

# Displaying G-BASE geochemical sample information in Google Earth

Land Use Planning and Development Programme Open Report OR/11/014



#### BRITISH GEOLOGICAL SURVEY

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# Displaying G-BASE geochemical sample information in Google Earth

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#### Keywords

G-BASE, soil, stream sediment, stream water, geochemistry, Google Earth.

#### Front cover

Example from computer screen showing Google Earth displaying sample sites and associated placemark label

#### Bibliographical reference

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Maps and diagrams in this book use topography based on Ordnance Survey mapping.

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# Summary

This report describes the Google Earth geochemical sample information delivery Project in which basic information about G-BASE geochemical samples is displayed in Google Earth. Information downloaded from the BGS corporate Geochemistry Database is converted into standardised data files, classified by country (England, Wales, Scotland and N. Ireland) and sample type (topsoil, deep soil, stream sediment and stream water). These files are then input into an application used to convert the data into Google Earth data files (KML format or KMZ for large files). The application to convert the information into KML files is written in the open source R script which is now widely use in geochemical applications. Some other similar data sets for the UK (*e.g.* from Tellus and FOREGS projects) have also been included in this work to demonstrate the applicability of the R script programs to other non G-BASE data sets.

A number of interpolated geochemical images generated from G-BASE data have also been included as a way of demonstrating how the G-BASE geochemical baseline information can be displayed in Google Earth. The KML files for creating and displaying the interpolated images are also generated using R script though further development work is required on the code used to generate the gridded images.

The KML/KMZ files are accessed through web pages, the initial landing page being a map of the UK from which the user selects the country of interest. This leads to country pages on which tables of available data sets (and interpolated images for England stream sediments) are linked to the KML/KMZ files. Clicking on the hyperlink starts up Google Earth, adding to the "Temporary Places" directory and displaying the location of sampling sites against an appropriately zoomed and centred satellite image. Placemark labels at each site show the information available for the associated sample along with hyperlinks to further information. Comprehensive documentation about G-BASE and other sample types is available from information links on the web pages.

The Google Earth is easy to use, available worldwide, and is increasingly being used to display spatial information about environmental data. Displaying information about the BGS G-BASE geochemical data holdings in Google Earth will make the data more accessible to the general public. It is also hoped that this may serve as an example project for how NERC can disseminate information on its environmental data holdings. Furthermore, many countries have similar geochemical data, for example that collected during the FOREGS and GEMAS projects in Europe. If they can be encouraged to generate KML files of their geochemical data holding from the freely available R scripts generated by this project, then a more global landing page to geochemical data information can be created.

# 1 Introduction

This report describes the British Geological Survey's (BGS) Google Earth Geochemical Information Delivery Project (project code NEE4082). This 2010-11 pilot project was funded from the BGS "opportunities fund" (see Appendix 1), a relatively small budget used to develop ideas that will delivery the BGS strategy (British Geological Survey, 2009). The project delivers all six of BGS strategic challenges and, by making BGS geochemical data more publicly available and readily accessible to a much wider audience than just geochemists, it specifically delivers on Challenges 1 and 2:

**Challenge 1**: Acquire, interpret and enhance the UK geoscience knowledge base and make it accessible and interoperable.

**Challenge 2**: Improve the communication of geoscience knowledge so that it can better support policy and decision-making by government and society.

The G-BASE (Geochemical Baseline Survey of the Environment) Project sample locations, with a limited amount of other information, have been available for more than five years on the internet through the BGS GeoIndex application<sup>1</sup>. However, this system is not intuitive to use, and for the non-geochemist looking for chemical information for the surface environment the language used (*e.g.* words like, geochemistry, baseline, G-BASE) does not make the information easy to discover or understand. Google Earth<sup>2</sup> is now widely used to display environmental data and information. It is a freely available and popular internet application used across a great variety of platforms and devices, including mobile phones. It is easy to use and data can be added to maps of the Earth's surface for the entire globe using KML or KMZ files. Keyhole Markup Language (KML) is a computer language scheme for expressing geospatial information in internet-based 2-D and 3-D Earth browsers. It was developed for use with Google Earth. KML files can be distributed/loaded on the internet as KMZ files – these are compressed (zipped) files with a .kmz extension.

The objective of this project is to generate KML files, using R scripts that show the location of sample sites with a certain amount of information attached to the placemark label.  $R^3$  is a language and environment for statistical computing and graphics increasingly being used to interpret and graphically present geochemical data (*e.g.* Reimann et al., 2008). Scripts for creating KML files are freely available and have been used as a basis for this project (see Section 3). The creation of a fairly elaborate KML file for display in Google Earth from a simple standardised data file using R scripts is central to this project (see Figure 1). By utilising a standard file format for the input data, the R scripts are freely available for any organisation and can be used to create and display their geochemical information in Google Earth in a similar manner.

A further objective of this pilot project was to demonstrate how interpolated geochemical images can be created using R scripts and the images can also be imported into Google Earth as KML files. Seven interpolated images have been created for stream sediments from England for a selected number of elements (As, Ca, Cr, Cu, Ni, Pb and Sr).

<sup>&</sup>lt;sup>1</sup> <u>http://www.bgs.ac.uk/GeoIndex/</u>

<sup>&</sup>lt;sup>2</sup> <u>http://www.google.co.uk/intl/en\_uk/earth/index.html</u>

<sup>&</sup>lt;sup>3</sup> <u>http://www.r-project.org/</u>



Figure 1: Work flow from the BGS Geochemistry Database through to Google Earth using R scripts to generate KML files

# 2 Geochemical sample information files format

All BGS geochemical data for the UK land surface is stored in an Oracle corporate database known as the Geochemistry Database (Coats and Harris, 1995). This database at the time of writing contains some 585,000 samples (rock, soil, sediment, water, mine waste *etc.*) and over 10 million analyte determinations. Retrieving geochemical data from the database can be a complex procedure requiring a good knowledge of the database dictionary codes and an understanding of the history of the data held therein.

For this pilot project a selected number of sample types (topsoil, deep soil, stream sediment and stream water) were selected for sites sampled by the G-BASE project. Other sample types are available, collected by a variety of projects, but the G-BASE samples are considered to be most relevant for environmental applications and represent the largest part of the Geochemistry Database. Summary information about these G-BASE samples is in Appendix 2.

During this pilot project, KML files for the Northern Ireland Tellus and the FOREGS project data have also been created. This was done to demonstrate the applicability of the R scripts to be used with non-G-BASE data. Tellus and FOREGS data is not stored in the Geochemistry Database and the sample information files are easily created from documentation associated with these projects.

# 2.1 DATA DOWNLOADED FROM THE BGS GEOCHEMISTRY DATABASE

For the G-BASE data sample site information was generated based on fields from the Geochemistry Database:

PROJECT CODE SAMPLE NUMBER SAMPLE TYPE EASTING NORTHING DATE OF SAMPLING ANALYTES DETERMINED OTHER DETERMINANDS FRACTION

The Geochemistry Database data was received as txt files from Alan Mackenzie, the Geochemistry Database Manager (gbase\_a\_kwa.txt, gbase\_c\_kwa.txt, gbase\_w\_kwa.txt and gbase\_S\_soils\_with\_fraction.txt). This data was imported into EXCEL 2007 files (note that earlier versions of EXCEL cannot cope with more than 65,536 rows of data), and modified as described in the following subsections. The modified files were imported into ArcGISv9.2 and partitioned into the different countries (England – ENG, Wales – WAL, Northern Ireland - NIR and Scotland – SCO).

# 2.1.1 Project Code, Sample Number and Sample type

These are three separate fields assigned to every geochemical sample in the Geochemistry Database and for the purpose of this project are concatenated to give a unique **sample\_id**. Sample type codes used in G-BASE are S (deep soil), A (topsoil), C (stream sediment) and W (stream water).



**Figure 2: Example of Google Earth placemark label used to describe corresponding sample site.** The Sample ID, Date Collected, Water Filter, Analytes Determined and Other Determinand sections come from the data rows of the standard data input csv file. Other information is based on the header rows from the input data file. The different analytical methods used for the analytes are indicated by a single character symbol suffix (see Table 1).

# 2.1.2 Easting and Northing

The BGS Geochemistry Database stores spatial coordinate data as Easting and Northing for the British National Grid, down to a 1m resolution. Google Earth requires the spatial coordinates to be in longitude and latitude. However, as long as the grid coordinate system is known and necessary parameters that define it are identified, R scripts can be used to convert the  $\mathbf{x}$  and  $\mathbf{y}$  coordinates to longitude and latitude. The FOREGS site data coordinates are already in latitude and longitude and the Tellus sites use the Irish National Grid. The R script program has been written to use different input coordinate systems by identifying from the input data file the project used to generate the data set.

A statement about the derivation of the grid coordinates and their spatial resolution is important and included prominently on the landing page. This states that "Locational data are based on British National Grid coordinates (Irish Grid in N Ireland) converted to longitude and latitude and derived either from Ordnance Survey maps or, since 2003, using GPS. Possible error in spatial locations is estimated at  $\pm 100$  m".

# 2.1.3 Date of sampling

The date the sample was collected (**Date** field) is an important piece of sample information so any results associated with it can be put into a time-line context. However, only since the Humber-Trent area G-BASE sampling has the field data been routinely entered into the Geochemistry Database though a record of the date of sampling is available on the hardcopy field form. Earlier G-BASE samples need to have the Date\_collected field attributed even though this might be a year rather than identifying the precise day. For the non-G-BASE data sets this has been entered only to the resolution of year.

# 2.1.4 Analytes determined

The **Analytes** field is a list of all the chemical elements determined on a particular sample. There are instances where the same sample has had the same element determined but by a different analytical method. A "default" method of analysis is determined for each data subset and this is stated on the placemark label - this would be the method by which the majority of samples have been analysed. Elements determined by the default method are just listed as the chemical symbol (*e.g.* Ag, Cu, Pb, ...). Those determined by methods otherwise or in addition to the default will have a single character suffix the chemical symbol (*e.g.* Ag, Ag\*, Cu, Cu~, Pb, Pb\*...). Table 1 lists the single character code translations used in the Google Earth labels with an explanation of the abbreviation based on the BGS Geochemistry Database "Analysis Method" domain table. An explanation of the analytical method abbreviations used on the placemark labels is also given on the web landing page in the list of further information describing the placemark label (see also Figure 2).

| BGS Database<br>Method Code | Explanation  |             |
|-----------------------------|--|-------------|
| AAS                         | Atomic Absorption Spectrometry                           | =           |
| COL                         | Colorimetric method                                      |             |
| DNA                         | Delayed Neutron Activation                               | +           |
| FICPMS                      | Fire Assay Inductively Coupled Plasma Mass Spectrometry  | %           |
| HYICP                       | Hydride Generation Inductively Coupled Plasma            | \$          |
| IC                          | Ion Chromotography                                       | 2           |
| ICP-AES                     | Inductively Coupled Plasma Atomic Emmission Spectrometry | *           |
| ICP-MS                      | Inductively Coupled Plasma Mass Spectrometry             | @           |
| ISE                         | Ion Selective electrode                                  | ۸           |
| LIFS                        | Laser Induced Fluorescence Spectrometry                  | u           |
| OES and DCOES               | Optical Emission Spectrophotometry                       | #           |
| XRFS                        | X-ray Fluorescence Spectrometry                          | <nul></nul> |
| <foregs data=""></foregs>   | Hg Analyser  |             |

# Table 1: Suffix codes added to the chemical symbol in the Google Earth used to give information about the analytical method

# 2.1.5 Other determinands

For the soil samples, where available, the results for LOI and pH determinations are added to the Google Earth placemark label. This information is extracted from various locations in the Geochemistry Database, originally stored in the overburdens data table but now for more recent samples stored in analyte\_determinations. Similarly, for pH, conductivity and bicarbonate in stream waters, this information is included where available (but only extracted from the analyte\_determinations data table). The data is downloaded from the Database as a numeric field for each determinand. This data is concatenated into a single text field (**Other**) for the R scripts input data file. This is done in Excel using the following formulae with careful attention to the number of decimal places used (pH value being in cell I6 and LOI in cell J6):

="pH="&TEXT(I6, "0.0")&" LOI="& TEXT(J6, "0.0")&"%"

# 2.1.6 Fraction

The fraction field contains the information regarding the fraction size used for the soil and sediment analysis. The same field is populated for waters to give the filter size used prior to

analyses of the elements (0.45  $\mu$ m). The fraction size for stream sediments has remained constant (<150 microns). All G-BASE topsoils are sieved to <2 mm but the deep soils have been sieved to either <2 mm or <150  $\mu$ m). The <150  $\mu$ m information was originally missing from the Geochemistry Database but has now been added, though this information is still missing for some of the earlier G-BASE soils collected. Information about G-BASE soil fractions is also provided as a pdf on the landing page under the list of further information.

# 2.2 STANDARD DATA FORMAT FOR FILES TO BE USED WITH THE R SCRIPTS

The data partitioned into different country files has been saved as comma separated variable (csv) files for use with the R scripts used to turn the data into a KML file. Such files are help to remove any font or style inconsistencies that may be associated with other file types and there is no limit on the number of records that can be held. The only identified problem with this format has been the use of " $\mu$ " which does not appear correctly in the csv files - the word microns has been used instead. It is important that the standard format is used as the successful running of the R script depends on a consistent and precise layout to the data to be input. Part of an example standard input file is shown below. Including field names, there are five rows of header information at the start of each data file before the data starts. The csv file is defined as having seven fields on each row so the first four rows, in which only the first field is used, should terminate with six commas.

ROW 1: G-BASE England topsoil samples,,,,,,

**ROW 2:** "All element analyses done by XRFS.",,,,,,

ROW 3: Loss-on-ignition (LOI) determined at 450degC over 24 hrs.,,,,,

**ROW 4:** Results available under licence contact enquiries@bgs.ac.uk. For more information about G-BASE see http://www.bgs.ac.uk/gbase/,,,,,,

**ROW 5:** Sample\_id,x,y,Date,Analytes,Other,Fraction

**ROW 6:** 50 380A,215100,92670,10/09/2002,"Ag,Al,As,Ba,Bi,Br,Ca,Cd,Ce,Co,Cr,Cs,Cu,Fe,Ga,Ge,Hf,I,K,La,Mg,Mn,Mo, Na,Nb,Nd,Ni,P,Pb,Rb,Sb,Sc,Se,Si,Sm,Sn,Sr,Ta,Te,Th,Ti,Tl,U,V,W,Y,Zn,Zr",LOI=9.08%,<2 mm

**ROW 7:** 50 449A,215170,86350,11/09/2002,"Ag,Al,As,Ba,Bi,Br,Ca,Cd,Ce,Co,Cr,Cs,Cu,Fe,Ga,Ge,Hf,I,K,La,Mg,Mn,Mo, Na,Nb,Nd,Ni,P,Pb,Rb,Sb,Sc,Se,Si,Sm,Sn,Sr,Ta,Te,Th,Ti,Tl,U,V,W,Y,Zn,Zr",LOI=10.48%,<2 mm

The sample\_id and x and y fields will always contain data. Other fields may be empty.

# 2.2.1 Row 1

This row contains a single text field that is used by the R script to set many of the parameters in the program. It is very important that a strict sequence of words is followed, each word separated by a single space. This text, which identifies the data set, is also included under the "Data Series" caption on the top of the placemark label (see Figure 2, "Data Series" label).

The **first word** of the text string should be the name of the project that has generated the data (*e.g.* G-BASE, TELLUS or FOREGS). In the R script the "Project" variable is used to identify the logo for the placemark label and calculates the required start-up zoom in Google Earth. For example, G-BASE is a high density sampling project so sites will initially be displayed at a larger scale than say the low-density FOREGS mapping.

The **second word** of the text string should be the name of the country the data series is from. The "Country" variable can be used by the R script to calculate where to open and centre the start up map in Google Earth. For England, Scotland, Wales and England these are: BGS Keyworth, BGS Edinburgh, BGS Cardiff and GSNI Belfast, respectively.

The **third word** of the text string is used by the R script to identify the sample type ("Samptype" variable in the R script) based on four words – topsoil, deep, stream or water representing: topsoil, deep soil, stream sediment or water. This variable selects the colour of the Google Earth placemark to be used in the KML file (Table 2). "Samptype" also determines whether to use the caption "Water Filter:" or "Fraction Analysed:" on the placemark label.

| Sample             | G-BASE<br>Code | Google Earth<br>placemark<br>colour | Hyperlink   |
|--------------------|----------------|-------------------------------------|---|
| Stream<br>water    | W              | Light blue                          | http://maps.google.com/mapfiles/kml/paddle/ltblu-circle.png |
| Stream<br>sediment | С              | Blue                                | http://maps.google.com/mapfiles/kml/paddle/blu-circle.png   |
| Topsoil            | А              | Red                                 | http://maps.google.com/mapfiles/kml/paddle/red-circle.png   |
| Deep soil          | S              | Yellow                              | http://maps.google.com/mapfiles/kml/paddle/ylw-circle.png   |

### Table 2 : Translations used from sample type code to Google Earth placemark colour

### 2.2.2 Row 2

This contains information about the analytical method used for the elements listed on the placemark label, usually declaring a default method of analysis plus additional methods used. The single character codes used to identify the methods are described in Table 1. An explanation of the analytical method abbreviations used on the placemark labels is also given under further information on the landing page in which the layout of the placemark label is described.

This header row, potentially containing a variety of symbols, has the potential to be quite problematic when being input into the R scripts. Certain symbols will cause the program to misinterpret the data input stream. For this reason this text string is enclosed within inverted quotes (*i.e.* ".....",,,,).

# 2.2.3 Row 3

This contains information about the other determinands data field, generally pH and loss on ignition for soils and pH, conductivity and bicarbonate for waters. It is a string field concatenated from numeric fields (see above).

# 2.2.4 Row 4

The final row of header text is used at the bottom of the placemark label to provide further information about the data series. This could contains one or more hyperlinks.

# 2.2.5 Row 5

This row contains the data field names, *i.e.* Sample\_id, x, y, Date, Analytes, Other, Fraction

# 2.2.6 Rows 6 to end

Rows 6 to the end contain all the data needed to populate the rest of the placemark label. The sample\_id is used as the title for the placemark label. The grid coordinates are in the x and y fields. For the G-BASE samples these are the British National Grid coordinates. Other data set

may use a different coordinate system (Tellus uses Irish National Grid and FOREGS longitude and latitude). The date is the date of sample collection the resolution of which may vary from day to year of sampling.

| File                     | G-BASE          | FOREGS | Tellus |
|--------------------------|-----------------|--------|--------|
| ENG_G-BASE_Water.csv     | 27,142          |        |        |
| ENG_G-BASE_Topsoil.csv   | 28,761          |        |        |
| ENG_G-BASE_Deepsoil.csv  | 25,894          |        |        |
| ENG_G-BASE_Sediment.csv  | 33,138          |        |        |
|                          |                 |        |        |
| SCO_ G-BASE_Water.csv    | 43 <i>,</i> 855 |        |        |
| SCO_ G-BASE_Topsoil.csv  | 1,622           |        |        |
| SCO_ G-BASE_Deepsoil.csv | 1,608           |        |        |
| SCO_ G-BASE_Sediment.csv | 51,238          |        |        |
|                          |                 |        |        |
| WAL_ G-BASE_Water.csv    | 9,985           |        |        |
| WAL_ G-BASE_Topsoil.csv  | 889             |        |        |
| WAL_G-BASE_Deepsoil.csv  | 1,138           |        |        |
| WAL_G-BASE_Sediment.csv  | 13,735          |        |        |
|                          |                 |        |        |
| ENG_FOREGS_Water.csv     |                 | 33     |        |
| ENG_FOREGS_Topsoil.csv   |                 | 33     |        |
| ENG_FOREGS_Deepsoil.csv  |                 | 33     |        |
| ENG_FOREGS_Sediment.csv  |                 | 33     |        |
|                          |                 |        |        |
| SCO_FOREGS_Water.csv     |                 | 18     |        |
| SCO_FOREGS_Topsoil.csv   |                 | 18     |        |
| SCO_FOREGS_Deepsoil.csv  |                 | 18     |        |
| SCO_FOREGS_Sediment.csv  |                 | 18     |        |
|                          |                 |        |        |
| WAL_FOREGS_Water.csv     |                 | 5      |        |
| WAL_FOREGS_Topsoil.csv   |                 | 5      |        |
| WAL_FOREGS_Deepsoil.csv  |                 | 5      |        |
| WAL_FOREGS_Sediment.csv  |                 | 5      |        |
|                          |                 |        |        |
| NIR_FOREGS_Water.csv     |                 | 4      |        |
| NIR_FOREGS_Topsoil.csv   |                 | 4      |        |
| NIR_FOREGS_Deepsoil.csv  |                 | 4      |        |
| NIR_FOREGS_Sediment.csv  |                 | 4      |        |
|                          |                 |        |        |
| NIR_TELLUS_Water.csv     |                 |        | 5,892  |

The number of data rows for each data set is shown in Table 3.

### Table 3 : Number of data records in each standardised format csv file

# 3 R scripts for writing Google Earth (KML) files

# 3.1 SAMPLE SITE INFORMATION

The R scripts used for creating the KML files have been written by Mark Cave (BGS) based on ideas from Hengl (2009). Additional KML code to "hardwire" into the R script has been provided by Ailsa Napier (BGS). Chris Johnson adapted the R scripts written by Mark Cave so that different country data sets, from different projects and covering different sample types could be created from a single script without the need of any editing. The geographical reference system data needed to convert grid coordinates to longitude and latitude comes from the European Petroleum Survey Group (EPSG) Geodetic Parameter Dataset which is available from <u>http://www.epsg.org/CurrentDB.html</u>. An updated copy of this is embedded in the R package "rgdal".

The R script was written using R version 2.12.2 and required the following libraries to be installed: rgdal, gstat, lattice, and maptools. The code (Standard\_csv2kml\_v1\_1.R) used to produce the first version of all the KML files is listed in Appendix 3. The flow of the program is summarised in Figure 3.



Figure 3: Flow of the R program to convert the standard csv data file into a Google Earth KML file

A listing of an example of the Google Earth file generated is given in Appendix 4. An example of the Google Earth view of the KML file with a label displayed is given in Figure 4.



Figure 4: Example of the Google Earth view of the KML file with a label displayed

# 3.2 INTERPOLATED GEOCHEMICAL IMAGES

The R code used to generate the interpolated geochemical images is given in Appendix 3 and an example of an in image displayed in Google Earth is shown in Figure 5a.

The R script for this project has been written by Mark Cave based on ideas from Hengl (2009) and uses the following libraries: geoR; gstat; sp; rgdal; gpclib; and maptools. It should be noted that the geometry computations in maptools depend on the package gpclib, which has a restricted licence. It is disabled by default; to enable gpclib, when it is run for the first time in an R session, type gpclibPermit().

Prior to generating the gridded images, a csv file was created for each element (As, Ca, Cr, Cu, Ni, Pb and Sr) for the stream sediment results from England. The results file used is the same as that used by Andreas Scheib the generate the UK geochemical images from stream sediments currently available on the G-BASE web pages<sup>4</sup> so a direct comparison could be made with some of the geochemical images generated by a different software application. Although the Tamar results from the SW England were included in the stream sediment element results files, when it came to the gridding process Tamar was excluded because having two unconnected areas to grid causes many additional and difficult challenges for the gridding program.

<sup>&</sup>lt;sup>4</sup> <u>http://www.bgs.ac.uk/gbase/regional.html</u>

The format for each single element csv files is a header row with the field names "PROJECT"; "SITENO", "EASTING"; "NORTHING"; "METHOD"; "ATLAS"; "Calcium". Subsequent rows contained the data though for this gridding application only the x/y coordinates in British National Grid Format (i.e. columns 3 & 4) and the element concentrations (i.e. column 7) is used.

The flow of the R code used (see Appendix 3 for listing) was:

- 1. The element data file is read
- 2. A polygon outlining the extent of the stream sediments is read. For England a polygon had to be created of the land area sampled so far.
- 3. Create a grid of 5000 m spacing based on the limits of the outlining data polygon.
- 4. A spatial data frame is created within a polygon defining the sampled area (in latitude and longitude coordinates).
- 5. Element results are prepared for gridding any results above the 99 percentile are reset to the 99 percentile to avoid the stretching of classes to a very high value (for some elements the 98 percentile was used).
- 6. IDW extrapolation of the sample points is done (with latitude/longitude conversion of British National Grid coordinates) with the maximum number of points used in the gridding set to the five nearest neighbours.
- 7. The image file as created as a "png" format file and the image coloured according to standard parameters/colour scheme (dark blue (low) to yellow (high)).
- 8. A KML file is written to overlay the generated image file in Google Earth.

The R codes for the gridding of the G-BASE results was a more challenging task than writing the scripts to create the KML files described earlier. By the end of the project gridded images, such as that shown in Figure 5a, could be generated and overlain in Google Earth. However, it is felt that there are still improvements that need to be made:

- The time taken to grid the large G-BASE data files was excessively long. The England stream sediment data (with approximately 37,000 records) took nearly 4 hours to grid. This time needs to be reduced.
- Currently the user has far less control over the gridding parameters and classification colouring than one has when using a GIS gridding application (e.g. the tools available in ArcGIS). More experimenting needs to be done with the options available via the gridding (idw) and image classification (image) functions in the R script.
- No key is generated with the current R script, the current legend just indicating the high to low colours has been added using an image editing program. The script for a key should be written so there is an option of a key in with the KML file overlay.

There was insufficient time available in this pilot project to address the above issues but the project succeeded in generating seven gridded element images for the stream sediment results from England. These could be compared with images generated from the same results by ArcGIS (compare Figures 5a and 5b). The broad regional trends were the same in images generated by the two different applications though currently the classification of results and colouring scheme is more satisfactory in the ArcGIS images.



Figure 5: (a) Example of an interpolated geochemical image (Cu in stream sediments from England) generated by R scripts (5 km cell, IDW). (b) The same results from part of the UK Cu in stream sediments map currently displayed on the internet (generated in ArcGISv9.2, 500m cell, IDW, 1.5 km search radius).

# 4 Google Earth (KML) files

The Google Earth (KML) files are generated entirely by the R script described in Section 3. The files begin with the standard KML code required by Google Earth. The main bulk of the code is taken up by the label and locational data associated with each sample placemark. The balloon label is defined at the start of the code and this gives much greater flexibility in displaying the information on the placemark label. The KML code at the first <LookAt> statement centres the Google Earth view on the BGS office appropriate for the country of the data set and with a zoom (*i.e.* appropriate <a href="https://www.auteuc.com">auteuc.com</a> stateuc.

As a further means of promoting the data sets and contact information, KML code for a placemark and associated label for the appropriate BGS office has been pasted into the start of the KML files (see Table 4) before the first sample site placemark.

```
<Placemark>
          <name>BGS Cardiff</name>
          <LookAt>
                <longitude>-3.241</longitude>
                <latitude>51.5295</latitude>
                <altitude>1500</altitude>
                <heading>-0.003904228203065869</heading>
                <tilt>0</tilt>
                <range>2503.068812447143</range>
                <altitudeMode>relativeToGround</altitudeMode>
                <gx:altitudeMode>relativeToSeaFloor</gx:altitudeMode>
          </LookAt>
          <styleUrl>#office</styleUrl>
          <ExtendedData>
                <Data name="office_name">
                     <value>British Geological Survey,</value>
                </Data>
                <Data name="office_description">
                     <value>Cardiff Office</value>
                </Data>
                <Data name="office_image">
                     <value>cardiff_thumb.jpg</value>
                </Data>
          </ExtendedData>
          <Point>
                <coordinates>-3.241,51.5295,0</coordinates>
          </Point>
     </Placemark>
```

Table 4: Example of the KML code used for the BGS Cardiff office placemark and label

# 5 Web pages

Web pages, including a landing page (see Figure 6), have been written for the project using the BGS website template and these have initially been placed on the BGS internet development server: <u>http://kwntsicms:81/research/geochemB/home.html</u>.

From the landing page the user is then directed to a web page that contains a table listing the available data sets for the selected country (country data set page). The sample types are listed in columns and the user by clicking on the required data set will start up Google Earth with the samples displayed by standard Google Earth placemarks coloured as described in Table 2. The user can return to the web browser to load further KML/KMZ files. Left-clicking on the hyperlink starts up Google Earth (*i.e.* runs the Google Earth application). Right-clicking on the KML/KMZ file hyperlink enables the user to save the file for use independent of the web browser.

For the UK there are four country data set pages – England, Scotland, N. Ireland and Wales. These are shown in Figure 7. From these pages the user can also select to view information about the data set, the sample information web pages illustrated in Appendix 2. For the pilot project, a selected number of elements for the G-BASE stream sediments have been presented as interpolated geochemical images which can be accessed from the England data set pages via a further web page which lists the KML images available.

There are more data sets listed on the country data set pages than are available as KML files. This includes the EuroGeoSurvey's GEMAS samples, the National Soil Inventory (NSI) samples (recently reanalysed by BGS), TELLUS project samples from N. Ireland and the Wolfson stream sediment samples (Imperial College, London). These data set are beyond the remit of this pilot project but information files have been included should extra time be available to prepare this data for the final internet implementation. These data sets would also require some external permissions to be granted in order to use them in this manner.

At the bottom of the landing page (Figure 6) are additional links to further useful information. This further information is included in Appendix 2.

#### Location index for chemical data in environmental samples

This is an index that displays the location in Google Earth of information on the chemistry of surface environmental samples (soil, stream water and stream sediment). Locations of samples are classified by the four nations of the UK. The results are from British Geological Survey and associated projects.

**Note.** Locational data are based on British National Grid coordinates (Irish Grid in N Ireland) converted to longitude and latitude and derived either from Ordnance Survey maps or, since 2003, using GPS. Possible error in spatial locations are estimated at ±100 m.

#### United Kindgom Country Index Map

Select Country for required sample locations



You will need Google Earth on your computer to use this application. Download Google earth

#### **Additional Information**

Example of Google Earth placemarker label with explanation of content Further information about G-BASE soil sample fraction sizes

**Figure 6: Landing page for the Google Earth sample information.** Users select the country where they want to find environmental sample information.

| England   |                 |              | Scotland  |                 |              |
|---|-----------------|--------------|---|-----------------|--------------|
| SOIL  | STREAM SEDIMENT | STREAM WATER | SOIL  | STREAM SEDIMENT | STREAM WATER |
| G-BASE topsoil<br>G-BASE deep soil<br>G-BASE deep soil<br>NSI<br>FOREGS topsoil<br>FOREGS deep soil<br>GEMAS<br>Comparison of the solution of the sol | G-BASE          | G-BASE       | G-BASE topsoil<br>G-BASE deep soil<br>FOREGS topsoil<br>FOREGS deep soil<br>GEMAS           | G-BASE          | G-BASE       |
| Wales   | 1               |              | Northern Ireland  |                 |              |
| SOIL  | STREAM SEDIMENT | STREAM WATER | SOIL  | STREAM SEDIMENT | STREAM WATER |
| SOIL<br><u>G-BASE top soil</u><br><u>G-BASE deep soil</u><br><u>O</u><br>NSI<br><u>FOREGS top soil</u><br><u>O</u><br><u>FOREGS deep soil</u>   | STREAM SEDIMENT | STREAM WATER | SOIL<br>Tellus top soil<br>Tellus deep soil<br>FOREGS top soil<br>FOREGS deep soil<br>GEMAS | STREAM SEDIMENT | STREAM WATER |

Figure 7: The four country data set tables (copied from the respective country home pages). Entries with hyperlinks load kml files of sample site information in Google Earth. "i" links to information pages and "M" links to interpolated maps.

# 6 Future developments

- 1. The Google Earth geochemical information delivery project needs to be moved from the internet development server so it is available externally on the internet. The position of links to the project landing page need to be determined and the success of the finding the pages in an internet search need to be maximised with appropriate tags to the landing page.
- 2. Additional KML files can be easily added to expand beyond the FOREGS and G-BASE data sets currently available. The main delay in implementing this will be getting external permissions to use the sample information from these data sets in this way.
- 3. This project has generated new information about the BGS soil sample holdings and these web pages should be linked into the NERC soils portal.
- 4. This work on the presenting an index for chemical data available on surface environment samples should be flagged up in future NERC national capability work on the knowledge exchange of environmental information.
- 5. The R scripts for generating the KML files should be made readily available to anyone who wishes to use them, something that can be achieved through having this report widely available through NORA. If other countries around the world can be encouraged to display their sample information in a similar manner then a more continental or global landing page can be created. The EuroGeoSurveys Expert Geochemistry Group, for example, could be encouraged to display all the FOREGS and GEMAS data in this manner.
- 6. The Google Earth label currently only gives data for field derived parameters such as water pH, conductivity and alkalinity or soil pH and LOI. This application could readily be adapted to display all the geochemical results should BGS policy change to make all the baseline geochemical data freely available.
- 7. The project has demonstrated that the gridded interpolated geochemical images can be generated using freely available R scripts and overlain in Google Earth. However, the functionality of the R scripts as used here is not yet as good as that found in ArcGIS and more development work on the gridding script is needed.

# References

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

BRITISH GEOLOGICAL SURVEY. 2009. British Geological Survey Strategy 2009-2014. Applied geoscience for our changing Earth. (Nottingham: British Geological Survey).

COATS, J.S. AND HARRIS, J.R. 1995. Database design in geochemistry: BGS experience. *In*: Giles, J.R.A. (ed.) *Geological Data Management*. Special Publication. Geological Society, London, 25 – 32.

HENGL, T. 2009. A Practical Guide to Geostatistical Mapping. November 2009. ISBN: 978-90-9024981-0 http://www.lulu.com/product/file-download/a-practical-guide-to-geostatistical-mapping/14938111

REIMANN, C., FILZMOSER, P., GARRETT, R.G. AND DUTTER, R. 2008. Statistical Data Analysis Explained. Applied Environmental Statistics with R. John Wiley & Sons Ltd., Chichester, England.

# Appendix 1 :Bid document for opportunities funding

# APPLICATION FOR SUPPORT FROM THE BGS OPPORTUNITIES FUND

Proposer name:Dr C C JOHNSONScience/Information team:Geochemistry Baselines and Medical Geology/Websystems

# **Description of proposed activity (200 words max):**

This project will deliver the sites of BGS geochemical baseline samples along with their metadata and a selected number of gridded geochemical images viewable in Google Earth. A standardised metadata file will be converted to Google Earth (kml) files using standard R scripts and these files will be made available through the BGS OpenGeoscience initiative. The objective is to make information about the geochemical data BGS holds more accessible to those that wish to use it and is a response to user consultation. It is a cross cutting project between the information and science directorates and will help to broaden the scope of the OpenGeoscience using data that of great environmental relevance. It builds on the existing GeoIndex system to give access to the geochemical data holdings in a more universally accessible manner with more information that in the future could be put into the context of other European and global geochemical baseline data and information. This could be the template for the dissemination of global geochemical baseline data and so maintain BGS's leading innovative role in this area of science and add to our competitive edge in international mapping projects.

### **Business case (200 words max):**

Nationally and globally there is a need for chemical data from the surface environment covering a wide range of applications that seek to tackle big challenges of our time (examples -sustainable natural resources; informed contribution to environmental legislation; efficient agricultural delivering nutritious crops with minimal fertiliser input; improving the quality of life and health in urban areas). The project delivers all six of BGS strategic challenges most notably challenges 1 and 2.

BGS holds a substantial resource of geochemical samples and data, which has cost many millions of pounds to create, and this needs to be exploited to realise its true value and deliver more collaborative science and commercial projects. To-date the effort and expense in collecting the geochemical data over 40 years not been matched by any substantial drive to exploit the samples and data - this project, representing a very small fraction of the sampling and analytical costs, will help to redress this fact.

The project will make use of experienced staff resources that will be available in the second half of fy 2010-11.

**Objectives in current FY (two bullet points, max 15 words each)** 

- Create R scripts to convert standardised spatially referenced sample information to a kml file
- Create R scripts to deliver gridded geochemical images of G-BASE data in Google Earth

Deliverables in current FY (two bullet points, max 15 words each)

- Metadata for G-BASE samples available for Google Earth accessible through OpenGeoscience and procedures reported.
- 20 gridded geochemical images of G-BASE data available for Google Earth

accessible through OpenGeoscience.

#### Requested budget (minimum £10k, maximum £50k) Staff: £15,400

Services: £0

Other recurrent: £250

Internal

# Project completion date: 1<sup>st</sup> March 2011. Anticipate main working period November 2010 – February 2011.

# Sustainability:

(The Opportunities Fund can only provide support for year 1 of projects. For longer projects, please confirm a source of longer term funds to complete the project).

The work can be sustained for geochemical data produced after this fy by incorporating the methodology into the current G-BASE/Geochemical Data management project procedures. Having designed and created standardised metadata formats and sets of R-scripts (documented in an Open File Report), generation of kml files for Google Earth will be simple and quick.

The project could act as a seed corn project for delivery of the global geochemical baseline information in a standardised manner and BGS could use the experience gained from this initiative to lever funding for involvement in more international projects (e.g. the US National Science Foundation funded iPlant cyber infrastructure collaborative) to make information about geochemical baselines globally available.

# **Supporting comments from Head(s) of Science/Information:**

I fully support and endorse this proposal as it will enable the geochemical baseline samples, along with their metadata, and a selected number of geochemical maps to be viewable in Google Earth through the OpenGeoScience www pages and data portal. On completion this will immediately raise the profile of the geochemical baseline data and information; making it more readily accessible and hence broaden the delivery of the data and information to a wider audience. It will also provide a template for other corporate BGS datasets to follow (e.g. National Geotechnical Properties or National Landslide Database) and keep BGS at the cutting edge of geoscientific data delivery.

#### Dr Helen Reeves (HoS Land Use, Planning & Development) Name: Date: 09.06.10

This is a great initiative and has my full support. OpenGeoscience is hungry for more open access information and it would be excellent to release some geochemical content to enhance and complement the geoscience materials already released (e.g. DiGmapGB-50 WMS). It is my aim to see materials from all areas of BGS science served through OpenGeoscience, and this would form an excellent example for that. OpenGeoscience has global visibility, and open access materials served for viewing through it are a proven way to attract interest in the underlying science and to encourage re-use and exploitation of the full underlying datasets (in this case the full G-BASE dataset). In the modern science and information world, it is important to give users 'something to play with' (a quote from a BBC editor regarding OpenGeoscience).

Name: Keith Westhead (HoI, Knowledge Exchange) Date: 11 June 2010 (emailed comments)

# **Confirmation from Skills/Facilities Leader(s):**

**₩**we confirm that staff/facilities are available to support this task:

Chris Johnson
 Alan Mackenzie
 Mark Cave
 Patrick Bell
 Emma Ball
 Gemma Nash-Ailsa Napier

**Name(s):** Dee Flight – Mark Cave up to 35 days available; Chris Johnson up to 5 days available.

Email from Simon Flowers (09/06/2010)

Chris,

No problem with these staff, except Gemma, who is nearly fully allocated. Emma has more free time, so could contribute 24 days, or Ailsa Napier is another possible alternative for Gemma.

Simon

# **Appendix 2** :Sample information web pages

#### **Soils Summary Information** 1

#### **G-BASE and Tellus Soils**

#### **Synopsis**

The British Geological Survey's Geochemical Baseline Survey of the Environment (G-BASE) project (Johnson et al., 2005) started to systematically collect soils as part of its UK regional geochemical mapping programme in the late 1980s. Between 1986-1988, over the Chalk of the Yorkshire Wolds, where there was no or poor drainage yielding very few stream sediments, soil samples (standard depth 30-40 cm, i.e. deep soils) were collected from 502 sites at a density of one site per km<sup>2</sup> (BGS, 1996). Similarly, between 1988-1990 in some lowland areas of Lancashire, Cheshire and parts of NE Wales, 2064 soil sites were sampled (standard depth 30-40 cm, i.e. deep soils) at a density of 1 site per 2 km<sup>2</sup> in areas where the low-order drainage was sparse (BGS, 1997). Further soil samples collected from eastern parts of Wales are described in BGS (2000).

Since the 1990s soil samples have become part of the systematic geochemical mapping of the UK both in rural and urban areas at sampling densities of 1 site per 2 km<sup>2</sup> and 4 sites per km<sup>2</sup>, respectively. A standard sampling methodology has been established and is described by Johnson (2005) and summarised below. Topsoils (5-20 cm) and deep soils (35-50 cm) are routinely collected from every site though generally only the topsoils are analysed for some 50 elements by X-ray fluorescence spectrometry (XRFS). Some geochemical images of a selected number of elements are available in the electronic atlas of central and eastern England.

A summary map of the soil sample sites from England, Scotland and Wales is available from the G-BASE website (download map). Northern Ireland was systematically sampled using G-BASE methodology (see Smyth, 2007) as part of the Tellus Project 2004-2007. As a result of the Tellus Project, Northern Ireland has the most comprehensive coverage of regional soil geochemical mapping of any nation of the UK and preparation of a geochemical atlas of the Tellus soil data (N Ireland) is in progress. On-going rural sample continues in England around the perimeter of Greater London as part of the "London Earth Project" and in Scotland as part of the "Clyde Basin Urban Super Project (CUSP)". During the London Earth Project an additional sample of surface soil (0 - 2 cm) was collected from the majority of sites though this sample has not been routinely analysed.

From an environmental perspective, the geochemical mapping of urban areas using soils as a sampling medium has become a priority, as exemplified by the London Earth Project. The urban work is described by Fordyce et al. (2005) and more recently by Flight and Scheib (2011). Urban geochemistry reports based on soil samples can be accessed from the G-BASE urban webpage. By the end of 2010 the following urban areas have been sampled: England - Corby, Coventry, Derby, Doncaster, Hull, Ipswich, Leicester, Lincoln, London, Manchester, Mansfield, Northampton, Nottingham, Peterborough, Scunthorpe, Sheffield, Stoke-on-Trent, Telford, Wolverhampton and York; Wales - Cardiff and Swansea; and Scotland - Glasgow. Belfast and Londonderry in Northern Ireland were sampled as part of the Tellus Project.

#### Soil Sampling Methodology



paper bags

Soils are collected using a Dutch The deeper soil samples are dried then sieved to -2 mm auger taking 5 subsamples at the and are only routinely analysed in areas where drainage is corners and centre of a 20 m square. absent. The topsoil samples are dried and sieved to 2 mm A topsoil (5 to 20 cm) and a deeper and pulverised in agate ball mills then pelletised for XRFS sample (35 to 50 cm) are taken at analyses of a wide range of trace and major elements (Ag, each site. Samples are collected from Al, As, Ba, Bi, Br, Ca, Čd, Ce, Co, Cr, Cs, Cu, Fe, Ga, Ge, alternate 1 km grid squares though in Hf, I, K, La, Mg, Mn, Mo, Na, Nb, Nd, Ni, P, Pb, Rb, Sb, Sc, urban areas sampling density is Se, Si, Sm, Sn, Sr, Ta, Te, Th, Ti, Tl, U, V, W, Y, Zn and increased to four samples every km². Zr). Loss-on-ignition (450°C) and pH is also routinely Samples are collected in Kraft<sup>TM</sup> measured.

#### **Data Availability**

Geochemical data, including the G-BASE soil results are available under licence from the British Geological Survey. There is a data licencing and handling charge plus a charge of £0.50 per data record (with discount for large numbers). Some or all of these charges can be waivered for academic use of the data. Contact <u>BGS Enquiries</u>. The G-BASE data licencing policy is being revised in May 2011 to coincide with the release of the London Earth soil data. The London Earth data will be available free-of-charge but with a fixed data licencing and handling fee of £150.

Excess sample powders have already found use in many research projects. These are archived at the National Geoscience Data Centre (NGDC), British Geological Survey, Keyworth, Nottingham, UK. Information concerning the availability of the Tellus Northern Ireland geochemical data can be found on the <u>Tellus data licensing</u> web page.

BGS data are protected by NERC copyright, Tellus data are protected by Crown Copyright.

#### **References and Links**

BGS. 1996. <u>Regional geochemistry of north-east England</u>. Keyworth, Nottingham. British Geological Survey. ISBN 0 85272 255 9.

BGS. 1997. <u>Regional geochemistry of parts of north-west England and North Wales</u>. Keyworth, Nottingham. British Geological Survey. ISBN 0 85272 307 5.

BGS. 2000. <u>Regional geochemistry of Wales and part of west-central England: stream sediment and soil.</u> Keyworth, Nottingham. British Geological Survey. ISBN 0 85272 378 4.

Flight, D.M.A. and Scheib, A.J. 2011. Soil Geochemical Baselines in UK Urban centres: The G-BASE Project. Chapter 13, 186-206. In: Mapping the Chemical Environment of Urban Areas. Johnson C.C., Demetriades, A., Locutura, J. and Ottesen, R.T. (Eds.). John Wiley & Sons, Ltd., Chichester, UK.

Fordyce, F.M., Brown, S.E., Ander, E.L., Rawlins, B.G., O'Donnell, K.E., Lister, T.R., Breward, N. and Johnson, C.C. 2005. <u>GSUE: urban geochemical mapping in Great Britain. Geochemistry: Exploration,</u> <u>Environment, Analysis</u>, 5 (4), 325-336.

Johnson, C.C. 2005. 2005 <u>G-BASE field procedures manual.</u> British Geological Survey, 65pp. (IR/05/097) (Unpublished).

Johnson, C.C., Breward, N., Ander, E.L. and Ault, L. 2005. <u>G-BASE: Baseline geochemical mapping of</u> <u>Great Britain and Northern Ireland</u>. Geochemistry: Exploration, Environment, Analysis, 5 (4), 347-357.

Smyth, D. 2007. Methods used in the Tellus Geochemical Mapping of Northern Ireland. British Geological Survey Open Report OR/07/022.

#### FOREGS

#### Synopsis

As its contribution to the <u>IUGS/IAGC Global Geochemical Baselines</u> Programme, the Forum of European Geological Surveys (FOREGS, now EuroGeoSurveys), through its component surveys, collected various environmental materials (including three types of soil - organic top layer, minerogenic top and sub soils) to create geochemical baseline maps for Europe. For the drainage samples and soils this was done at a scale that averages out to about one sample per 4700 km<sup>2</sup>. A two part geochemical atlas of Europe has been published (Salminen et al., 2005; De Vos et al., 2006) and databases, maps and atlases are readily and freely available from web pages hosted by the Geological Survey of Finland (GTK).

Sample site selection was based on the Global Reference Network (GRN) grid cells developed for the purpose of Global Geochemical Baseline Mapping (Darnley et al., 1995), each cell being 160 x 160 km. The soil sampling procedure is described in detail in Salminen et al. (1998) and summarised below. The target was to collect from five "random" sites within each cell.

The British Geological Survey collected the FOREGS samples for the UK in August-October 1998. Sixty top and sub soil samples were collected and 28 humus samples.

#### Soil Sampling and Analytical Methodology

A large variety of sampling media were used in this project including:

- Residual soil, upper horizon (topsoil) 0 25 cm without the top organic layer (<2 mm)
- Residual soil, lower (C) horizon (subsoil); a 25 cm layer within a depth range of 50 200 cm (<2 mm)</li>
- Humus where present

Samples in the UK were collected with a stainless steel trowel and stored in Kraft paper bags. Suitable sampling sites were selected in an area where 3 - 5 pits could be dug to observe and sample the soil

profile. Each sample was a composite of 3 - 5 samples, the minimum distance between any two subsamples being 5 m. Living surface vegetation, fresh litter, big roots and rock fragments (stones) were removed. Samples were dried at a temperature not higher than 40°C, disaggregated in a porcelain bowl, sieved through a 2 mm nylon screen and subsequently pulverised to <0.063 mm in an agate disc mill.

Top and sub soils were analysed at various laboratories across Europe by XRFS-WD, ICP-MS (following mixed acid extraction), ICP-AES (following *aqua regia* extraction), Hg analyser and a granulometric method for total organic carbon (TOC).

#### **Data Availability**

Geochemical results and maps are available from the <u>atlas site</u> hosted by the Finnish Geological Survey (GTK). Data files take the form of a collection of zipped MS Excel files from which individual country subsets can be extracted using the country code field. Excess sample powders were transferred in 2009 to the National Geoscience Data Centre (NGDC), British Geological Survey, Keyworth, Nottingham, UK.

#### **References and Links**

Darnley, A.G., Bjorklund, A., Bolviken, B. et al. 1995. A Global Geochemical Database for Environmental and Resource Management, Earth Science Series No. 19, UNESCO Publishing, Paris, 122 pp.

De Vos, W. and Tarvainen, T. (ed.) et al. 2006. <u>Geochemical Atlas of Europe. Part 2 - Interpretation of Geochemical Maps</u>, Additional tables, Figures, Maps, and Related Publications. Geological Survey of Finland, Otamedia Oy, Espoo, 692 pp.

Salminen, R., Tarvainen, T., Demetriades, A. et al., 1998. <u>FOREGS Geochemical Mapping Field Manual</u>. Geological Survey of Finland, Guide 47.

Salminen, R. (chief ed.) et al. 2005. <u>Geochemical Atlas of Europe. Part 1 - Background Information,</u> <u>Methodology and Maps.</u> Geological Survey of Finland, Otamedia Oy, Espoo, 525 pp.

#### GEMAS

#### Synopsis

The Geochemical Mapping of Agricultural Soils (GEMAS) is a European-wide project between the component geological surveys of the <u>EuroGeoSurveys</u> and <u>Eurometaux</u> (European Association of Metals). The aim of the project is to produce one of the best harmonized and directly comparable datasets on soil quality and metals in soils that exists at the EU scale. In 2008 across Europe, 2211 samples of arable soil (0-20 cm) and 2118 samples of grazing land soil (0-10 cm) were collected at an average sampling density of 1 sample per 2500 km<sup>2</sup>. The extensive analytical programme determined more than 50 elements by ICP following an aqua regia extraction and more than 40 elements determined by XRFS.

The British Geological Survey collected the UK soil samples for this project (see <u>G-BASE webpage</u>). Sampling sites were based on 50 x 50 km cells with 65 sites in England, 51 in Scotland, 14 in Wales and 8 in Northern Ireland. Samples were collected according to an agreed protocol (EGS Geochemistry Working Group, 2008) which is summarised below.

#### Soil Sampling Methodology

| stainless steel spade is used for collection. |  | Each sample is a composite of a<br>minimum of 5 subsamples yielding a<br>2-2.5 kg sample collected in a<br>RILSAN bag. Subsamples are<br>collected from the corners and<br>centre of a 10 x 10m square. A<br>stainless steel spade is used for<br>collection. | The arable sample is taken from the ploughing layer (0-20 cm), whilst the grazed land sample is collected from the top 10 cm (removing any living surface vegetation). Samples are dried at a max of 40°C, disaggregated as necessary and sieved to < 2 mm using a nylon screen. |
|---|--|---|--|
|---|--|---|--|

#### Data Availability

Results for the UK are freely available from the country representative on the GEMAS Project, namely Andreas Scheib (BGS). There are some restrictions for some elements (e.g. Au) and analysis is currently in progress. In January 2011, for arable and grazing soils the ICP *aqua regia*, pH, CEC and TOC results were available. XRFS results were additionally available for the grazing land soils.

#### **References and Links**

EGS Geochemistry Working Group. <u>2008. EuroGeoSurveys Geochemical mapping of agricultural and grazing land soil of Europe (GEMAS) - Field manual.</u> Report for EuroGeosurveys/Eurometaux. Report No. 2008.038. Geological Survey of Norway (NGU), 46pp. NGU, Trondheim, Norway.

Reimann, C., Demetriades, A., Eggen, O.A., Filzmoser, P. et al. 2009. <u>The EuroGeoSurveys geochemical</u> <u>mapping of agricultural and grazing land soils project (GEMAS) - Evaluation of quality control results of</u> <u>aqua regia extraction analysis</u>. Report No. 2009.049. Geological Survey of Norway (NGU), 94pp. NGU, Trondheim, Norway.

#### NSI

#### Synopsis

<u>National Soil Inventory</u> (NSI) samples cover England and Wales on a 5 km grid (6,127 sites). The original sampling was from around 1980 and there have been partial resamplings in the mid-1990s. NSI data includes erosion, land use and lithological information. NSI profile information gives a very detailed description including stone abundance, root descriptions and boundary information. The NSI topsoil data gives detailed measurements of over 20 elements from the soils, in addition to pH. This information is held by Cranfield University in their Landis database.

Archived material was recently re-analysed at the British Geological Survey by X-ray fluorescence spectrometry (XRFS) yielding new analytical results for more than 50 chemical elements.

A similar set of data also referred to as the <u>National Soil Inventory</u> exists for Scotland (James Hutton Institute, formerly until April 2011 the Macaulay Land Use Research Institute) on a 5 km grid (total 3,094 sites). Sites on a 10 km grid (770) include chemical analyses.

#### Soil Sampling and Analytical Methodology

NSI soil sampling sites were collected at the intersects of a 5-km orthogonal grid (a grid offset 1 km north and east of the British Ordnance Survey National Grid so sites did not fall on the margin of printed map sheets. The principal interest was agricultural land and did not specifically target urban areas. From 6,127 sites visited 5,691 soil samples were collected between 1978 and 1983.

Soil sampling was restricted to the uppermost 15 cm of mineral soil (less if bedrock was encountered). Twenty-five cores of soil were taken using a mild-steel, screw-type auger at the nodes of a 4 m grid within a 20 m x 20 m square centred on the site location. These soil cores were bulked and the target sample weight was 450 g. Samples were double-bagged in food-grade polythene bags and refrigerated on the day of sampling. Within two weeks the soils were air dried on Kraft paper, after which each sample was split into two equal portions. One portion was kept as a reference sample, the other was milled in a mild-steel roller-mill to pass a 2-mm aperture sieve. A further 25g sub-sample was taken from the <2mm airdry sample by coning and quartering, and ground to <150 micrometres in an all-agate planetary ball mill. This sample was used for the determination of Al, Ba, Cd, Ca, Cr, Co, Cu, Fe, Pb, Mg, Mn, Ni, P, K, Na, Sr and Zn extracted by *aqua regia*, and determined by ICP-AES. The unground <2 mm fraction was also determined for pH (soil-water suspension); organic carbon (dichromate oxidation); available K, Mg (1M ammonium nitrate extraction), and P (0.5 M sodium bicarbonate extraction); and extractable Cd, Co, Cu, Pb, Ni, and Zn (0.05 M ammonium-EDTA extraction).

The 2010 BGS XRFS reanalysis was undertaken on a subsample of ground material upon which the original *aqua regia* digests were undertaken yielded a large number of total element concentrations for: Ag, Al, As, Ba, Bi, Br, Ca, Cd, Ce, Cl, Cl, Co, Cr, Cs, Cu, Fe<sub>2</sub>O<sub>3</sub>, Ga, Ge, Hf, I, In, K, La, Mg, Mn, Mo, Na Nb, Nd, Ni, P, Pb, Pd, Rb, S, Sb, Sc, Se, Si, Sm, Sn, S, Sr, Ta, Te, Th, Ti, Ti, TI, U, V, W, Y, Yb, Zn and Zr.

#### Data Availability

The new BGS XRFS data will be released as an electronic atlas in October 2011 and the raw data will become freely available from October 2013.

NSI site and sample information availability (England and Wales) is described on the National Soil Resources Institute (Cranfield University) web page "Information on NSI data products". More information on the Scottish NSI can be obtained by contacting <u>MLURI</u>.

#### **References and Links**

Cranfield University Landis (Land Information System) home web page

James Hutton Institute (formerly Macaulay Land Use Research Institute) <u>Scottish NSI web page</u> McGrath, S. P. and Loveland, P. J. 1992. The Soil Geochemical Atlas of England and Wales, Blackie Academic and Professional, Glasgow.

### 2 Stream Sediments Summary Information

#### **G-BASE and Tellus**

#### Synopsis

The British Geological Survey's Geochemical Baseline Survey of the Environment (<u>G-BASE</u>) project (Johnson et al., 2005) started to systematically collect stream sediments as part of its UK regional geochemical mapping programme in the late 1960s (see <u>History of G-BASE</u>). Fine stream sediments from small streams are used to define the regional geochemical baseline as sediments derived from the drainage catchment above the sampling site generally give an excellent approximation of the concentrations of the chemical elements in the surface environment. In excess of 105,000 stream sediments have been collected from Great Britain and Northern Ireland with some 85% of the area being sampled - only southern England remains unsampled (<u>download map</u>). The western part of Northern Ireland was systematically sampled using G-BASE methodology in the mid 1990s (Flight et al., 1995) and the whole country completed as part of the <u>Tellus Project</u> 2004-2007 (Smyth, 2007).

Systematic sampling southwards across England ceased in 2007. On-going rural stream sediment sampling continues in England around the perimeter of Greater London as part of the "London Earth Project" and in Scotland as part of the "Clyde Basin Urban Super Project (CUSP)".

Stream sediment is sieved at site through a nylon sieve to <150 µm and collected from small (low order) streams at a high average sampling density of 1 site every 1 - 2 km<sup>2</sup> (see Johnson, 2005; Johnson et al., 2008). This high density of sampling enables the regional geochemical baseline to be interpreted at a local scale. Stream water samples and heavy mineral panned concentrates are also collected from each site. Since the project commenced "total" element concentrations have been determined, firstly by direct current optical emission spectroscopy (DCOES) and more recently X-ray fluorescence spectrometry (XRFS). The current methodology, a combination of wavelength-dispersive (WD) and energy-dispersive (ED) XRFS delivers results for some 50 chemical elements.

The stream sediment results have been published in a series of geochemical atlases (see <u>Geochemical</u> <u>maps and atlases</u>) in which the results for the most recent atlases are presented as interpolated geochemical images. Central and eastern England stream sediment data for a selected number of elements is presented as an <u>electronic geochemical atlas</u>. A geochemical atlas of the Tellus stream sediment data (N Ireland) is in preparation.

#### Soil Sampling and Analytical Methodology

| Sediment is collected from the actidrainage channel of 1st or 2nd ord streams. The sediment is wet siew firstly through a 2 mm nylon screthen a 150 µm nylon sieve. The fistream sediment is collected in Kraft <sup>TM</sup> paper bag. Sampling dens varies according to land use a drainage pattern but averages one sample every one to two squakilometre. | Sediments are dried initially by air drying then freeze drying<br>before being pulverised in agate ball mills. Samples are<br>pelletised ready for XRFS analyses at the BGS laboratories<br>in Keyworth, UK. A combination of emission and dispersive<br>techniques gives a wide range of elements (Ag, Al, As, Ba,<br>Bi, Br, Ca, Cd, Ce, Co, Cr, Cs, Cu, Fe, Ga, Ge, Hf, I, K, La,<br>Mg, Mn, Mo, Na, Nb, Nd, Ni, P, Pb, Rb, Sb, Sc, Se, Si, Sm,<br>Sn, Sr, Ta, Te, Th, Ti, TI, U, V, W, Y, Zn and Zr)<br>at<br>re |
|--|--|
|--|--|

#### **Data Availability**

Geochemical data, including the G-BASE stream sediment results are available under licence from the British Geological Survey. There is a data licencing and handling charge plus a charge of £0.50 per data record (with discount for large numbers). Some or all of these charges can be waivered for academic use of the data. Contact <u>BGS Enquiries</u>.

Excess sample powders have already found use in many research projects. These are archived at the National Geoscience Data Centre (NGDC), British Geological Survey, Keyworth, Nottingham, UK.

Information concerning the availability of the Tellus Northern Ireland geochemical data can be found on the <u>Tellus data licensing</u> web page.

BGS data are protected by NERC copyright, Tellus data are protected by Crown Copyright.

#### **References and Links**

Flight, D.M.A., Christie, J.L., Lister, T.R., Simpson, P.L. and Smith, B. 1995. Results of a pilot geochemical survey, Northern Ireland, Geological Survey of Northern Ireland Technical report No. GSNI/95/6., Geological Survey of Northern Ireland, Belfast. March 1995.

Johnson, C.C. 2005. <u>2005 G-BASE field procedures manual</u>. British Geological Survey, 65pp. (IR/05/097) (Unpublished).

Johnson, C.C., Breward, N., Ander, E.L. and Ault, L. 2005. <u>G-BASE: Baseline geochemical mapping of</u> <u>Great Britain and Northern Ireland.</u> Geochemistry: Exploration, Environment, Analysis, 5 (4), 347-357.

Johnson, C.C., Flight, D.M.A., Ander, E.L., Lister, T.R., Breward, N., Fordyce, F.M. and Nice, S.E., 2008. <u>The collection of drainage samples for environmental analyses from active stream channels.</u> In: B. de Vivo, H.E. Belkin and A. Lima (Editors), Environmental Geochemistry: Site characterisation, data analysis and case histories. Elsevier, Oxford, pp. 59-92.

Smyth, D. 2007. Methods used in the Tellus Geochemical Mapping of Northern Ireland.{insert NORA hyperlink} British Geological Survey Open Report OR/07/022.

#### Wolfson (Imperial College London)

#### Synopsis

The first comprehensive geochemical mapping in the UK was carried out by the Applied Geochemistry Research Group at Imperial College London. This remains the only completed high density regional geochemical stream sediment survey of England. A rapid field sampling programme, carried out in the space of just one year (1969), collected stream sediments from 49,464 sites in England and Wales giving an approximate sampling density of one sample every 3 square kilometres. However, this density does not account for the unsampled urban areas and regions of no surface drainage (e.g. over chalk). The results are presented as interpolated geochemical images in the Wolfson Geochemical Atlas of England and Wales (Webb et al., 1978).

#### Soil Sampling and Analytical Methodology

At each drainage site, composite samples were collected from a stretch of the active drainage channel at least 20 m upstream from the road used to access the stream. Samples were dried at 60-80°C . After disaggregation the sample was sieved to minus 80-mesh (c. 200 µm). The majority of elements were determined by direct current optical emission spectrometry (DCOES) (AI, Ba, Co, Cr, Cu, Fe, Ga, Li, Mg, Mn, Ni, Pb, Sc, Si, Sr, Ti and V. The following elements were also determined but rejected on the basis of poor quality: Ag, Bi, Be, La, Zr and W). Zinc and Cd were determined by atomic adsorption spectrophotometry (AAS). Following a nitric acid extraction, Mo and As were determined colorimetrically after a potassium hydrogen sulphate fusion.

#### **Data Availability**

Enquiries about the geochemical data should be directed to Imperial College, London.

#### **References and Links**

WEBB, J.S., THORNTON, I., THOMPSON, M., HOWARTH, R.J. & LOWENSTEIN, P.L., 1978. The Wolfson geochemical atlas of England and Wales. Clarendon Press, Oxford.

#### FOREGS

#### Synopsis

As its contribution to the <u>IUGS/IAGC Global Geochemical Baselines</u> Programme, the Forum of European Geological Surveys (FOREGS, now EuroGeoSurveys), through its component surveys, collected various environmental materials (including stream sediments) to create geochemical baseline maps for Europe. For the drainage samples and soils this was done at a scale that averages out to about one sample per 4700 km<sup>2</sup>. A two part geochemical atlas of Europe has been published (Salminen et al., 2005; De Vos et al., 2006) and databases, maps and atlases are freely available from web pages hosted by the Geological Survey of Finland (GTK).

Sample site selection was based on the Global Reference Network (GRN) grid cells developed for the purpose of Global Geochemical Baseline Mapping (Darnley et al., 1995), each cell being 160 x 160 km. The soil sampling procedure is described in detail in Salminen et al. (1998) and summarised below. The target was to collect from five "random" sites within each cell.

The British Geological Survey collected a total of sixty stream sediment samples for FOREGS in the UK between August-October 1998.

#### Stream Sediment Sampling and Analytical methodology

At selected drainage sites stream sediment and water was collected. Active stream sediment was collected from the small, second order drainage basins (catchment areas <100 km<sup>2</sup>). Each sample was a composite of sample taken from 5-10 points over a stretch of 250-500 m along the stream. The sediment is wet sieved, firstly through a 2 mm nylon screen, then a 150  $\mu$ m nylon sieve, and the resulting fine sediment collected in a wooden gold pan. The fine stream sediment is collected in a Kraft<sup>TM</sup> paper bag. A minimum of 500 g of sediment (dry weight) was collected at each site.

The stream sediments were determined at a number of laboratories across Europe by a variety of analytical techniques: XRFS-WD, ICP-MS (following mixed acid extraction), ICP-AES (following aqua regia extraction), Hg analyser and a granulometric method for total organic carbon (TOC).

#### **Data Availability**

Geochemical results and maps are freely available from the <u>atlas site</u> hosted by the Finnish Geological Survey (GTK). Data files take the form of a collection of zipped MS Excel files from which individual country subsets can be extracted using the country code field. Excess sample powders were transferred in 2009 to the National Geoscience Data Centre (NGDC), British Geological Survey, Keyworth, Nottingham, UK.

#### **References and Links**

Darnley, A.G., Bjorklund, A., Bolviken, B. et al. 1995. A Global Geochemical Database for Environmental and Resource Management, Earth Science Series No. 19, UNESCO Publishing, Paris, 122 pp.

De Vos, W. and Tarvainen, T. (ed.) et al. 2006. <u>Geochemical Atlas of Europe. Part 2 - Interpretation of Geochemical Maps</u>, <u>Additional tables</u>, <u>Figures</u>, <u>Maps</u>, <u>and Related Publications</u>. Geological Survey of Finland, Otamedia Oy, Espoo, 692 pp.

Salminen, R., Tarvainen, T., Demetriades, A. et al., 1998. <u>FOREGS Geochemical Mapping Field Manual</u>. Geological Survey of Finland, Guide 47.

Salminen, R. (chief ed.) et al. 2005. <u>Geochemical Atlas of Europe. Part 1 - Background Information</u>, <u>Methodology and Maps</u>. Geological Survey of Finland, Otamedia Oy, Espoo, 525 pp.

### 3 Stream Waters Summary Information

#### **G-BASE and Tellus**

#### **Synopsis**

The British Geological Survey's Geochemical Baseline Survey of the Environment (G-BASE) project (Johnson et al., 2005) started to systematically collect stream waters as part of its UK regional geochemical mapping programme in the late 1960s (see History of G-BASE). Stream waters were initially collected just for pH, conductivity, F and U determination (i.e. from N Scotland). With improved analytical techniques stream waters became part of the suite of samples collected from each drainage sample site. These are collected from small streams (1st and 2nd order) and approximately 85% of Great Britain and Northern Ireland has been sampled. Only southern England remains unsampled (download map), plus areas of chalk and limestone (e.g. Yorkshire Wolds in NE England) were there are no surface streams to sample. The Tellus Project (Smyth, 2007) completed the national survey of stream water sampling begun in 1994 by the British Geological Survey (BGS) on behalf of the Department of Economic Development and Department of Environment (Flight et al., 1995).

Systematic sampling southwards across England ceased in 2007. On-going rural stream water sampling continues in England around the perimeter of Greater London as part of the "London Earth Project" and in Scotland as part of the "Clyde Basin Urban Super Project (CUSP)".

Stream waters are collected at every G-BASE drainage site at a high average sampling density of 1 site every 1 - 2 km<sup>2</sup> (see Johnson, 2005; Johnson et al., 2008). This high density of sampling enables the regional geochemical baseline to be interpreted at a local scale. As sampling is done in the summer months, occasionally during very dry periods, water could not be collected even though dry stream sediment could, hence there are some drainage sites with no waters.

The stream water results are generally presented in the series of geochemical atlases (see Geochemical maps and atlases) as interpolated geochemical images. A geochemical atlas dedicated to stream waters from Wales and parts of west-central England was published in 1999 (BGS, 1999). Central and eastern England stream water data for a selected number of elements is presented as an electronic geochemical atlas. A geochemical atlas of the Tellus water data (N Ireland) is in preparation.

#### **Stream Water Sampling and Analytical Methodology**



Filtered (0.45 µm cellulose Alkalinity (by colorimetric titration), pH and conductivity determined filter) and unfiltered waters are on unfiltered samples, on location. Filtered samples analysed at collected from the same site BGS. ICP-MS: Li, Be, B, Na, Mg , Al, Si, P, S, K, Ca, Ti, V, Cr, Mn, as the drainage sediment. Fe, Co, Ni, Cu, Zn, Ga, As, Se, Rb, Sr, Y, Zr, Nb, Mo, Ag, Cd, Sn, in Sb, Cs, Ba, La, Ce, Pr, Nd, Sm, Eu, Tb, Gd, Dy, Ho, Er, Tm, Yb, and Lu, Hf, Ta, W, TI, Pb, Th & U [56 elements]. Ion Chromatography: acidified as required by the Br, Cl, F, NO2, NO3, SO4, PO4 [7 ions]. TIC/TOC analyser for Nonanalytical method. Filtered purgeable organic carbon (NPOC)

#### **Data Availability**

Geochemical data, including that for G-BASE stream waters, are available under licence from the British Geological Survey. There is a data licencing and handling charge plus a charge of £0.50 per data record (with discount for large numbers). Some or all of these charges can be waivered for academic use of the data. Contact BGS Enquiries.

Excess water samples collected since 2000 are archived in a cold store at the National Geoscience Data Centre (NGDC), British Geological Survey, Keyworth, Nottingham, UK. Information concerning the availability of the Tellus Northern Ireland geochemical data can be found on the Tellus data licensing web page.

BGS data are protected by NERC copyright, Tellus data are protected by Crown Copyright.

stored bottles

#### References and Links

BGS (1999). Regional geochemistry of Wales and part of west-central England: stream water. Keyworth, Nottingham. British Geological Survey. ISBN 0 85272 363 6.

Flight, D.M.A., Christie, J.L., Lister, T.R., Simpson, P.L. and Smith, B. 1995. Results of a pilot geochemical survey, Northern Ireland, Geological Survey of Northern Ireland Technical report No. GSNI/95/6., Geological Survey of Northern Ireland, Belfast. March 1995.

Johnson, C.C. 2005. <u>2005 G-BASE field procedures manual</u>. British Geological Survey, 65pp. (IR/05/097) (Unpublished).

Johnson, C.C., Breward, N., Ander, E.L. and Ault, L. 2005. <u>G-BASE: Baseline geochemical mapping of</u> <u>Great Britain and Northern Ireland</u>. Geochemistry: Exploration, Environment, Analysis, 5 (4), 347-357.

Johnson, C.C., Flight, D.M.A., Ander, E.L., Lister, T.R., Breward, N., Fordyce, F.M. and Nice, S.E., 2008. <u>The collection of drainage samples for environmental analyses from active stream channels.</u> In: B. de Vivo, H.E. Belkin and A. Lima (Editors), Environmental Geochemistry: Site characterisation, data analysis and case histories. Elsevier, Oxford, pp. 59-92.

Smyth, D. 2007. Methods used in the Tellus Geochemical Mapping of Northern Ireland. British Geological Survey Open Report OR/07/022.

#### FOREGS

#### Synopsis

As its contribution to the IUGS/IAGC Global Geochemical Baselines Programme, the Forum of European Geological Surveys (FOREGS, now EuroGeoSurveys), through its component surveys, collected various environmental materials (including stream waters) to create geochemical baseline maps for Europe. For the drainage samples and soils this was done at a scale that averages out to about one sample per 4700 km<sup>2</sup>. A two part geochemical atlas of Europe has been published (Salminen et al., 2005; De Vos et al., 2006) and databases, maps and atlases are freely available from web pages hosted by the Geological Survey of Finland (GTK).

Sample site selection was based on the Global Reference Network (GRN) grid cells developed for the purpose of Global Geochemical Baseline Mapping (Darnley et al., 1995), each cell being 160 x 160 km. The water sampling procedure is described in detail in Salminen et al. (1998) and summarised below. The target was to collect from five "random" sites within each cell.

The British Geological Survey collected a total of sixty stream water samples for FOREGS in the UK between August-October 1998.

#### Stream Water Sampling and Analytical methodology

At the selected drainage sites running stream water was collected from the small, second order streams (catchment areas <100 km<sup>2</sup>). During sampling disposable plastic gloves were worn on both hands. The following sub-samples were separately collected at each site:

- 500 mL polyethylene bottle of unfiltered water for major ion analysis (Ion Chromatography, IC)
- 100 mL polyethylene bottle filtered (0.45 μm) water for ICP-MS and ICP-AES analysis (acidified)
- 120 mL Nalgene<sup>™</sup> bottle unfiltered water for Hg analysis (acidified) (Hg Analyser)
- 100 mL polyethylene bottle filtered (0.45 µm) water for dissolved organic carbon analysis (DOC)

The pH and electrical conductivity were measured by meters on location, as was the water alkalinity (determined by titration). Samples were kept cool using a cool box and refrigerator.

The stream waters were analysed at a number of laboratories across Europe by a variety of analytical techniques as listed above.

#### Data Availability

Geochemical results and maps are easily and freely available from the atlas site hosted by the Finnish Geological Survey (GTK). Data files take the form of a collection of zipped MS Excel files from which individual country subsets can be extracted using the country code field.

#### **References and Links**

Darnley, A.G., Bjorklund, A., Bolviken, B. et al. 1995. A Global Geochemical Database for Environmental and Resource Management, Earth Science Series No. 19, UNESCO Publishing, Paris, 122 pp.

De Vos, W. and Tarvainen, T. (ed.) et al. 2006. Geochemical Atlas of Europe. Part 2 - Interpretation of Geochemical Maps, Additional tables, Figures, Maps, and Related Publications. Geological Survey of Finland, Otamedia Oy, Espoo, 692 pp.

Salminen, R., Tarvainen, T., Demetriades, A. et al., 1998. FOREGS Geochemical Mapping Field Manual. Geological Survey of Finland, Guide 47.

Salminen, R. (chief ed.) et al. 2005. Geochemical Atlas of Europe. Part 1 - Background Information, Methodology and Maps. Geological Survey of Finland, Otamedia Oy, Espoo, 525 pp.

# Appendix 3 : R scripts

# SCRIPTS FOR GENERATING SITE INFORMATION

# Requirements for standard input data file and further information in BGS Open Report OR/11/014

#Choose standard input data file
f.name<-file.choose()</pre>

#Read in header data H.data<-read.table(file=f.name,nrows=4,sep=",",header=F,stringsAsFactors=F) project.dat<-H.data\$V1[1] #samptype.dat<-H.data\$V2[1] Anal.dat<-H.data\$V1[2] other.dat<-H.data\$V1[3] ipr.dat<-H.data\$V1[4]</pre>

# Set program controls based on header line project title
Project<-strsplit(project.dat," ")[[1]] [1]
Country<-strsplit(project.dat," ")[[1]] [2]
Samptype<-strsplit(project.dat," ")[[1]] [3]</pre>

# set Google Earth placemark according to sample type - default is blank yellow balloon
placemark<-"<href> http://maps.google.com/mapfiles/kml/paddle/ylw-blank.png </href>"
if(Samptype=="deep")placemark<-"<href> http://maps.google.com/mapfiles/kml/paddle/ylw-circle.png </href>"
if(Samptype=="topsoil")placemark<-"<href> http://maps.google.com/mapfiles/kml/paddle/red-circle.png </href>"
if(Samptype=="stream")placemark<-"<href> http://maps.google.com/mapfiles/kml/paddle/blu-circle.png </href>"
if(Samptype=="stream")placemark<-"<href> http://maps.google.com/mapfiles/kml/paddle/blu-circle.png </href>"
if(Samptype=="stream")placemark<-"<href> http://maps.google.com/mapfiles/kml/paddle/blu-circle.png </href>"
if(Samptype=="water")placemark<-"<href> http://maps.google.com/mapfiles/kml/paddle/ltblu-circle.png </href>"

# set label logo according to Project - default is white circle logo<-"blank\_logo.gif"</pre>

```
if(Project=="FOREGS")logo<-"EGS logo ico small.jpg"
if(Project=="GEMAS")logo<-"EGS logo ico small.jpg"
if(Project=="TELLUS")logo<-"GSNI.gif"
if(Project=="G-BASE")logo<-"bgs c t 50x50.gif"
# set altitude for zoom according to Project so sample sites appear at a reasonable density on start up
zoom<-" <altitude>150000</altitude>"
if(Project=="FOREGS")zoom<-" <a href="https://www.ifitudescore-complexity.com">altitudescore-complexity.com</a>
if(Project=="GEMAS")zoom<-" <a href="littude"><a href="littude"</a>
if(Project=="TELLUS")zoom<-" <a href="littude"><a href="littude"</a>
if(Project=="G-BASE")zoom<-" <a href="mailto:</a href="mailto:searched">altitude>"</a>
#Set kml <look at> longitude and latitude based on country - default BGS Keyworth
longit<-" <longitude>-1.078098</longitude>"
latit<-" <latitude>52.876000</latitude>"
#set possible countries
Location <- c("England", "Scotland", "Wales", "N.Ireland")
#England (Keyworth)
if(Country==Location[1]){
longit<-" <longitude>-1.078098</longitude>"
latit<-" <latitude>52.876000</latitude>"
#N.Ireland (Belfast)
if(Country==Location[4]){
longit<-" <longitude>-5.9325</longitude>"
latit<-" <latitude>54.5771</latitude>"
                  }
#Wales (Cardiff)
if(Country==Location[3]){
longit<-" <longitude>-3.2387</longitude>"
latit<-" <latitude>51.5291</latitude>"
                  }
#Scotland (Edinburgh)
if(Country==Location[2]){
longit<-" <longitude>-3.1792</longitude>"
latit<-" <latitude>55.9242</latitude>"
                  }
```

# filename to write kml code - take input filename, strip off file extension and replace with kml extension filename<-f.name

filename<-paste(substr(filename,1,nchar(filename)-3),"kml",sep="")</pre>

# set kml <name> field
kmlname<-paste("<name>",project.dat,"</name>",sep="")

# Now read in the rest of the data
# start at line 5 (skip=4)
# Name and path of the file
C.data<-read.table(file=f.name,skip=4,sep=",",header=T,stringsAsFactors=F)</pre>

C.data\$Fraction<-sub("<", "&lt;", C.data\$Fraction) # replace < so kml can read sign C.data\$Analytes<-gsub(",",", ",C.data\$Analytes) # change seperator to be a comma plus space

loops<-length(C.data\$x) # number of times to loop round to write kml data for each sample

# Load the packages library(rgdal) library(gstat) library(lattice) library(maptools)

#Transform coordinates according to project

#GEMAS and FOREGS use lat/long, G-BASE uses British National Grid, Tellus uses Irish National Grid #The Geographical reference system data comes from the EPSG Geodetic Parameter Dataset #which is available from http://www.epsg.org/CurrentDB.html

Csp.data<-C.data coordinates(Csp.data)<-~x+y

if(Project=="FOREGS")proj4string(Csp.data)<-CRS("+proj=longlat +datum=WGS84") if(Project=="GEMAS")proj4string(Csp.data)<-CRS("+proj=longlat +datum=WGS84") if(Project=="TELLUS")proj4string(Csp.data) <- CRS("+init=epsg:29902") if(Project=="G-BASE")proj4string(Csp.data) <- CRS("+init=epsg:27700")</pre>

Csp.II<-spTransform(Csp.data,CRS("+proj=longlat +datum=WGS84"))

#open file to write kml code
filename<-file(filename,"w")</pre>

# now start writing the kml code
# Header lines
write("<?xml version=\"1.0\" encoding=\"UTF-8\"?>",filename)

```
write("<kml xmlns=\"http://earth.google.com/kml/2.1\">",filename,append=TRUE)
write("<Document>",filename,append=TRUE)
write(paste(kmlname),filename,append=TRUE)
write("
       <Style id=\"simple\">",filename,append=TRUE)
write("
         <IconStyle>",filename,append=TRUE)
            <scale>1.1</scale>",filename,append=TRUE)
write("
write("
            <Icon>",filename,append=TRUE)
write(paste(placemark), filename, append=TRUE)
write("
            </Icon>",filename,append=TRUE)
write("
         </IconStyle>",filename,append=TRUE)
write("
         <LabelStyle>",filename,append=TRUE)
            <color>00ffffff</color>",filename,append=TRUE)
write("
         </LabelStyle>",filename,append=TRUE)
write('
         <BalloonStyle>",filename,append=TRUE)
write("
write("
            <text><![CDATA[",filename,append=TRUE)
write("<div style=\"background-color:#DDDDDD; width:400; font-family:helvetica;\" align=\"center\" >",filename,append=TRUE)
write("",filename,append=TRUE)
write("<strong>SAMPLE ID $[SAMPLE ID]</strong>
write("<strong>Data series: </strong>$[description]",filename,append=TRUE)
write("<strong>Date Collected: </strong>$[DATE_COLLECTED] ",filename,append=TRUE)
if(Samptype=="water")write("<strong>Water Filter: </strong>$[FRACTION ANALYSED]",filename,append=TRUE)else {
write("<strong>Fraction Analysed: </strong>$[FRACTION ANALYSED]",filename,append=TRUE)
write("<strong>Analytes Determined: </strong>$[Analytes determined]",filename,append=TRUE)
write("<strong>Other Determinands: </strong>$[Other]",filename,append=TRUE)
write("<strong>Analytical Method: </strong>$[MAIN METHOD]",filename,append=TRUE)
write("<tr><td>$[Other Analysis]<math><filename,append=TRUE)
write("$[IPR statement]",filename,append=TRUE)
#Paste in correct logo
write("<tr><td align=\"center\"><imq src=",filename,append=TRUE)
write(paste(logo),filename,append=TRUE)
write("
write("",filename,append=TRUE)
write("</div>",filename,append=TRUE)
write("
                   ]]></text>",filename,append=TRUE)
         </BalloonStyle>",filename,append=TRUE)
write("
       </Style> ",filename,append=TRUE)
write("
# Write all sample points and labels in a loop
for(i in 1:loops){
write(" <Placemark id=\"1\">",filename,append=TRUE)
# Now start adding the data
```

```
write(paste("<name>",C.data$Sample_id[i],"</name>",sep=""),filename,append=TRUE)
                  <description>",project.dat,"</description>",sep=""),filename,append=TRUE)
 write(paste("
 write("
            <styleUrl>#simple</styleUrl>",filename,append=TRUE)
 write("
           <ExtendedData> ",filename,append=TRUE)
                       <Data name=\"DATE COLLECTED\">",C.data$Date[i],"</Data> ",sep=""),filename,append=TRUE)
 write(paste("
                      <Data name=\"SAMPLE_ID\">",C.data$Sample_id[i],"</Data>",sep=""),filename,append=TRUE)
 write(paste("
 write(paste("
                       <Data name=\"Analytes determined\">",C.data$Analytes[i],"</Data>",sep=""),filename,append=TRUE)
                       <Data name=\"FRACTION_ANALYSED\">",C.data$Fraction[i],"</Data>",sep=""),filename,append=TRUE)
 write(paste("
                      <Data name=\"Other\">",C.data$Other[i],"</Data>",sep=""),filename,append=TRUE)
 write(paste("
                      <Data name=\"MAIN METHOD\">",Anal.dat,"</Data>",sep=""),filename,append=TRUE)
 write(paste("
                      <Data name=\"Other_Analysis\">",other.dat,"</Data>",sep=""),filename,append=TRUE)
 write(paste("
                       <Data name=\"IPR_statement\">",ipr.dat,"</Data>",sep=""),filename,append=TRUE)
 write(paste("
 write("
           </ExtendedData>",filename,append=TRUE)
                                                     <Point><coordinates>",coordinates(Csp.II)[[i,1]],",",coordinates(Csp.II)[[i,2]],"</coordinates></Point>
 write(paste("
</Placemark>",sep=""),filename,append=TRUE)
write("<LookAt id=\"ID\">",filename,append=TRUE)
#Set correct start up location based in country
write(paste(longit),filename,append=TRUE)
write(paste(latit),filename,append=TRUE)
#Set the correct altitute for the data set to be viewed
write(paste(zoom),filename,append=TRUE)
write(" <heading>0</heading>",filename,append=TRUE)
write(" <tilt>0</tilt>",filename,append=TRUE)
write(" <altitudeMode>relativeToGround</altitudeMode>",filename,append=TRUE)
write("</LookAt>For",filename,append=TRUE)
write("</Document>",filename,append=TRUE)
write("</kml>",filename,append=TRUE)
close(filename)
```

#### SCRIPTS FOR GENERATING INTERPOLATED GEOCHEMICAL IMAGES

\*\*\*\*\*\* # Code to create interpolated geochemical images as an overlay kml file # Written by Mark Cave with modifications from Chris Johnson. 20th June 2011 # # Read in the element results from a csv file # This example is for arsenic (As)in stream sediments from England SSAs.dat<-read.table(file="C:/GoogleEarthProject/GBASE As SED ENG.csv" ,sep=",",header=T,stringsAsFactors=F,na.strings=" ") # Read in the outline of sample coverage, here for stream sediments in England OL.dat<-read.table(file="C:/GoogleEarthProject/ENG sediments.csv" ,sep=",",header=T,stringsAsFactors=F) # create a grid of the correct shape library(geoR) library(gstat) # pred grid sets up a grid of spacing by=5000 using limits from OL.dat) gr<-pred grid(OL.dat,by=5000)</pre> #locations.inside pulls out the grid within the bounding area gr<-locations.inside(gr,OL.dat)</pre> # adding an extra column to gr so it can be accepted as a spatial data frame data<-matrix(nrow=(nrow(gr)),ncol=1)</pre> qr<-cbind(qr,data)</pre> #now set up gr as a spatial data frame  $coordinates(qr) = \sim Var1 + Var2$ 

#now convert it to a SpatialPixelsDataFrame gr<-as(gr,"SpatialPixelsDataFrame")

#Make a polygon to bound the study area and project it to geographical coordinates
#(lat/long from British National Grid)
library(sp)
library(rgdal)
library(gpclib)
library(maptools)

# gpclibPermit() # needs to be run first time in a new session

grd <- as(gr, "SpatialPolygons")
proj4string(grd) <- CRS("+init=epsg:27700")
grd.union <- unionSpatialPolygons(grd, rep("x", length(slot(grd, "polygons"))))
II <- CRS("+proj=longlat +datum=WGS84")
grd.union.II <- spTransform(grd.union, II)</pre>

\*\*\*\*

### See page 97 of Applied Spatial Data Analysis for this bit (Hengl,2009)

# Now set up the Element data El.data<-cbind(SSAs.dat[,c(3,4,7)]) # Remove the Tamar data as this is a discrete area we don't wish to grid El.dat<-subset(El.data,EASTING>300000) plot(El.dat\$EASTING,El.dat\$NORTHING)

# Reset highest As results to 98th percentile TL < -quantile(El.dat \$Arsenic, 0.98, na.rm = T)IND=El.dat\$Arsenic>=TL El.dat\$Arsenic[IND==T]<-TL # set up as a spatial data frame  $coordinates(El.dat) = \sim EASTING + NORTHING$ # now do the idw interpolation proj4string(El.dat) <- CRS("+init=epsg:27700")</pre> SSEI II <- spTransform(El.dat, CRS("+proj=longlat +datum=WGS84")) # perform idw extrapolation IISPix\$pred <- idw(Arsenic~1, SSEL II, IISPix,</pre> idp = 2.0, max = 5, debug. level = -1) \$var1. pred ###Output the data to a png raster graphics file png(file="EngSSAs IDW.png", width=llGRD\$width, height=llGRD\$height, bg="transparent") par(mar=c(0,0,0,0), xaxs="i", yaxs="i") image(IISPix, "pred", col=bpy.colors(10)) dev.off() # Create the kml overlav file for Google earth kmlOverlay(IIGRD, "EngSSAs IDW.kml", "EngSSAs IDW.png")

# Appendix 4 :Example of Google Earth KML file generated by R script

The KML file below (WAL\_FOREGS\_SEDIMENT.KML) has been generated by the R script (listed in Appendix 3)

The standard csv input data file used to generate this is also listed at the end of this Appendix. Note that this KML file contains only four samples. The G-BASE sample files can contain in excess of 50,000 samples. Google earth opens centred on the appropriate BGS office and this is achieved by inserting the placemark code immediately before the first sample placemark entry -example for BGS Cardiff is given in Table 4.

```
<?xml version="1.0" encoding="UTF-8"?>
<kml xmlns="http://earth.google.com/kml/2.1">
<Document>
<name>FOREGS Wales stream sediment samples</name>
 <Style id="simple">
   <IconStyle>
     <scale>1.1</scale>
     <Icon>
<href> http://maps.google.com/mapfiles/kml/paddle/blu-circle.png </href>
     </Icon>
   </IconStyle>
   <LabelStyle>
     <color>00ffffff</color>
   </LabelStyle>
   <BalloonStyle>
     <text><![CDATA]
<div style="background-color:#DDDDDD; width:400; font-family:helvetica;" align="center" >
<strong>SAMPLE ID $[SAMPLE ID]</strong>
<strong>Data series: </strong>$[description]
<strong>Date Collected: </strong>$[DATE_COLLECTED] 
<strong>Fraction Analysed: </strong>$[FRACTION_ANALYSED]
<strong>Analytes Determined: </strong>$[Analytes_determined]
<strong>Other Determinands: </strong>$[Other]
<strong>Analytical Method: </strong>$[MAIN_METHOD]
$[Other_Analysis]
$[IPR statement]
<img src=
EGS_logo_ico_small.jpg
</div>
]]></text>
```

</BalloonStyle> </Style> <Placemark id="1"> <name>N35W02S2</name> <description>FOREGS Wales stream sediment samples</description> <styleUrl>#simple</styleUrl> <ExtendedData> <Data name="DATE\_COLLECTED">1998</Data> <Data name="SAMPLE\_ID">N35W02S2</Data> <Data name="Analytes\_determined">Al, As, As\*, Ba, Ba\*, Be@, Ca, Cd@, Ce@, Co, Co\*, Cr, Cr\*, Cs, Cu, Cu\*, Dy@, Er@, Eu@, Fe, Fe\*, Ga, Gd@, Hf@, Hg\, Ho@, K, Li@, Lu@, Mg, Mn, Mn\*, Na, Nb, Nd@, Ni, Ni\*, P, Pb, Pb\*, Pr@, Rb, S\*, Sb@, Si, Sm@, Sn, Sr, Ta@, Tb@, Th, Ti, Tl@, Tm@, U, V, W@, Y@, Yb@, Zn, Zn\*, Zr</Data> <Data name="FRACTION ANALYSED">&lt;0.150 mm</Data> <Data name="Other">TOC=1.33%</Data> <Data name="MAIN\_METHOD">Default method XRFS (Total), some elements (\*) by ICP-AES after aqua regia extraction; ICP-MS (@) following peroxide fusion/acid extraction; Hg-Analyser ().</Data><Data name="Other Analysis">Total Organic Carbon (TOC) by carbon analyser.</Data> <Data name="IPR statement">Data freely available - see http://www.gsf.fi/foregs/geochem/</Data> </ExtendedData> <Point><coordinates>-3.36.52.31</coordinates></Point> </Placemark> <Placemark id="1"> <name>N35W02S3</name> <description>FOREGS Wales stream sediment samples</description> <styleUrl>#simple</styleUrl> <ExtendedData> <Data name="DATE\_COLLECTED">1998</Data> <Data name="SAMPLE ID">N35W02S3</Data> <Data name="Analytes\_determined">Al, As, As\*, Ba, Ba\*, Be@, Ca, Cd@, Ce@, Co, Co\*, Cr, Cr\*, Cs, Cu, Cu\*, Dy@, Er@, Eu@, Fe, Fe\*, Ga, Gd@, Hf@, Hg\, Ho@, K, Li@, Lu@, Mg, Mn, Mn\*, Na, Nb, Nd@, Ni, Ni\*, P, Pb, Pb\*, Pr@, Rb, S\*, Sb@, Si, Sm@, Sn, Sr, Ta@, Tb@, Th, Ti, Tl@, Tm@, U, V, W@, Y@, Yb@, Zn, Zn\*, Zr</Data> <Data name="FRACTION\_ANALYSED">&lt;0.150 mm</Data> <Data name="Other">TOC=1.59%</Data> <Data name="MAIN METHOD">Default method XRFS (Total), some elements (\*) by ICP-AES after agua regia extraction; ICP-MS (@) following peroxide fusion/acid extraction; Hg-Analyser ().</Data><Data name="Other Analysis">Total Organic Carbon (TOC) by carbon analyser.</Data> <Data name="IPR\_statement">Data freely available - see http://www.gsf.fi/foregs/geochem/</Data> </ExtendedData> <Point><coordinates>-3.49.51.89</coordinates></Point> </Placemark> <Placemark id="1"> <name>N36W02S2</name> <description>FOREGS Wales stream sediment samples</description> <styleUrl>#simple</styleUrl> <ExtendedData> <Data name="DATE\_COLLECTED">1998</Data> <Data name="SAMPLE\_ID">N36W02S2</Data> <Data name="Analytes\_determined">Al, As, As\*, Ba, Ba\*, Be@, Ca, Cd@, Ce@, Co, Co\*, Cr, Cr\*, Cs, Cu, Cu\*, Dy@, Er@, Eu@, Fe, Fe\*, Ga, Gd@, Hf@, Hg\, Ho@, K, Li@, Lu@, Mg, Mn, Mn\*, Na, Nb, Nd@, Ni, Ni\*, P, Pb, Pb\*, Pr@, Rb, S\*, Sb@, Si, Sm@, Sn, Sr, Ta@, Tb@, Th, Ti, Tl@, Tm@, U, V, W@, Y@, Yb@, Zn, Zn\*, Zr</Data>

<Data name="FRACTION ANALYSED">&lt;0.150 mm</Data> <Data name="Other">TOC=2.32%</Data> <Data name="MAIN\_METHOD">Default method XRFS (Total), some elements (\*) by ICP-AES after aqua regia extraction; ICP-MS (@) following peroxide fusion/acid extraction; Hg-Analyser ().</Data><Data name="Other\_Analysis">Total Organic Carbon (TOC) by carbon analyser.</Data> <Data name="IPR\_statement">Data freely available - see http://www.gsf.fi/foregs/geochem/</Data> </ExtendedData> <Point><coordinates>-4.51.53.33</coordinates></Point> </Placemark> <Placemark id="1"> <name>N36W02S3</name> <description>FOREGS Wales stream sediment samples</description> <styleUrl>#simple</styleUrl> <ExtendedData> <Data name="DATE\_COLLECTED">1998</Data> <Data name="SAMPLE\_ID">N36W02S3</Data> <Data name="Analytes\_determined">Al, As, As\*, Ba, Ba\*, Be@, Ca, Cd@, Ce@, Co, Co\*, Cr, Cr\*, Cs, Cu, Cu\*, Dy@, Er@, Eu@, Fe, Fe\*, Ga, Gd@, Hf@, Hg\, Ho@, K, Li@, Lu@, Mg, Mn, Mn\*, Na, Nb, Nd@, Ni, Ni\*, P, Pb, Pb\*, Pr@, Rb, S\*, Sb@, Si, Sm@, Sn, Sr, Ta@, Tb@, Th, Ti, Tl@, Tm@, U, V, W@, Y@, Yb@, Zn, Zn\*, Zr</Data> <Data name="FRACTION\_ANALYSED">&lt;0.150 mm</Data> <Data name="Other">TOC=3.82%</Data> <Data name="MAIN\_METHOD">Default method XRFS (Total), some elements (\*) by ICP-AES after aqua regia extraction; ICP-MS (@) following peroxide fusion/acid extraction; Hg-Analyser ().</Data><Data name="Other\_Analysis">Total Organic Carbon (TOC) by carbon analyser.</Data> <Data name="IPR\_statement">Data freely available - see http://www.gsf.fi/foregs/geochem/</Data> </ExtendedData> <Point><coordinates>-3.87,52.73</coordinates></Point> </Placemark> <LookAt id="ID"> <longitude>-3.2387</longitude> <latitude>51.5291</latitude> <altitude>150000</altitude> <heading>0</heading> <tilt>0</tilt> <altitudeMode>relativeToGround</altitudeMode> </LookAt>For </Document> </kml>

#### Standard format csv file (WAL\_FOREGS\_SEDIMENT.CSV) used to generate KML file listed above

FOREGS Wales stream sediment samples,,,,,,

"Default method XRFS (Total), some elements (\*) by ICP-AES after aqua regia extraction; ICP-MS (@) following peroxide fusion/acid extraction; Hg-Analyser (\).",,,,,,

Total Organic Carbon (TOC) by carbon analyser.,,,, Data freely available - see http://www.gsf.fi/foregs/geochem/,,,,, Sample\_id,x,y,Date,Analytes,Other,Fraction

#### N35W02S2,-3.36,52.31,1998,

"Al,As,As\*,Ba,Ba\*,Be@,Ca,Cd@,Ce@,Co,Co\*,Cr,Cr\*,Cs,Cu,Cu\*,Dy@,Er@,Eu@,Fe,Fe\*,Ga,Gd@,Hf@,Hg\,Ho@,K,Li@,Lu@,Mg,Mn,Mn\*,Na,Nb,Nd@,Ni,Ni\*,P,Pb,Pb\*, Pr@,Rb,S\*,Sb@,Si,Sm@,Sn,Sr,Ta@,Tb@,Th,Ti,Tl@,Tm@,U,V,W@,Y@,Yb@,Zn,Zn\*,Zr",TOC=1.33%,<0.150 mm N35W02S3,-3.49,51.89,1998,

"Al,As,As\*,Ba,Ba\*,Be@,Ca,Cd@,Ce@,Co,Co\*,Cr,Cr\*,Cs,Cu,Cu\*,Dy@,Er@,Eu@,Fe,Fe\*,Ga,Gd@,Hf@,Hg\,Ho@,K,Li@,Lu@,Mg,Mn,Mn\*,Na,Nb,Nd@,Ni,Ni\*,P,Pb,Pb\*, Pr@,Rb,S\*,Sb@,Si,Sm@,Sn,Sr,Ta@,Tb@,Th,Ti,Tl@,Tm@,U,V,W@,Y@,Yb@,Zn,Zn\*,Zr",TOC=1.59%,<0.150 mm

N36W02S2,-4.51,53.33,1998,

N36W02S3,-3.87,52.73,1998,

"Al,As,As\*,Ba,Ba\*,Be@,Ca,Cd@,Ce@,Co,Co\*,Cr,Cr\*,Cs,Cu,Cu\*,Dy@,Er@,Eu@,Fe,Fe\*,Ga,Gd@,Hf@,Hg\,Ho@,K,Li@,Lu@,Mg,Mn,Mn\*,Na,Nb,Nd@,Ni,Ni\*,P,Pb,Pb\*, Pr@,Rb,S\*,Sb@,Si,Sm@,Sn,Sr,Ta@,Tb@,Th,Ti,Tl@,Tm@,U,V,W@,Y@,Yb@,Zn,Zn\*,Zr",TOC=3.82%,<0.150 mm

### Example of code generated for kml interpolated image file (Eng\_As\_seds.kml)

<?xml version='1.0' encoding='UTF-8'?>

<kml xmlns='http://earth.google.com/kml/2.0'>

<GroundOverlay>

<name>R image</name>

<Icon><href>As.png</href><viewBoundScale>0.75</viewBoundScale></Icon>

 $<\!\!LatLonBox\!\!<\!\!north\!\!>\!\!55.7888866202127<\!\!/north\!\!>\!\!south\!\!>\!\!51.6526826669131<\!\!/south\!\!>\!\!east\!\!>\!\!1.78655642462359<\!\!/east\!\!>\!\!east\!\!>\!\!east\!\!>\!\!east\!\!>\!\!1.78655642462359<\!\!/east\!\!>\!\!east\!\!\!east\!\!>\!\!east\!\!\!east\!\!\!east\!\!>\!\!east\!\!>\!\!east\!\!\!east\!\!>$ 

3.60749228911763</west></LatLonBox>

</GroundOverlay></kml