate distribution histograms of the gridded data and percentiles information as text output, and this is usually included with the geochemical image.

For more hands-on interpretive use, higher resolution greyscale geochemical images can be produced which may be fed into an image-processing package to detect geochemical gradients, produce linear geochemical profiles or examine and, for example, create geostatistical signatures for particular geological formations. Feedback from the image to the stored database allows data for individual samples to be examined.

Useful additional information may be obtained by combining three elements together as a colour-addition image. This is achieved using image-processing software such as NIH-Image™ or Adobe Photoshop™ and allocating a percentile-classified element image to each of the red, green and blue image channels. The resulting image uses Red-Green-Blue (RGB) primary colour addition logic such that, for example, red+green=yellow, red+blue=magenta, green+blue=cyan and red+green+blue=white, at full saturation. The technique allows the concentrations of different groups or combinations of elements to be clearly displayed, and an example from southern Scotland is given below (Figure 29). Element ratios may also be gridded in a similar way to normal concentration data, and can also yield valuable information.

Gridded images from G-BASE for a selected number of elements are available on the internal GDI.

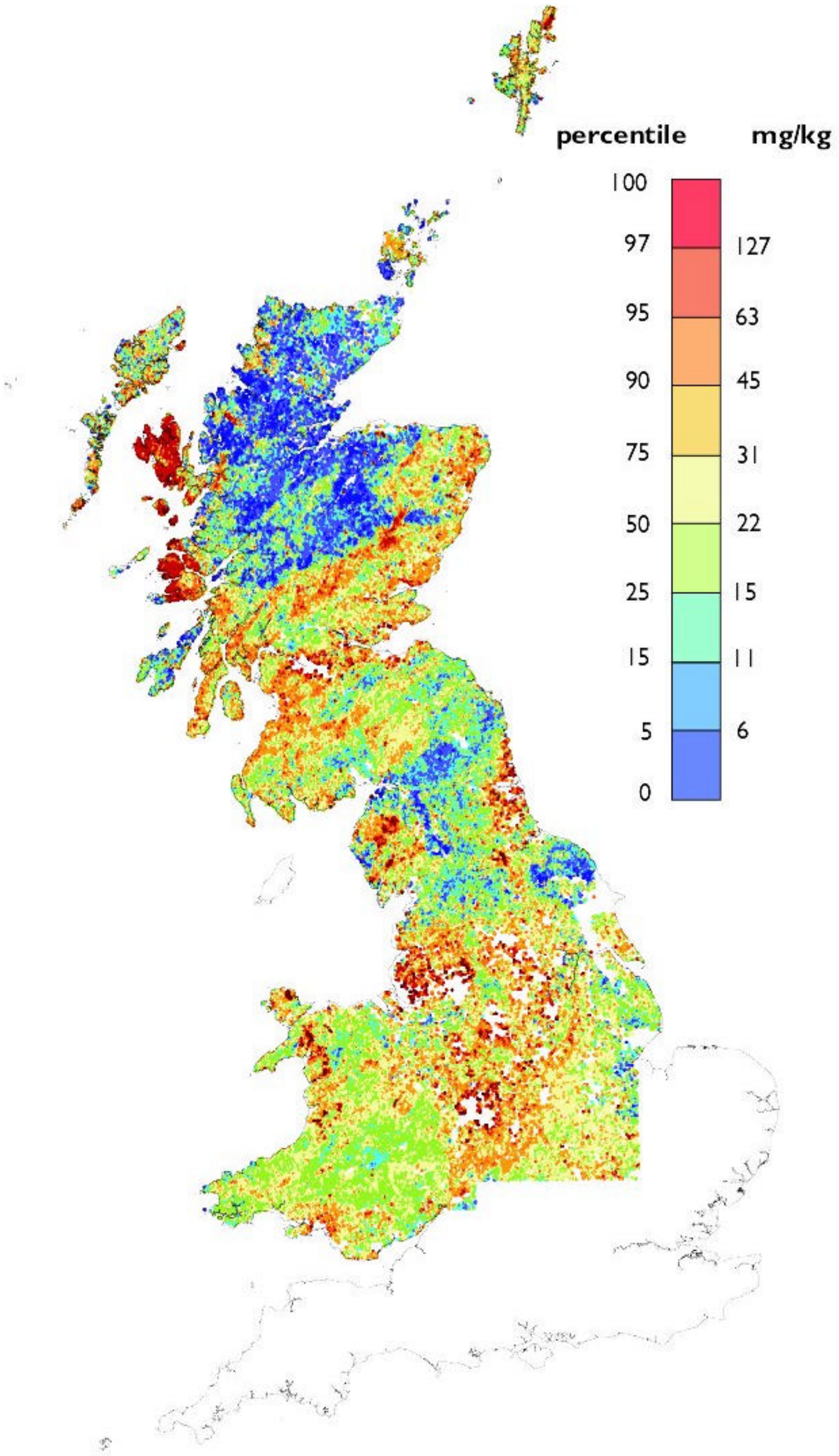


Figure 28: A standard G-BASE geochemical image showing the distribution of copper in stream sediments

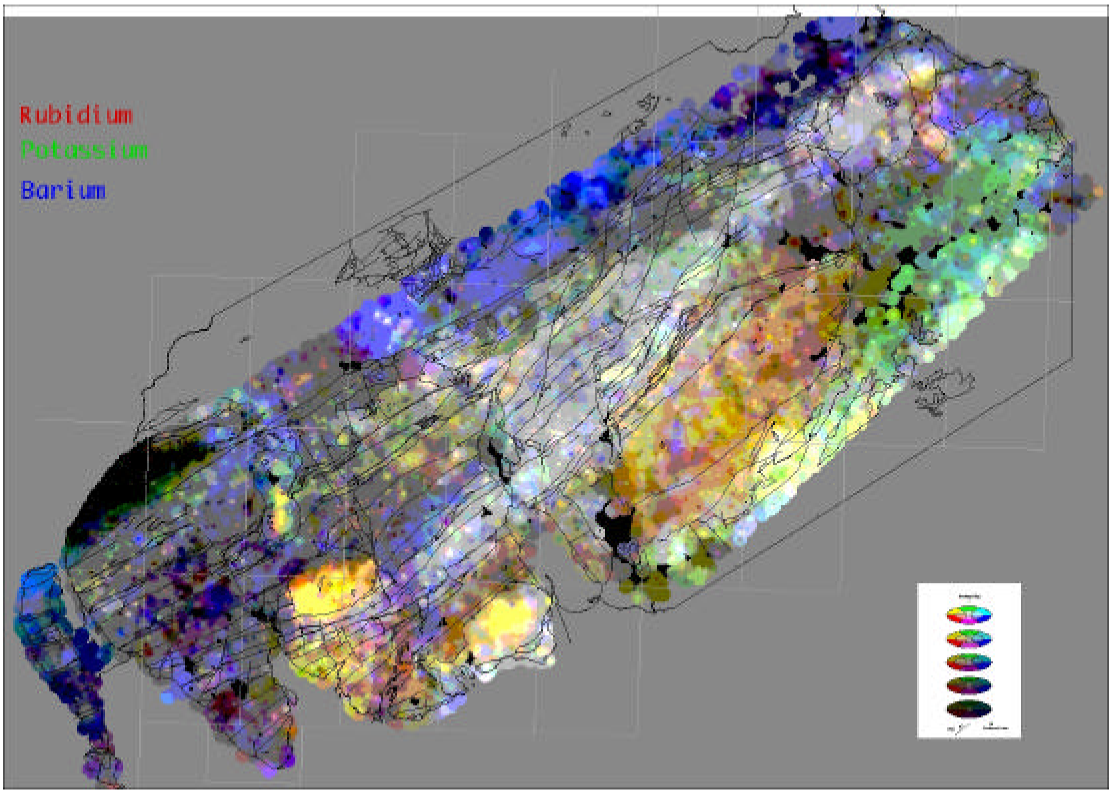


Figure 29: An example of a three component colour image for Rb, K and Ba in stream sediments from southern Scotland

8 Sources of Geochemical Information

8.1 WEB LINKS

G-BASE	http://www.bgs.ac.uk/gbase/
Geochemistry Database	http://www.bgs.ac.uk/mineralsuk/data/geochemistry/
W M White Geochemistry text book in pdf format	http://www.geo.cornell.edu/geology/classes/geo455/Chapters.HTML
Web Elements Periodic Table	http://www.webelements.com/
Association of Exploration Geochemists (AEG)	http://www.aeg.org/
AEG web page of Geochemistry related links	http://www.aeg.org/Links/newlinks.htm
BGS Intranet Data Access (from Keyworth)	http://intranet/resources/data/ida/idamain.htm
Alan Mackenzie's Cold fusion application to retrieve data from the Geochemistry Database (from Keyworth)	http://kwnts99:82/scripts/ida/geog/geog2_combformb.cfm
BGS internal GDI (from Keyworth)	Q:\Gdi\gdi31.apr
BGS International Geochemistry CD-ROMs	http://www.bgs.ac.uk/geochemcd

8.2 CONTACTS

General Geochemistry enquiries: N Breward - nbr@bgs.ac.uk (Keyworth extn 3479)

BGS Geochemistry data licensing: B G Rawlins - bgr@bgs.ac.uk (Keyworth extn 3140)

Geochemistry Database Development and Applications Manager: A C Mackenzie - acma@bgs.ac.uk (Keyworth extn 3516)

Geochemistry Database Administrator: S F Hobbs - sfh@bgs.ac.uk (Keyworth extn 3579)

G-BASE Project Leader and Geochemistry Database Manager: C C Johnson - ccj@bgs.ac.uk (Keyworth extn 3372)

Appendix 1 Summary of Important Fields used for retrievals in the Geochemistry Database

The Geochemistry Database has many Oracle tables (see Figure 9) with similar fields that in many instances can be found in several tables. A user unfamiliar to the Geochemistry Database will need to ask the question "where do I find …..?". Appendix 3 gives a worked example of how to download analytical results. The following looks at the important fields in the database that can be used in selective criteria. The discussions below assume the user has the skills to construct a Query in MS Access.

1. How do I select G-BASE samples?

Use the field NUMBERING_SYSTEM which can be found in the site tables (BGS_DTA_ DRAINAGE_SITES, BGS_DTA_NORMAL_SITES, or BORE_SITES). The codes for the numbering system are found in the domain table BGS_MTA_DOM_NUMBERING_SYSTEM (see Appendix 2(d)) and for G-BASE the code is 4.

2. How do I know if the data I want to assess is confidential?

There is a field called CONFIDENTIALITY which is defined in the domain table BGS_MTA_DOM_CONFIDENTIALITY (see Appendix 2(e)) and is found in the sites tables listed above and the BGS_DTA_ BATCHES table. Confidential data is coded with a 4 or 5 in this field. These codes are somewhat outdated and would not fit within the current BGS IPR scheme. A review of geochemistry data confidentiality is recommended. The default value, if assigned, is usually 4 (confidential). Any doubts about data confidentially should be referred to the Geochemistry Database Manager.

3. How do I select a particular type of sample?

The sample type is defined as a single character code and keyfield SAMPLETYPE in the BGS_DTA_ANALYTE_DETERMINATIONS, BGS_DTA_PROJECT_BATCHES, and several other data tables and is defined by the domain table BGS_MTA_DOM_ SAMPLE_TYPE (see Appendix 2(f)). Retrieval is usually done on the BGS_DTA_ ANALYTE_DETERMINATIONS table as shown in the example in Appendix 3.

4. How do I select data for a specified geographical area?

Methods of retrieving data from the Geochemistry Database are described in Section 3.1 and different methods are more appropriate to the shape and size of an area than others. The standard type of search would use a rectangle defined by full British National Grid coordinates. The Coldfusion form application described in Section 3.1.2 is suitable for this or it can be done with greater flexibility using MS Access (Section 3.1.6). The EASTING and NORTHING fields of the site tables are used for retrieval where the full metre grid reference should be used. For polygon areas ArcView can be employed to select samples from predefined polygonal areas such as local authority or lithological boundaries.

5. When I download analytical results why do I get several different analyses for the same sample

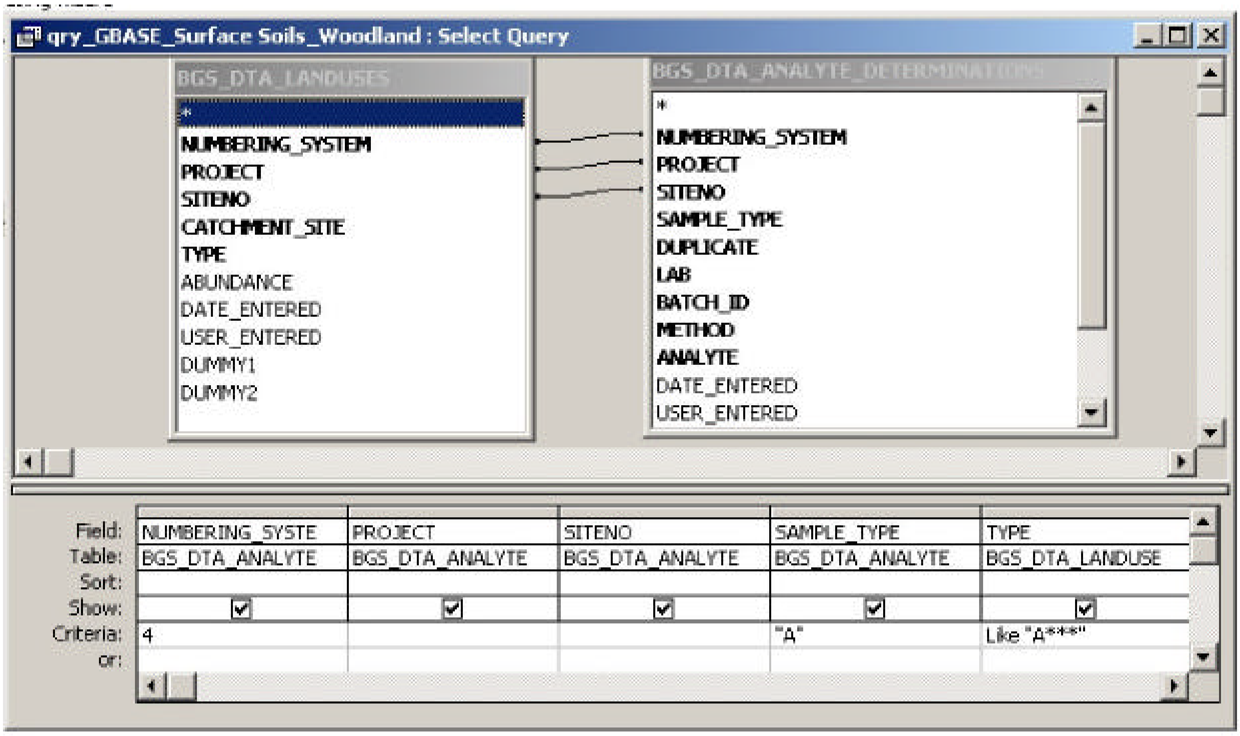
Some of the samples loaded in the Geochemistry Database may have been analysed by several different analytical methods and if you do not specify a particular method then results for all methods will be retrieved. It is necessary, if this is the case, to specify a selection criteria for the method used. The METHOD is a keyfield in the BGS_DTA_ ANALYTE_DETERMINATIONS table and codes are defined in the BGS_MTA_DOM_ANALYSIS_METHOD table (see Appendix 2(c)). For example, if only analyses done by optical emission spectroscopy are required then the code "OES" in the METHOD field should be used for retrieval.

6. Where do I find sample pH?

For waters this is considered as a property and can be found in the PH field of the BGS_DTA_ WATERS table along with conductivity and other water properties. Unfortunately, there is no way of indicating in the database how the pH determination was done (e.g. on site with pH stick or in fieldbase with pH meter). Soil pH results can be found in the BGS_MTA_DOM_ OVERBURDENS table where it is listed as a property. Loss-on-ignition, which for G-BASE samples is requested at the same time as soil pH determinations, is considered as a method ("LOI450") and is found in the BGS_DTA_ ANALYTE_DETERMINATIONS table.

7. How do I retrieve samples associated with a particular land use?

Land use is information entered on geochemistry field slips (Figure 11) and this would generally be more accurate and up-to-date than land use maps that may be available. LANDUSE is a field in found in the BGS_DTA_ LANDUSE database table and defined in the domain table BGS_MTA_DOM_ LANDUSE. Land use codes are hierarchical so "wildcard" characters can be used to search for more general grouping. For example, to list all surface soils from G-BASE associated with woodlands (which may be classified as deciduous, mixed, coniferous etc.) use "A***" as criteria for land use. The query for this example is shown in Figure 30.



Field:	NUMBERING_SYSTE	PROJECT	SITENO	SAMPLE_TYPE	TYPE
Table:	BGS_DTA_ANALYTE	BGS_DTA_ANALYTE	BGS_DTA_ANALYTE	BGS_DTA_ANALYTE	BGS_DTA_LANDUSE
Sort:					
Show:	☑	☑	☑	☑	☑
Criteria:	4			"A"	Like "A***"
or:					

Figure 30: Example of a land use query using 'wildcard' characters

8. How do I retrieve samples associated with contamination?

Twenty columns are available on the G-BASE field cards to record site contamination which becomes nine fields of coded information (often supported by free text comments in the field database). In the Geochemistry Database codes are translated to conform with entries in the domain table BGS_MTA_DOM_ CONTAMINANT. A simple select query on the BGS_DTA_ CONTAMINANTS table can identify the samples of a particular sample type that are associated with contamination (use 'Is not null' in the contaminant field). A crosstab query is needed to list on a single row all the different contamination associated with a particular sample.

9. How do I retrieve samples associated with a particular lithology?

Geochemical sample field forms record the geology at site and of the catchment area. This is recorded by student collectors who would usually take the geology from the published geological map. Classifying drainage or overburden samples by a lithological code is probably best done using the Arc GIS interface to the Geochemistry Database and using GIS functionality to intersect sample sites with the BGS digital geology map polygons.

10. How do I get a list of samples collected by a particular sampler?

The sample collector is a field (COLLECTOR) in the BGS_DTA_ DRAINAGE_SITES and BGS_DTA_ NORMAL_SITES tables. Sampling is usually done in pairs and the samplers initials are entered in the COLLECTOR field, i.e. there is usually more than one person identified in this field. For example, to select all the samples collected by CCJ, then the select criteria should be "*CCJ*". Note that it is standard G-BASE procedure for the form filler's initials to be recorded first and the collector's initials second. From 2003 onwards sampler IDs are recorded in the annual field campaign report.

Appendix 2 Summary of Important Codes used in the Geochemistry Database

The following tables list some of the more important codes used in the Geochemistry Database that are frequently used to selectively retrieve data from the database. The codes are stored in domain tables (sometimes referred to as "look-up tables") identified on kwdbase as BGS_MTA_DOM_*********. A more comprehensive listing can be found in Harris and Coats (1992) though many of the domain tables are updated in a revised version available from Sue Hobbs. Latest versions of the domain tables can be assessed on kwdbase.

(a) BGS_MTA_DOM_ATLAS - geochemistry atlas area.

Codes from Scotland generally refer to quarter inch geology map areas and are not completely consistent with the G-BASE atlas sheet boundaries. For example, the southern Scotland and part of northern England atlas contains results from CLYD and BORD and the NW England atlas contains data from LIVB and WALE.

CODE	TRANSLATION	DEFINED_AS
ARGL	Argyll - Tiree	
BORD	Borders-Farne	
CATH	Caithness	
CLYD	Clyde-Maine	
EMID	East Midlands	
EANG	East Anglia	
GLEN	Great Glen	
HEBS	Hebrides	
HUMB	Humber-Trent	
LAKE	Lake District	
LIVB	Liverpool Bay	
MOBU	Moray-Buchan	
MWAL	Mid Wales	
ORKN	Orkney	
SEEN	SE England	
SHET	Shetland	
SUTH	Sutherland	
SWEN	SW England	
TYFH	Tay-Forth	
TYNE	Tyne Tees	
WALE	Wales	

(b) BGS_MTA_DOM_ANALYSIS_QUALIFIER - analysis qualifier

This is a single character code that qualifies the analyte abundance. It is an important field that should be down loaded with analyte abundance.

CODE	TRANSLATION	DEFINED_AS
>	Probably high	Not determined due to interference probably high.
<	Probably low	Not determined due to interference probably low.
^	No estimate possible	Not determined due to interference no estimate possible
*	Dubious quality	The value has a documented quality control issue that should restrict its use.

(c) BGS_MTA_DOM_ANALYSIS_METHOD - analytical method used to determine abundance

CODE	TRANSLATION	DEFINED AS
AAS	Atomic Absorption Spectrometry	Atomic Absorption Spectrometry.
AFS	Atomic Fluorescence	Atomic Fluorescence
AQTOC	Shimadzu 5000	
BERYL	Beryllometry	Gamma excitation of Beryllium and detection of neutrons.
BETAP	Beta Probe	Direct electron excitation X-ray spectrometry.
CE1500	CARLO ERBA 1500 CHNS Analyser	
COL	Colorimetric Method	Colorimetric Method
COLHEX	Colorimetric Hot Extractable	Colorimetric Hot Extractable
CVAAS	Cold Vapour AAS	Cold Vapour Atomic Absorption Spectrometry
DCOES	Direct Reading OES	Direct Reading Optical Emission Spectroscopy
DNA	Delayed Neutron Activation	Delayed Neutron Activation
ETAAS	Electrothermal AAS	Electrothermal Atomic Absorption Spectrometry
FAAS	Fire Assay AAS	Fire Assay Atomic Absorption Spectroscopy
FDCP	Fire Assay Direct Coupled Plasma	Fire Assay Direct Coupled Plasma.
FICP	Fire Assay ICP-AES	Fire Assay Inductively Coupled Plasma Atomic Emission Spectrometry
FICPMS	Fire Assay ICP-MS	Fire Assay Inductively Coupled Plasma Mass Spectrometry
FLAAS	Flame AAS	Flame Atomic Absorption Spectrometry
FLAES	Flame Atomic Emission Spectrometry	Flame Atomic Emission Spectrometry
FNA	Fire Assay Neutron Activation	Fire Assay Neutron Activation
GRAV	Gravimetric method	Gravimetric method
HYICP	Hydride Generation ICP	Hydride Generation Inductively Coupled Plasma
ICP	Inductively Coupled Plasma	Inductively Coupled Plasma
ICPAES	ICP Atomic Emission Spectrometry	Inductively Coupled Plasma Atomic Emission Spectrometry
ICPMS	ICP Mass Spectrometry	Inductively Coupled Plasma Mass Spectrometry
ISE	Ion Selective Electrode	Ion Selective Electrode
LAICP	Laser Ablation ICP-MS	Laser Ablation Inductively Coupled Plasma Mass Spectrometry
LECO	LECO CHNS Analyser	LECO CHNS Analayser
LIFS	Laser Induced Fluorescence Spec	Laser Induced Fluorescence Spectroscopy using Scintrex machine
LOI105	Loss on ignition at 1050C	Gravimetric method to determine organic carbon content
LOI450	Loss on ignition at 450C	Gravimetric method to determine H2O content
NA	Neutron Activation	Neutron Activation
NPOC	Non-purgeable organic carbon	measurement by non-dispersive infra red of the CO2 from combusted sample that had been acidified and put on Pt Column at 680c
OES	Optical Emission Spectroscopy	Optical Emission Spectroscopy
PE240	PERKIN-ELMER 240 CHNS Analyser	
SPPHOT	Spectrophotometric method	Spectrophotometric method
TITRE	Titrimetric method	Titrimetric method
XRF	X-Ray Fluorescence Pressed Pellets	X-Ray Fluorescence Pressed Pellets
XRFB	X-Ray Fluorescence On Fused Beads	X-Ray Fluorescence On Fused Beads
XRFED	X-Ray Fluorescence ED spectrometry	XRFS using emission dispersion
XRFWD	X-Ray Fluorescence WD spectrometry	XRFS using wave dispersion

(d) BGS_MTA_DOM_NUMBERING_SYSTEM - sample numbering system used

This field can be used to distinguish data generated by different projects.

CODE	TRANSLATION	DEFINED_AS
1	Min Pet	Mineralogy & Petrology system
2	Bio Strat	Biostratigraphy system
3	MRP	Mineral Reconnaissance Programme
4	GSP	G-BASE formerly GSP

(e) BGS_MTA_DOM_CONFIDENTIALITY - confidentiality of the data

When downloading data users should retrieve this information so the confidentiality of the data set is known. This domain table needs modernising to bring it up-to-date with BGS IPR issues. Codes 0 - 3 need to be redefined, codes 4 and 5 indicate care is needed over the confidentiality of the data. The table shows confidentiality levels as defined in August 1997 and is need of revision.

CODE	TRANSLATION	DEFINED_AS
0	Published	Outside published data from BGS or other sources.
1	Published	Freely available published BGS data in openfile report.
2	Unpublished, retrieval charge	Supplementary information to open file report, not published. Charged at retrieval cost.
3	Unpublished, retrieval charge	Supplementary information to open file report, not published. Charged at retrieval cost.
4	Confidential	Confidential, normal BGS data not released or work in progress.
5	Highly confidential	Highly confidential, Commercial-in-Confidence.

(f) BGS_MTA_DOM_SAMPLE_TYPE - sample type identifier

CODE	TRANSLATION	DEFINED_AS
A	Shallow GBASE soil sample.	Shallow GBASE soil sample. Standard depth 0-15 cm
C	Stream Sediment	Stream Sediment
D	Drill core	Drill core
E	Mineral	Mineral
F	Float sediment (Fines)	Float sediment (Fines)
G	Gas	Gas
H	Panned Rock	Panned Rock
J	Marine sediment	Marine sediment.
M	Drill mud (Sludge)	Drill mud (sludge)
N	Panned sludge	Panned sludge
P	Panned stream sediment	Panned stream sediment
R	Rock	Rock
S	Soil	Shallow overburden altered by soil forming processes. (GBASE soil 30 - 45 cm)
T	Deep overburden	Deep overburden unaltered by soil forming processes (often a till in northern Britain)
U	Panned overburden or soil	Panned overburden or soil
V	Vegetation	Vegetation
W	Water	Water

Appendix 3 Worked Examples in downloading G-BASE geochemical data from the Geochemistry Database

Examples prepared for the Geochemistry Database Workshop on 23rd January 2004 by Dr J S Coats.

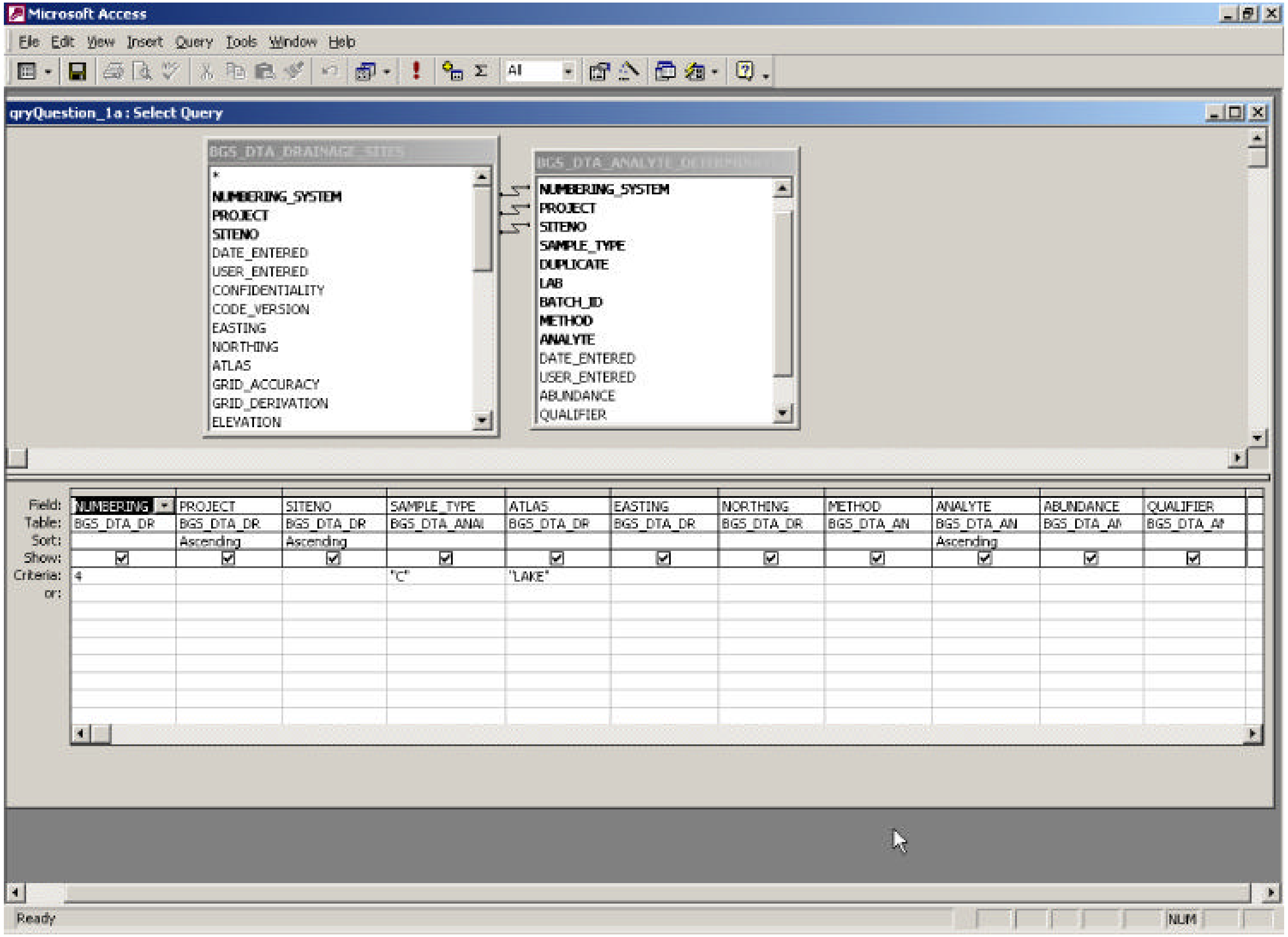
EXAMPLE 1: How do I retrieve all the G-BASE stream sediment samples with Easting, Northing, and analytical results for the Lake District Atlas area?

1. Firstly create a query in MS Access to down load the stream sediment data from the G-BASE project for the Lake District atlas area. This is shown in Figure 31. The BGS.DTA_DRAINAGE_SITES and BGS.DTA_ANALYTE_DETERMINATIONS tables are linked and the following selection criteria applied: NUMBERING_SYSTEM = 4 (for G-BASE samples); SAMPLE_TYPE = "C" for stream sediments; and ATLAS = "LAKE" for Lake District.

NUMBERING_SYSTEM	PROJECT	SITENO	SAMPLE_TYPE	ATLAS	EASTING	NORTHING	METHOD	ANALYTE	ABUNDANCE	QUALIFIER
4	30	208	C	LAKE	399100	565670	DCOES	Ag	0	
4	30	208	C	LAKE	399100	565670	DCOES	Al	53534.8	
4	30	208	C	LAKE	399100	565670	DCOES	B	49	
4	30	208	C	LAKE	399100	565670	DCOES	Ba	615.402	
4	30	208	C	LAKE	399100	565670	DCOES	Be	1.3	
4	30	208	C	LAKE	399100	565670	DCOES	Bi	0	
4	30	208	C	LAKE	399100	565670	DCOES	Ca	32215.74278	
4	30	208	C	LAKE	399100	565670	DCOES	Cd	0.4	
4	30	208	C	LAKE	399100	565670	DCOES	Ce	0	
4	30	208	C	LAKE	399100	565670	DCOES	Co	28.0751	
4	30	208	C	LAKE	399100	565670	DCOES	Cr	151.0051	
4	30	208	C	LAKE	399100	565670	DCOES	Cu	14.4361	
4	30	208	C	LAKE	399100	565670	DCOES	Fe	31629.05705	
4	30	208	C	LAKE	399100	565670	DCOES	Ga	9.00854	
4	30	208	C	LAKE	399100	565670	DCOES	K	14446.31364	

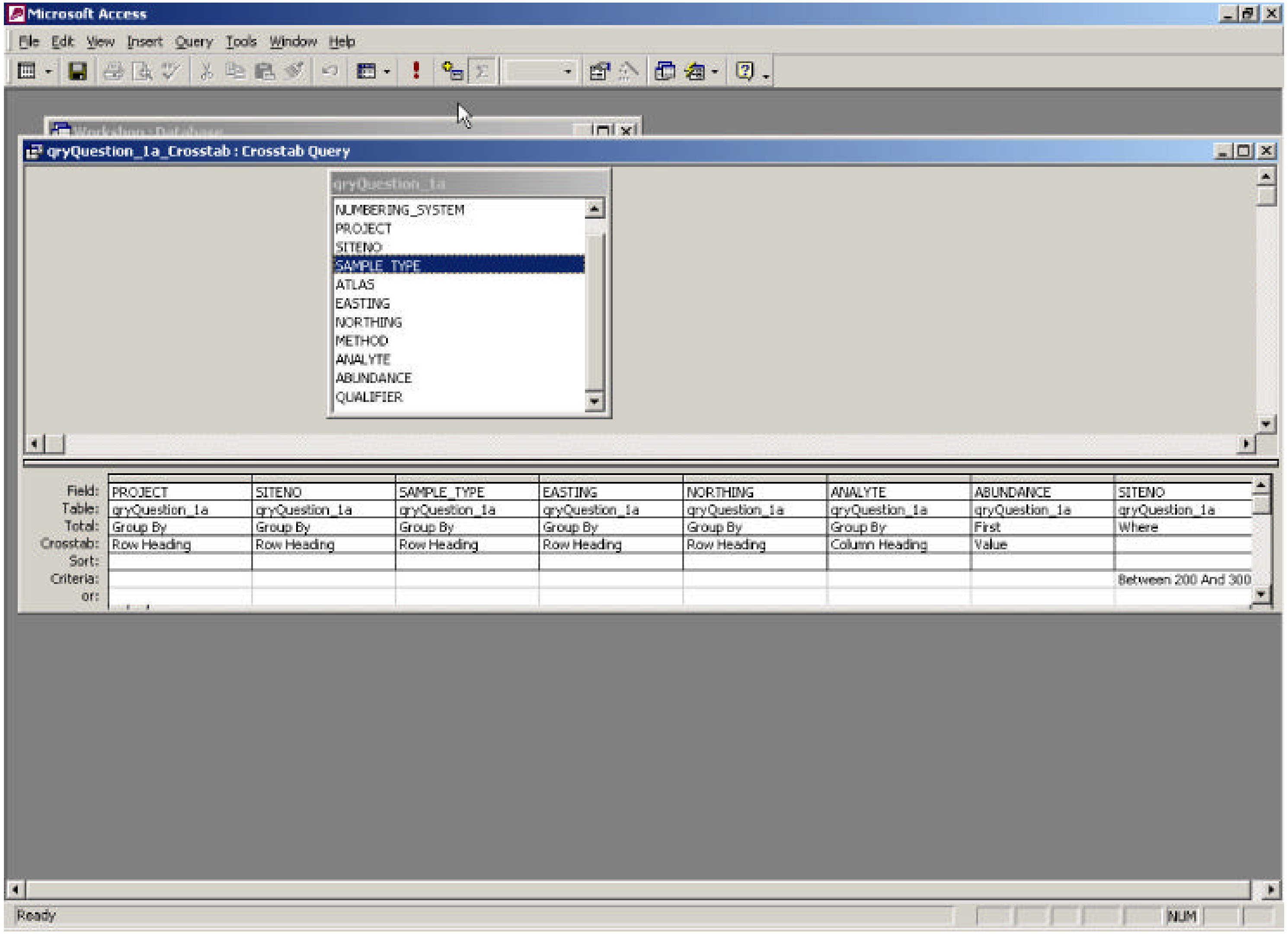
Table 5: Listing of results produced by the select query in example 1

2. This query produces a very large data table listing each analyte (element) determination for each site on a separate row. An example of the first few records is given above. Note that a sample may have been determined by several different methods. The abundances are not yet rounded to a sensible number of decimal places as original data has been levelled by a correction factor in the database. There is also a "qualifier" field which should contain information about the 'correctness' of the abundance value, e.g. < to indicate less than detection. This field has not been utilised much in the past but will be populated following a recent audit of the database which highlighted the problem of listing less than detection values as 0. In order to produce a more readable table, sample should be represented by a single row with column headings. This can be done by using a 'Crosstab Query' based on the 'Select Query' used above.



Field:	NUMBERING	PROJECT	SITENO	SAMPLE_TYPE	ATLAS	EASTING	NORTHING	METHOD	ANALYTE	ABUNDANCE	QUALIFIER
Table:	BGS_DTA_DR	BGS_DTA_DR	BGS_DTA_DR	BGS_DTA_ANAI	BGS_DTA_DR	BGS_DTA_DR	BGS_DTA_DR	BGS_DTA_AN	BGS_DTA_AN	BGS_DTA_AN	BGS_DTA_AN
Sort:		Ascending	Ascending						Ascending		
Show:	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑	☑
Criteria:	4			"C"	"LAKE"						
or:											

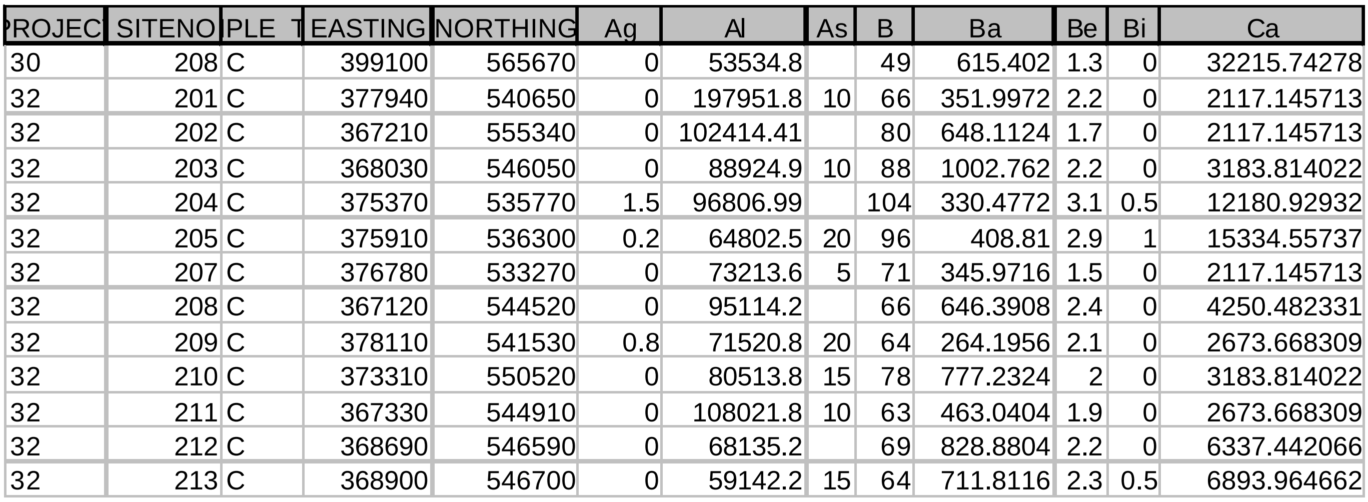
Figure 31: Example 1 - query to download analyte data for G-BASE Lake District stream sediments



Field:	PROJECT	SITENO	SAMPLE_TYPE	EASTING	NORTHING	ANALYTE	ABUNDANCE	SITENO
Table:	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a
Total:	Group By	Group By	Group By	Group By	Group By	Group By	First	Where
Crosstab:	Row Heading	Row Heading	Row Heading	Row Heading	Row Heading	Column Heading	Value	
Sort:								
Criteria:								Between 200 And 300
or:								

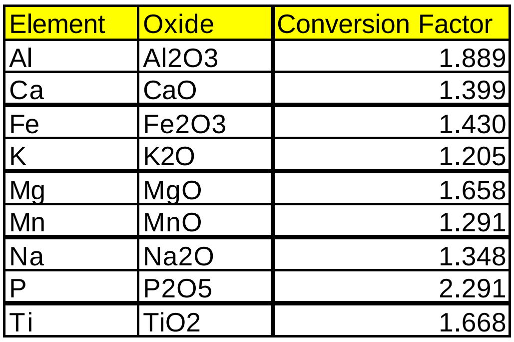
Figure 32: Example 1 - Crosstab Query using the Select Query created in the first part of the example

3. To create the Crosstab query selected 'create a query in design view" and add the query created in step one to the top window and create the query as shown in Figure 32. An example of part of the selected data is listed below in Table 6 (exported to Excel). Note that element concentrations (all listed in ppm) have not yet been formatted to the correct number of decimal places. Elements usually quoted in G-BASE as percentage oxide (e.g. Al and Ca) will need converting to oxide concentrations. Conversion factors for commonly used oxides are given in Table 7.



ROJEC	SITENO	PLE T	EASTING	NORTHING	Ag	Al	As	B	Ba	Be	Bi	Ca
30	208	C	399100	565670	0	53534.8		49	615.402	1.3	0	32215.74278
32	201	C	377940	540650	0	197951.8	10	66	351.9972	2.2	0	2117.145713
32	202	C	367210	555340	0	102414.41		80	648.1124	1.7	0	2117.145713
32	203	C	368030	546050	0	88924.9	10	88	1002.762	2.2	0	3183.814022
32	204	C	375370	535770	1.5	96806.99		104	330.4772	3.1	0.5	12180.92932
32	205	C	375910	536300	0.2	64802.5	20	96	408.81	2.9	1	15334.55737
32	207	C	376780	533270	0	73213.6	5	71	345.9716	1.5	0	2117.145713
32	208	C	367120	544520	0	95114.2		66	646.3908	2.4	0	4250.482331
32	209	C	378110	541530	0.8	71520.8	20	64	264.1956	2.1	0	2673.668309
32	210	C	373310	550520	0	80513.8	15	78	777.2324	2	0	3183.814022
32	211	C	367330	544910	0	108021.8	10	63	463.0404	1.9	0	2673.668309
32	212	C	368690	546590	0	68135.2		69	828.8804	2.2	0	6337.442066
32	213	C	368900	546700	0	59142.2	15	64	711.8116	2.3	0.5	6893.964662

Table 6: Listing of part of the results produced by the crosstab query of Example 1

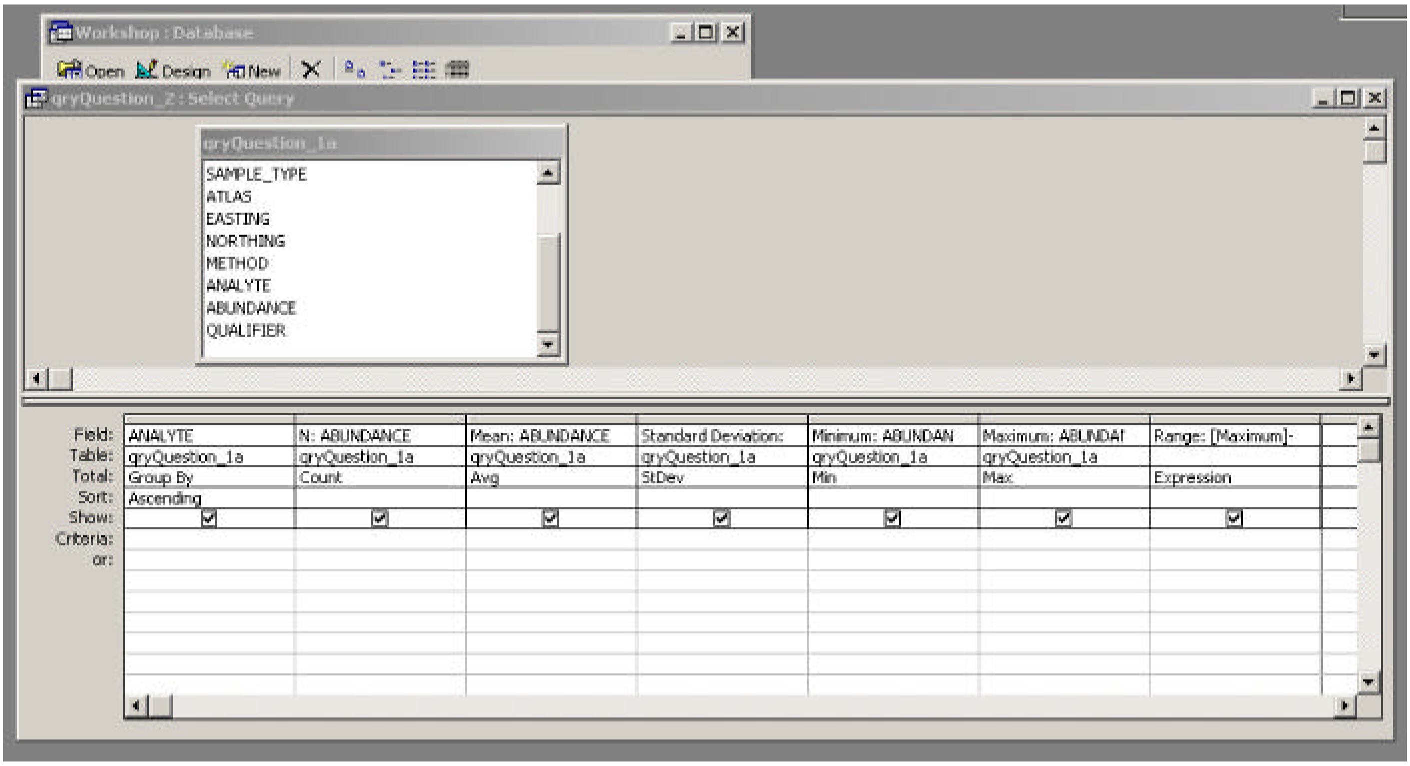


Element	Oxide	Conversion Factor
Al	Al2O3	1.889
Ca	CaO	1.399
Fe	Fe2O3	1.430
K	K2O	1.205
Mg	MgO	1.658
Mn	MnO	1.291
Na	Na2O	1.348
P	P2O5	2.291
Ti	TiO2	1.668

Table 7: Table of the most commonly used oxide conversion factors

EXAMPLE 2: How do I calculate simple statistics for each element on a group of samples?

1. Build a new query using the Select Query created at the beginning of Example 1 (see Figure 33).
2. Create a Summary Query by selecting '?' on the menu bar and complete as shown in Figure 33.
3. An example of the basic summary statistics generated by this Summary Query is shown in Table 8.



Field:	ANALYTE	N: ABUNDANCE	Mean: ABUNDANCE	Standard Deviation:	Minimum: ABUNDAN	Maximum: ABUNDAI	Range: [Maximum]-
Table:	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	qryQuestion_1a	
Total:	Group By	Count	Avg	StDev	Min	Max	Expression
Sort:	Ascending						
Show:	☑	☑	☑	☑	☑	☑	☑
Criteria:							
or:							

Figure 33: Example 2 - Summary Query based on a select Query

ANALYTE	N	Mean	Standard Deviation	Minimum	Maximum	Range
Ag	6120	0.168578	1.2974907	0	66.8	66.8
Al	6201	100278	45857.716	529	417010.7	416481.7
As	3339	31.19197	102.73083	0	3000	3000
B	6116	69.54349	39.02314	0	567	567
Ba	6201	674.3338	875.70521	90.314	10685.9	10595.59
Be	6201	2.629592	1.3958672	0.3	18	17.7
Bi	6180	1.028398	2.1702787	0	93.5	93.5
Ca	6201	7522.405	13699.058	2117.146	235068.2	232951.1
Cd	6111	0.957503	1.9720458	0	14.3	14.3

Table 8: Simple summary statistics output for Example 2

Appendix 4 Geochemistry Discovery Metadata

Identifier	GBASEGEOCHEM		
Description	Geochemical Baseline Survey of the Environment (G-BASE)		
Abstract			
The G-BASE project involves systematic sampling and the determination of chemical elements in samples of stream sediment, stream water and, locally, soil, to build up a picture of the surface chemistry of the UK. The average sample density for stream sediments and water is about one site per 1.5-2 km square. Analytical precision is high with strict quality control to ensure countrywide consistency. Results have been standardised to ensure seamless joins between geochemical sampling campaigns. The data provide baseline information on the natural abundances of elements, against which anomalous values due to such factors as mineralisation and industrial contamination may be compared. Analytical data for the 150 microns fraction of soil and stream sediment samples are available for some or all of: Ag, As, B, Ba, Bi, Be, Ca, Ce, Cd, Co, Cr, Cs, Cu, Fe, Ga, K, La, Li, Mg, Mn, Mo, Nb, Ni, P, Pb, Rb, Sb, Se, Sn, Sr, Th, Ti, U, V, Y, Zn, and Zr. Most water samples have been analysed for alkalinity, pH, conductivity, F and U and some for multi-element analyses including Al, Cl, Na, Si, SO_4,NO_3, and TOC.			
Start Date Comment	Regional geochemical Mapping commenced in the Caithness and South Orkney area carried out by the Institute of Geological Sciences (IGS -now BGS).		
Start Date	01-01-1968	**End Date**	ongoing
End Date Comment	Projected completion 2015		
Update Frequency Comment	Updated on a yearly basis.		
Completeness	80% complete for Scotland, Wales, Northern England, Humber-Trent and Central England. East Anglia ongoing. Southern England yet to be started.		
Level of Spatial Detail	Samples av. 1 per 1.75 km square collected using 1:50 000 OS base maps.		
Logical Consistency	Geochemical mapping carried out according to International Geochemical Sampling methods described by IGCP 259.		
Lineage	Project initially called Regional Geochemical Reconnaissance Programme (RGRP) and subsequently Geochemical Survey Project (GSP).		
Metadata Entered	19-04-1999	**Metadata Updated**	21-03-2003
Access Constraints	Data distributed under licence.		
Use Constraints	Copyright control.		
Spatial Reference System	BRITISH NATIONAL GRID		
Bounding Coordinates			
West	50000	**East**	550000
North	1220000	**South**	160000
Areal Extent	ENGLAND	**Areal Extent Type**	COUNTRY
Areal Extent	SCOTLAND	**Areal Extent Type**	COUNTRY
Areal Extent	WALES	**Areal Extent Type**	COUNTRY
Areal Extent	UNITED KINGDOM	**Areal Extent Type**	KINGDOM
Storage Format	ORACLE		
Delivery Format	ATLAS , DIGITAL FILE FORMATS		
Language	ENGLISH		
Supplier	BRITISH GEOLOGICAL SURVEY		

Appendix 5 Detailed Information on G-BASE geochemical data summarised by atlas area

8. Argyll

17. East Anglia

7. East Grampians

16. East Midlands

6. Great Glen

5. Hebrides

13. Humber-Trent

10. Lake District

11. NE England

20. Northern Ireland (west)

12. NW England & N Wales

2. Orkney

1. Shetland

Shetland Follow-up

3. South Orkney & Caithness

18. SE England

9. S Scotland

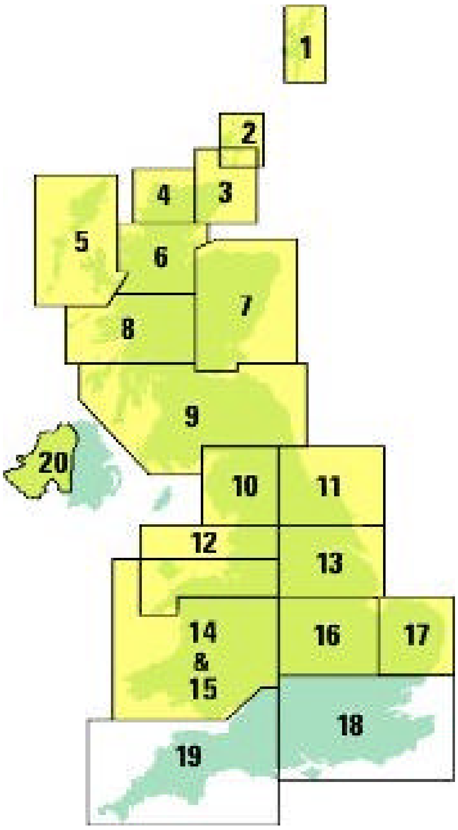
19. SW England

4. Sutherland

14. Wales & W Midlands (soil, sediment)

15. Wales & W Midlands (water)

[Atlases listed in grey are to be completed, yellow-shaded areas on map have been sampled. The Tamar drainage catchment (part of area 19) was completed in 2002]



ATLAS:	**Argyll**
REFERENCE:	British Geological Survey (1990). Regional Geochemical Atlas: Argyll. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 190 0
Sheet boundaries:	Min Easting: 092000 Max Easting: 279000 Min Northing: 680000 Max Northing: 799000
Sampling period:	Summer 1976 and 1977
Sampling density:	1 sample per 1.6 km^2
Project/Sample code:	CP/20/21 CZ/22
No. of sites	9560
Sample type (no. sites sampled)	Stream sediment (9560), Stream waters (8680), Heavy mineral panned concentrates (approx. 70% of sediment sites)
Sample preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ba, Be, Bi, B, Ca, Cr, Co, Cu, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Sr, Sn, Ti, V, Y, Zn and Zr (DR-ES); Sb and As (5215 samples were analysed by acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis). The pH and conductivity in surface waters determined at 1500 sites.
Atlas content	Interpretative maps using proportional vector symbols and accompanying text are presented for 28 elements; Sb, As, Ba, Be, Bi, B, Ca, Cr, Co, Cu, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Sr, Sn, Ti, U, V, Y, Zn and Zr in sediment and for pH, conductivity and U in water.
Notes:	Sponsored by the Department of Trade and Industry.

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ATLAS:	**East Grampians**
REFERENCE:	British Geological Survey (1991). Regional geochemistry of the East Grampians area. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 198 6
Sheet boundaries:	Min Easting: 275000 Max Easting: 420000 Min Northing: 677000 Max Northing: 900000
Sampling period:	Summer 1977-1980
Sampling density:	1 sample per 1.6 km^2
Project/Sample code:	BP/10/18 CZ/22 CW/23 CX/24

No. of sites	9920
Sample type *(no. sites sampled)*	Stream sediment (9920), stream waters (4230), heavy mineral panned concentrates (9920).
Sample preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, V, Y, Zn and Zr (DR-ES); Sb and As (5338 samples were analysed by acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis).
Atlas content	Interpolated geochemical maps and accompanying text are presented for 30 elements; Sb, As, Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, U, V, Y, Zn and Zr in sediment and for pH, conductivity, bicarbonate, fluoride and U in water.
Notes:	Initially sponsored by the Department of Trade and Industry. Funded to completion by Department of Education and Science

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ATLAS:	**Great Glen**
REFERENCE:	British Geological Survey (1987). Regional Geochemical Atlas: Great Glen. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 085 8
Sheet boundaries:	Min Easting: 167000 Max Easting: 295000 Min Northing: 791500 Max Northing: 907000
Sampling period:	July - September 1974
Sampling density:	1 sample per 1.5 km^2
Project/Sample code:	AP/04 SN/06 FN/05 DP/07 BP/10 TZ/12 TB/13 TD/14 TA/15 SR/16 TX/17 CP/20
No. of sites	7270
Sample type *(no. sites sampled)*	Stream sediment (7270), Stream waters (6933), Heavy mineral panned concentrates (approx. 70% of sediment sites).
Sample preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ba, Be, B, CaO, Cr, Co, Cu, Fe, La, Li, MgO, Mn, Mo, Ni, K_2O, Rb, Sr, Sn, TiO_2, V, Y and Zr (DR-ES); Pb and Zn (acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis). The pH and conductivity in surface waters determined at 424 sites.
Atlas content	Interpretative maps using proportional vector symbols and accompanying text are presented for 25 elements; Ba, Be, B, CaO, Cr, Co, Cu, Fe, La, Pb, Li, MgO, Mn, Mo, Ni, K_2O, Rb, Sr, Sn, TiO_2, U, V, Y, Zn and Zr in

	sediment and for pH, conductivity and U in water.
Notes:	Sponsored by the Department of Trade and Industry.

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ATLAS:	**Hebrides**
REFERENCE:	Institute of Geological Sciences (1983). Regional Geochemical Atlas: The Hebrides. London, Institute of Geological Sciences. ISBN 0 85272 078 5
Sheet boundaries:	Min Easting: 053000 Max Easting: 180000 Min Northing: 780000 Max Northing: 967000
Sampling period:	July and September 1975
Sampling density:	1 sample per 1.5 km^2
Project/Sample code:	DP/07 (Lewis)
No. of sites	3370
Sample type (no. sites sampled)	Stream sediment (3370) Stream waters (3370) Heavy mineral panned concentrates (approx. 70% of sediment sites)
Sample Preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ba, Be, B, CaO, Cr, Co, Cu, Fe, La, Pb, Li, MgO, Mn, Mo, Ni, K_2O, Rb, Sr, Sn, TiO_2, V, Y, Zn and Zr (DR-ES); U (delayed neutron activation analysis).
Atlas content	Interpretative maps using proportional vector symbols and accompanying text are presented for 25 elements; Ba, Be, B, CaO, Cr, Co, Cu, Fe, La, Pb, Li, MgO, Mn, Mo, Ni, K_2O, Rb, Sr, Sn, TiO_2, U, V, Y, Zn and Zr in sediment and for pH, conductivity and U in water. (pH and conductivity determined at only 455 sites)
Notes:	Sponsored by the Minerals, Metals extraction and reclamation Executive Committee of the Department of Industry.

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ATLAS:	**Lake District**
REFERENCE:	British Geological Survey (1992). Regional geochemistry of the Lake district and adjacent areas. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 225 7
Sheet boundaries:	Min Easting: 298000 Max Easting: 400010 Min Northing: 455000 Max Northing: 572000
Sampling period:	Summer 1978 – 1980
Sampling density:	1 sample per 1.6 km^2

Project/Sample code:	32
No. of sites	6200
Sample type *(no. sites sampled)*	Stream sediment (6200), stream waters (2585), heavy mineral panned concentrates (6200)
Sample preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, V, Y, Zn and Zr (DR-ES); Sb and As (5338 samples were analysed by acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis).
Atlas content	Interpolated geochemical maps and accompanying text are presented for 30 elements; Sb, As, Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, U, V, Y, Zn and Zr in sediment and for pH, conductivity, bicarbonate, fluoride and U in water.
Notes:	Initially sponsored by the Department of Trade and Industry. Funded to completion by Department of Education and Science (Office of Science and Technology).

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ATLAS:	**North-east England**
REFERENCE:	British Geological Survey (1996). Regional geochemistry of north-east England. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 255 9
Sheet boundaries:	Min Easting: 400000 Max Easting: 525000 Min Northing: 455000 Max Northing: 572000
Sampling period:	Summer 1986 – 1988
Sampling density:	1 sample per 1.5 sq km
Project/Sample code:	30
No. of sites	4306
Sample type *(no. sites sampled)*	Stream sediment (4306), stream waters (2153), heavy mineral panned concentrates (4306). Soils: Due to the absence of surface drainage channels in the area underlain by chalk in the Yorkshire Wolds, soil samples were collected from 502 sites at a sample density of 1 per 1 km^2. Over other areas of poor drainage density over the vales of York and Pickering, soils were also collected at a density of 1 per 2 sq km. Soils were collected on a grid basis, one from every 1 km national grid square over the chalk and from every second grid square in other areas. Soils were collected at a standard depth of 30 – 40 cm with a hand auger.
Sample	The < 150 micron fraction was ground until 95 % was < 53 micron using an

preparation:	agate ball mill.
Determinands (methods):	Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, V, Y, Zn and Zr (DR-ES); Sb and As were analysed by acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS in all samples; U (delayed neutron activation analysis).
Atlas content	Interpolated geochemical maps and accompanying text are presented for 30 elements; Sb, As, Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, U, V, Y, Zn and Zr in sediment, all except Sb and As in soil and for pH, conductivity, bicarbonate, fluoride and U in water.
Notes:	Initially sponsored by the Department of Trade and Industry. Funded to completion by Department of Education and Science (Office of Science and Technology).

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ATLAS:	**North-west England and North Wales**
REFERENCE:	British Geological Survey (1997). Regional geochemistry of parts of north-west England and North Wales. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 307 5
Sheet boundaries:	Min Easting: 210000 Max Easting: 400000 Min Northing: 320000 Max Northing: 464000
Sampling period:	Summer 1988 – 1990
Sampling density:	1 sample per 1.5 sq km
Project/Sample code:	35
No. of sites	5203
Sample type (no. sites sampled)	Stream sediment (5203), stream waters (3000), heavy mineral panned concentrates (5203). Soils: Due to the absence of surface drainage channels in some of the lowland areas of Lancashire and Cheshire, soil samples were collected from 2064 sites at a sample density of 1 per 2 sq km. Soils were collected on a grid basis, one from every second 1 km national grid square. Soils were collected at a standard depth of 30 – 40 cm with a hand auger.
Sample preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, V, Y, Zn and Zr (DR-ES); Sb and As were analysed X-ray fluoresence (XRF) in all samples; U (delayed neutron activation analysis).
Atlas content	Interpolated geochemical maps and accompanying text are presented for 30 elements; Sb, As, Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, U, V, Y, Zn and Zr in sediment and soil and for pH, conductivity, bicarbonate, fluoride and U in water.
Notes:	Initially sponsored by the Department of Trade and Industry. Funded to completion by Department of Education and Science (Office of Science and

	Technology).

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ATLAS:	**Orkney**
REFERENCE:	Institute of Geological Sciences (1978). Regional Geochemical Atlas: Orkney. London, Institute of Geological Sciences. ISBN 0 85272 060 2
Sheet boundaries:	Min Easting: 281964 Max Easting: 383404 Min Northing: 900779 Max Northing: 1065125
Sampling period:	July 1970
Sampling density:	1 sample per 1.14 km^2
Project/Sample code:	AR/03
No. of sites	672
Sample type *(no. sites sampled)*	Stream sediment (437) Stream waters (672)
Sample preparation:	The < 150 micron fraction ground until 95 % was < 100 micron using a mechanical agate mortar
Determinands (methods):	Ba, Be, B, Cr, Co, Fe, Mn, Mo, Ni, Sn, V and Zr (OES); Cu, Pb and Zn (acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis)
Atlas content	Interpretative maps using proportional vector symbols and accompanying text are presented for 15 elements; Ba, Be, B, Cr, Co, Cu, Fe, Pb, Mn, Mo, Ni, U, V, Zn and Zr in sediment and U in surface water. Only 88 sites determined for pH and conductivity of surface water. Interpreted images for Sn were not presented due to the detection of a significant level of within site variance.
Notes:	Sponsored by the Department of Industry through its Chemical and Minerals Requirement Board. Second in the series of atlases to be published

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ATLAS:	**Shetland**
REFERENCE:	Institute of Geological Sciences (1978). Regional Geochemical Atlas: Shetland. London, Institute of Geological Sciences. ISBN 0 85272 061 0
Sheet boundaries:	Min Easting: 384412 Max Easting: 514315 Min Northing: 1045053 Max Northing: 1236642
Sampling period:	August and September 1970
Sampling density:	1 sample per 1.16 km^2
Project/Sample	AS/01

code:	
No. of sites:	1254
Sample type *(no. sites sampled)*	Stream sediment (1254) Stream waters (1254)
Sample preparation:	The < 150 micron fraction ground until 95 % was < 100 micron using a mechanical agate mortar.
Determinands (methods):	Ba, Be, B, Cr, Co, Fe, Mn, Mo, Ni, Sn, V and Zr (OES); Cu, Pb and Zn (acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis).
Atlas content	Interpretative maps using proportional vector symbols and accompanying text are presented for 15 elements; Ba, Be, B, Cr, Co, Cu, Fe, Pb, Mn, Mo, Ni, U, V, Zn and Zr in sediment and U in surface water. Only 124 sites determined for pH and conductivity of surface water. Interpreted images for Sn were not presented due to the detection of a significant level of within site variance.
Notes:	Sponsored by the Department of Industry through its Chemical and Minerals Requirement Board. Follow up regional survey conducted in 1990 (see Shetland follow-up). First in the series of atlases to be published

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ATLAS:	**Shetland Follow-up**
REFERENCE:	
Sheet boundaries:	
Sampling period:	Summer 1990
Sampling density:	
Project/Sample code	83
No. of sites	1240
Sample type *(no. sites sampled)*	Stream sediment (1240 + 124 in pilot study) Stream waters (1240 + 124 in pilot study) Heavy mineral panned concentrates (1240 + 124 in pilot study).
Sample preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ag, As, Al_2O_3, B, Ba, Be, Bi, Ce, CaO, Cd, Co, Cr, Cu, Fe_2O_3, Ga, K_2O, La, Li, MgO, Mn, Mo, Nb, Nd, Ni, P, Pb, Rb, Sb, SiO_2, Sn, Sr, TiO_2, U, V, W, Y, Zn and Zr (DR-ES and XRF); alkalinity, conductivity, F (specific ion method); pH; U (laser-induced fluorometry).
Atlas content	Interpolated geochemical maps and accompanying text are presented for As, Ba, Cu and Zn in stream sediments and fluoride in stream water.

Notes:	Project run by Ms Dee Flight in collaboration with the Shetlands Islands Council and Highlands and Islands Enterprise.

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ATLAS:	**South Orkney and Caithness**
REFERENCE:	Institute of Geological Sciences (1978). Regional Geochemical Atlas: South Orkney and Caithness. London, Institute of Geological Sciences. ISBN 0 85272 064 5
Sheet boundaries:	Min Easting: 281800 Max Easting: 360000 Min Northing: 902700 Max Northing: 1014000
Sampling period:	July 1969
Sampling density:	1 sample per 2.3 km^2
Project/Sample code:	AR/02 AQ/03 AP/04 FN/05 SN/06
No. of sites	1287
Sample type *(no. sites sampled)*	Stream sediment (1287) Stream waters (1287)
Sample preparation:	The < 150 micron fraction ground until 95 % was < 100 micron using a mechanical agate mortar.
Determinands (methods):	Ba, Be, B, Cr, Co, Fe, Mn, Mo, Ni, Sn, Ti, V and Zr (OES); Cu, Pb and Zn (acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis). Only 104 sites determined for pH and conductivity of surface water.
Atlas content	Interpretative maps using proportional vector symbols and accompanying text are presented for 16 elements; Ba, Be, B, Cr, Co, Cu, Fe, Pb, Mn, Mo, Ni, Ti, U, V, Zn and Zr in sediment and for pH, conductivity and U in water. Interpreted images for Sn were not presented due to the detection of a significant level of within site variance.
Notes:	Sponsored by the Department of Industry through its Chemical and Minerals Requirement Board. Third in series of atlases published

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ATLAS:	**Southern Scotland**
REFERENCE:	British Geological Survey (1991). Regional geochemistry of southern Scotland and part of northern England. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 229 X
Sheet boundaries:	Min Easting: 117000 Max Easting: 440000 Min Northing: 531000 Max Northing: 685000
Sampling period:	Summer 1977, 1981 – 1986
Sampling	1 sample per 1.5 km^2

density:	
Project/Sample code:	27 28 29 34 39
No. of sites	9920
Sample type *(no. sites sampled)*	Stream sediment (19 000), stream waters (4230), heavy mineral panned concentrates (19 000)
Sample preparation:	The < 150 micron fraction was ground until 95 % was < 53 micron using an agate ball mill.
Determinands (methods):	Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, V, Y, Zn and Zr (DR-ES); Sb and As (sites to the west of 4°W were analysed by acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS). To the east of 4°W Sb and As were analysed by X-ray fluorescence); U (delayed neutron activation analysis)
Atlas content	Interpolated geochemical maps and accompanying text are presented for 30 elements; Sb, As, Ba, Be, Bi, B, Ca, Cr, Co, Cu, Ga, Fe, La, Pb, Li, Mg, Mn, Mo, Ni, K, Rb, Ag, Sr, Sn, Ti, U, V, Y, Zn and Zr in sediment and for pH, conductivity, bicarbonate, fluoride and U in water.
Notes:	Initially sponsored by the Department of Trade and Industry. Funded to completion by Department of Education and Science

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ATLAS:	**Sutherland**
REFERENCE:	Institute of Geological Sciences (1982). Regional Geochemical Atlas: Sutherland. London, Institute of Geological Sciences. ISBN 0 85272 068 8
Sheet boundaries:	Min Easting: 19500 Max Easting: 284000 Min Northing: 903000 Max Northing: 975000
Sampling period:	Summer 1968 – 1972
Sampling density:	1 sample per 1.8 km^2
Project/Sample code:	AP/03 AP/04 FN/05 SN/06
No. of sites	2620
Sample type *(no. sites sampled)* *[results in database]*	Stream sediment (2460) [2461] Stream waters (2622) [2564]
Sample preparation:	The < 150 micron fraction ground until 95 % was < 100 micron using a mechanical agate mortar.
Determinands (methods):	Ba, Be, B, Cr, Co, Fe, Mn, Mo, Ni, Sn, V and Zr (OES); Cu, Pb and Zn (acid attack (ammonium persulphate with 75% hydrochloric acid) followed by solvent extraction AAS); U (delayed neutron activation analysis).

Atlas content	Interpretative maps using proportional vector symbols and accompanying text are presented for 14 elements; Be, B, Cr, Co, Cu, Fe, Pb, Mn, Mo, Ni, U, V, Zn and Zr in sediment and for pH, conductivity and U in water (pH and conductivity on only 155 sites). Interpreted images for Sn were not presented due to the detection of a significant level of within site variance and Ba was also omitted due to concern over a change in background level thought to be attributable to analytical error.
Notes:	Sponsored by the Department of Industry through its Chemical and Minerals Requirement Board. Four standards for every batch of 100 samples.

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ATLAS:	**Wales and West Midlands – Sediments and Soil**
REFERENCE:	British Geological Survey (2000). Regional geochemistry of Wales and west-central England: stream sediment and soil. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 378 4
Sheet boundaries:	Min Easting: 170000 Max Easting: 400000 Min Northing: 160000 Max Northing: 400000
Sampling period:	summer 1988 – 1994
Sampling density:	1 sample per 1.5 sq km
Project/Sample code:	36 37 38
No. of sites	18 927
Sample type *(no. sites sampled)*	Stream sediment (18 927) and soils (3800). Soils were collected at a standard depth of 30 – 40 cm with a hand auger.
Sample preparation:	Stream sediments and 35 – 45 cm soil sample < 150 micron fraction ground until 95 % was < 53 micron using an agate ball mill; surface soils (10 – 20 cm) were oven dried, sieved to –2mm and ground until 95% was less than 53µm using an agate planetary ball mill.
Determinands (methods):	Mg, P, K, Ca, Ti, Mn, Fe, V, Cr, Co, Ba, Ni, Cu, Zn, Ga, As, Se, Rb, Sr, Y, Zr, Nb, Mo, Pb, Bi, Th, U, Ag, Cd, Sn, Sb, Cs, La, Ce (XRF); Sb and As were analysed X-ray fluorescence (XRF) in all samples; Soil pH determined on all subsoil samples in a slurry of 0.01 M $CaCl_2$ (10 g air-dried soil to 25 ml 0.01 M $CaCl_2$).
Atlas content	Interpolated geochemical maps for the stream sediments and accompanying text are presented for 34 elements; Sb, As, Ba, Bi, B, Ca, Cd, Ce, Cr, Co, Cu, Ga, Fe, La, Pb, Mg, Mn, Mo, Ni, Nb, P, K, Rb, Se, Ag, Sr, Th, Sn, Ti, U, V, Y, Zn and Zr , and all these elements except Bi, Cd and Ag in soil
Notes:	Office of Science and Technology (Department of Education and Science)

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ATLAS:	**Wales and West Midlands – Water**
REFERENCE:	British Geological Survey (1999). Regional geochemistry of Wales and west-central England: stream water. Keyworth, Nottingham, British Geological Survey. ISBN 0 85272 363 6
Sheet boundaries:	Min Easting: 170000 Max Easting: 400000 Min Northing: 160000 Max Northing: 400000
Sampling period:	Summer 1988 – 1994
Sampling density:	1 sample per 1.5 sq km
Project/Sample code:	36 37 38
No. of sites	13 444
Sample type(no. sites sampled)	Stream water (13 444) from 1st and 2nd order streams
Sample preparation:	none
Determinands (methods):	ICP-AES used to determine 27 elements: Sr, Cd, Ba, Si, Mn, Fe, P S (as SO_4^{2-}), B, Mg, V, Na, Mo, Al, Be, Ca, Zn, Cu, Pb, Li, Zr, Co, Ni, Y, La, K and Cr. Automated colorimetric methods were used to determine Cl and NO_3^-. Ion selective electrode was used to determine F. Laser-induced fluorescence was used to determine U.
Atlas content	Interpolated geochemical maps and accompanying text are presented for; pH, conductivity, Al, Ba, Bicarbonate, B, Cd, Ca, Cl, F, Fe, Pb, Li, Mg, Mn, Mo, Ni, NO_3^- , P, K, Si, Na, Sr, SO_4^{2-}, U, V, and Zn . Many thematic multi-element maps are included.
Notes:	Office of Science and Technology (Department of Education and Science)

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References

ANDER, E.L. 2004. Baseline concentrations of metals in stream waters and sediments. Commissioned Report Series CR/04/035, British Geological Survey, Keyworth, Nottingham, UK.

BREWARD, N. 2003. Heavy-metal contaminated soils associated with drained fenland in Lancashire revealed by BGS Geochemical Survey. *Applied Geochemistry*, Vol. 18, 1663-1670.

BREWARD, N, and HERD, R. 1998. Report on the development of the NIH-Image program for processing and examining geochemical data. *British Geological Survey*, BGS Technical Report No. WP/97/07.

BRITISH GEOLOGICAL SURVEY. 1999. *Regional geochemistry of Wales and part of west-central England: stream water*. (Keyworth, Nottingham: British Geological Survey.) ISBN 085272363 6

CEC. 2000. Water Framework Directive. *Commission of the European Communities*.

COATS, J S. 2004. The BGS Geochemistry Database: history, design and current usage. *British Geological Survey*, Internal Report Number IR/04/033

COATS, J S, and HARRIS, J R. 1995. Database design in geochemistry: BGS experience. 25-32 in *Geological Data Management*. GILES, J R A (editor). No. 97. (Geological Society of London Special Publication.)

COOPER, A., KESSLER, H., FORD, J. PRICE, S. HALL, M. and PHARAOH, T. 2004. The Vale of York. Multidisciplinary survey and geographical information system. *Earthwise*. ISSUE. 20. 8-9. British Geological Survey, Keyworth, Nottingham, UK.

DAVIS, J C. 1986. *Statistics and data Analysis in Geology* (Second edition). (New York: John Wiley & Sons.) ISBN 0-471-08079-9

DEFRA, and ENVIRONMENT AGENCY. 2002. Assessment of risks to human health from land contamination. An overview of the development of soil guideline values and related research. *UK Department for Environment Food and Rural Affairs and Environment Agency*, ISBN: 1 857 05732 5.

DETR. 2000. Environmental Protection Act 1990: Part IIA. *Department of Environment, Transport and the Regions*, DETR Circular 02/2000.

FORDYCE, F M. 2003. A bibliographic review of regional geochemical mapping for Quaternary studies. *British Geological Survey*, BGS Internal Report No IR/03/169R.

FORDYCE, F M, and ANDER, E L 2003. *Urban Geochemistry GIS - A Case Study from Stoke-on-Trent*. Internal Report Series. No. IR/01/35/R. (Keyworth, Nottingham: British Geological Survey.)

FORDYCE, F M, ZHANG, G., GREEN, K., LIU, X. 1998. Soil grain and water chemistry and human selenium imbalances in the Enshi district, Hubei Province, China. *British Geological Survey, Overseas Geology Series*, WC/96/54.

FREESTONE, S E, O'DONNELL, K E, and BROWN, S E 2002. Geochemical baseline data for the urban area of Sheffield. *British Geological Survey, Keyworth, UK*, Internal Report No. IR/02/084.

HARRIS, J R, and COATS, J S. 1992. Geochemistry Database: Data Analysis and Proposed Design. *British Geological Survey*, Mineral Reconnaissance Programme Report No. 125.

HASLAM, H W, CAMERON, D G, and EVANS, A D. 1990. The Mineral Reconnaissance Programme 1990. *British Geological Survey*, Mineral Reconnaissance Programme Report No. 114.

HOBBS, S F. 2004. ArcView digitising and connecting to Oracle databases guide. *British Geological Survey*, Internal Report No. IR/04/03.

HOBBS, S F, KIMBELL, S F, COATS, J S, and FORTEY, N J. 2000. BGS databases for mineral exploration: status in 2000. *British Geological Survey*, Research Report RR/00/11. DTI Minerals Programme Publication No. 6.

HOWARD, A S, WATERS, C N, and MARSH, S H. In Prep. Recommendations for handling and managing geological survey baseline data: Summary Report. *British Geological Survey*, Internal Report No. IR/04/***.

HOWARTH, R J, (editor) 1983. *Statistics and Data Analysis in Geochemical Prospecting*. Handbook of Exploration Geochemistry. No. 2. (Amsterdam: Elsevier.)

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

JOHNSON, C C. 2002. Within site and between site nested analysis of variance (ANOVA) for Geochemical Surveys using MS EXCEL. *British Geological Survey, Keyworth, UK*, Internal Report No. IR/02/043.

JOHNSON, C C, and BREWARD, N. 2004. GBASE: The UK Geochemical Baseline Survey of the Environment. *British Geological Survey*, BGS Report Number CR/04/016N.

JOHNSON, C C, BROWN, S E, and LISTER, T R. 2003a. G-BASE Field Procedures Manual version 1.1. *British Geological Survey, Keyworth, UK*, Internal Report No. IR/03/096.

JOHNSON, C C, FORDYCE, F M, and STEWART, A G 2003b. The geochemistry of iodine and its application to environmental strategies for reducing the risks from iodine deficiency disorders (IDD). *British Geological Survey*, Commisioned Report CR/03/057N.

JONES, R C, and COATS, J S. 1993. Sources of geochemical data collected by the International Division since 1965. *British Geological Survey*, Technical Report WC/97/49.

LISTER, T R. 2002. Analysis of Variance (ANOVA) of G-BASE sub-surface soil data from 11 urban centres in England and Wales. *British Geological Survey, Keyworth, UK*, Internal Report No. IR/02/009.

LISTER, T R, STAINES, R, and JOHNSON, C C. In Prep. G-BASE data conditioning procedures for stream sediment and soil chemical analyses. *British Geological Survey*, BGS Internal Report Number IR/04/***.

MACHALI MUCHSIN, A, JOHNSON, C C, CROW, M J, DJUMSARI, A, and SUMARTONO. 1997. *Geochemical Atlas of Southern Sumatra. Regioanl Geochemical Atlas Series of Indonesia No. 2.* (Keyworth, Nottingham, UK/Bandung, Indonesia: Directorate of Mineral Resources/British Geological Survey.)

O'DONNELL, K E, and RAWLINS, B G. 2003. Soil geochemical signatures in UK urban environments *poster presentation at International Symposium on Environmental Geochemistry 2003 conference*, September 2003, Edinburgh.

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.

REIMANN, C, FILZMOSER, P, and GARRET, R G. 2002. Factor analysis applied to regional geochemical data: problems and possibilities. *Applied Geochemistry*, Vol. 17, 185-206.

STEVENSON, A G, TAIT, B A R, RICHARDSON, A, SMITH, R T, NICHOLSON, R A, and STEWART, H R. 1995. The geochemistry of sea-bed ssediments of the United Kingdom Continetal Shelf; the North Sea, Hebrides and West Shetland shelves, and the Malin-Hebrides sea area. *British Geological Survey*, Technical Report WC/95/28C.

STONE, P, BREWARD, N, and MERRIMAN, R. 2003. Mineralogical controls on metal distribution in stream sediment derived from the Caledonides of the Scottish Southern Uplands and English Lake District. *Mineralogical Magazine*, Vol. 67, 893-906.

STONE, P, GREEN, P.M., LINTERN, B.C., PLANT J.A., SIMPSON, P.R., BREWARD, N. 1991. Geochemistry characterizes provenance in southern Scotland. *Geology Today*, Vol. 7, 177-181.

THORNTON, I, and PLANT, J.A. 1980. Regional geochemical mapping and health in the United Kingdom. *Journal of the Geological Society of London*, Vol. 137, 575-586.

WILLIAMS, T M. 1997. DFID-TDR project R6491. Mining-related arsenic hazards: Thailand case-study summary report. *British Geological Survey*, Overseas Geology Series Technical Report WC/97/49.