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Geochemistry@BGS: A guide to geochemical data at the British Geological Survey

Environmental Geoscience Baselines/
Information Management Programme
Open Report OR/09/028

BRITISH GEOLOGICAL SURVEY

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Geochemistry@BGS: A guide to geochemical data at the British Geological Survey

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BRITISH GEOLOGICAL SURVEY

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We publish an annual catalogue of our maps and other publications; this catalogue is available online or from any of the BGS shops.

The British Geological Survey carries out the geological survey of Great Britain and Northern Ireland (the latter as an agency service for the government of Northern Ireland), and of the surrounding continental shelf, as well as basic research projects. It also undertakes programmes of technical aid in geology in developing countries.

The British Geological Survey is a component body of the Natural Environment Research Council.

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Summary

This report reviews the main activities in the British Geological Survey (and previously as the Institute of Geological Sciences) that have generated geochemical data. Included are; the mineral reconnaissance programme; regional geochemical mapping; groundwater geochemistry; marine and estuarine surveys; environmental geochemistry and health; radiometric surveys; isotopic geochemistry; lithogeochemical investigations; organic geochemistry laboratories; and many international activities involving geochemical sampling. An indication is given as to where the data resides and who is currently responsible for managing it. An objective of this report is to give better access to the geochemical results and information both for the internal and external users of geochemical data. A list of recommendations are proposed to help give a more corporate and joined up approach to BGS provision of geochemical data and information. The presentation of the geochemical data to the public should be done in a less project-orientated manner. The corporate Geochemistry Database is rather a misnomer as it only contains geochemical data generated by a small number (although very sizable) projects. Other geochemical databases exist but they are not particularly accessible. There is still a lot of geochemical data that is not captured to any corporately supported database. Internal and external reports are one of the major sources of geochemical data and information and this report contains a comprehensive reference list to key BGS geochemical publications.

1 Introduction

This report is a guide to the geochemical data, samples and associated information that have been produced in BGS. It seeks to better inform geochemical data users (both internal and external) as to the range of geochemical data holdings and how to access them. BGS has a wealth of geochemical data generated by numerous applied geochemical projects over the past 50 years both in the UK and internationally. The report does not claim to have captured all the information regarding geochemistry at BGS. For example, a major area of BGS geochemical work excluded from this report is the commissioned projects on radioactive waste disposal and fluid processes as the majority of this work was done as “commercial-in-confidence”. The BGS analytical laboratories are a principal source of the geochemical data generated but are not discussed in any detail unless the laboratory is an integral part of the science project as is the case for NERC Isotopic Geoscience Laboratory (NIGL) and the organic geochemistry laboratory.

The geochemical data is a sub-set of BGS’s environmental data set and it continues to underpin many parts of the BGS strategy (British Geological Survey, 2009). The collection and analysis of samples, and their interpretation and presentation is considered to be part of BGS’s national capability. As a result BGS has a good international reputation in the field of applied geochemistry and it is well positioned to compete for and win commission projects (or external income EI). The take up, application and exploitation of the geochemical data is generally encapsulated in BGS’s research programmes, for example, modelling and understanding soil processes, human health and contaminated land studies, and investigations of groundwater vulnerability. A better understanding of the BGS geochemical data heritage will improve its exploitation and application. BGS has a wealth of geochemical data that has cost millions of pounds to generate yet it remains a greatly under-utilised resource.

The following definitions seek to describe the scope of the BGS geochemical data holdings:

1. ***A measurement of a chemical element or compound***.

A chemical element will be one of the 117 elements of the Periodic Table. An analyte may be a mixture or single isotope, cation or anion, or a compound consisting of a combination of two or more elements. The definition therefore covers both inorganic and organic compounds and in the database the chemical element or compound will be referred to as an analyte. The measurements must have a defined unit of measurement and the analyte determined will be associated with a defined analytical method.

2. ***A measurement made by direct or remote contact with a material being analysed which may be in situ or a sample removed for analysis elsewhere***.

This will include measurements made by non-destructive analysis such as XRFS or neutron activation where a specific sample has been used for analysis. Data generated by remote geophysical techniques such as airborne or sea-bed gamma-ray spectrometer can also be considered as geochemical data though here there is considerable overlap with data more generally considered as geophysical measurements.

3. ***A measurement that has been made or commissioned by BGS***.

Geochemical data in this report refer to measurements made by or commissioned by the BGS. The ownership and IPR rights will vary according to the project that generated the data. The provision of geochemical data to users must be accompanied by a clear definition of ownership and the IPR rights. For data generated through commissioned work there are likely to be restrictions on how the data can be used. Third party data donated or otherwise to BGS are not considered in this report.

4. ***A measurement with a unique identifier and spatial coordinates defined with a temporal reference*.**

   The spatial coordinates will define whether the geochemical data is classified as being from the UK land area (on-shore), UK territorial waters (off-shore), or classified as an "International" measurement. This threefold geographical definition is the initial criterion used to classify BGS geochemical data. Note that anything collected from below the marine high water mark in UK territorial waters is considered as off-shore data and this would include the results of the BGS estuarine projects.

The geochemical data may be accompanied by measurements of other parameters that help to understand or interpret the chemical concentrations. These could include measurements such as pH, Eh, conductivity or temperature. These measurements alone do not constitute geochemical data.

The samples collected for geochemical analysis should also be considered as part of the BGS geochemistry data holdings. BGS has an extensive UK collection of soil, rock, drill core and drainage samples, including stream water samples in cold storage. The storage of the samples is the responsibility of the National Geoscience Data Centre (NGDC) at Keyworth.

The management of geochemical data is the responsibility of the Information Management Programme of BGS. Within this programme there is a data management team which leads data management projects. Geochemistry data management (IM4) is one of these projects and this project is primarily responsible for UK land surface geochemistry (*i.e.* excluding hydrogeology (IM3) and marine geology data (IM6)). In recent years, as part of project start up, new projects are required to write a data management plan and in the case of geochemical projects this should involve storage of excess samples in the NGDC and input of geochemical results into a corporate database. This is what should happen but in practice databases are not able to accept data for analytes extracted and determined by methods not defined in the database tables (*e.g.*, a lot of the chemical information generated by bioaccessibility studies of G-BASE soil samples). The geochemical data and its storage must conform to corporate database and dictionary standards. Legacy geochemical data will invariably have some non-conformity with current standards *e.g.* because of revision of dictionary codes. It is important that any translations of legacy data to fit with corporate standards are documented.

The British Geological Survey (BGS) has been actively generating geochemical data for the UK from "treetop to bedrock" since the 1960s in support of special surveys, the principal of which have been for mineral exploration (Mineral Reconnaissance Programme, Haslam *et al.*, 1990), baseline geochemical mapping (G-BASE, Johnson *et al.*, 2005), natural quality of groundwater (Edmunds *et al.*, 2003), offshore sea-bed sediment geochemistry (Stevenson *et al.*, 1995), estuary studies (Ridgway and Shimmield, 2002 and Jones *et al.*, 2004), environmental radioactivity studies (especially radon) onshore (*e.g.* Miles and Appleton, 2005), uranium exploration (*e.g.* Bowie *et al.*, 1973), and seabed gamma spectrometry for a range of applications (*e.g.* Jones, 2001). Outside of the UK substantial amounts of geochemical data have been generated by development projects (mainly supported by the Overseas Development Administration (ODA) and its successor Department for International Development (DfID). These international data are generally not in corporate databases (with the exception of hydrogeochemical data) but are published in reports and geochemical atlases (*e.g.* Sumatra, Indonesia, Muchsin *et al.*, 1997) or made available on CD-ROMs.

2 Geochemical data in BGS

2.1 GEOCHEMICAL DATA FOR UK MINERAL EXPLORATION

Geochemical data from BGS projects relating to UK mineral exploration are held in the corporate Geochemistry Database. There is no non-BGS (*i.e.* third party) exploration data held in this database. The BGS Mineral Reconnaissance Programme (MRP) (1972-1997) collected stream sediments, panned concentrates, soils, tills, rocks and drill core samples which were determined for a wide range of chemical elements. Uranium exploration work that predates the MRP is described in Section 2.8.1. Haslam *et al*. (1990) describe the work of the MRP up to 1990 and the geochemical data that the programme generated is summarised by Hobbs *et al*. (2000). This multidisciplinary programme involved targeted mineral exploration and so the associated geochemical results tend to be site specific. However, there were also a number of regional reconnaissance surveys over large areas (*e.g.* Northumberland, Bateson and others, 1983). 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 finished in April 2004 and now most BGS metalliferous exploration projects are those carried out overseas.

The MRP was the driving force behind the creation of BGS's first corporate ORACLE database, the Geochemistry Database (Harris and Coats, 1992 and Coats, 2004). The entity diagram for the Geochemistry Database is shown in Figure 1 and a breakdown of the MRP samples available in the database is given in Table 1. A comprehensive series of MRP reports means that the sampling methodology and analytical background to the geochemical data is well documented and during the 1990s resources were available to populate the database with MRP results. There is no longer any active BGS UK geochemical work associated with minerals and there has been no MRP geochemical data routinely loaded to the Geochemistry Database since 2000. Whilst much of the chemical data has been captured there is a lot of site and sample information that has not been loaded. The hardcopy data is archived in the NGDC (National Geoscience Data Centre), the MRP fields cards are on aisle 61 and information about the chemical analysis in aisle 62. Aisle 151 also contains some hardcopy MRP information.

Project	**Soils and tills**	**Stream sediments**	**Panned mineral concs.**	**Surface waters**
MRP	82265	28655	33383	9499
G-BASE	49658	100356	75942	74871
OTHERS	328	0	0	0
Total	132251	129011	38271	84370

Table 1: Summary of the most common sample types in the Geochemistry Database categorised by Project

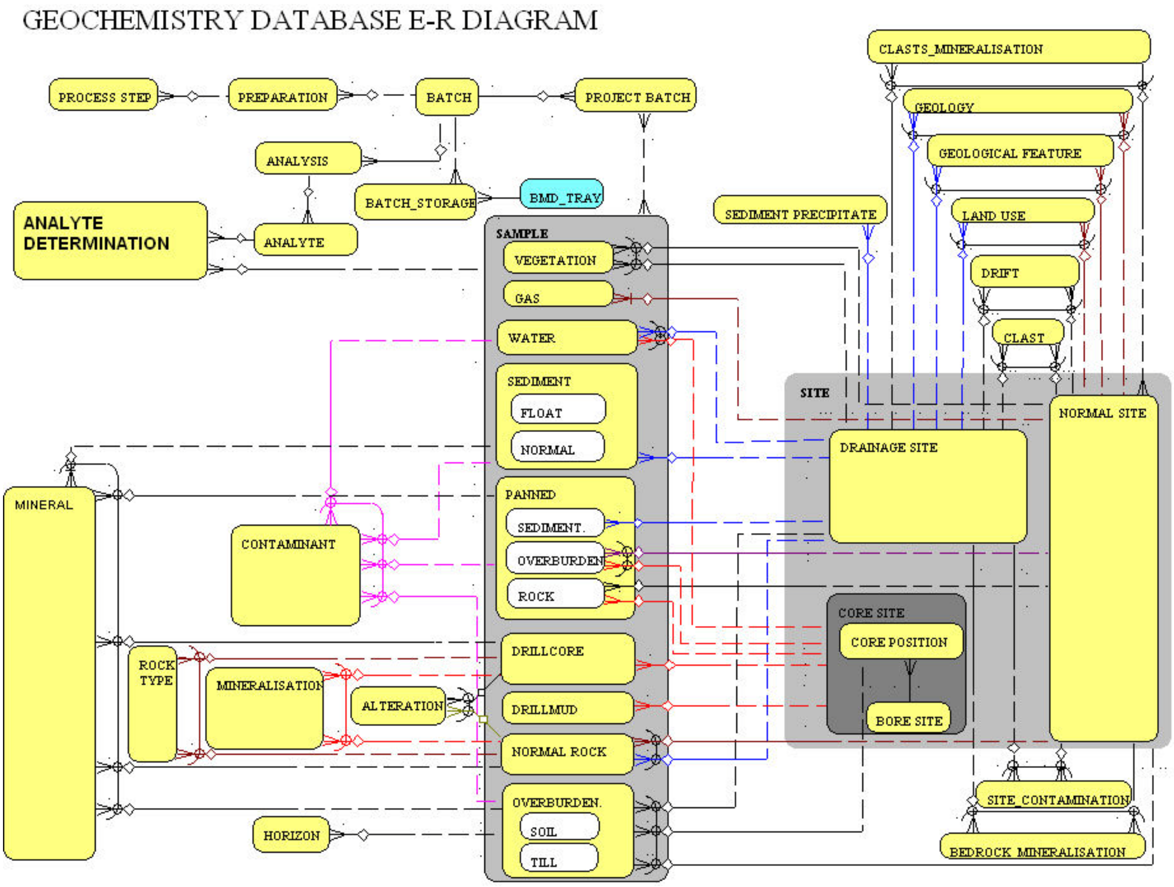

Figure 1: Entity diagram for the Geochemistry Database

Information about MRP geochemical data can be accessed through the MRP reports which are listed through the ‘publications’ link on the MineralsUK[1] web site. The BGS online bookshop[2] gives a list of all the MRP reports and information on how to purchase them (under the “Minerals Publications” category). BGS staff can access scanned MRP reports through GEOLIB[3]. The MRP reports covering geochemical surveys generally contain summary geochemical information and maps. Some also contain listings of the locational and analytical data for each sample (*e.g.* Bateson and Johnson, 1984). Availability of geochemical data for MRP samples is shown on the geochemistry layer of the BGS GeoIndex[4]. Figure 2 gives an example screen showing the spatial distribution of MRP samples in a selected area of the UK and an associated information query. The BGS Enquiries desk[5] should be the initial channel for any external enquiries relating to BGS MRP information, data availability or pricing. These will be forwarded by enquiries to: (a) the “Minerals for Development” Team Leader of the BGS Minerals theme for enquiries relating to BGS metalliferous minerals projects; and (b) Digital licencing and Sales for enquiries concerning the licencing of MRP data. The current BGS pricing policy covering data in the Geochemistry Database is summarised in Box 1.

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[1] http://www.bgs.ac.uk/mineralsuk/home.html

[2] http://shop.bgs.ac.uk/bookshop/

[3] http://geolib.bgs.ac.uk/cgi-bin/webview.sh

[4] http://www.bgs.ac.uk/geoindex/index.htm

[5] enquiries@bgs.ac.uk

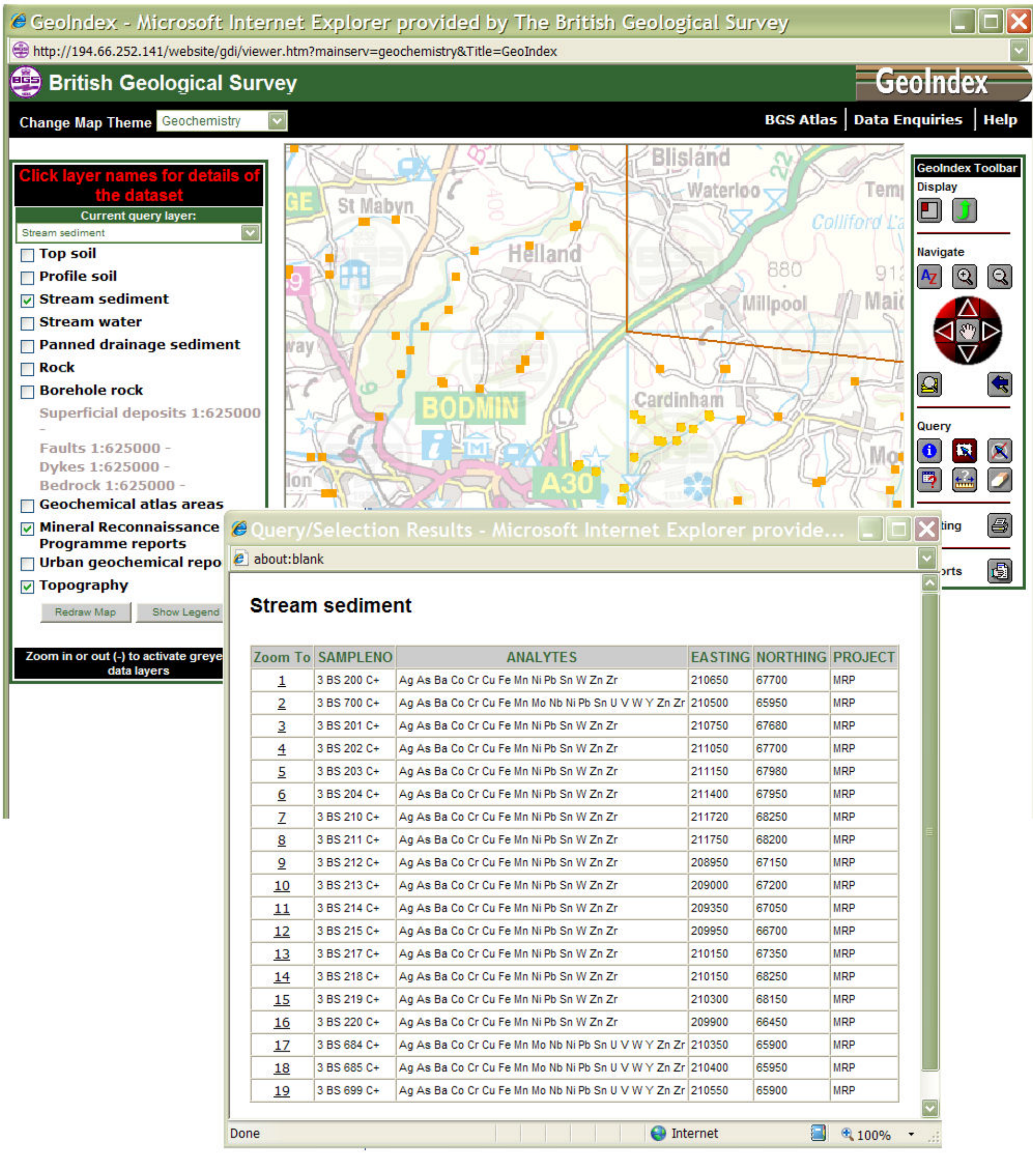
BOX 1: Pricing policy for digital data from the Geochemistry Database

Digital data from the Geochemistry Database is licenced, not sold, on the basis of the number of records of data required, regardless of the number of analyte fields. All the field and analytical data for a particular sample type from a site is defined as a record. The licence fee comprises three elements:

- Licence Administration Charge (LAC)
- Data Preparation and Delivery Charge (DPC)
- Data Use Charge (DUC)

The LAC is £150 and the DPC is a minimum of £150 but can be higher for large or complex data sets. The DUC is based on the following equation:

DUC = (C x N x Y x S x D) where C is a £0.50 charge per record; N is the number of records; Y is the length of licence (1- 5 years); S = number of licence seats factor; and D is a discount factor applied when N > 2000)



Click layer names for details of the dataset

Current query layer: Stream sediment

☐ Top soil
☐ Profile soil
☑ Stream sediment
☐ Stream water
☐ Panned drainage sediment
☐ Rock
☐ Borehole rock
Superficial deposits 1:625000 -
Faults 1:625000 -
Dykes 1:625000 -
Bedrock 1:625000 -
☐ Geochemical atlas areas
☑ Mineral Reconnaissance Programme reports
☐ Urban geochemical repo
☑ Topography

Redraw Map | Show Legend

Zoom in or out (-) to activate greye data layers

Stream sediment

Zoom To	SAMPLENO	ANALYTES	EASTING	NORTHING	PROJECT
1	3 BS 200 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	210650	67700	MRP
2	3 BS 700 C+	Ag As Ba Co Cr Cu Fe Mn Mo Nb Ni Pb Sn U V W Y Zn Zr	210500	65950	MRP
3	3 BS 201 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	210750	67680	MRP
4	3 BS 202 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	211050	67700	MRP
5	3 BS 203 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	211150	67980	MRP
6	3 BS 204 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	211400	67950	MRP
7	3 BS 210 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	211720	68250	MRP
8	3 BS 211 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	211750	68200	MRP
9	3 BS 212 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	208950	67150	MRP
10	3 BS 213 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	209000	67200	MRP
11	3 BS 214 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	209350	67050	MRP
12	3 BS 215 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	209950	66700	MRP
13	3 BS 217 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	210150	67350	MRP
14	3 BS 218 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	210150	68250	MRP
15	3 BS 219 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	210300	68150	MRP
16	3 BS 220 C+	Ag As Ba Co Cr Cu Fe Mn Ni Pb Sn W Zn Zr	209900	66450	MRP
17	3 BS 684 C+	Ag As Ba Co Cr Cu Fe Mn Mo Nb Ni Pb Sn U V W Y Zn Zr	210350	65900	MRP
18	3 BS 685 C+	Ag As Ba Co Cr Cu Fe Mn Mo Nb Ni Pb Sn U V W Y Zn Zr	210400	65950	MRP
19	3 BS 699 C+	Ag As Ba Co Cr Cu Fe Mn Mo Nb Ni Pb Sn U V W Y Zn Zr	210550	65900	MRP

Figure 2: BGS Internet GeoIndex page showing information about MRP stream sediment samples east of Bodmin.

All BGS staff have read access to the BGS Oracle Geochemistry Database. However, the complex and numerous dictionary and data tables (documented in Harris and Coats, 1992) makes it very difficult for staff without a detailed knowledge of the Geochemistry Database to download data. Johnson *et al*. (2004) in a report for the SIGMA project gives worked examples on how to download geochemical data from the database. However, such is the rapidity in which software applications are being updated and replaced that instructions rapidly become out-of-date. In 2006 query layers to interrogate the Geochemistry Database were written – these are summarised in Table 2. However, it must be noted that the query layers were written to access more frequently used G-BASE rather than MRP data. The "numbering_system" field in the Geochemistry Database is the quickest way to identify MRP samples (see Table 3).

Key fields for the MRP geochemical samples are the Numbering_System (see Table 3), the Project Code (alphanumeric character code up to 3 characters in length), the Siteno (integer number of 5 digits length between 00000 and 99999), and Sample_type (see Table 4). Spatial referencing of sites is given by the Easting and Northing fields, the British National Grid reference in metres and numeric field of 6 and 7 in length respectively). These are the minimum number of fields required for identifying and locating samples.

Query Layer Name	Description
QL_GEOCHM_DEEPSOIL	G-BASE "S" (deep soil) analyses
QL_GEOCHM_PANCONC	All panned concentrate analyses
QL_GEOCHM_MINE	Environmental project contaminated land analyses
QL_GEOCHM_STRSED	All G-BASE stream sediment analyses
QL_GEOCHM_DRLCORE	All drill core analyses
QL_GEOCHM_STRWATER	All G-Base stream water analyses
QL_GEOCHM_TOPSOIL	G-BASE "A" (top soil) analyses

Table 2: Summary of query layers for interrogating the Geochemistry Database

CODE	TRANSLATION	DEFINED_AS
1	Min Pet	Mineralogy and Petrology
2	Bio Strat	Biostratigraphy
3	MRP	Mineral Reconnaissance Programme
4	GBASE	Geochemical Baseline Survey of the Environment
5	Environmental surveys	Environmental surveys
6	Sustainable Soils	Sustainable Soil
7	Rothhamsted Soils	Rothamsted samples acquired to supplement G-BASE

Table 3: Explanation of the numbering_system code in the Geochemistry Database (from BGS_MTA_DOM_NUMBERING_SYSTEM)

CODE	TRANSLATION	DEFINED_AS
A	Shallow G-BASE soil sample	Shallow G-BASE soil sample. Standard depth 5-20cm.
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.
K	Suspended particulate	Suspended paticulate collected from fluid (air or wate).
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. G-BASE sample generally 35-50cm.
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.
X	G-BASE surface soil	Surface soil from 0-2cm depth collected by G-BASE.
Z	Mine Waste	Tailings etc

Table 4: Sample type codes from the Geochemistry Database domain table (from BGS_MTA_DOM_SAMPLE_TYPE)

2.2 REGIONAL GEOCHEMICAL MAPPING OF THE UK LAND AREA

Baseline geochemical data for regional and urban areas of the UK are also held in the BGS Geochemistry Database. Such data are not site specific investigations and the samples collected contribute to high resolution regional and urban baselines. The main source of funding for this systematic baseline survey has been from government departments and in recent years co-funded work has contributed to the progression of the geochemical mapping, *e.g.* with the Environment Agency in the Tamar drainage catchment, SW England, and DETI (Department of Enterprise, Trade and Investment) in Northern Ireland for the Tellus Project. The current geochemical mapping projects are part of the Geochemical Baseline and Medical Geology Team of the Environmental Geoscience Baselines science theme area and funded through national capability budget.

The current Geochemical Baseline Survey of the Environment (G-BASE) project is a continuation of previous regional geochemical mapping projects that have been mapping the geochemical surface environment of the UK land mass since 1969. At present work is currently focused on the London urban area carried out as the “London Earth Project”. G-BASE is described by Johnson *et al.* 2005 and the GSUE project (Geochemical Surveys of the Urban

Environment), which now exists as a task within G-BASE, but between 2003 to 2005 was a separate project, is described by Fordyce *et al*. 2005. The history of the G-BASE project and a generalised account of the project's work (Johnson and Breward, 2004) are available as downloadable pdf files from the project's internet web page[6]. A summary of the main sample types collected and the analytes determined is given in Table 5.

	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 kilometre.	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, UK. A combination of emission and dispersive techniques gives a range of 52 elements (Ag, Al, As, Ba, Bi, Br, Ca, Cd, Ce, Cl, Co, Cr, Cs, Cu, Fe, Ga, Ge, Hf, I, In, K, La, Mg, Mn, Mo, Na, Nb, Nd, Ni, P, Pb, Rb, S, Sb, Sc, Se, Si, Sm, Sn, Sr, Ta, Te, Th, Ti, Tl, U, V, W, Y, Yb, Zn and Zr)
 Panned concentrate	The -2mm+150µm 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.
 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 top soil sample (5 to 20 cm) and a deeper sample (35 to 50 cm) are taken at each site. Samples are collected from alternate 1 km grid squares though in urban areas sampling density is increased to four samples every 1 km^2. Commencing in 2008 a surface sample (0 to 5 cm) is also collected in urban areas. Samples are collected in Kraft™ paper bags	The deeper soil samples are dried then sieved to -2 mm. These deep 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 (450ºC) and pH is also routinely measured for soils.

Table 5: Summary of the sample types collected by the G-BASE project and the analytes determined

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[6] http://www.bgs.ac.uk/gbase/downloads.html

The principal objective of the BGS regional geochemical mapping programme is to create a complete geochemical baseline of the UK surface land area. The main sampling medium in order to achieve this is drainage sediments but since the 1990s when geochemical mapping became more environmentally relevant, and the project was mapping lowland agricultural areas and urban centres, soils have also become an important sample medium. Improvements to analytical methodology for water samples over the past decade have also meant that stream waters are also an important part of the G-BASE UK geochemical baseline. Progress with sampling is shown in Figure 3 and Figure 4.

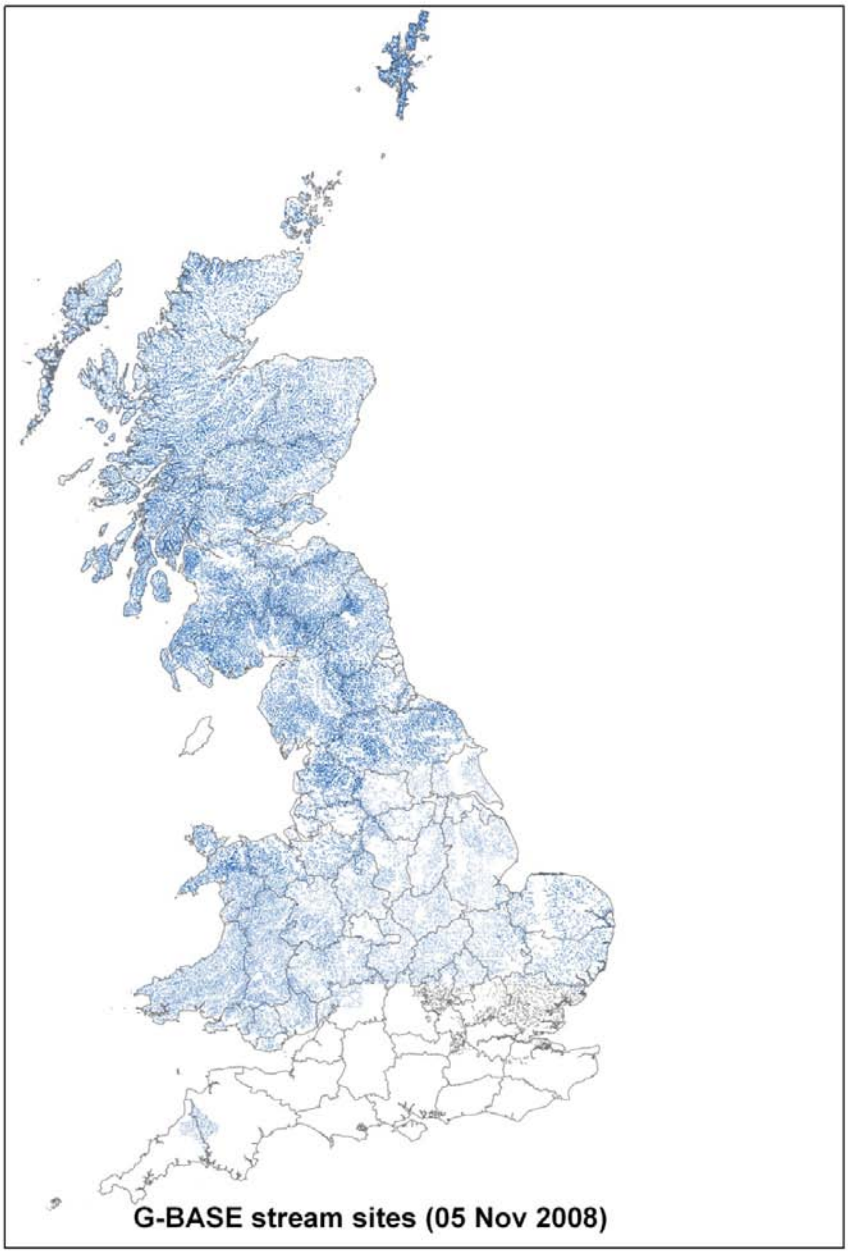


Figure 3: Progress with regional geochemical sampling until end of 2008 – drainage sites (sediment and waters)

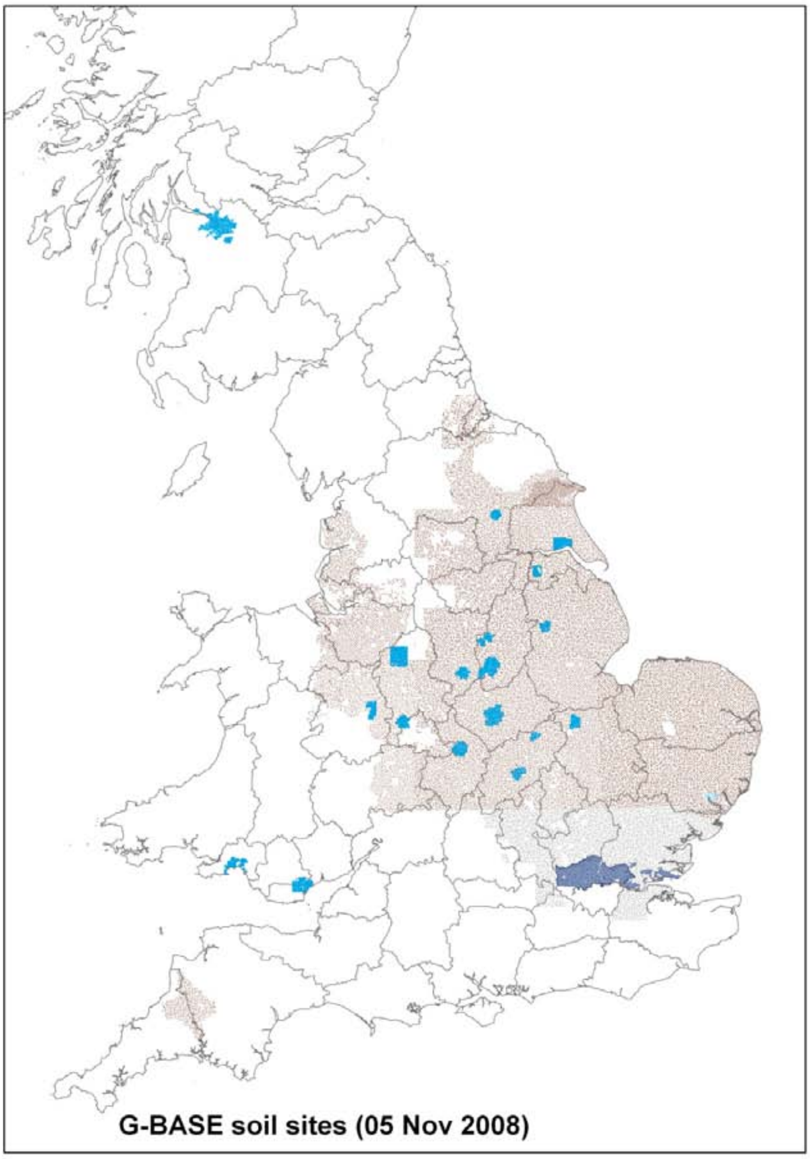


Figure 4: Progress with regional geochemical sampling until end of 2008 – soils. Blue colour represents urban samples.

A MicroSoft ACCESS field database of site and sample information is created during the field campaign from the field forms recorded at each sample site (Lister *et al*., 2005). Field measurements carried out at the field base (water pH, conductivity and alkalinity) are also entered into the field database. A campaign report is prepared by each field team leader at the end of each field campaign (*e.g.* Knights *et al*., 2007) which includes important information such as student sampler ID codes and sample number ranges. Within several weeks of the fieldwork being completed the field database is loaded to the Geochemistry Database using an application called MS ACCESS LOADER (Mackenzie and Johnson, 2006). This is a far from simple process because whilst G-BASE field information and coding has remained pretty consistent since the 1970s, BGS corporate codes have evolved and the LOADER program translates G-BASE codes into permissible BGS codes. An example of this is soil colour, the G-BASE project uses a restricted list of permissible colours but for the database these have to be translated to Munsell colour codes. The complexity of transferring the G-BASE field data to the Geochemistry Database is shown by Table 6 which maps the fields of the G-BASE field card to numerous different data tables in the Geochemistry Database.

Samples collected during a summer field campaign are generally analysed by the following March. Since 2006 stream sediment and soil results (where X-Ray Fluorecence Spectrometry (XRFS) is the principal method of analysis) are loaded directly via the BGS Laboratory Information Management System (LIMS) to raw data tables in the Oracle database. Control sample information and laboratory and batch information tables are exported to the database at the same time (Ault *et al.*, 2006). Earlier analytical data in digital format had to be loaded manually to the database using the LOADER application or manually using standard SQL direct into ORACLE. Stream water data is usually received as digital MS EXCEL files and also has to be manually loaded to the Geochemistry Database using the LOADER application.

The "raw" soil and sediment data needs to be subjected to a data conditioning process (Lister and Johnson, 2005 and Johnson *et al.*, 2008) so data is fully quality controlled, the accuracy and precision assessed, and, where necessary, levelled with respect to earlier results so seamless national geochemical maps can be produced from data spanning four decades. Conditioned data is loaded to the Geochemistry Database using the LOADER application to the Analyte_Determinations table (see Table 7). It is a deficiency of the Geochemistry Database that geochemical data from a variety of different projects exists in the Analyte_Determinations table but only someone with a good knowledge of the project that generated it will know the amount of quality control and levelling that data has been subjected to.

The location of G-BASE samples can be determined from the BGS internet GeoIndex (*e.g.* Figure 5) and this information is now generally updated soon after the completion of a field campaign. Whilst raw analytical data is generally available within six months of sample collection, G-BASE data are not generally released until they have undergone the rigorous data conditioning process, which in its entirety may take up to three years to complete. This is because the final process of the data conditioning, to level the data between analytical batches and different field campaigns, is best done on larger data sets covering atlas sheet areas. At the current rate of sampling, atlas sheet areas are taking many years to complete. The GeoIndex will show that analytical data is available for completed atlas areas but gives no indication that raw unqualified analytical data is available. The data conditioning process is important in confirming the data quality and during this process analyte determinations can be qualified by use of qualifier codes in the qualifier field of the Analyte_Determinations table. An example of this would be the replacement of semi-quantitative below detection results with a specified value by a method indicated by the qualifier code, *e.g.* a value one half of the analysts specified detection limit. Such data conditioning and qualification of the data is essential if customers that are non-geochemists are using the data.

Field forms for all G-BASE samples are either kept in metal "punch-card" drawers in P006 and are still actively used by several projects (East Midlands and East Anglia atlas areas and the most recent sampling) or archived to aisle 129 in the NGDC. All G-BASE field data since 1994 has been captured to the Geochemistry Database following the publication of the protocols covering the field database (Lister *et al.*, 2005). The history of G-BASE field forms and databases is documented in Lister *et al*. 2005. Much of the pre-1994 G-BASE field data has not been loaded to the database and exists only in analogue form. Analytical data is now reported in digital format, either directly to the ORACLE database as in the case of the soil and sediment results or as MS EXCEL files for stream water data. There are therefore no longer any primary hardcopy data files. Before 2004 all data was reported to the G-BASE data manager who maintained hardcopy records of G-BASE data. There are no hardcopy data records from 1996- 2002 and since then records are stored in the Data Manager's office (Bob Lister P005) or P006. Hardcopy analytical data from before 1996 is patchy but generally well documented in notes and files now stored in aisle 128 of the NGDC records room. There are no hardcopy or digital records of the earliest raw data on which much of the Scottish G-BASE results in the Geochemistry Database are based.

Field Card fields for transfer to GD	Data Type	Loading Size	GD column name and conditional arguments	GD tables fields are loaded to
Project_Code	Text	3	PROJECT	ALL TABLES THAT HAVE A 'PROJECT' COLUMN
Site_Number	Integer	16	SITENO	ALL TABLES THAT HAVE A 'SITENO' COLUMN
Sampling_Protocol	Text	5	SAMPLING_PROTOCOL	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Code_Version	Number	6,2	CODE_VERSION	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Duplicate			None	
Samp_C	Text	1	SAMPLE_TYPE	DTA_SEDIMENTS
Samp_P	Text	1	SAMPLE_TYPE	DTA_PANS
Samp_W	Text	1	SAMPLE_TYPE	DTA_WATERS
Samp_A	Text	1	SAMPLE_TYPE	DTA_OVERBURDENS
Samp_S	Text	1	SAMPLE_TYPE	DTA_OVERBURDENS
Samp_Std	Text	4	SAMP_STD	DTA_SEDIMENTS, DTA_WATERS, DTA_OVERBURDENS
Easting	Double	8	Easting	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Northing	Double	8	Northing	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Ref_map	Double	8	MAP_SHEET	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Map_Scale	Integer	5	MAP_SCALE	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Collectors	Text	100	Collectors	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Date	Date/Time	8	DATE_VISITED	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Rel_Samp	Integer	5	REL_SAMP	DTA_SEDIMENTS, DTA_WATERS, DTA_OVERBURDENS
Stm_order	Integer	2	STREAM_ORDER	DTA_DRAINAGE_SITES
Drain_type	Integer	4	DRAINAGE_TYPE	DTA_DRAINAGE_SITES
Drain_cond	Integer	4	DRAINAGE_CONDITION	DTA_DRAINAGE_SITES
Weather	Integer	4	WEATHER	DTA_DRAINAGE_SITES
PPT_orange	Integer	4	COLOUR (as 'OR'), abundance if ([ppt_orange]=3,1,[ppt_orange]=1,3)	DTA_SEDIMENT_PPT
PPT_brown	Integer	4	COLOUR (as 'BR'), abundance if ([ppt_brown]=3,1,[ppt_brown]=1,3)	DTA_SEDIMENT_PPT
PPT_black	Integer	4	COLOUR (as 'BK'), abundance if ([ppt_black]=3,1,[ppt_black]=1,3)	DTA_SEDIMENT_PPT
Sed_colour	Text	5	Munsell Colour Columns	DTA_SEDIMENTS
Sed_clay	Text	5	CLAY . abundance= if([SED_CLAY]=3,1,[SED_CLAY]=1,3)	DTA_SEDIMENTS
Sed_organic	Text	5	ORGANIC abundance= if([SED_ORGANIC]=3,1,[SED_ORGANIC]=1,3)	DTA_SEDIMENTS
Contam1	Text	6	CONTAMINANT relative abundance 1	DTA_SITE_CONTAMINANTS
Contam2	Text	6	CONTAMINANT relative abundance 2	DTA_SITE_CONTAMINANTS
Contam3	Text	6	CONTAMINANT relative abundance 3	DTA_SITE_CONTAMINANTS
Contam4	Text	6	CONTAMINANT relative abundance 4	DTA_SITE_CONTAMINANTS
Contam5	Text	6	CONTAMINANT relative abundance 5	DTA_SITE_CONTAMINANTS
Contam6	Text	6	CONTAMINANT relative abundance 6	DTA_SITE_CONTAMINANTS
Contam7	Text	6	CONTAMINANT relative abundance 7	DTA_SITE_CONTAMINANTS
Contam8	Text	6	CONTAMINANT relative abundance 8	DTA_SITE_CONTAMINANTS
Contam9	Text	6	CONTAMINANT relative abundance 9	DTA_SITE_CONTAMINANTS
Land_use1	Text	6	TYPE . sets catchment_site='S', abundance=1	DTA_LANDUSES
Land_use2	Text	6	TYPE . sets catchment_site='S', abundance=2	DTA_LANDUSES
Land_use3	Text	6	TYPE . sets catchment_site='S', abundance=3	DTA_LANDUSES
Clast1	Text	6	TYPE. sets abundance=1	DTA_CLASTS
Clast2	Text	6	TYPE. sets abundance=2	DTA_CLASTS
Clast3	Text	6	TYPE. sets abundance=3	DTA_CLASTS
Clast4	Text	6	TYPE. sets abundance=4	DTA_CLASTS
Clast5	Text	6	TYPE. sets abundance=5	DTA_CLASTS
Clast6	Text	6	TYPE. sets abundance=6	DTA_CLASTS
Clast7	Text	6	TYPE. sets abundance=7	DTA_CLASTS
Clast8	Text	6	TYPE. sets abundance=8	DTA_CLASTS
Bedrock	Text	6	VISIBLE_BEDROCK	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Drift1	Text	255	TYPE. sets abundance=1 catchment_site='S'	DTA_DRIFTS
Drift2	Text	6	TYPE. sets abundance=2 catchment_site='S'	DTA_DRIFTS
Drift3	Text	6	TYPE. sets abundance=3 catchment_site='S'	DTA_DRIFTS
Drift4	Text	6	TYPE. sets abundance=4 catchment_site='S'	DTA_DRIFTS
Relief	Integer	1	RELIEF	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES
Site_geol1	Text	6	TYPE. sets abundance=1 catchment_site='S'	DTA_GEOLOGYS
Site_geol2	Text	6	TYPE. sets abundance=2 catchment_site='S'	DTA_GEOLOGYS
Cat_geol1	Text	6	TYPE. sets abundance=1 catchment_site='C'	DTA_GEOLOGYS
Cat_geol2	Text	6	TYPE. sets abundance=2 catchment_site='C'	DTA_GEOLOGYS
Pan_min1	Text	6	TYPE. sets abundance=1	DTA_MINERALS #
Pan_min2	Text	6	TYPE. sets abundance=2	DTA_MINERALS #
Pan_min3	Text	6	TYPE. sets abundance=3	DTA_MINERALS #
Pan_min4	Text	6	TYPE. sets abundance=4	DTA_MINERALS #
Pan_min5	Text	6	TYPE. sets abundance=5	DTA_MINERALS #
Pan_min6	Text	6	TYPE. sets abundance=6	DTA_MINERALS #
Min_bed1	Text	6	TYPE. sets abundance=1	DTA_BEDROCK_MINERALISATION
Min_bed2	Text	6	TYPE. sets abundance=2	DTA_BEDROCK_MINERALISATION
Min_bed3	Text	6	TYPE. sets abundance=3	DTA_BEDROCK_MINERALISATION
Min_clast1	Text	6	TYPE. sets abundance=1	DTA_CLASTS_MINERALISATION
Min_clast2	Text	6	TYPE. sets abundance=2	DTA_CLASTS_MINERALISATION
Min_clast3	Text	6	TYPE. sets abundance=3	DTA_CLASTS_MINERALISATION
Minbed_Style	Text	1	MINERALISATION_STYLE Default = 0 (undifferientated)	DTA_BEDROCK_MINERALISATION
Wat_colour	Text	6	Munsell Colour Columns	DTA_WATERS
Susp_solid	Text	6	SUSPENDED_SOLIDS	DTA_WATERS
SoilA_colour	Text	6	Munsell Colour Columns	DTA_OVERBURDENS

Field Card fields for transfer to GD	Data Type	Loading Size	GD column name and conditional arguments	GD tables fields are loaded to
SoilS_colour	Text	6	Munsell Colour Columns	DTA_OVERBURDENS
SoilA_text	Text	6	TEXTURE	DTA_HORIZONS
SoilS_text	Text	6	TEXTURE	DTA_HORIZONS
Depth_A	Text	6	BOTTOM_DEPTH*	DTA_NORMAL_SITES
Depth_S	Text	6	BOTTOM_DEPTH*	DTA_NORMAL_SITES
Organic_A	Number	1	ORGANIC_CONTENT	DTA_OVERBURDENS
Organic_S	Number	1	ORGANIC_CONTENT	DTA_OVERBURDENS
A_clast1	Text	6	TYPE. sets abundance=1	DTA_CLASTS
A_clast2	Text	6	TYPE. sets abundance=2	DTA_CLASTS
A_clast3	Text	6	TYPE. sets abundance=3	DTA_CLASTS
A_clast4	Text	6	TYPE. sets abundance=4	DTA_CLASTS
A_clast5	Text	6	TYPE. sets abundance=5	DTA_CLASTS
A_clast6	Text	6	TYPE. sets abundance=6	DTA_CLASTS
S_clast1	Text	6	TYPE. sets abundance=1	DTA_CLASTS
S_clast2	Text	6	TYPE. sets abundance=2	DTA_CLASTS
S_clast3	Text	6	TYPE. sets abundance=3	DTA_CLASTS
S_clast4	Text	6	TYPE. sets abundance=4	DTA_CLASTS
S_clast5	Text	6	TYPE. sets abundance=5	DTA_CLASTS
S_clast6	Text	6	TYPE. sets abundance=6	DTA_CLASTS
A_moist	Text	6	SOIL_MOISTURE	DTA_OVERBURDENS
S_moist	Text	6	SOIL_MOISTURE	DTA_OVERBURDENS
Ph@	Number	6,2	PH (recorded to 1 dec place e.g. 7.2)	DTA_WATERS
Conduct@	Number	5	Conduct	DTA_WATERS
Bicarb	Double	8	BICARBONATE	DTA_WATERS
Comments	Text	255	COMMENTS	DTA_NORMAL_SITES,DTA_DRAINAGE_SITES

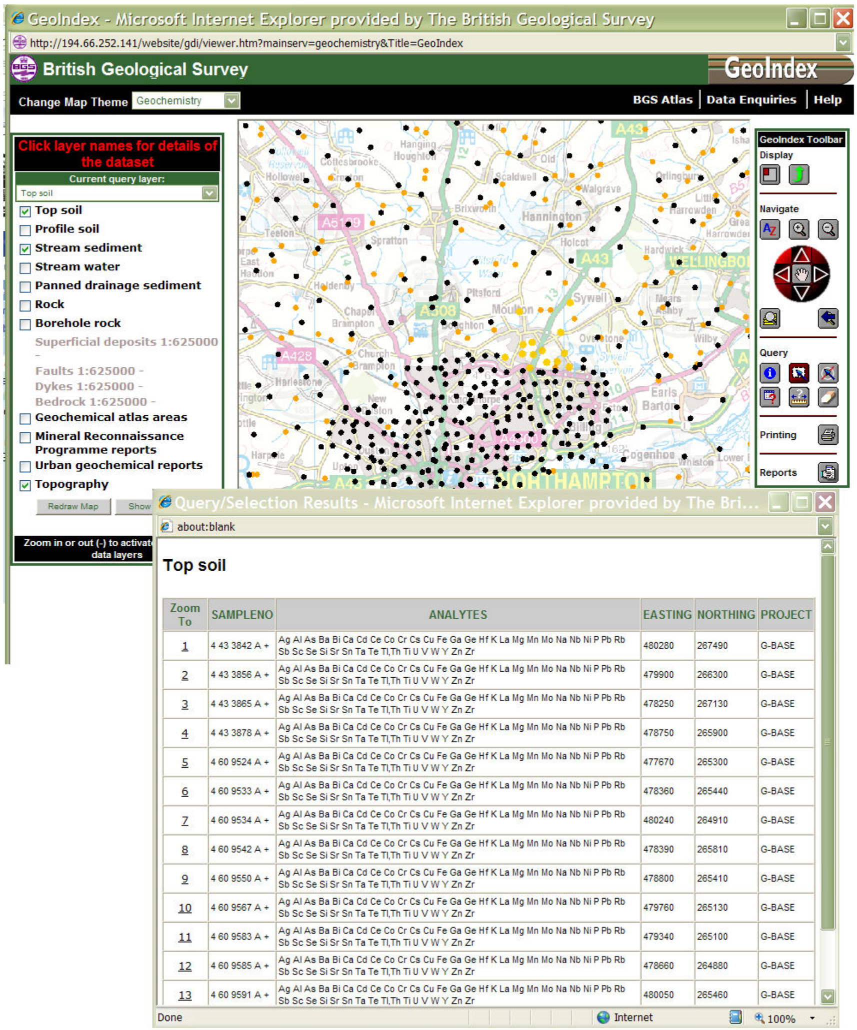
$ = Default from loading screen
# = where samp_p is not null
@=entered in field database but not on field card
~ = duplicate is indicated by 1,2,3 etc non duplicates as +
* Top_depth is derived by subtracting 0.15m

Table 6: A table showing how fields of the G-BASE field card map to Geochemistry Database data tables

CODE	TRANSLATION	DEFINED_AS
Ac	Actinium	Actinium
Ag	Silver	Silver
Al	Aluminium	Aluminium
Am	Americium	Americium
Ar	Argon	Argon
As	Arsenic	Arsenic
As(III)	As oxidation state 3	As(III)
As(V)	As oxidation state 5	As(V)
As.3+	arsenite	As+3
As.5+	arsenate	As+5
At	Astatine	Astatine
Au	Gold	Gold
B	Boron	Boron
B4O7.2-	tetraborate	B4O7-2
BO2.-	metaborate	BO2-
BO3.3-	borate	BO3-3
Ba	Barium	Barium
Be	Beryllium	Beryllium
Bi	Bismuth	Bismuth
Bk	Berkelium	Berkelium
Br	Bromine	Bromine
Ge	Germanium	Germanium
H	Hydrogen	Hydrogen
H.3	tritium	3H
H2O.+	combined water	H2O+
H2O.-	moisture	H2O-
H2PO4.-	dihydrogen orthophosphate	H2PO4-
H2S	hydrogen sulphide	H2S
HCO3.-	bicarbonate	HCO3-
HPO4.2-	hydrogen orthophosphate	HPO4-2
He	Helium	Helium
Hf	Hafnium	Hafnium
Hg	Mercury	Mercury
Ho	Holmium	Holmium
Humic	humic acids	Humic
I	Iodine	Iodine
I.-	iodide	I-
IO3.-	iodate	IO3-
In	Indium	Indium
Ir	Iridium	Iridium
K	Potassium	Potassium
Kr	Krypton	Krypton
Pr	Praseodymium	Praseodymium
Pt	Platinum	Platinum
Pu	Plutonium	Plutonium
Ra	Radium	Radium
Ra.226	radium - 226	226Ra
Rb	Rubidium	Rubidium
Re	Rhenium	Rhenium
Rh	Rhodium	Rhodium
Rn	Radon	Radon
Rn.222	radon - 222	222Rn
Ru	Ruthenium	Ruthenium
S	Sulphur	Sulphur
S2O3.2-	thiosulphate	S2O3-2
SO3.2-	sulphite	SO3-2
SO4.2-	sulphate	SO4-2
Sb	Antimony	Antimony
Sc	Scandium	Scandium
Se	Selenium	Selenium
Se(IV)	Se oxidation state four	Se(IV)
Se(VI)	Se oxidation state six	Se(VI)
Se.4+	selenite	Se+4

Br.-	bromide	Br-
BrO3.-	bromate	BrO3-
C	Carbon	Carbon
C.14	carbon - 14	14C
CEC	Cation exchange capacity	Cation exchange capacity
CN.-	cyanide	CN-
CO3.2-	carbonate	CO3-2
Ca	Calcium	Calcium
Cd	Cadmium	Cadmium
Ce	Cerium	Cerium
Cf	Californium	Californium
Cl	Chlorine	Chlorine
Cl.-	chloride	Cl-
ClO3.-	chlorate	ClO3-
Cm	Curium	Curium
Co	Cobalt	Cobalt
Conduct	Conductivity	Electrical conductivity
Cr	Chromium	Chromium
Cr2O7	dichromate	Cr2O7
CrO4.2-	chromate	CrO4-2
Cs	Caesium	Caesium
Cu	Copper	Copper
DIC	Dissolved InorganicCarbon	DIC
DOC	Dissolved Organic Carbon	DOC
Dy	Dysprosium	Dysprosium
Er	Erbium	Erbium
Es	Einsteinium	Einsteinium
Eu	Europium	Europium
F	Fluorine	Fluorine
F.-	fluoride	F-
Fe	Iron	Iron
Fe.2+	ferrous	Fe+2
Fe.3+	ferric	Fe+3
Fm	Fermium	Fermium
Fr	Frankium	Frankium
Fulvic	fulvic acids	Fulvic
Ga	Gallium	Gallium
Gd	Gadolinium	Gadolinium
LOI	loss on ignition	loss on ignition
LOI1000	Loss on ignition at 1000 ºC	LOI 1000 ºC
LOI1050	loss on ignition at 1050 ºC	LOI 1050 ºC
LOI450	loss on ignition at 450 ºC	LOI 450 ºC
La	Lanthanum	Lanthanum
Li	Lithium	Lithium
Lr	Lawrencium	Lawrencium
Lu	Lutecium	Lutecium
Md	Mendelevium	Mendelevium
Mg	Magnesium	Magnesium
Mn	Manganese	Manganese
MnO4.-	permanganate	MnO4-
MnO4.2-	manganate	MnO4-2
Mo	Molybdenum	Molybdenum
N	Nitrogen	Nitrogen
NH3	ammonia	NH3
NH4.+	ammonium	NH4+
NO2.-	nitrite	NO2-
NO3.-	nitrate	NO3-
Na	Sodium	Sodium
Nb	Niobium	Niobium
Nd	Neodymium	Neodymium
Ne	Neon	Neon
Ni	Nickel	Nickel
No	Nobelium	Nobelium
Np	Neptunium	Neptunium
O	Oxygen	Oxygen
OH.-	hydroxide	OH-
Os	Osmium	Osmium
P	Phosphorus	Phosphorus
P-o	Olsen Phosporous	Olsen Phosporous
P-r	Reactive P	Reactive P
PO4.3-	phosphate	PO4-3
Pa	Protactinium	Protactinium
Pb	Lead	Lead
Pd	Palladium	Palladium
Pm	Promethium	Promethium
Po	Polonium	Polonium
Se.6+	selenate	Se+6
Si	Silicon	Silicon
Sm	Samarium	Samarium
Sn	Tin	Tin
Sr	Strontium	Strontium
TDS	total dissolved solids	TDS
TIC	total inorganic carbon	TIC
TOC	total organic carbon	TOC
TON	total oxidised nitogen	TON
TOT_ALK	Total alkalinity	Total alkalinity
Ta	Tantalum	Tantalum
Tb	Terbium	Terbium
Tc	Technetium	Technetium
Te	Tellurium	Tellurium
Th	Thorium	Thorium
Th.230	thorium - 230	230Th
Th.232	thorium - 232	232Th
Ti	Titanium	Titanium
Tl	Thallium	Thallium
Tm	Thulium	Thulium
U	Uranium	Uranium
U.234	uranium - 234	234U
U.238	uranium - 238	238U
V	Vanadium	Vanadium
W	Tungsten	Tungsten
Xe	Xenon	Xenon
Y	Yittrium	Yittrium
Yb	Yitterbium	Yitterbium
Zn	Zinc	Zinc
Zr	Zirconium	Zirconium
d18O	delta oxygen eighteen	d 18O
d2H	delta deuterium	d 2H
pH	pH	pH

Table 7: Analyte_Determinations domain Table from the Geochemistry Database (BGS_MTA_DOM_ANALYTE)



☑ Top soil
☐ Profile soil
☑ Stream sediment
☐ Stream water
☐ Panned drainage sediment
☐ Rock
☐ Borehole rock
Superficial deposits 1:625000 -
Faults 1:625000 -
Dykes 1:625000 -
Bedrock 1:625000 -
☐ Geochemical atlas areas
☐ Mineral Reconnaissance Programme reports
☐ Urban geochemical reports
☑ Topography

Top soil

Zoom To	SAMPLENO	ANALYTES	EASTING	NORTHING	PROJECT
1	4 43 3842 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	480280	267490	G-BASE
2	4 43 3856 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	479900	266300	G-BASE
3	4 43 3865 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	478250	267130	G-BASE
4	4 43 3878 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	478750	265900	G-BASE
5	4 60 9524 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	477670	265300	G-BASE
6	4 60 9533 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	478360	265440	G-BASE
7	4 60 9534 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	480240	264910	G-BASE
8	4 60 9542 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	478390	265810	G-BASE
9	4 60 9550 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	478800	265410	G-BASE
10	4 60 9567 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	479760	265130	G-BASE
11	4 60 9583 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	479340	265100	G-BASE
12	4 60 9585 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	478660	264880	G-BASE
13	4 60 9591 A +	Ag Al As Ba Bi Ca Cd Ce Co Cr Cs Cu Fe Ga Ge Hf K La Mg Mn Mo Na Nb Ni P Pb Rb Sb Sc Se Si Sr Sn Ta Te Tl,Th Ti U V W Y Zn Zr	480050	265460	G-BASE

Figure 5: BGS Internet GeoIndex page showing information about G-BASE samples

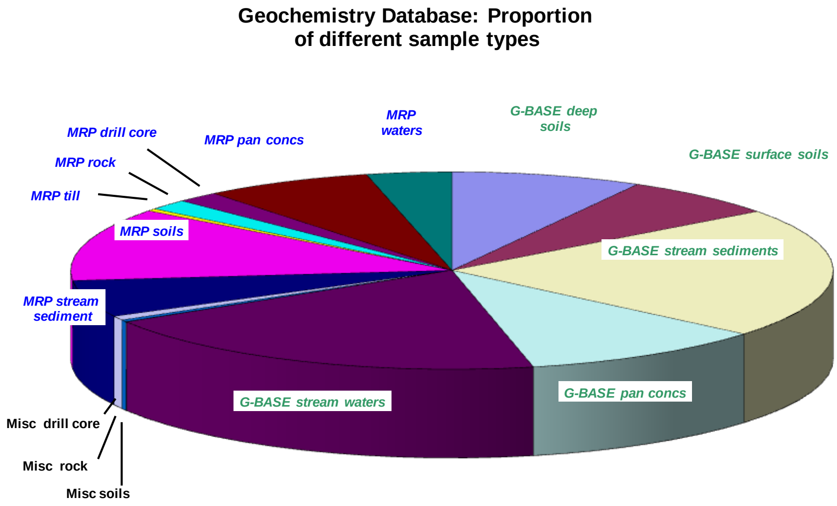


Figure 6: Pie chart showing the main contributing projects to the BGS Geochemistry Database (based on 2005 data)

Keyfields for the G-BASE data are as for those described for the MRP data. G-BASE identifies soils in a different way to that used in MRP projects with an additional sample types “A” for topsoils (5-20 cm) and “X” for surface soils (0-2 cm). Whereas G-BASE will have “A”, “S” and “X” soil samples collected from a single site, the MRP would assign all samples as “S” but assign a different site number (Siteno) for soils collected at different depths down a soil profile.

In 2007 a major ground geochemical survey was completed by the Tellus Project in Northern Ireland which extended the area sampled by G-BASE in the 1990s. The geochemical sampling was directed by the G-BASE project and the data will be loaded to the BGS Geochemistry Database when all the data conditioning is complete (this work was still in progress in early 2010). However, the principal first contact point for Northern Ireland geochemical data or samples should be the Geological Survey of Northern Ireland (GSNI) office in Belfast. All other regional and urban geochemical data for the UK is managed by the BGS Geochemistry Data Manager.

The pricing policy for digital geochemical data is the same as that previously described for MRP data (Box 1). Internal use of baseline geochemical data should be coordinated through the BGS Geochemistry Data Manager. External enquiries should initially be routed through the BGS enquiries desk who will forward enquires about digital data licencing and IPR to the BGS digital licencing manager. Any other enquiries about the availability of regional or urban baseline geochemical data will be forwarded to the Geochemistry Baselines and Medical Geology Team Leader.

The G-BASE project is now the only project that is routinely adding geochemical data to the Geochemistry Database. Two-thirds of the samples in the database have originated from the G-BASE project (see Figure 6). It is somewhat misleading that there are many active BGS projects generating geochemical data that are not captured to the corporate Geochemistry Database because the database was specifically designed for MRP, G-BASE and mineralogy/petrology data only. As one of the earliest BGS Oracle databases the Geochemistry Database was a divisional rather than a corporate initiative and so the Geochemistry Database is more-or-less exclusive to the MRP and G-BASE projects.

All BGS staff have read access to the Geochemistry Database and samples and results can be accessed using the query layers mentioned in the previous sub-section (see also Table 2). Baseline geochemistry results can be retrieved using Numbering_System code = 4.

Regional geochemistry atlases are the main published source of information for the baseline data. G-BASE also has a substantial record of peer-reviewed publications and these can be found referenced in the G-BASE project EndNote bibliography located on the Geochemistry Baselines Team area of the SAN (access to internal BGS users only). Urban data was reported in the BGS Internal Report series until 2007 but are now presented in the new BGS Open Report series. Urban geochemical data is presented in BGS reports as summary statistics for each element and the preferred method of data presentation is as proportional symbol maps. In 2009 all the G-BASE/GSUE urban geochemistry reports were added to NERC Online Research Archive NORA[7] and can also be downloaded from the G-BASE internet web pages. The internet GeoIndex (geochemistry data layer) graphically displays the reporting areas (with a bibliographic reference) for atlases and urban reports. As described previously, the GeoIndex identifies baseline sample sites for all the different sample media and using the information tool users can identify site numbers and analytes determined. External customers have no direct access to the chemical results. For collaborative projects baseline data are often provided in an ArcGIS project as an IDW gridded tiff image (*e.g.* Figure 7) and use of these images in publications is an issue of copyright rather than one of data licencing.

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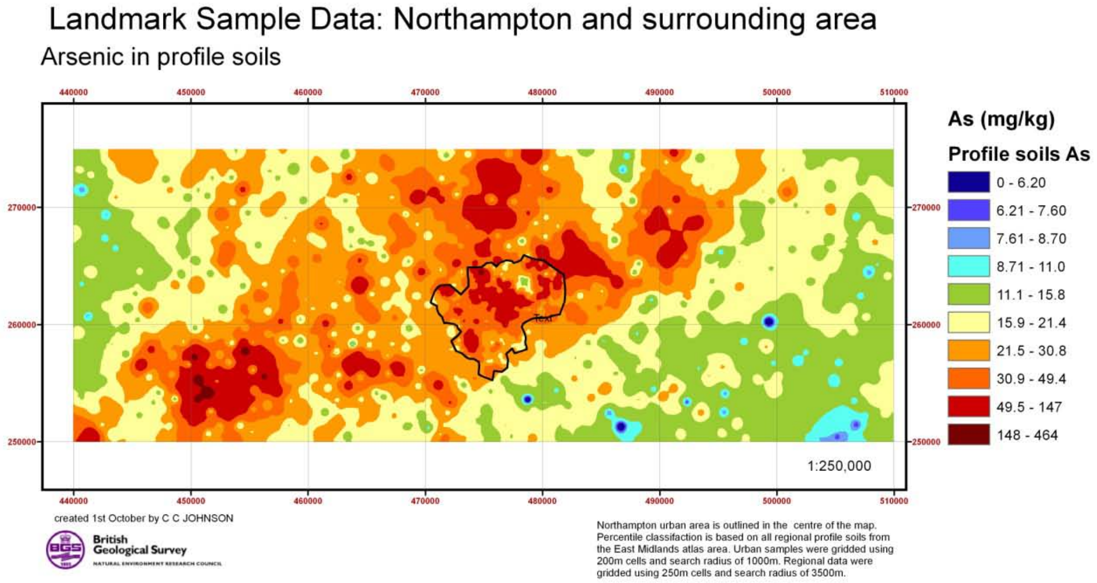
[7] NORA (NERC Open Research Archive) http://nora.nerc.ac.uk/


Landmark Sample Data: Northampton and surrounding area

Arsenic in profile soils

created 1st October by C C JOHNSON

Northampton urban area is outlined in the centre of the map. Percentile classifaction is based on all regional profile soils from the East Midlands atlas area. Urban samples were gridded using 200m cells and search radius of 1000m. Regional data were gridded using 250m cells and search radius of 3500m.

Figure 7: Example of typical G-BASE geochemical image generated by IDW gridding in ArcGIS

The Regional Geochemical Atlas series was the main means of disseminating the regional geochemical data and a list of these atlases is given in Appendix 1. Summary statistics for each element are presented in each atlas and the earlier atlases had regional geochemical maps based on proportional symbols. Since the publication of the East Grampians Atlas in 1991 the standard method of presenting the regional geochemical data has been the gridded geochemical images.

2.3 SURFACE WATER GEOCHEMISTRY

Stream water geochemical data have been generated by the G-BASE project, and minor contributions on surface water geochemistry are also available from the MRP.

2.4 GROUNDWATER GEOCHEMISTRY

The bulk of BGS geochemical data for groundwater has originated from the work of BGS Wallingford. UK-based hydrogeochemical work spans several decades and the scope of projects is varied. Clients include BGS science projects, government departments, Environment Agency, and numerous water companies and the varied data holdings reflect this diversity. Data from 1998 are stored in the Wallingford hydrochemical laboratory database, which is structured to include appropriate spatial information. Earlier data are stored electronically in two historical formats, and also in paper records. Work to convert all these data into a single database on the corporate Oracle platform is well advanced. The combined dataset will hold all BGS groundwater chemistry data, including international data (Section 2.11.2), from 1967 to date. Some additional work is needed to attribute confidentiality restrictions, after which it is intended to make this resource available to staff (internal to BGS) via the GeoIndex.

Following the reorganisation of laboratories between Wallingford and Keyworth in March 2009, the Wallingford laboratory database was closed to new data. A mechanism for capture of future groundwater chemistry data from the BGS laboratory to the new Oracle tables is under active consideration between the laboratory Facility Leader and the groundwater science programme.

Of the numerous UK-based projects undertaken in groundwater chemistry, one of the largest is the ‘Baseline’ project (The natural quality of groundwater in England and Wales). The first phase of this project was conducted during 1996–1998 and produced eight regional reports based on hydrogeochemical interpretation from existing data. A subsequent phase, carried out during 1999–2005 involved the production of reports for 24 more aquifers or aquifer blocks in England and Wales, with the scope expanding to include sampling and analysis of newly-collected groundwater samples. Both these project phases were co-funded by BGS science budget and the Environment Agency. A summary report was also produced on completion of this series (Shand *et al*., 2007). From 2006, the Baseline project has continued with science budget only funding. Groundwater geochemical data are presented diagrammatically in these reports, for example as box plots (see Figure 8) and cumulative-probability plots. A list of baseline reports is given in Appendix 2.

A parallel project on the Baseline quality of groundwater in Scotland has been ongoing since 2004, in part with co-funding from Scottish Environment Protection Agency (SEPA). Reports produced as a result of this project are also listed in Appendix 2. Information on the Baseline Scotland project is available via the intranet and internet web pages have also been set up[8].

Many other non-confidential hydrogeochemical reports encompassing groundwater pollution, residence time, groundwater resources and fundamental processes can be downloaded via the intranet. Some are also available in NORA and some via the Groundwater Portal[9] (BGS intranet).

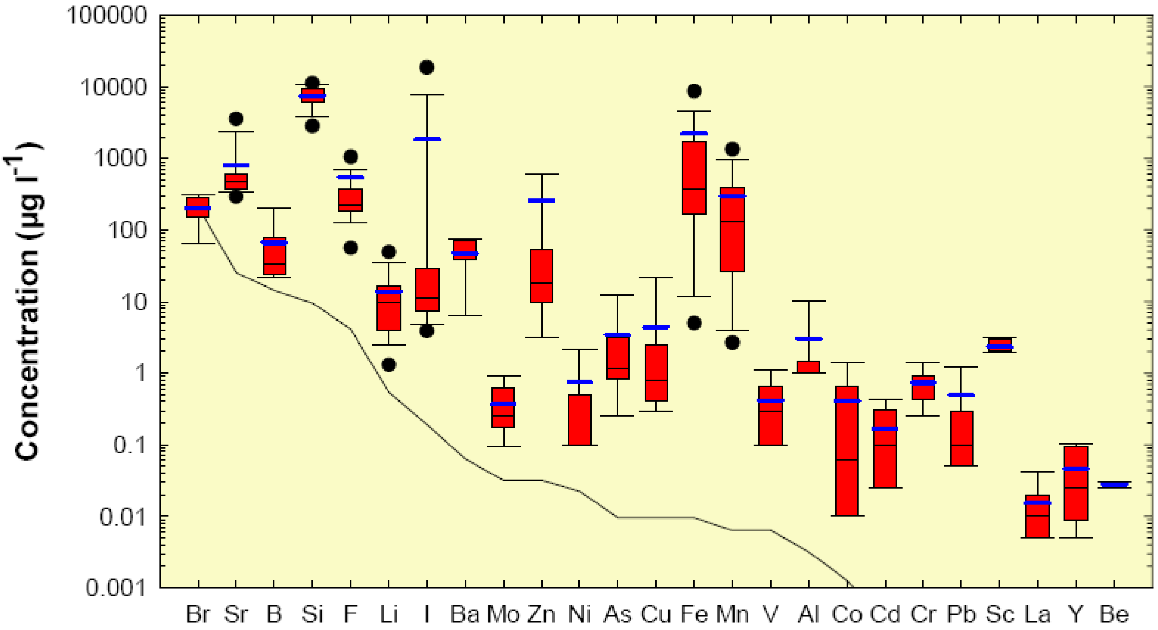


Figure 8: Boxplot of minor and trace elements in the Crag groundwaters (after Ander *et al*., 2006)

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[8] http://www.bgs.ac.uk/data/baselineScotland/home.html

[9] http://bgsintranet/groundwater_portal/default.shtml

2.5 OFFSHORE/MARINE GEOCHEMISTRY

This section is concerned with offshore geochemical investigations in UK territorial waters – international offshore geochemical studies are briefly discussed in Section 2.11.4. The history of the BGS offshore geochemistry programme is described by Stevenson *et al*. (1995) and summarised below. This report was originally classified as commercial in confidence but has now been declassified and can be made publically available through the BGS library. More recently Fordyce *et al*. (2004) have reviewed BGS offshore (and onshore) geochemical data in relation to contaminant transport investigations. BGS has carried out geochemical investigations in a number of estuaries in the UK and although such work should be classified as offshore or marine geochemistry it is discussed in a separate section (see Section 2.6). Furthermore, much of the sea-bed sediment sampling was conducted concurrently with the offshore radiometric surveys described in Section 2.8.2.

In the 1970s there was growing concern about the levels of mercury in fish. The analytical chemistry unit of the BGS (or Institute of Geological Sciences (IGS) as it was then called) was asked to look at trace metal contents, particularly mercury, in waters and sediments around the British Isles. Initial work in the tidal reaches of the River Thames was published by Smith *et al*. (1971). This was followed by a study of the Thames Estuary sediments in conjunction with the City of London Polytechnic (Smith *et al*., 1973).

In 1971, IGS commenced its sea-bed radioactivity work (see Section 2.8.2) and at the same time sea-bed sediments were collected across the Forth Estuary and southwards along the North Sea coast to Flamborough Head. Samples were collected using a Shipek grab and analysed for Cu, Pb, Zn, Cd, Mn, Hg and loss-on-ignition. Results are reported by Nicholson and Moore (1978).

Sampling of the sea-bed continued with the support of various government departments and in 1977 the BGS Marine Geology Group carrying out a UK Continental Shelf survey (funded by the Department of Energy) suggested that their offshore sampling should be combined with that of the Analytical Chemistry Group. As a result sampling rate and sample density increased significantly. Progress with work is described in the IGS Annual reports from this period (see Figure 9).

Collaboration surveys between Marine Geology and Analytical Chemistry groups continued until completion of the regional offshore survey in 1986 (see FIGURE 10). During the period 1968-1986 approximately 30,000 sea-bed samples were collected from the UK Continental Shelf. About 9,000 of these samples were analysed for 38 geochemical elements, 31 of which are reported by Stevenson *et al*. (1995) (see Table 8). In this report a description of the distribution of each element is given along with a histogram, summary descriptive statistics and percentile classified gridded image (FIGURE 11). As a test for combining different datasets within a GIS Neil Breward and Graham Wiggans experimented in combining on- and offshore sediment data and produced gridded images for Cu, Pb and Zn. These combined images have been used in posters and publicity material.

The offshore geochemical database consists of two Oracle tables, BGS.GEOCHEMICAL_DATA and BGS.GEOCHEMICAL_CORRECTED_DATA, but there is no documentation to accompany these tables. The data tables are currently under the custodianship of the Marine Geological Mapping team through data manager Paul Henni. The BGS corporate Coastal and Marine Database (CMD)[10] is designed to be populated with geochemical data but has yet to be populated with the sea-bed sediment data and this is not considered to be a high priority task for this database.

The charging policy for the marine sediment geochemical data is not published externally but can be found by BGS staff on the GeoScience Twiki site[11]. Data are supplied either as an ESRI

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[10] http://kwxvcs.ad.bgs.ac.uk/twiki/bin/view/BGS/CoastalandMarineDatabase

[11] http://kwxvcs/twiki/bin/view/BGS/GeochemicalDataCharging

interpolated grid for each chemical element (£250 ex. VAT) or as a data file for plotting point data (£500 for each element, ex. VAT). Text information about the data is available in Stevenson (2001).

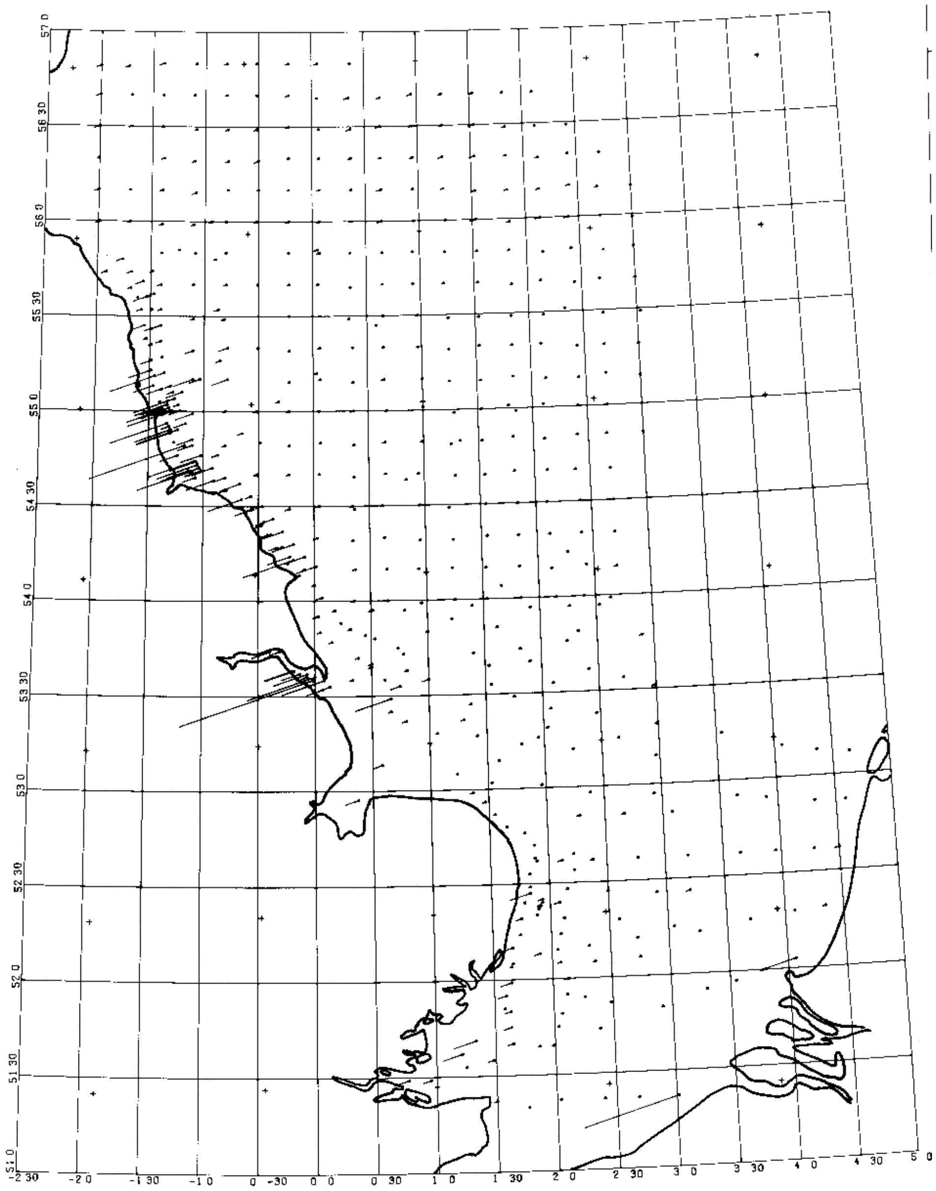

Figure 9: Distribution of mercury in sediments on the sea-bed of the North Sea (from IGS Annual Report, 1979)

(length of symbol arm is proportional to the Hg concentration though scale and units not given in original diagram)

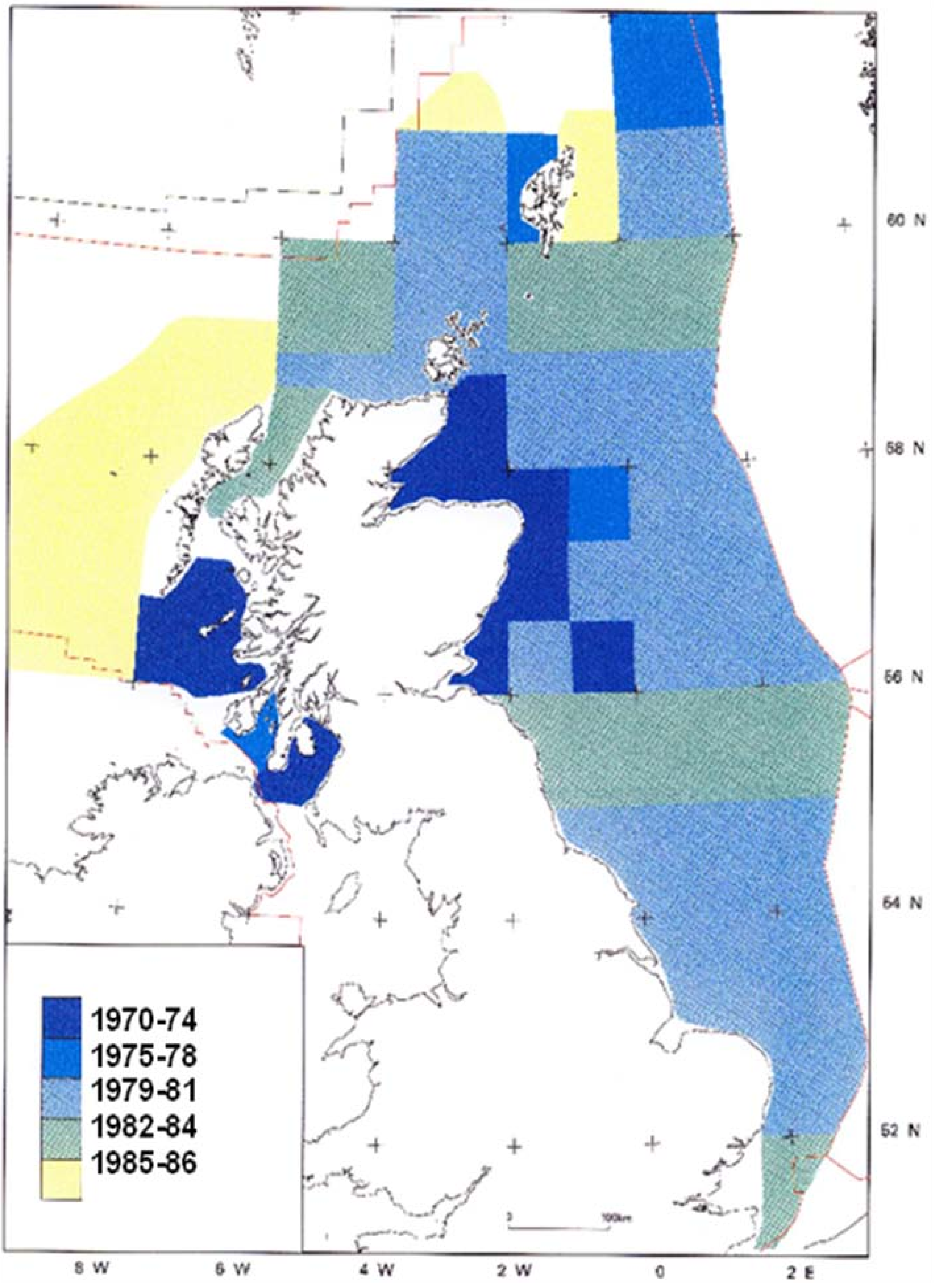

Figure 10: Figure showing the chronology of the sea-bed sediment sampling (after Stevenson *et al*. 1995)

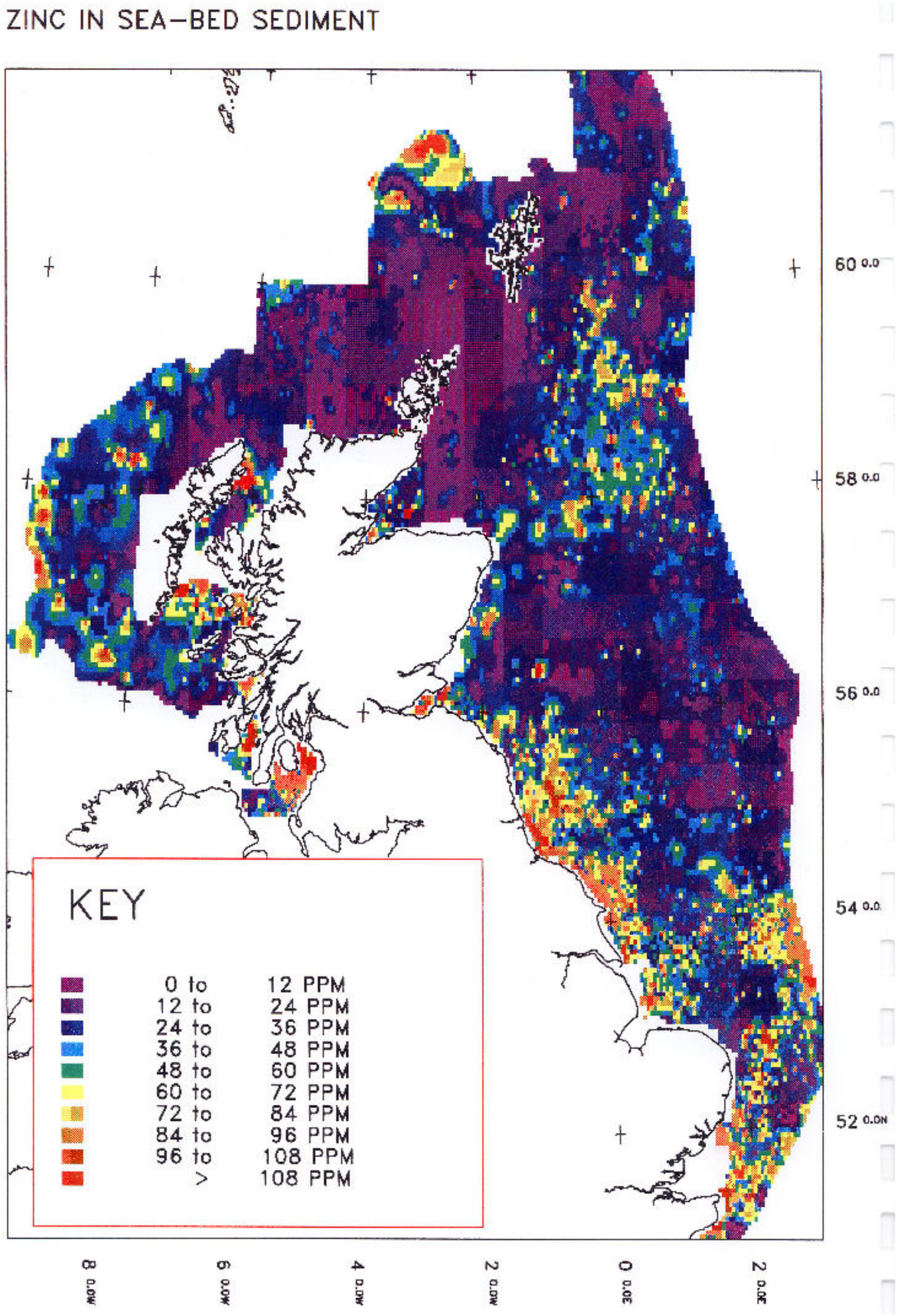

Figure 11: Geochemical image for zinc in sea-bed sediments (from Stevenson *et al*. 1995)

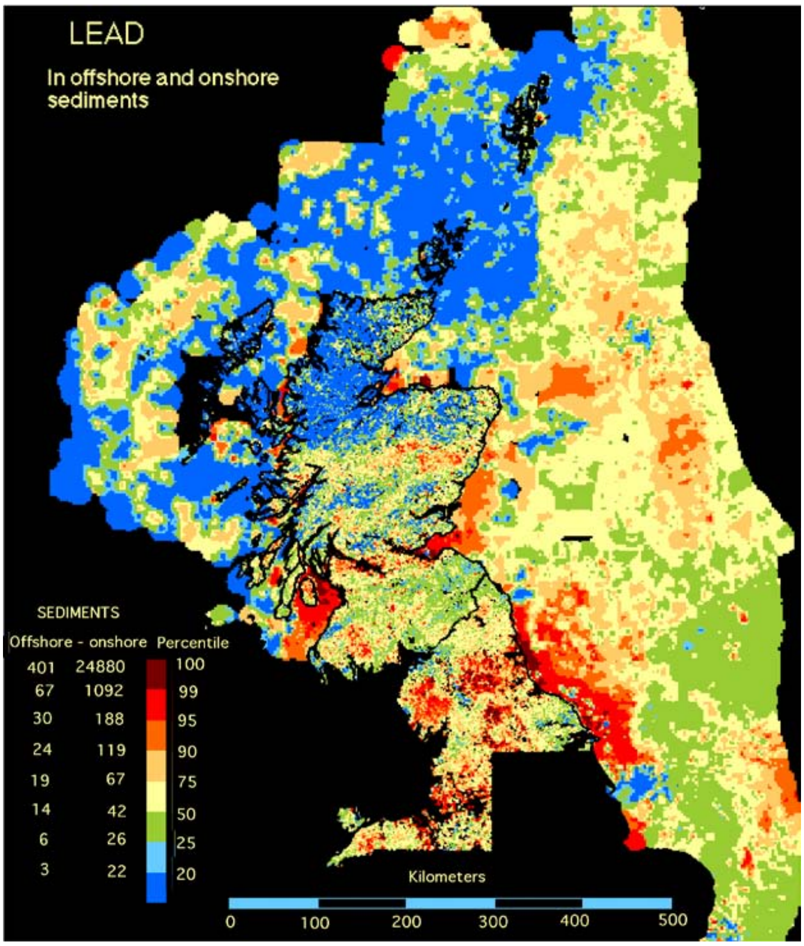

Figure 12: Geochemical image for Pb for the combined offshore sea-bed sediments and the onshore stream sediments

Aluminium	Iron	Potassium
Barium	Lanthanum	Rubidium
Beryllium	Lead	Strontium
Bismuth	Lithium	Titanium
Boron	Magnesium	Uranium
Cadmium	Manganese	Vanadium
Calcium	Mercury	Yttrium
Chromium	Molybdenum	Zinc
Cobalt	Nickel	Zirconium
Copper	Niobium	
Gallium	Phosphorous	

All elements determined by direct reading emission spectrometry except U (delayed neutron activation) and Hg (flameless atomic absorption spectrometry)

Table 8: Elements determined on the sea-bed sediments reported by Stevenson *et al*. (1995)

2.6 ESTUARINE GEOCHEMISTRY

Systematic studies of estuarine contamination have been undertaken since 1999, originally under the Coastal Geoscience Programmes and currently under Marine Geoscience. The main areas studied are the Mersey Estuary (Ridgway *et al*., In press; Vane *et al*., 2007b), the Tawe Estuary in South Wales (no published reference) and ongoing work on the Clyde Estuary (Jones *et al*., 2004; Vane *et al*., 2007a). Earlier projects have studied aspects of the geochemistry of individual estuaries or estuaries in particular geographic areas *e.g.* the Tees and Humber estuaries, studied as part of the NERC-funded Land-Ocean Interaction Project (Plater *et al*., 1998; Rees *et al*., 1998a), several Irish Sea estuaries examined for a Department of the Environment, Transport and the Regions (DETR)-funded project on distinguishing natural and anthropogenic inputs to the Irish Sea (Ridgway *et al*., 2001; Ridgway *et al*., 2003) and a more general study of the effects of different processes on contaminants (with the emphasis on radio-nuclides) in the Irish Sea for the Department for Environment, Food and Rural Affairs (DEFRA) (Jones *et al*., 2002; Jones *et al*., 2007).

Funding for the systematic surveys has been on a co-funding basis, with a mix of science budget (SB) and commissioned research (CR) inputs, including contributions from the Environment Agency for England and Wales (EA), Associate and British Ports (ABP), Glasgow City Council and SEPA. Other specific projects have been NERC research topics or CR as outlined above.

The estuarine geochemical work involves the assessment of the contamination of the sediments by both inorganic and organic substances. An important part is the distinguishing between the natural background and anthropogenic components. The geochemical results are placed in the context of the longer term evolution of the estuary, provided by geophysical studies (*e.g.* single or multibeam bathymetry, sidescan sonar and shallow seismic reflection) and sampling. Surface sediment and core samples are collected by a variety of methods. Intertidal sediments have normally been collected at low tide from hovercraft or on foot, the surface material by trowel, deeper sediments by hand coring or the use of vibrocorers or a Marlow corer. Subtidal sampling is achieved by the use of grab samplers from survey vessels, including Van Veen, Shipek and Day grabs to obtain surface sediments, and different corers (*e.g.* gravity, Mackereth and Craib) to sample to greater depth. A cruise report is typically prepared after each survey.

A brief general description of the samples is made in the field at all sites and sample site photographs taken at intertidal sites. A recent development (2007-8) has been geochemical screening of the cores. The first stage of this is the gamma logging of the intact core in its plastic liner. This provides an initial assessment of the distribution of natural radioactivity (K, U and Th) down the core and of the anthropogenic ^{137}Cs, which is useful for indicating the part of the core subject to relatively recent contamination; ^{137}Cs was introduced into the environment by man in significant quantities only from the 1950s as a product of nuclear power, weapons testing and accidents such as Chernobyl. After this screening the cores are sliced in half longitudinally, a descriptive log made and photographs taken (sometimes including X-ray images). The second stage of screening involves the use of portable XRF on the cut core surface. The results from this analysis, and the earlier gamma logging, are used to select cores for further study.

Surface sediment samples and depth slices from the cores are then freeze dried, sieved to remove the >2 μm fraction and further prepared as necessary for analysis. An inorganic suite of elements, very similar to that used for G-BASE, is measured by XRFS. In addition Hg and a range of organic substances are also analysed (TOC, TPH, PAH, PCB).

Sequential extractions are made on a small selection of samples, followed by determination of a range of inorganic analytes. The particle size of the sediments is obtained by sieving and Sedigraph analysis and the mineralogy and petrology by XRD (whole sediment and <2 μm fraction) and microscopy (optical and SEM). These studies help to understand the phases with which different elements are associated in the sediments, their availability and the diagenetic and other processes operating.

The data are provided as MS Excel files from the analysts and then as tables in MS Access. As full a range as possible of the data can be viewed within the project GIS along with other information for the estuary. Basic information on the geophysics and samples are held in the BGS Marine Database and can be viewed using the Marine and Coastal GIS or using GeoIndex. There has been ongoing discussion about incorporating the analytical data into the Marine database or the Geochemistry Database, and this remains an aspiration. Currently estuarine geochemical data is neither "owned" by onshore or offshore corporate geochemistry databases and because of this there is a danger that it will get neglected.

Quality control is maintained by the analysis of monitor samples (from the Mersey Estuary) with each batch. There have rarely been any issues of data levelling because the data for each estuary have been generated over a relatively short time span using the same methods.

There is no formal pricing policy for licencing of offshore data, although it is likely that data would be released on a similar basis as that applying to G-BASE and other datasets. Data has been provided as part of co-funding arrangements, for example to Glasgow City Council and SEPA in return for their providing direct and indirect (ship time) funding for the work. At present information about estuarine geochemical data is dealt with on a personal level through enquiries directed either to Dave Jones or Bob Lister at BGS Keyworth.

2.7 ENVIRONMENTAL GEOCHEMISTRY

BGS work on environmental geochemistry and health goes back to the early days of the G-BASE project and peer-reviewed publications demonstrate this fact (*e.g.* Plant and Moore, 1979). *Ad hoc* projects were carried out investigating contaminated land by the Geochemistry Group before the BGS matrix came into operation in 2000 (*e.g.* Appleton *et al*. (1991), and Breward and Cheney (1995)). BGS has also carried out major research projects internationally in the field of mining contamination and studies of trace element deficiencies and toxicities and their impact on human health (see Section 2.11.3).

This section essentially reports on the environmental geochemistry data generated by the abandoned mine and contaminated land team and the medical geology team. After the BGS reorganisation in 2000 this was initially work done under the Chemical and Biological Hazard (CBH) Programme, later renamed the "Environment & Health" Theme, matching the new NERC theme "Environment, Pollution and Human Health" from the "Next Generation Science for Planet Earth" Strategy 2007-2012. The Environment & Health theme area of BGS ceased to exist after April 2009 and this work was dispersed across many teams throughout BGS. The emphasis on geochemical data acquisition is in order to understand the fate and transport of inorganic and organic pollutants in the terrestrial environment and their impact on human health. The data type, mostly geo-referenced but not always, tends to be site-specific and often focussed to explaining water-rock interaction processes.

Under this general remit, a number of projects have produced geochemical data in specific areas which are described in the following paragraphs. The geochemical raw and processed data are scattered throughout various BGS Reports, peer reviewed papers and PhD thesis which are listed in the Chemical and Biological Hazards (CBH) EndNote database. However, as this programme and its successor (Environment & Health Theme) no longer exist there is currently no obvious location for this EndNote library on the SAN.

2.7.1 Geochemical data for the Abandoned Mine and Contaminated Land Team

This Team's projects have involved targeted areas, known for their mining related contamination, and, therefore, the acquired geochemical data are site-specific.

SW England.The geochemical survey at Devon Great Consols Mine comprises total chemical analysis of soil, mine waste and surface water samples (Klinck *et al*. 2005; Palumbo-Roe *et al*. 2007; Palumbo-Roe and Klinck 2007). This dataset has been loaded to the Geochemistry Database. Geochemical data have also been obtained from chemical sequential extractions of selected samples, aimed at the characterisation of the elemental distribution in different mineralogical phases.

Central Wales.A reconnaissance survey over the abandoned mines of the central Wales orefield consists of soil, water and mine waste sample collection and chemical analysis (Palumbo and Klinck 2002). Site specific investigation of two abandoned mines, Grogwynion and Frongoch mines, has been carried out with chemical analysis of soil, waste, surface water and pore water samples. Geochemical data have also been obtained from chemical sequential extractions of selected samples, aimed at the characterisation of the elemental distribution in different mineralogical phases.

Batch and column leaching experiments have been carried out on composite samples representing the mine tailings material and provide geochemical data on the leaching properties of the material (Palumbo-Roe *et al*. 2009).

This dataset will be entered into the Geochemistry Database, once the research project is completed.

Northern Pennines.A reconnaissance survey on the impact of mining and ore smelting in the Rookhope area in Weardale consists of vegetation, soil, mine waste and freshwater sample collection and chemical analysis. This dataset has been loaded to the Geochemistry Database. Three synoptic water samplings (June 2007 - January 2008) and river flow measurement of the Rookhope catchment have produced a dataset of water chemistry and element loads for the Rookhope Burn.

2.7.2 Geochemical data for the Medical Geology Team

One of the aims of the Team is to investigate the exposure of different receptors (*i.e.* humans and groundwaters) to potentially harmful elements (PHE) in soils. This work is centred on the mobility of key inorganic elements such as arsenic, chromium, cadmium, nickel and lead and organic compounds polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls (PCBs) which are priority contaminants of concern. A number of methods are employed to determine contaminant mobility, with the choice of methodology being dependant on the receptor under investigation. One such methodology employed, for assessing human exposure to soil contaminants via the oral ingestion routes, is in vitro bioaccessibility testing. The term bioaccessibility is used to describe the fraction of the total elemental concentration that is soluble in the human stomach and gut and as a result is available for systemic uptake. An in vitro test, the physiologically based extraction test (PBET) has been used in BGS to simulate the leaching of a solid matrix in the human stomach and gastrointestinal tract (Oomen *et al*. 2004). In addition to assessing the mobility of contaminants from point sources, the medical geology team also use the available methodologies to assess this form of contaminant mobility on a spatial scale. To date, the spatial coverage of bioaccessibility data focussed on areas where either the natural background soil concentration or mining-impacted soil concentration of PHEs is above the recommended soil guidelines values. Research in this area includes investigation of arsenic bioaccessibility in soils developed over Jurassic ironstones in eastern England (Palumbo-Roe *et al*., 2005; Wragg, 2005), in mineralised soils in SW England (Klinck *et al*., 2005) and lead mobility (bioaccessibility) investigations in lead mining areas in central Wales (Palumbo and Klinck, 2002; Wragg and Klinck, 2007).

Other geochemical data are integrated with the bioaccessibility data to study the relationship between natural geological factors and health in man and animals, and the influence of ordinary environmental factors on the geographical distribution of such health problems. In particular, the Chemometric Identification of Substrates and Element Distribution (CISED) test, a simple and quick multi-elemental sequential extraction methodology is used to identify the chemical forms of potentially harmful elements that are present in contaminated soils (Cave *et al.*, 2004; Palumbo-Roe *et al.*, 2005; Palumbo-Roe *et al.*, 2007; Wragg *et al.*, 2007).

The Medical Geology Team has domestic and international links with other research groups investigating the area of soil PHE mobility, in particular bioaccessibility. An aim of the Team is to strengthen these links by collaborative research projects with UK Universities and Local Authorities, whereby resources and skills can be pooled in order to achieve a common goal. Ongoing research opportunities include the application of a structured informatic approach to hazard/risk assessment of PHEs in UK soils where existing G-BASE data (soil, stream sediments and water) and the collection of additional geochemical data is used predict and model the bioaccessibility of PHE's in UK soils. The international links made whilst serving as Secretary and Chair of the Bioaccessibility Research Group of Europe (BARGE) are strengthened through international research projects investigating the measurement of the solid phase distribution and bioaccessibility of PHEs in old Dutch Town soils in collaboration with RIVM and TNO in the Netherlands. Similarly, the measurement of the solid phase distribution of PHEs, in this case As and Sb, features in a collaboration with INERIS, France. The outcomes of both collaborations will influence local policy decisions on contaminant mobility and ultimately the risk assessment process in the respective countries.

2.8 RADIOMETRIC DATA

Radiometric data for the UK have been acquired over many years, for both onshore and offshore areas. This extends back at least to the search for uranium at the end of the Second World War and continued into the Mineral Reconnaissance Programme (*e.g.* Bowie *et al.*, 1971; Haslam *et al.*, 1990). Many new measurements were obtained in conjunction with the mapping of indoor radon and for SB and CR projects in environmental radioactivity (*e.g.* Appleton and Ball, 1995, 2002; Ball *et al.*, 1992; Miles and Appleton, 2005).

Resource exploration (primarily for uranium) involved both field measurements and the laboratory analysis of samples. Field techniques included radon in soil gas and gamma-ray methods, initially as total count (or exposure/dose) and later providing K, U and Th data by gamma spectrometry. Many of the instruments used were developed for the programme in collaboration with Harwell. This was also true of the original seabed gamma spectrometer (Eel) systems, developed from the 1970s onwards (Jones, 2001), which produced data on continuous traverses of the sea floor. Similar traverses were made with car-borne and airborne gamma systems, in addition to point measurements on the ground. For the early regional geochemical surveys (predecessors to G-BASE) measurements of gamma ray exposure (in $\mu R\ h^{-1}$) were made at each site, although the data were never entered into a digital database and results can be found on the original field cards stored in NGDC (aisle 128).

Radon in soil gas methods were used to produce radon potential maps of several areas of the UK with European and UK government funding (*e.g.* Department of Environment), the driver being the hazard to health posed by indoor radon. Extensive datasets of soil gas radon and in situ gamma spectrometry were produced during these studies for parts of Derbyshire, Somerset, Devon, Cornwall, Northamptonshire and elsewhere. These types of studies were continued under the Natural Environmental Radioactivity Survey project, which compiled and collected new data for map sheets of Liverpool Bay, Lake District and East Midlands, and its successor the Environmental Radioactivity Project, and has been ongoing, on a smaller scale, up to the present. Enquiries about Radiometric data are currently directed to Dave Jones.

2.8.1 Onshore

Data from the earliest uranium exploration work is not readily accessible, except when tabulated in old reports of the Atomic Energy Division or Radiogeology and Rare Minerals Unit (RRMU)/Radioactivity and Metalliferous Minerals Unit (RMMU) or included in published papers (*e.g.* Bowie *et al*., 1966, 1979; Bowie and Plant, 1983; Miller and Taylor, 1966; Miller, 1967; Miller and Ball, 1968; Plant *et al*., 1983). Mineral Reconnaissance Programme data is generally included in the Geochemistry Database although some may only be available within MRP reports (listed in Haslam *et al*., 1990).

The later radon and gamma spectrometer data (*e.g.* Appleton and Ball, 1995; Emery *et al*., 2003, 2005) are generally held in digital form as MS Excel or Access files, but compilation into a single database was never achieved. The raw radon in soil gas data are converted into activity concentrations (Bg L^{-1} = kBq m^{-3}) by calibration of the instrument and individual counting cells using a known radon concentration from the FRED (Fast Radon Exposure Device) facility at the Health Protection Agency. The field gamma spectrometer data are converted to concentrations of K, eU and eTh using calibrations based on concrete pads of known concentration. The eU and eTh are equivalent U and Th, because the measurements are of the decay products of these radioelements and equilibrium in the decay chain is assumed. Data have also been generated for the anthropogenic radionuclide ^{137}Cs in certain areas, particularly from surveys around the Irish Sea coasts, where this fission product was discharged in the past from the Sellafield reprocessing plant.

More recent borehole logging suites include the Spectral Gamma Ray (Gamma spectrometer) tool, rather than just providing the gamma (*i.e.* total gamma tool) and the Geochemical Logging Tool (GLT). Thus for certain boreholes information on K, U and Th content is available and, from the GLT, Al, Si, Ca, Fe, Ti, Gd, H and Cl. Information on BGS holdings can be obtained by BGS staff through the IDA (BGS Intranet Data Access Application).

Airborne gamma spectrometer data exist for parts of the UK – much of this data was gathered as part of the HiRES project and these areas can be found in the geophysics layer of the GeoIndex[12]. These are directly analogous to the ground-based measurements except for being an averaged reading over a larger area. As they are often acquired with other airborne geophysical data (*e.g.* magnetic and electromagnetic) these results are dealt with in BGS as part of geophysical datasets and are therefore not discussed further here.

2.8.2 Offshore

The BGS towed seabed gamma spectrometer (Eel) was developed originally in the 1970s with Harwell with later versions being produced through continued collaboration with Harwell, KVI Groningen and the German company Antares (Jones, 2001; Miller and Symons, 1973; Miller *et al*., 1977). Surveys were carried out on the UK continental shelf between 1971 and 1991, covering different areas, including regional surveys of the Irish Sea and North Sea with wide line spacing (10 km or greater) and more detailed local surveys (line spacing typically 1-5 km) covering specific areas or long individual lines or groups of lines such as the corridors along pipeline and cable routes.

The early data were typically collected over 1 minute intervals and were often averaged over 10 minutes when converted into radioelement concentrations (K, U and Th as well as total gamma count rates). This conversion was made by reference to counts on calibration pads with known radioelement contents or buried point sources of known strength. When present (particularly in the Irish Sea), the concentrations of anthropogenic radionuclides, such as ^{137}Cs, were also calculated.

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[12] http://www.bgs.ac.uk/GeoIndex/index.htm

The older data (up to *ca*1980) are usually tied to Decca Navigator System positions, so that positional errors could be as great as several hundred metres. The post-1980 results were more usually located using more accurate methods such as Trisponder, Motorola Miniranger or GPS, with errors typically of a few metres. Other geophysical techniques were often run in conjunction with the Eel, such as echo sounder, shallow seismic (sparker, boomer, pinger) and sidescan sonar. Samples of seabed sediments and bedrock were also normally taken for calibration and interpretational purposes, most frequently by Shipek grab, cone dredge and gravity corer, although other techniques were used on certain surveys. The samples were commonly analysed for radionuclides and often particle size analysis and inorganic geochemistry was undertaken.

In general the locations of the Eel and geophysical survey lines were incorporated into the BGS Offshore database along with the basic sample descriptions, but some survey information may not be recorded in that way. There has not been a systematic check that all information was provided from every cruise and it is probable that basic data for some surveys is missing. The geophysical results exist only as analogue records, held in the National Geoscience Data Centre (NGDC) although for many surveys the depth at fix points was included in digital files and, in a few cases, was tidally corrected. The Eel data was all held digitally at some point. However, the early survey data was recorded on punched tape or punch cards. The ultimate computer files may not have been transferred in all cases from one BGS computer system to the next (*e.g.* across old mainframe system such as the GEC and VAX to PCs). It is possible that some data exist only as computer printout or may have been lost. The more recent data exists as digital files, usually as text files or spreadsheets.

The UK Eel cruises are summarised in an Excel spreadsheet held by David Jones This was compiled in 2003 and contains incomplete information on the data collected on each survey. This task was not finished because of insufficient time being available. At a similar time a lot of sorting of paper records was undertaken as part of the archiving of coastal data by Tony Crosby. He incorporated a lot of basic plots and maps from the Eel surveys into the NGDC and summarised what he did in Word documents. In addition to UK surveys, Eel work was carried out overseas with surveys in Belgium, the Netherlands, Philippines, S. Korea and the USA.

2.9 ISOTOPIC GEOCHEMISTRY

Although the status of the NERC Isotopic Geoscience Laboratory (NIGL) has meant that in the past it has generally not been considered part of BGS it does nevertheless generate geochemical data at the BGS Keyworth site and it is necessary to know what data is held by NIGL when we receive external enquiries.

NIGL[13] employ a wide range of isotopic methods to a variety of applications including solid earth geoscience, geochronology, pollution, hydrology, climate change, archaeology and forensic/medical studies. There is no single database of isotope data and the isotope geochemists would explain that the raw data itself is of little value out of context.

Ian Millar currently has data management responsibilities in NIGL which is structured around the four sections of NIGL:

i. U/Th/Pb dating [Stephen Noble]
ii. Tracers (Sr/Nd/Pb/Hf etc.) [Matthew Horstwood]
iii. Stable Isotopes (CHOS – carbon-hydrogen-oxygen-silicon isotope facility) [Melanie Leng]
iv. Stable isotopes (CAL – combustion and laser analysis facility) [Tim Heaton]

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[13] http://www.bgs.ac.uk/nigl/index.htm

Policy is to publish data in scientific publications so this is the principal source of isotope data in NIGL. To this end NIGL have a very comprehensive and well maintained EndNote bibliography but as with the CBH EndNote bibliography described in Section 2.7 there are problems of providing read-only access to this resource.

2.10 LITHOGEOCHEMISTRY

Significant studies of lithogeochemistry have been carried out for a number of BGS projects including those involved with mineral exploration and geological mapping in the UK.

A study of U and other elements in Lower Palaeozoic shales was made during uranium exploration activities (Bowie *et al.*, 1979). The samples collected for this study remain in the NGDC and were reanalysed for a wider range of elements as part of a subsequent work on buried carbonate-hosted mineralisation (Jones and Plant, 1989). That study also included new sampling and analysis (by XRFS) of Lower and Upper Palaeozoic (Carboniferous: Visean-Namurian) shales from boreholes in the East Midlands. A subsequent extension of that work across northern England included further XRFS analysis of Carboniferous mudstones from sampling of boreholes held by BGS (Plant and Jones, 1999). The work also involved a reappraisal of the geochemistry of limestones undertaken previously as part of limestone assessment projects (Harrison, 1982; Harrison and Adlam, 1985) and other mineral exploration activities, including a small number of new analyses. Ball and Merriman (1989) published a BGS research report on the petrology and geochemistry of the Ordovician Llewelyn Volcanic Group.

A study of the Cheshire Basin also involved significant lithogeochemical studies of the Permo-Triassic basin fill (Plant *et al.*, 1999). A more limited appraisal of red beds in the UK had been carried out by Haslam and Sandon (1991).

	Numbering System					
	1:MinPet	2:BioStrat	3:MRP	4:GBASE	5:Environment	Totals
Normal Rock Samples with XY data	1532	0	7917	0	0	9449
Normal Rock Samples without XY data	1296	0	245	0	0	1541
Drainage Rock Samples with XY data	0	0	9	0	0	9
Core Rock Samples with XY data	3104	0	8228	0	0	11332
Core Rock Samples without XY data	28	0	159	0	0	187
Totals	5960	0	16558	0	0	22518

Table 9: Number of rock and core samples in the Geochemistry Database (using the NORMAL_ROCKS and CORE_POSITIONS tables)

	Numbering System					
	1:MinPet	2:BioStrat	3:MRP	4:GBASE	5:Environment	Totals
Normal Rock Samples with XY data	1471	0	6216	0	0	7687
Normal Rock Samples without XY data	21	0	71	0	0	92
Drainage Rock Samples with XY data	0	0	9	0	0	9
Core Rock Samples with XY data	14	0	170	0	0	184
Core Rock Samples without XY data	0	0	0	0	0	0
Analysed Rock Samples without sample data*	57	0	4876	0	0	4933
Totals	1563	0	11342	0	0	12905

**Rock sample in the ANALYTE_DETERMINATION table without a corresponding record in NORMAL_ROCK, CORE_POSITION or DRILLCORE tables*

Table 10: Number of rock and core samples defined in Table 9 that have associated Analyte Determinations

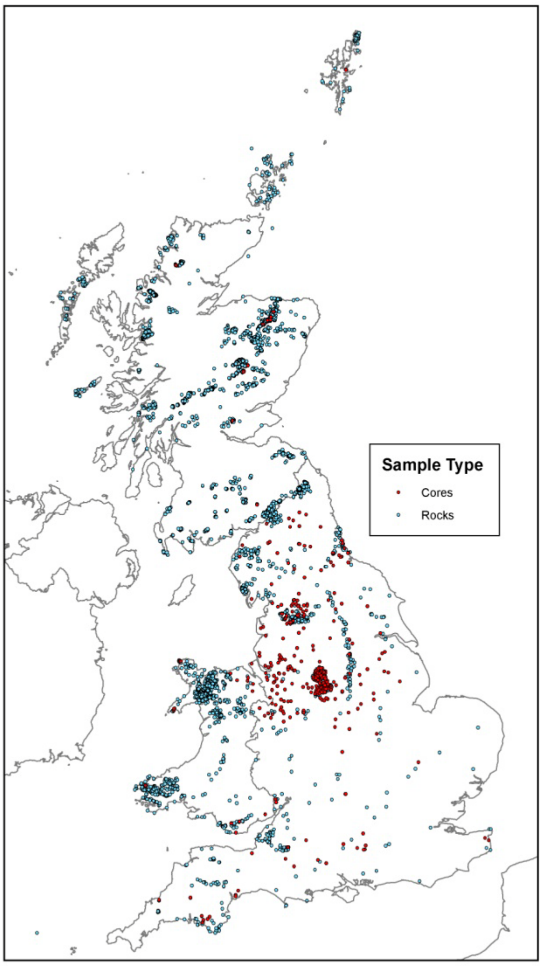

Figure 13: Distribution of rock and core sample sites in the Geochemistry Database (after Hulbert, 2007)

The availability of lithogeochemical data in the BGS Geochemistry Database was investigated by Hulbert (2007) (Table 9 and Table 10 are from this report, as is Figure 13). The databasing of lithogeochemical data was the responsibility of the Geochemistry Division Database Group pre-2000. It is part of the "corporate memory loss" (notably when Robert Jones, Stan Coats and Henry Haslam retired) that the history and whereabouts of the stand alone lithogeochemistry database (UK-IGBA) is not clearly known. This is thought to have become the responsibility of someone in Leicester University. The fate of this lithogeochemistry database to which BGS contributed needs to be investigated. IGBA (IGneous dataBAse) and the national geochemical data bank are described by Le Bas *et al*. (1983).

Lithogeochemistry was also a part of BGS mapping projects and reference should be made to relevant reports. For example the work carried out by Derek Cooper and Brett Beddoe-Stephens for the multidisciplinary Lake District project (*e.g.* Allen and Cooper, 1986; Allen *et al*., 1987 ; Beddoe-Stephens, 1991, 1997; Beddoe-Stephens *et al*., 1995; Cooper *et al*., 1988, 2004).

2.11 INTERNATIONAL GEOCHEMISTRY

2.11.1 Geochemical Mapping and Mineral Exploration

A good summary of international exploration and baseline mapping work (1965 -1993) is presented by Jones and Coats (1993). A draft report focusing on BGS international minerals related data holdings has also been prepared by Pitfield (2001). Much of the early BGS international work was done as technical assistance projects supported by the British Overseas Development Administration (ODA). However, overseas geochemical work since 1994 has either been as commissioned projects sponsored by organisations such as the World Bank or national governments or ODA TDR/DFID KAR (Knowledge and Research) projects.

National geochemical mapping commissioned by national governments (*e.g.* Ecuador, Morocco, Mauritania, Madagascar, Nigeria and Zambia) have generated large geochemical data sets that belong to the respective national governments and should be available from the national geological surveys either in map or digital form. Some of these have been described in peer-reviewed publications *e.g.* Williams *et al*. (2000) (Ecuador) and Key *et al*. (2004) (Zambia). International geochemical research projects have also been published in peer reviewed publications such as Ball *et al*. (1990) and Ridgway *et al*. (1991). Non-confidential maps and reports on this geochemical work should be available from the BGS library and in some instances, *e.g.* Morocco, CD-ROMs of project data and reports are still retained in BGS (*e.g.* Direction de la Géologie, 2001). Although BGS had no involvement in the sample collection for the Hong Kong geochemical atlas, BGS was commissioned to prepare the geochemical images and interpret the data (Johnson and Breward, 1997).

Hardcopy files relating to pre-1994 international geochemistry projects are stored in Aisle 128 of NGDC, and these often include analytical results and sample information. Many of the national geochemical mapping surveys produced geochemical atlases and reports that are available in the BGS library and these are an important source of geochemical information (*e.g.* Uganda – Reedman, 1973; North Sumatra – Stephenson *et al*., 1982; Solomon Islands – Ridgeway, 1983; Eastern Bolivia – Appleton and Llanos, 1985; Southern Sumatra – Muchsin *et al*., 1997). Some geochemical samples from these projects (*e.g.* split of the stream sediments from Bolivia) are stored in NGDC.

A large amount of geochemical data for rock samples was generated by the SE Asia tin granites project (Cobbing *et al*., 1992). This Overseas Development Administration (ODA)-funded project between 1981-88 provided data on 11 major oxides plus loss-on-ignition and 28 trace elements for 171 samples from Peninsular Malaysia, 83 samples from the Indonesian tin islands, 225 samples from Thailand and 150 samples from Burma (Myanmar). The collection of granites from Burma was made by Bob Beckinsale during a technical cooperation project in 1977.

The most comprehensively compiled database of BGS international geochemical data holdings is the International Regional Geochemistry CD-ROM series[14] which was launched in 1999 as an "innovation funding" project and relaunched at the end of 2007 with updated file formats and contact information. This is a series of six CD-ROMs (Table 11) available for purchase from the BGS online bookshop[15]. Geographically referenced sample data (mainly stream sediments) are presented in xls, cvs or dbf format along with all the project information available including bibliographic references for further information.

No.	Title	Release date
1	Indonesia: Sumatra	Sep 2007
2	Zimbabwe: Harare, Rushinga and Nyamapanda, and Makaha	Sep 2007
3	Bolivia: Eastern Bolivia	Sep 2007
4	Peru: Northern Peru	Sep 2007
5	Kenya: Sambura – Marsabit	Sep 2007
6	Solomon Islands: Choiseul and New Georgia	Sep 2007

Table 11: List of International Regional Geochemistry CD-ROMs available for purchase from the BGS online book shop

2.11.2 Groundwater chemistry

International groundwater chemistry work over the last 10–15 years has encompassed estimations of recharge in semi-arid regions, geothermal geochemistry, applications of stable isotopes in hydrogeological investigations, impacts of groundwater pollution from urbanisation and diffuse agricultural pollutants and relationships between naturally-occurring trace elements and human health. These themes have been covered in various projects with a number of funding agencies (principally DFID/ODA) and in numerous countries. Each has associated project reports and external publications. Data in most cases are stored on the Wallingford hydrochemistry laboratory database (except where analysed elsewhere). Project details include recharge estimations in *e.g.* Sudan, Senegal and Libya, investigated principally by Mike Edmunds and local partners. Applications of stable isotope techniques cover numerous countries (*e.g.* Iceland, Mexico, Costa Rica), while geothermal studies have focused principally on east Africa (Kenya). Each of these has been led by George Darling. Impacts of urbanisation include landfill leachate risk assessments in Jordan, Mexico and Thailand (Ben Klinck) and urban groundwater quality deterioration in Mexico, Thailand and Bolivia (Brian Morris). Diffuse pollution studies include impact of wastewater reuse in Mexico, Jordan and Thailand (John Chilton and David Kinniburgh), nitrate pollution in Malta (Marianne Stuart) and nitrate and pesticides in India (Adrian Lawrence). Studies of the impacts of naturally-occurring trace elements of health concern in groundwater include arsenic (Argentina, Bangladesh, Burkina Faso, China, Ghana, Mexico), fluoride (Argentina, Ghana, Sri Lanka, Tanzania) and iodine (Ghana). These were carried out under various projects, mainly led by Pauline Smedley. DFID funded a major investigation of arsenic in Bangladesh (1998–2000) in which BGS collaborated principally with the Bangladesh Government. This project was led by David Kinniburgh. The full groundwater dataset from the Bangladesh project is available for free download from the internet[16].

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[14] http://www.bgs.ac.uk/geochemcd/home.html

[15] http://shop.bgs.ac.uk/Bookshop/category.cfm?CAT_ID=6E

[16] www.bgs.ac.uk/arsenic

A summary of some international groundwater pollution projects is given in Table 12 and groundwater in relation to human health projects in Table 13.

Project/Duration	Project Leader	Funded by	Description
Preliminary study on the identification of the sources of nitrate contamination in groundwater in Malta. Study completed in 2009	Marianne Stuart	Rural Development Programme of Malta	Data and literature review and strategy design, sampling for nitrate stable isotopes and other indicators, results and conclusions, policy implications. 3 reports. Reports and data confidential
Human health risk in relation to landfill leachate. 3 yrs ending in 1999	Ben Klinck	DFID	Designed and produced catalogue of leachate quality based on climate, waste type etc. Collected groundwater and leachate quality from landfill sites in Jordan, Mexico and Thailand . Commonly occurring leachate components identified and risk assessments carried out for these for selected study sites. Options for mitigating human health risk evaluated. 3 case study reports, landfill leachate catalogue and final summary report. Marianne Stuart has originals of leachate data
Impact of wastewater reuse on groundwater in the Mezquital valley, Hidalgo State, Mexico. 3 yrs ending in 1998	John Chilton	DFID	Programme of regular groundwater sampling, canal leakage studies, microbiological risk assessment water balance model, options for improved management. Final report and data annex. Marianne Stuart has the whole stock. Data in Wallingford laboratory database.
Protecting groundwater beneath wastewater recharge sites. 3 yrs ending in 1998	David Kinniburgh	DFID	Four case study - Mezquital and Leon, Mexico; Wadi Dhuleil, Jordan and Hat Yai, Thailand. Objective to assess extent of detection and persistence of trace organic compounds where water infiltration has occurred. Analysed wastewater and groundwater for inorganics and broad scan organics. 3-part final report, Final summary, analytical results and broadscan gcms spectra. Marianne Stuart has copies. Data in report and in Wallingford laboratory database.
Follow -on project Assessment of pollution risk to deep groundwaters from urban wastewater. 3 yrs ending in 1997	Brian Morris	DFID	Sites as for initial project. Case study reports plus summary. Marianne Stuart has copies of most of them. Samples analyses at Wallingford so should be in laboratory database
Effects of wastewater reuse on urban groundwater resources, Leon Mexico. 3 yrs ending in 1996	John Chilton	ODA/EC	Programme of regular water level and quality measurements, surface geophysics, soil profiling and installation of piezometers. Assessment of impatcs and risks and evaluation of options for improvement. 2 progress reports and final report Marianne Stuart has the whole stock. Data in Wallingford laboratory database.
Impact of urbanisation on groundwater quality. 3 yrs ending in 1994	Brian Morris	ODA	Case study sites in Yucatan, Mexico; Hat Yai, Thailand and Santa Cruz, Bolivia. Case study reports for each site, including a final summary for each plus an overall project summary report - Marianne Stuart has copies of most of them. Samples analyses at Wallingford so should be in lab database
Impact of agriculture on groundwater quality in the alluvial aquifers of Madras, India. Completed 1993	Adrian Lawrence	ODA	Assessment of the impact of rice cultivation in terms of nitrate and pesticide leaching. Installation and monitoring of piezometers. Studies of carbofuran leaching and metabolites. Marianne Stuart has report.
Impact of agriculture on groundwater quality: Kalpitiya Peninsula Sri Lanka. Completed 1992	Adrian Lawrence	ODA	Assessment of the impact of horticulture in terms of nitrate and pesticide leaching. Installation and monitoring of piezometers and lysimeters. Studies of carbofuran leaching and metabolites. Marianne Stuart has report.

Table 12: Summary of some international groundwater/pollution projects from past 16 years (compiled by Marianne Stuart, BGS Wallingford)

Project	Description	Reference
ODA-TDR project Vulnerability of shallow groundwater quality due to natural geochemical environment 1993-1995	Field studies in Ghana and Sri Lanka. Investigations of As in groundwater in mining areas, F in groundwater and I deficiency	Edmunds and Smedley, 1995 Smedley *et al*., 1995
ODA-KAR project - Arsenic in Groundwaters from major aquifers: sources, effects and potential mitigation	Field studies in Argentina, Bangladesh and China. Spawned the larger DFID-funded project on arsenic in Bangladesh (1998-2001)	Smedley *et al*. 2000a, 2000b
DFID Groundwater Studies for Arsenic Contamination in Bangladesh	Rapid Investigation Phase – mapping and prelim assessment; subsequent detailed phase – cont'd mapping, hydrogeological/chemical interpretation and flow and geochemical modelling	DFID/BGS/MML, 1999 BGS and DPHE, 2001
DFID KAR project – Minimising fluoride in drinking water in problem aquifers	Field investigations in Ghana, Tanzania. Phase I completed, phase II not (DFID funding cuts).	Smedley *et al*. 2002

Table 13: Summary of some BGS-ODA/DFID projects concerning groundwater and human health, carried out in developing countries

2.11.3 Geochemistry and Health

In addition to the groundwater chemistry projects associated with human health as described in the previous sub-section, BGS has carried out many DFID/ODA projects concerning geochemistry and health. These have either been connected to mining contamination or natural trace element deficiencies or toxicities. Whilst some of this work has been published in peer reviewed publications the principal source of the geochemical data and information is in the internal BGS Overseas Geology report series. Many of these are summarised in Table 14 but are generally not readily accessible. Much more effort needs to be put into making this wealth of geochemical information available in NORA or as down-loadable reports from the internet.

2.11.4 Offshore geochemistry

As with the international onshore geochemistry and health and groundwater projects, BGS work in the offshore geochemistry area has been supported by the ODA. This was principally project R6191 Land-Ocean Contamination Study (LOCS). There were three locations where this work was carried out: Mombasa, Kenya (Rees *et al*., 1996); Jakarta Bay, Indonesia (Williams *et al*., 1997, first of three volumes); and Sepetiba Bay, Rio de Janeiro, Brazil (Rees *et al*., 1998b). As part of a DFID funded project (R7111) Rawlins *et al*. (1998) reviewed available information on the movement of sediments and pollutants of agricultural origin into the coastal zone in the Caribbean.

Project	Description	Reference
DFID KAR project R7411. Environmental Controls in Iodine deficiency Disorders	Field studies in China and Morocco. Study of the behaviour of iodine in the surface environment and the connection with IDD	Johnson *et al.* 2003 (This report lists all project reports and outputs)
DFID KAR project R6227. Prediction and remediation of Se imbalances	Se distribution in villages of the Keshan Disease Belt (Se deficiency), Zhangjiakou District, China. Se deficiency (Keshan Disease) and Se toxicity in Enshi District of China. Se deficiency in the environment & oesophageal cancer, Cixian, China. Se status of the environment in IDD areas of Sri Lanka	Johnson *et al.* 2000 Fordyce *et al.* 2000 Appleton *et al.* 2006 Fordyce *et al.* 2000
DFID KAR project R6226. Mitigation of mining-related mercury pollution hazards	Field studies in Mindanao (Au mining) and Palawan (Hg mining), Philippines. Field studies in Nambija and Ponce Enríquez (Au mining), Ecuador.	Appleton and Williams, 1998 (Summary Report -This report lists all project reports and outputs)
DFID TDR project R6228. Cerium and endomyocardial fibrosis (EMF) in tropical terrains	Literature review and fieldwork in Uganda to test hypothesis that linked EMF, Mg deficiency and exposure to Ce	Smith, 1998 (Summary Report)
DFID TDR project R6491. Environmental arsenic exposure: Health risks and geochemical solutions	Mining-related arsenic hazards: Thailand case-study Summary report	Williams, 1997
ODA TDR project 92/10 (R5557). Geochemistry and toxicity of naturally occurring aluminium	Coupling geochem. mapping and modelling techniques to predict the potential for enhanced Al concs. And resulting adverse environmental impacts	Smith, 1995 (Summary Report)
ODA TDR project R5547. Environmental Geochemical Mapping	Stream sediment, soil and forage chemistry as indicators of cattle mineral status in northeast Zimbabwe	Fordyce *et al.* 1994
ODA TDR project 91/16. Environmental Geochemical Mapping	Geochemical characteristics of soil, surface water and vegetation in the Fothergill Island area, Matusadona National Park, Zimbabwe	Williams, 1994
ODA TDR project 92/6. Environmental impacts of gold and complex sulphide mining	Preliminary field trial of a method for the rapid assessment of invertebrate stress from mining-related arsenic and heavy metal contamination: Wanderer gold mine, Zimbabwe	Weeks and Williams, 1994

Table 14: Summary of some BGS-ODA/DFID geochemistry and health projects – including groundwater - carried out in developing countries

2.12 ORGANIC GEOCHEMISTRY

2.12.1 Overview

Organic Geochemistry within BGS is led by Chris Vane and provides a scientific understanding of natural organic matter and anthropogenic organic compounds in soils, sediments and waters. The objectives of are four fold:

1. Provide data and interpretations that underpin NERC Strategy 2007-2012 “Next Generation Science for Planet Earth”;
2. Provide data and interpretations in support of BGS projects and themes;
3. Conduct commercial analyses to generate income;
4. Research and development for 1-3.

The science ranges from simple bulk measurements to complex series of molecular analyses designed to meet the needs of research projects. Organic geochemistry is now widely considered one of the most scientifically active areas within the BGS analytical chemistry facilities as evidenced by the quality and quantity of peer reviewed publications, BGS reports and a growing national/international reputation. Furthermore, organic geochemistry supplies both data and associated interpretations to nine of the twelve BGS science themes.

The organic geochemistry at BGS can be broadly divided into the four areas (with loss-on-ignition being determined as part of the general chemistry function of the laboratory):

1. **Baseline Pollution Studies and Environmental Forensics**

   Quantification of persistent organic pollutants (POPs) in soils, sediments and waters including total non-volatile hydrocarbons (saturate/aromatic and NSO compound classes) by TLC-FID (Iatroscan), Total Petroleum Hydrocarbons (TPH) by GC-FID, 15 of the 16 US EPA “priority pollutant” polycyclic aromatic hydrocarbons (PAH) by HPLC with fluorescence detection, Polychlorinated Biphenyls (PCB) reported as individual ICES 7 PCB and the sum of: tri, tetra, hepta, hexa and hepta homologues as well as the sum of PCB congeners by GC/MS. Values can be normalised to Total Organic Carbon (TOC) to enable direct sample comparison. Additional expertise in the analysis of volatile organic compounds such as BTEX and TCE by headspace GC/MS, pesticides such as mecoprop, atrazine and diuron, organo-metallic species such as tributyl-tins (TBT) and xenoestrogens. The laboratory is also capable of quantification of explosives formulations HMX, RDX and TNT in sediments by HPLC and quantification of sewage sterols to track sewage/faecal matter in the environment by GC/MS.

2. **Terrestrial and Marine Palaeoenvironmental Analysis**

   Application of analytical Pyrolysis combined with Gas Chromatography-Mass-Spectrometry (Py-GC/MS), Chemolysis-GC/MS and Infrared Spectroscopy (FTIR), to characterise structural polymers and macromolecules such as polysaccharides, lignin, suberin and tannin as well geomacromolecules such as kerogens and coal in order to reconstruct palaeoenvironment, determine biotic and abiotic alteration and understand biochemical evolution. The O&GC section is also competent in the quantification of Black Carbon (BC) in soils and sediments by chemothermo/oxidation method and in the isolation of dissolved organic carbon (DOC) in groundwaters by Tangential Flow Ultrafiltration (TFU).

3. **Climate Change**

   Estimation of palaeotemperature and palaeoclimate using biomarkers “fossil biological molecules”. Sedimentary organic matter that is soluble in organic solvent is removed by accelerated solvent extraction (ASE) fractionated by column chromatography and analysed by GC/MS operated in either full scan or selected ion monitoring mode. The range of biomarkers analysed for includes *n*-alkanes, *n*-alkanols, carboxylic acids, sterols (palaeoecology and atmospheric transport), highly branched isoprenoids (palaeosalinity) as well as alkenones for the *U*K37 and *U*K37 sea-surface temperature proxy.

4. Hydrocarbon Exploration and Reservoir Studies

Oil-source rock correlations, oil-oil correlations and reservoir studies using TOC and Iatrosan screening for saturate, aromatic and polar (NSO) fractions, quantification of saturate fraction using GC-FID evaluation of *n*-alkane envelop, CPI, pristine/*n*-C17 ratio, Pr+Ph / *n*-alkanes to indicate maturation, migration, biodegradation. A more detailed picture of oil chemistry is obtained by analysing the saturate fraction by GC/MS in SIM mode for specific biomarkers such as steranes, triterpanes and a variety of other compound classes.

2.12.2 Data Storage

The geochemical data generated by the organic geochemists at BGS takes many forms: quantitative, semi-quantitative and qualitative data. The worked up data is held by the relevant projects and some raw data where appropriate also stored in the UKAS central filing system in BGS (room U113). Due to the nature of organic geochemistry, data is not generally sold to internal or external clients in raw form, indeed many of the raw outputs (mass spectra and chromatograms are only compatible with specific forms of software). Moreover, the organic analysts supply interpretations of the data as part of projects which are published in reports and where appropriate academic journals/book chapters.

2.12.3 Sources of Organic Geochemical Information

The primary source of information concerning organic geochemistry in BGS is in the form of reports and publications. A comprehensive selection of these is given in Appendix 3.

3 Sources of Geochemical Data in BGS

Past and present projects generating a broad range of geochemical data are described in the preceding section. The principal sources of this geochemical data, classified by the main theme areas described in Section 2, are summarised in Table 15. It is immediately apparent from this table that there are numerous different geochemical data sources in BGS. With the exception of the BGS GeoIndex, references to internet links are surprisingly absent in Table 15. Although the different science areas of BGS have informative internet pages with links to geochemical content (*e.g.* G-BASE[17]), the different threads of geochemistry are not joined up and searching for BGS geochemistry content on the internet site is a frustrating challenge. The BGS web site needs a high level link that points directly to a page that covers all the areas of geochemistry discussed in this report.

Principal databases are the Geochemistry Database administered in Keyworth (mainly for UK drainage samples, soils and rocks) and the Hydrogeochemistry Database (MS ACCESS) at Wallingford. The Marine Geology Database whilst designed to receive geochemical data has not yet been populated. Many areas of geochemical data (*e.g.* estuarine geochemical results) are represented by *ad hoc* databases (*e.g.* as Excel spreadsheets) administered by individuals and remnants from now defunct projects. The position is further confused by the fact that the BGS corporate Geochemistry Database is actually only populated with data from a few specific projects in BGS. For someone looking for geochemical data it would be reasonable to assume that the BGS corporate Geochemistry Database would be the definitive starting point but it is clearly not. Furthermore, because of the nature of geochemical data, which is always tied to a number of quality and usage issues, it is very difficult for non-specialist geochemists to access digital data directly. Requests for geochemical data (internal and external) usually have to be dealt with by one or two trained individuals who have a good understanding of all the caveats concerning the data usage. Whilst the introduction of "Query Layers" for searching the Oracle Geochemistry Database removes the complexity of linking numerous data tables, it still fails as a satisfactory system for delivering geochemical data to those who wish to use it.

Much of BGS geochemical data is published in reports and external publications. EndNote bibliographies are therefore a valuable first stage into finding geochemical data but there is no corporate system that allows access to and the sharing of these important bibliographies. When programmes and theme areas in BGS have disappeared, the bibliographies have disappeared with them.

BGS can be seen as having several warehouses for geochemical data. Generally that data is well collated and organised and much legacy data is available for future generations of scientists to use. However, only specialist users have the key to accessing the data. More effort needs to be put into delivering the geochemical data from the disparate BGS sources in a format that potential users can access and download more easily. The Information Products team have to some extent started this process. For example, by taking various different data sets (using different sample media) a complete "predictive" arsenic map for England and Wales has been created (Appleton *et al.*, 2008). A module using soil geochemical data has been prepared for Landmark as an option for the "Home Owners Pack" that highlights the risk of contaminated land.

The creation of a series of International Regional Geochemistry CD-ROMs (see Table 11) was an excellent example of providing data in a format that was readily useable by external customers. The innovation project that created the CD-ROMs received c.£5k and CD sales to mineral exploration companies exceeded £30k within 3 years. The CD-ROMs are now sold

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[17] http://www.bgs.ac.uk/gbase/home.html

directly through the BGS online bookshop and does not require a specialist geochemist to be involved in delivering the data to the user.

Information Products are primarily concerned with generating income for BGS. However, geochemical data is fundamental to underpinning much of the science that is done in BGS so the delivery of geochemical data for science users must also be of great importance. The BGS intranet (for internal data users) and internet (for external data users) is key to delivering the data in a format that is easily useable. Hydrogeochemistry is well documented through the Groundwater Portal[18] on the BGS intranet (under data and information), particularly with regards to information and access to publications. Easy access to BGS geochemistry reports and publications is essential to enable the wide range of our geochemical work to be disseminated and particularly important for those areas which rely on publications for the distribution of geochemical data (*e.g.* NIGL and organic geochemistry). The NERC Open Research Archive (NORA) is growing to be a useful resource for the world to access BGS geochemistry reports (*e.g.* the urban geochemistry reports for UK cities). However, more effort has to be made to declassify reports and get them loaded into NORA.

New databases and derived products (*e.g.* gridded geochemical images for use in GIS) need to be delivered over the web. Users should not be concerned with the complexities of which database the data is derived from or what project generated it. The products should come with clear information regarding the quality of the data and limitations on its use.

The flow chart of Figure 14 attempts to classify the different sources of geochemical data into three main groups; UK Onshore; UK Offshore; and International geochemical data. The data is further subdivided into the theme areas to match with those identified in Section 2 and Table 15. The subdivision for the flow chart is based on key questions an enquirer may have concerning the geochemical data required. The BGS science area responsible for the data is also identified. Whilst the chart is a simplification of many different geochemical data sources where there is overlap between themes, it should inform enquirers as to what geochemical data BGS holds and where to go to get the data or further information.

Someone seeking geochemical data, information or samples from BGS (that have been generated or commissioned by the BGS) should firstly know the geographical site or area for which data is sought. At the highest level this may be a country or region of the world, or at a more detailed level the geographical coordinates (*e.g.* Eastings and Northings for the UK land area). If the geochemical data has not been gathered by remote sensing (as in the case of radiometric data) then the enquiry should relate to a specific sample media type or the nature of the investigation that generated it. With this information to hand an enquiry about geochemical data should then follow the flow paths shown in Figure 14.

A further source of information concerning BGS geochemical data holdings is the discovery metadata accessible from the BGS internet site[19]. A search using the keyword “geochemistry” will return metadata for some 35 datasets. This is a useful starting point to find some geochemical information but not all areas of BGS geochemistry are represented by the available metadata, titles for the metadata sets are not systematic or particularly informative and minor small projects are given equal status to major programmes.

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[18] http://intranet/groundwater_portal/default.shtml

[19] http://www.bgs.ac.uk/discoverymetadata/index.html

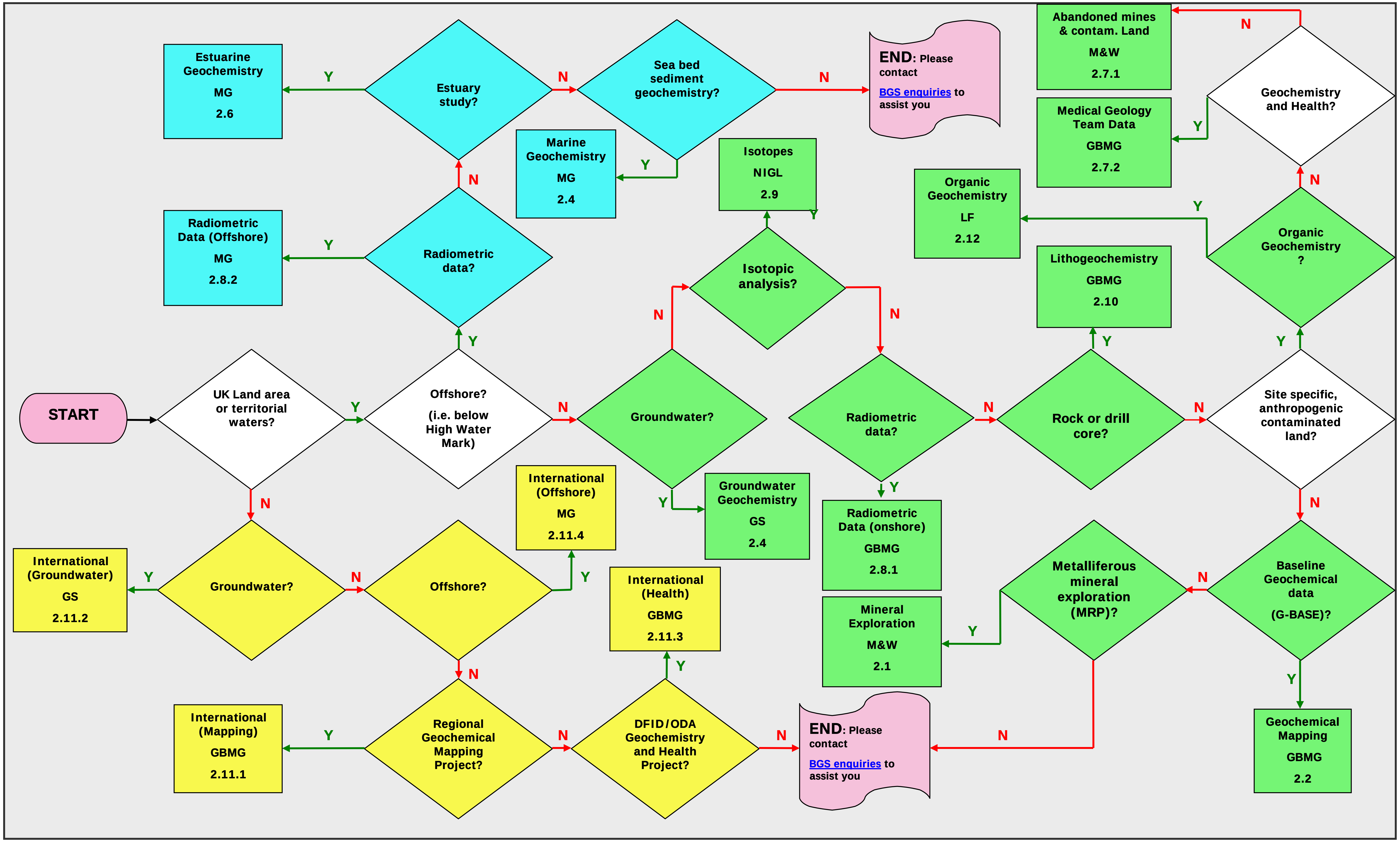

Figure 14: Flow chart to inform enquiries regarding sources of geochemical data in BGS. The main classifications of geochemical data are colour-coded: International – yellow; UK Offshore –blue; and UK Onshore –green. The white diamonds represent key questions in the enquiry flow. The boxes identify the key data sets with a hyperlink to the relevant section of text, The area of BGS science is coded: GS – Groundwater Science; GBMG – Geochemical Baselines and Medical Geology; MG – Marine Geosciences; M&W – Minerals and Wastes; LF – Laboratory facilities; and NIGL – NERC Isotopic Geoscience Laboratory.

Category (including section no. in this report)	**Sources of Information**
Mineral Exploration (2.1)	BGS Geochemistry Database
	MRP Report Series
	BGS GeoIndex (Geochemistry theme)
Regional and Urban Geochemical Mapping (2.2)	BGS Geochemistry Database
	Field forms
	Regional Geochemical Atlas Series
	BGS Internal Report Series & Geochem. Database Note Series
	G-BASE EndNote Bibliography
	BGS GeoIndex (Geochemistry theme)
Groundwater Geochemistry (2.4)	Wallingford Laboratory and Hydrogeochemistry Database
	BGS Commissioned Reports
	Web Portal (internal to BGS staff)
	BGS internet
Offshore/Marine Geochemistry (2.5)	BGS Commissioned Report (Stevenson *et al*. 1995)
	BGS GeoIndex (Offshore UK theme – Seabed samples layer)
Estuarine Geochemistry (2.6)	BGS Offshore database
	BGS Internal Report Series
	BGS GeoIndex (Offshore UK theme)
Environmental Geochemistry (2.7)	BGS Geochemistry Database
	BGS Internal Report Series
	CBH EndNote Bibliography
Radiometric Data (Offshore) (2.8.2)	BGS Offshore database
	BGS Internal Report Series
	BGS Geoindex (Offshore UK theme)
Radiometric Data (Onshore) (2.8.1)	Atomic Energy Division reports
	Internal BGS, MRP, RRMU and RMMU reports
	BGS Geoindex (Boreholes &Geophysics themes)
Isotopic Geochemistry (2.9)	NIGL EndNote publications bibliography
	Journal Publications
Lithogeochemistry (2.10)	BGS Geochemistry Database
	BGS GeoIndex (Geochem. theme – Rock & Borehole Rock layers)
	Limestone Assessment Reports
	Geological Memoirs
International Geochemistry (2.11)	International Regional Geochemistry CD-ROMs
	Atlases
	BGS Commissioned Technical and Internal reports
Organic Geochemistry (2.12)	Reports and publications (see Appendix 3)

Table 15: A summary of sources of geochemical data in BGS

Geochemical Baseline Survey Of The Environment (G-BASE) For The UK.

Dataset description

The G-BASE programme involves systematic sampling and the determination of chemical elements in samples of stream sediment, stream water and 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 1.5-2km square, and for soils one site per 2km 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, SO4,NO4, and TOC. The project now routinely determines the elements listed in the <2mm fraction of surface soils.

Constraints

Data sold under licence. Copyright control. Landowners permission given for non-site specific survey.

For more information please contact :

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Associated dataset(s)

Acidity of stream water
Arsenic in soil
Copper in stream sediment.
Fluoride in stream water
Geochemical Baseline Survey Of The Environment (G-BASE) For UK Soils In Urban Areas.
Metal Speciation And Bioavailability For Risk Assessment And Remediation.
Results From The Regional Geochemical Mapping Of Britain
Uranium in stream sediment.

Reviewed 17th March 2009

Figure 15: Example of some geochemistry discovery metadata available from the BGS internet site

Recommendations for making BGS geochemical data more accessible to users

The following recommendations are made to increase the accessibility of BGS geochemical data and information for both internal and external users so as to better contribute to the delivery of the BGS strategy;

1. Project Data Management plans need to be managed and enforced to ensure projects generating geochemical data conform to corporate standards for the storage of samples and data. This should be a function of the Geochemistry Data Management Project but will only be successful if projects are provided with clear guidance and policies as to what they should do with the data that is generated.
2. With the exception of the GeoIndex, links on the BGS internet about geochemical data and information are dispersed and hard to find. There is an absence of any high level entry point providing links to the existing geochemical resources. The removal of the word "geochemistry" from all parts of the organisational structure leaves users without any reference point to start from. A search on "Geochemistry" gives a long list of unjoined-up links that is an unhelpful overview of geochemistry at BGS. It is suggested that links to all the geochemical theme areas in this report are focused from within one specific science area of BGS.
3. It is misleading to have something called the corporate BGS Geochemistry Database that only receives a small part of BGS's geochemical data. External (and indeed internal users) are misled into believing this is BGS's only source of geochemical data. Whilst it would be good to have all BGS geochemical data in one place this would be impractical (see below). It is suggested that the term "corporate BGS Geochemical Database" be qualified to reflect its true content, *e.g.* corporate BGS Geochemical Database for the UK land surface.
4. Ideally all BGS geochemical data should be accessed via linked Oracle databases. However, this would require the investment of a lot of resources to replace and revamp adequate databases that already exist in different areas across BGS. The more pragmatic approach is to focus on delivery of data to the users. This will mean the creation of derived geochemical products delivered via the internet. An example of this would be a set of ArcGIS geochemical images for UK baseline geochemical data downloadable from the BGS web site.
5. The licensing of land surface geochemical data for the UK has been operating satisfactorily for many years. There needs to be a consistent pricing policy for all geochemical data, particularly with regard to the provision of geochemical data for external academic research.
6. Some particular areas that have generated geochemical data need support to capture legacy data and information before it is lost. Currently much of the data from estuarine, radiometric and raw G-BASE geochemical data is dependent upon the custodianship of individuals rather than corporate systems. The capture of these data sets to corporate systems needs to be addressed in the information management delivery plan.
7. Currently estuary geochemical data is neither "owned" by the Marine Geology or Environmental Geoscience Baselines themes and as a consequence, data from estuarine projects is in danger of becoming neglected. This report defines offshore as being below the high water mark and consequently estuary data is considered as being "offshore".

8. Information regarding the igneous rock geochemical database (UK-IGBA) no longer resides within BGS. Retired staff should be contacted so the status and whereabouts of this database can be re-established.
9. This report has demonstrated that in many areas of geochemical data generation it is publications and reports that play an important part in information dissemination. This is particularly the case for isotopic, organic and international research projects. The hydrogeology portal gives excellent access to downloadable pdfs of many hydrogeochemistry reports but this is restricted to BGS intranet users only. Bibliographic lists like those provided in the hydrogeology portal should be made available from the BGS internet site with associated links to free downloadable reports. There is a great wealth of geochemical information and data in inaccessible, non-digital internal and technical BGS reports, particularly for international research projects. These should be scanned and made available over the intranet.
10. EndNote bibliographies provide useful and comprehensive lists of reports that detail geochemical information and data. A corporate approach to the use and sharing of EndNote bibliographies is required. Valuable EndNote libraries are lost when programmes/Science theme areas are reorganised.
11. The confidential classification on many BGS technical and internal geochemical reports needs to be reviewed and wherever possible removed. Many of the geochemical theme areas are already making good use of the NERC Online Research Archive (NORA) but more geochemical reports should be added.
12. Team Leaders associated with the various geochemical theme areas should be providing more “geochemical data awareness” lectures within BGS and externally (for example to university departments). There is also scope for the provision of a training course to educate non-specialist geochemists in the use and interpretation of geochemical data.

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Appendix 1 :List of UK Regional Geochemistry Atlases

Listed in year order.

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

INSTITUTE OF GEOLOGICAL SCIENCES. 1978. *Regional Geochemical Atlas: Orkney***.** (London: Institute of Geological Sciences).

INSTITUTE OF GEOLOGICAL SCIENCES. 1978. *Regional Geochemical Atlas: South Orkney and Caithness***.** (London: Institute of Geological Sciences).

INSTITUTE OF GEOLOGICAL SCIENCES. 1982. *Regional Geochemical Atlas: Sutherland***.** (London: Institute of Geological Sciences).

INSTITUTE OF GEOLOGICAL SCIENCES. 1983. *Regional Geochemical Atlas: The Hebrides***.** (London: Institute of Geological Sciences).

BRITISH GEOLOGICAL SURVEY. 1987. *Regional Geochemical Atlas: Great Glen***.** (Keyworth, Nottingham: British Geological Survey).

BRITISH GEOLOGICAL SURVEY. 1990. *Regional Geochemical Atlas: Argyll***.** (Keyworth, Nottingham: British Geological Survey).

BRITISH GEOLOGICAL SURVEY. 1991. *Regional geochemistry of the East Grampians area***.** Regional Geochemistry (Keyworth, Nottingham: British Geological Survey).

BRITISH GEOLOGICAL SURVEY. 1992. *Regional geochemistry of the Lake District and adjacent areas***.** Regional Geochemistry (Keyworth, Nottingham: British Geological Survey).

BRITISH GEOLOGICAL SURVEY. 1993. *Regional geochemistry of southern Scotland and part of Northern England***.** Regional Geochemistry (Keyworth, Nottingham: British Geological Survey).

BRITISH GEOLOGICAL SURVEY. 1996. *Regional geochemistry of north-east England***.** Regional geochemistry (Keyworth, Nottingham: British Geological Survey).

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

BRITISH GEOLOGICAL SURVEY. 2000. *Regional geochemistry of wales and part of west-central England: stream sediment and soil***.** (Keyworth, Nottingham: British Geological Survey).

Appendix 2 :Groundwater Baseline Reports

The following list is taken from the BGS intranet.

England and Wales

Abesser C, Shand P and Ingram J. 2005. Baseline report series: 18. The Millstone Grit of northern England. British Geological Survey Commissioned Report CR/05/015N.

Abesser C, Shand P and Ingram J. 2005. Baseline report series 22: The Carboniferous Limestone of northern England. British Geological Survey Commissioned Report CR/05/076N.

Abesser, C. and Smedley, P.L. 2008. Baseline groundwater chemistry: the Carboniferous Limestone aquifer of the Derbyshire Dome. BGS Open Report OR/08/028.

Ander E L, Shand P, Griffiths K J, Lawrence A R, Hart P and Pawley J. 2004. Baseline Report Series: 13. The Great Ouse Chalk Aquifer, East Anglia. British Geological Survey Commissioned Report CR/04/236N.

Ander E L, Shand P and Wood S. 2006. Baseline Report Series: 21. The Chalk and Crag of north Norfolk and the Waveney Catchment. British Geological Survey Commissioned Report CR/06/043N Brewerton, L J and Edmunds, W M. 1997. The Magnesian Limestone of Yorkshire and Northumbria. British Geological Survey, WD/97/58.

Cobbing J E, Moreau M, Shand P and Lancaster A. 2004. Baseline Report Series 14: The Corallian of Oxfordshire and Wiltshire. British Geological Survey Commissioned Report CR/04/262N.

Edmunds, W M and Brewerton, L J. 1997. The Chalk of the South Downs. British Geological Survey, WD/97/55 (Environment Agency Project Record W6/i7222/4/A).

Edmunds, W M and Brewerton, L J. 1997. The Chalk of Berkshire and the Chilterns. British Geological Survey, WD/97/57 (Environment Agency Project Record W6/i7222/6/A).

Edmunds, W M, Brewerton, L J, Shand, P and Smedley, P L. 1997. Part 1: A guide to the natural (baseline) quality study. British Geological Survey, WD/97/51.

Edmunds W M, Doherty P, Griffiths K J and Shand, P. 2002. Baseline Report Series: 4. The Chalk of Dorset. British Geological Survey Commissioned Report CR/02/268N.

Griffiths K J, Shand P and Ingram I. 2002. Baseline Reports Series: 2. The Permo-Triassic Sandstones of west Cheshire and the Wirral. British Geological Survey Commissioned Report CR/02/109N.

Griffiths K J, Shand P and Ingram J. 2003 Baseline Report Series: 8. The Permo-Triassic Sandstones of Manchester and east Cheshire. British Geological Survey Commissioned Report CR/03/265C.

Griffiths K J, Shand P and Ingram J. 2005. Baseline report series: 19. The Permo-Triassic Sandstones of Liverpool and Rufford. British Geological Survey Commissioned Report CR/05/131N.

Griffiths K J, Shand P and Marchant P. 2006. Baseline report series: 23. The Lincolnshire Limestone. British Geological Survey Commissioned Report CR/06/060N.

Griffiths K.J., Shand, P. and Marchant, P. 2006. The Lincolnshire Limestone. BGS Report CR/06/060N; Environment Agency Report NC/99/74/23.

Moreau M, Shand P, Wilton P, Brown S and Allen D. 2004. Baseline Report Series: 12. The Devonian aquifer of south Wales and Herefordshire. British Geological Survey Commissioned Report CR/04/185N.

Neumann I, Brown S, Smedley P L and Besien T. 2003. Baseline Report Series: 7. The Great and the Inferior Oolite of the Cotswold district. British Geological Survey Commissioned Report CR/03/202N.

Neumann I, Cobbing J E, Tooth A and Shand P. 2004. Baseline Report Series: 15. The Palaeogene of the Wessex Basin. British Geological Survey Commissioned Report CR/04/245N.

Shand, P and Brewerton, L J. 1997. The Culm of south west England. British Geological Survey, WD/97/53 (Environment Agency Project Record W6/i722/2/A).

Shand, P and Brewerton L J. 1997. The Triassic Sandstones of Cumbria. British Geological Survey, WD/97/54 (Environment Agency Project Record W6/i722/3/A).

Shand P, Tyler-Whittle R A, Morton M, Simpson E, Lawrence A R and Hargreaves R L. 2002. Baseline Report Series: 1. The Triassic Sandstones of the Vale of York. British Geological Survey Commissioned Report CR/02/102N.

Shand P, Tyler-Whittle R, Besien T, Lawrence A R and Lewis O H. 2003 Baseline Report Series: 6. The Chalk of the Colne and Lee river catchments. British Geological Survey Commissioned Report CR/03/069N.

Shand P, Cobbing J E, Tyler-Whittle R, Tooth, A and Lancaster A. 2003. Baseline Report Series: 9. The Lower Greensand of southern England. British Geological Survey Commissioned Report CR/03/273C.

Shand P, Ander E L, Griffiths K J, Doherty P and Lawrence A R. 2004. Baseline Report Series: 11. The Bridport Sands of Dorset and Somerset. British Geological Survey Commissioned Report CR/04/166N.

Shand P, Abesser C, Farr G, Wilton N, Lapworth D J, Gooddy D C, Haria A and Hargreaves R L. 2005. Baseline report series:17. The Ordovician and Silurian meta-sedimentary aquifers of central and south-west Wales. British Geological Survey Commissioned Report CR/05/034N.

Shand, P., Edmunds, W.M., Lawrence, A.R., Smedley, P.L. and Burke, S. 2007. The natural (baseline) quality of groundwater in England and Wales. BGS Report RR/07/06; Environment Agency Report NC/99/74/24.

Smedley P L and Allen D. 2004. Baseline Report Series: 16. The Granites of south-west England. British Geological Survey Commissioned Report CR/04/255N.

Smedley, P L, and Brewerton, L J. 1997. The Chalk of Lincolnshire. British Geological Survey, WD/97/56 (Environment Agency Project Record W6/i722/5/A).

Smedley, P L, and Brewerton, L J. 1998. The Triassic Sherwood Sandstone of the East Midlands and South Yorkshire. British Geological Survey, WD/97/52 (Environment Agency Project Record W6/i722/1/A).

Smedley P L, Griffiths K J and Tyler-Whittle R. 2003. Baseline Report Series: 5. The Chalk of north Downs, Kent and east Surrey. British Geological Survey Commissioned Report CR/03/033N.

Smedley P L, Neumann I and Farrell R. 2004. Baseline Report Series: 10. The Chalk aquifer of Yorkshire and North Humberside. British Geological Survey Commissioned Report CR/04/128N.

Smedley P L, Neumann I and Brown S. 2005. Baseline report series: 20. The Permo-Triassic Sandstones of Shropshire. British Geological Survey Commissioned Report CR/05/061N.

Tyler-Whittle R, Brown S and Shand P. 2002. Baseline Report Series: 3. The Permo-Triassic Sandstones of south Staffordshire and north Worcestershire. British Geological Survey Commissioned Report CR/02/119N.

Scotland

MacDonald A M and Ó Dochartaigh B É. 2005. Baseline Scotland: an overview of available groundwater chemistry data for Scotland. British Geological Survey Commissioned Report CR/05/239N.

Ó Dochartaigh, B. É., Smedley, P.,L. MacDonald, A. M. and Darling, W. G. (2004) Baseline Scotland: the Lower Devonian aquifer of Strathmore. Commissioned Report, CR/06/250N. British Geological Survey.

Northern Ireland

Griffiths K J, McConvey P and Shand P. 2006. Natural (baseline) variations in the groundwater quality of the Palaeogene Antrim Lava Group, Northern Ireland. British Geological Survey Commissioned Report CR/06/059C. This report is confidential so no pdf is available at present.

Some Groundwater reports –British

Edmunds, W M, Cook, J M, Kinniburgh, D G, Miles, D L, and Trafford, J M. 1989. Trace element occurrence in British groundwaters. British Geological Survey, Research Report SD/89/3.

Groundwater other reports – environment and health

BGS and DPHE 2001. Arsenic Contamination of Groundwater in Bangladesh. Eds: Kinniburgh, D G and Smedley, P L. British Geological Survey Technical Report, WC/00/19. Four Volumes. Graphosman, Dhaka.

DPHE/BGS/MML 1999. Groundwater studies for arsenic contamination in Bangladesh. Phase I: Rapid Investigation Phase. BGS/MML Technical Report to Department for International Development (UK), Six volumes.

Edmunds W M and Smedley P L 1995. Vulnerability of shallow groundwater quality due to natural geochemical environment. 1: Water, geochemistry and health - an overview. British Geological Survey Report WC/95/43, 37 pp.

Smedley P L, Edmunds W M, West J M, Gardner S J and Pelig-Ba K B. 1995. Vulnerability of shallow groundwater quality due to natural geochemical environment. 2: Health problems related to groundwater in the Obuasi and Bolgatanga areas, Ghana. British Geological Survey Report WC/95/43, 122 pp.

Smedley P L, Macdonald D M J, Nicolli H B, Barros A J, Tullio J O and Pearce J M 2000. Arsenic and other quality problems in groundwater from northern La Pampa Province, Argentina. BGS Technical Report WC/99/36, 176 pp.

Smedley P L, Nicolli H B, and Luo Z 2000. Arsenic in groundwaters from major aquifers: sources, effects and potential mitigation. BGS Technical Report WC/99/38, 42 pp.

Smedley, P.L., Nkotagu, H., Pelig-Ba, K., MacDonald, A.M., Tyler-Whittle, R., Whitehead, E.J. and Kinniburgh, D.G. 2002. Fluoride in groundwater from high-fluoride areas of Ghana and Tanzania. CR/02/316.

Appendix 3 : Reports and Publications containing information and data from BGS Organic Geochemistry

ACADEMIC PAPERS 2001-2008

2001

G.M.Williams, I.Harrison, D.J.Noy, O.Crowley & R.M.Kalin. (2001). The use of enantiomeric ratios to assess the fate of mecoprop in groundwater. Pesticide behaviour in soils and water. *British Crop Protection Council Symposium Proceedings,* No 78, 211 –216.

M.J.Spence, S.H.Bottrell, J.J.W.Higgo, I.Harrison & A.E. Fallick. (2001). Denitrification and phenol degradation in a contaminated aquifer. *Journal of Contaminant Hydrology*, **53** (3-4), 305-318.

I.Harrison, G.M.Williams, J.J.W.Higgo, R.U.Leader, A.W. Kim & D.J. Noy. (2001). Microcosm studies of microbial degradation in a coal tar distillate plume. *Journal of Contaminant Hydrology*, **53** (3-4), 319-340.

2002

Drage, T.C., Vane, C.H., Abbott, G.D. 2002. The closed system pyrolysis at 300°C of β-O-4 lignin substructure model compounds. Organic Geochemistry: 33, 1523-1531.

Vane, C.H. 2003. The molecular composition of lignin in spruce decayed by white-rot fungi (Phanerochaete chrysosporium and Trametes versicolor) using Pyrolysis–GC-MS and Thermochemolysis with Tetramethylammonium Hydroxide. International Biodeterioration and Biodegradation: 51, 1, 67-75.

G.M.Williams, I.Harrison, D.J.Noy, S.Dumpleton, C.A.Carlick, O.Crowley & R.M.Kalin. (2002). Natural attenuation of chiral mecoprop in a fractured limestone aquifer. *Geochimica et Cosmochimica Acta*, **66** (15A), A838-A838 Suppl.

G.M.Williams, I.Harrison, D.J.Noy, O.Crowley & R.M.Kalin. (2002). The use of enantiomeric ratios to identify natural attenuation of chiral mecoprop in the Lincolnshire Limestone. Published in *Groundwater Quality: Natural and Enhanced Restoration of Groundwater Pollution- ed. S.F.Thornton & S.E.Oswald* IAHS (International Association of Hydrological Sciences) Publication No. 275, pp.295-300.

D.C.Gooddy, P.J.Chilton & I.Harrison (2002). A field study to assess the degradation and transport of diuron and its metabolites in a calcareous soil. *Science of the Total Environment,* **297** (1-3), 67-83.

2003

Vane, C.H., Drage, T.C., Snape, C.E. 2003. Biodegradation of Oak (Quercus alba) wood during growth of the Shiitake Mushroom (Lentinula edodes): A Molecular Approach. Journal of Agriculture and Food Chemistry: 51, 4, 947-956.

Vane, C.H. 2003. Monitoring decay of black gum (Nyssa sylvatica) wood during growth the shiitake mushroom (Lentinula edodes) using DRIFT spectroscopy. Applied Spectroscopy: 57, 5, 514-517.

I.Harrison, G.M.Williams & C.A.Carlick (2003). Enantioselective biodegradation of mecoprop in aerobic and anaerobic microcosms. *Chemosphere,* 53 (5), 539-549.

G.M.Williams, I.Harrison, C.A.Carlick & O.Crowley (2003). Changes in enantiomeric fraction as evidence of natural attenuation of mecoprop in a limestone aquifer. *Journal of Contaminant Hydrology,* 64 (3-4), 253-267.

2004

Beramendi-Orosco, L.E., Castro-Diaz, M., Snape C.E., Vane C.H., Large, D.J. 2004. Application of catalytic hydropyrolysis for the rapid preparation of lignin concentrates from wood. Organic Geochemistry: 35, 61-72.

Meridith, W., Russell, C.A., Cooper, M., Snape, C.E., Love, G.D., Fabbri, D., Vane C.H. 2004. Trapping hydropyrolysates on silica and their subsequent thermal desorption to facilitate rapid fingerprinting by GC/MS. Organic Geochemistry: 35, 73-89.

2005

Vane, C.H., Drage, T.C., Snape, C.E. Stephenson. M.H. Foster C.B. 2005 Decay of cultivated apricot wood (Prunus armeniaca) by the ascomycete Hypocrea sulphurea using solid state ^{13}C NMR and Off-line TMAH thermochemolysis with GC-MS. International Biodeterioration and Biodegradation, 55, 175-185.

Stephenson, M. H., Leng, M. J., Vane, C.H., Osterloff P.L., Arrowsmith. C. 2005. Investigating Permian climate change from argillaceous sediments, Oman, Geological Society of London, 162, 1-11.

Vane C.H. and Trick J.K. 2005. Evidence of adipocere in a burial pit from the foot and mouth epidemic of 1967 using gas chromatography-mass spectrometry. Forensic Science International, 154,1, 19-23

Langston, W.J., Burt, G.R. Chesman, B.S, and Vane, C.H. 2005. Partitioning, bioavailability and effects of oestrogens and xen-oestrogens in the aquatic environment. Journal of the Marine Biological Association: 85, 1-30.

2006

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Beramendi-Orosco LE , Vane C.H, Cooper M, Sun CG, Large DJ, Snape CE. 2006. Evaluation of errors associated with □^{13}C analysis of lignin-derived TMAH thermochemolysis products by Gas Chromatography-Combustion-Isotope Ratio Mass Spectrometry. Journal of Analytical and Applied Pyrolysis, 76, 88-95.

Rawlins, B Simon, K., Hodgkinson, E.H., Riding, J., Vane,C.H., Poulton, C. Freeborough, K.. 2006. The potential and pitfalls of establishing the provenance of earth-related samples in forensic investigations. Journal of Forensic Science 51, 4, 832-845.

Stephenson, M.H., Leng, M.L. Michie, U and Vane, C.H. 2006. Palaeolimnology of Palaeozoic lakes, focussing on a single lake cycle in the Middle Devonian of the Orcadian Basin, Scotland. Earth Science Reviews, 75, 177-197.

2007

Vane, C.H., Harrison; I and Kim, A.W. 2007. Polycyclic aromatic hydrocarbons (PAHs) and polychlorinated biphenyls (PCBs) in sediments from the Mersey Estuary, U.K. Science of the Total Environment 374, 112-126.

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Gooddy D.G., Mathias S.A., Harrison I., Lapworth D.J. and Kim A.W. 2007. The significance of colloids in the transport of pesticides through chalk. *Science of the Total Environment*, 385, 1-3, 262-271.

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