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User Guide for the British Geological Survey Stream Sediment Geochemistry (500m Grid) dataset

Open Report OR/17/004



BRITISH GEOLOGICAL SURVEY

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National Grid Reference

SW corner 2880,13440
NE corner 653885,1217750

Front cover

Example map of K₂O concentrations in UK stream sediments. Visualised with the perceptually uniform 'Inferno' colour scale. Brighter = higher concentration, histogram equalised.

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

C Kirkwood, R Lister, F Fordyce, R Lawley

BRITISH GEOLOGICAL SURVEY

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The London Information Office also maintains a reference collection of BGS publications, including maps, for consultation.

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

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

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

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Foreword

This report is the user-guide to the content and application of the national scale Stream Sediment Geochemistry maps produced by the British Geological Survey (BGS) at a 500m grid. This map release, referred to as 'BGS_SedGC_500m', provides the spatial distribution of element concentrations across the United Kingdom as measured and interpolated from the chemical analysis of stream sediments. The purpose of this user guide is to enable those downloading this dataset to have a better appreciation of how the dataset has been created and therefore a better understanding of the potential applications and limitations that the dataset may have.

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Summary

This report explains the methods used by the British Geological Survey (BGS) in the production and visualisation of the national scale Stream Sediment Geochemistry maps (BGS_SedGC_500m).

Acknowledgements

The geochemical data that supports the BGS_SedGC_500m maps has been collected and maintained by the British Geological Survey's Geochemical Baseline Survey of the Environment (G-BASE) project (for samples collected in Scotland, England and Wales) and by the Geological Survey of Northern Ireland's TellusNI project (for samples collected in Northern Ireland). The success of both projects would not have been possible without the efforts of a vast number of volunteer field workers. The released maps represent the combined efforts of the G-BASE, TellusNI and products teams.

1 Introduction

Founded in 1835, the British Geological Survey (BGS) is the world's oldest national geological survey and the United Kingdom's premier centre for earth science information and expertise. The BGS provides expert services and impartial advice in all areas of geoscience. Our client base is drawn from the public and private sectors both in the UK and internationally.

Our innovative digital data products aim to help describe the ground surface and what's beneath across the whole of Great Britain. These digital products are based on the outputs of the BGS survey and research programmes and our substantial national data holdings. This data coupled with our in-house Geoscientific knowledge are combined to provide products relevant to a wide range of users in central and local government, insurance and housing industry, engineering and environmental business, and the British public.

The source data for the product is;

1. Stream sediment analytical data generated by the G-BASE Project (and its predecessors) of the British Geological Survey between 1968 and 2013.
2. Stream sediment analytical data generated by the Tellus NI Project of the Geological Survey of Northern Ireland between 1994 and 2006.

Throughout the lifetime of the G-BASE and Tellus NI projects, strict quality control procedures have been in place at all stages from sample collection to analytical data reporting. Analytical data have been closely monitored to ensure continuity during numerous field campaigns and between different analytical methods. All data have been conditioned with respect to primary reference materials in order to provide both accurate and precise element concentrations with a high degree of confidence.

Further information on all the digital data provided by the BGS can be found on our website at <http://www.bgs.ac.uk/data/digitaldata/digitaldata.cfm> or by contacting:

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2 About the BGS_SedGC_500m Dataset

2.1 BACKGROUND

This dataset represents the first publication of complete national maps from the Geochemical Baseline Survey of the Environment (G-BASE) and TellusNI projects, whose aim was to conduct a national geochemical survey of the United Kingdom in order to improve understanding of our geology and environment and provide quantitative evidence against which to gauge future environmental change.

This dataset consists of a series of interpolated raster (ASCII grid) maps displaying the concentrations of a suite of chemical elements in the stream sediments of the United Kingdom.

2.2 WHO MIGHT REQUIRE THIS DATA?

This dataset is for users who are seeking information about the baseline geochemistry of the United Kingdom at national to regional scales. This quantification of the chemical composition of the ground beneath our feet provides an important source of information for geoscience, environmental science, mineral exploration, and research into the impacts of geology on society; for example on agricultural productivity and human health.

2.3 WHAT THE DATASET SHOWS?

This dataset shows the spatial variation in element concentrations across the United Kingdom. The source data has been interpolated from stream sediment analyses using ordinary kriging. Variations in stream sediment element concentrations are controlled by a combination of underlying geology and surficial environmental processes.

The data are presented as ASCII raster grids covering the landmass of the United Kingdom using a regular grid with a 500m cell size (see figure 1).

For each element, two grids are provided; one containing predicted concentration values and a second grid containing standard deviation values, which provide an indication of the uncertainty associated with the predicted concentrations. These can be viewed simply by dragging and dropping into a GIS package such as QGIS, ArcMap or MapInfo (or using these platforms to convert the ASCII data into their own proprietary grid formats). Colour scales can be assigned according to personal preference, or the traditional classified G-BASE colour scheme can be assigned using the provided colour lookup tables.

The data covers a suite of 18 elements and oxides (in the case of major elements); those included are shown in Table 1 alongside their units of measurement and lower limits of detection, i.e. the lowest concentration that could be reliably measured.

In addition to the 18 elements presented in this dataset, baseline stream sediment data are available for a more extensive suite of elements, however data coverage is incomplete for the entire UK landmass.



Figure 1. Example map of K_2O concentrations in UK stream sediments. Visualised with the perceptually uniform 'Inferno' colour scale. Brighter = higher concentration, histogram equalised.

Table 1 Elements / oxides included in the dataset

Element / oxide	Units	Lower limit of detection (in given units)
As	mg/kg	0.9
Ba	mg/kg	1.0
CaO	weight %	0.050
Cr	mg/kg	3.0
Co	mg/kg	1.5
Cu	mg/kg	1.3
Fe ₂ O ₃	weight %	0.010
La	mg/kg	1.0
Pb	mg/kg	1.3
MgO	weight %	0.3
MnO	weight %	0.005
Ni	mg/kg	1.3
K ₂ O	weight %	0.010
Rb	mg/kg	1.0
U	mg/kg	0.5
V	mg/kg	3.0
Zn	mg/kg	1.3
Zr	mg/kg	1.0

3 Technical Information

3.1 DEFINITIONS

The following definitions apply to the BGS_SedGC_500m dataset.

ORDINARY KRIGING: The interpolation method used to produce the maps is ordinary kriging, a geostatistical method that attempts to provide optimal unbiased predictions according to the spatial autocorrelation of the input data. For this product, the input data are the point-sampled element concentrations.

SPATIAL AUTOCORRELATION: The degree to which a variable e.g. element concentration correlates with itself through space. In nature things that are close together tend to be more similar than things that are far apart, as stated in Tobler's first law of geography – "everything is related to everything else, but near things are more related than distant things". Ordinary kriging constructs a model of how this autocorrelation varies with distance, and uses this to calculate optimal predictions.

CONCENTRATION: The proportion of a material, by weight, that a particular element occupies. This is either reported in mg/kg (equivalent to parts per million) or weight %, depending on the abundance of the element.

STANDARD DEVIATION: A measure of the variation or dispersion of a set of data values. These provide an indication of the uncertainty associated with the predicted concentration value for each grid cell.

3.2 SCALE

The BGS_SedGC_500m dataset provides geochemical predictions on a regular 500x500m grid: each cell covers 0.25km². The original point samples were collected at around one sample per 2.2km². As a result, the data should not be interpreted beyond its original scale of capture.

3.3 FILE DESCRIPTIONS

The BGS_SedGC_500m dataset contains two ASCII grids and a CSV colour table for each element. These are described in table 2 below. Further details about the data can be found in section 3.4 below. An example visualisation of both concentration and uncertainty by two-channel composite map is shown in Appendix 1.

Table 2 File descriptions

FILE NAME	FILE TYPE	DESCRIPTION
UK_Kriged_* element *_concentration_in_stream sediments.asc	ASCII grid containing float value e.g. 23.4	The predicted mean concentration of the element in stream sediments within the grid cell. Units are either mg/kg or weight % (see Table 1 for details of each element).
UK_Kriged_* element *_stdev(uncertainty)_in_stream sediments.asc	ASCII grid containing float value e.g. 7.0	The predicted standard deviation of the element's concentration in stream sediments within the grid cell. An indication of the uncertainty associated with the prediction.
UK_Kriged_* element *_concentration_in_stream sediments_classified_colour_table.csv	CSV table	Table showing the concentration ranges and colours required to replicate our traditional 'G-BASE' colour scheme, which uses percentiles from the point samples, not the map. Colours are provided as both HEX and RGB.

3.4 CREATION OF THE DATASET

The data in the BGS_SedGC_500m dataset has been interpolated from the original stream sediment geochemistry point sample data collected by the G-BASE and TellusNI projects using ordinary kriging.

Ordinary kriging makes use of a variogram – a model of the spatial autocorrelation within the data – in order to optimise the weights given to surrounding sample points when interpolating concentrations to new locations (in this case the cell centres of the output grid). Figure 2 shows the variogram for potassium oxide in the stream sediments of the UK. We can see that the semi-variance (a measure of the difference between values) increases with the distance between sample sites.

While semi-variance is lower at short distances (i.e. neighbouring samples are more similar than distant samples) it never reaches zero, even at zero distance. This difference in values even at the finest scales is known as the nugget effect. For the BGS_SedGC_500m datasets we have handled this nugget effect as measurement error in order to produce a non-exact interpolation (in which the surface does not pass precisely through the data points) to prevent overfitting to noise/outliers.

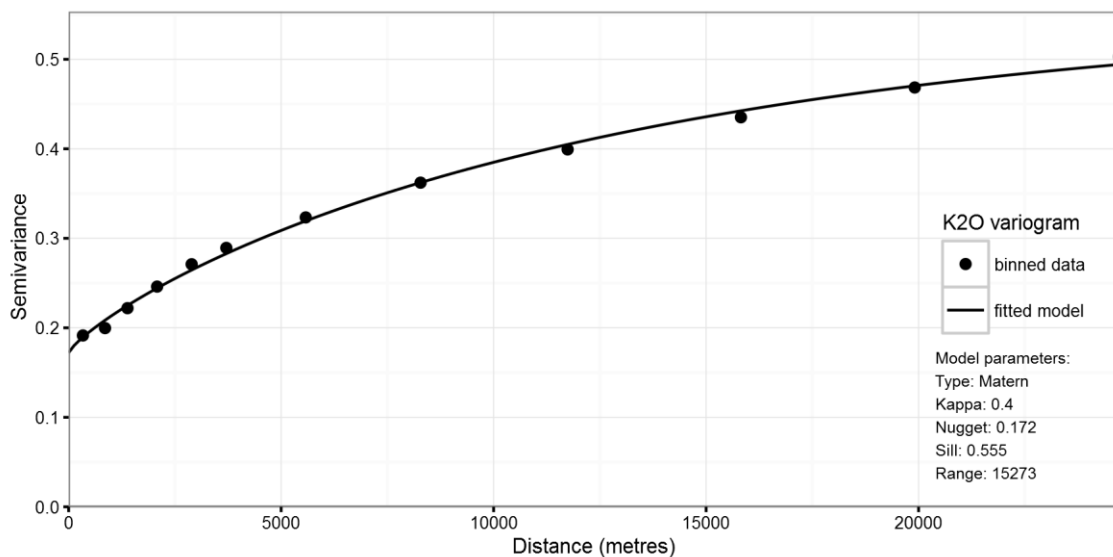
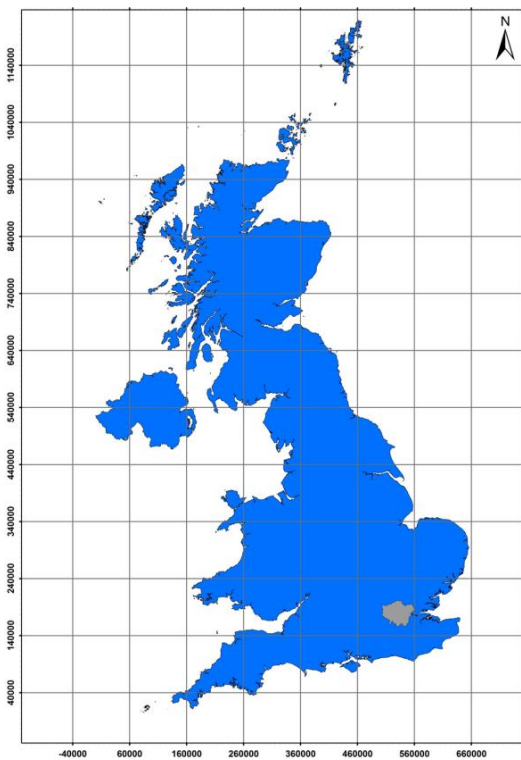


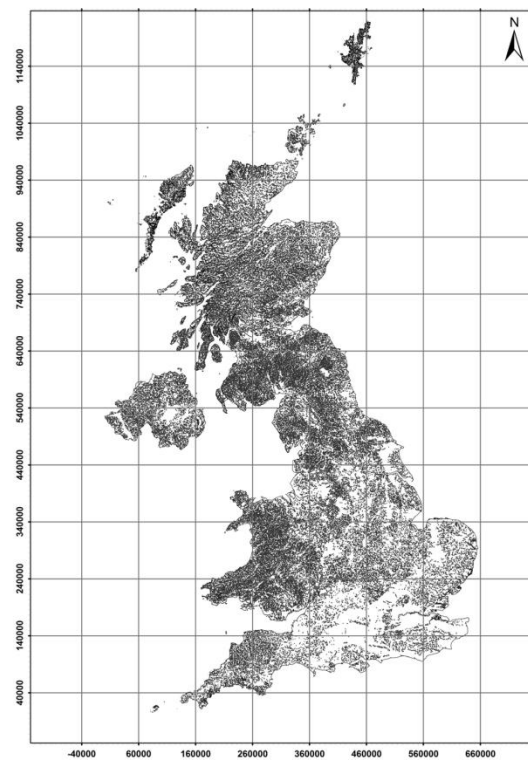
Figure 2. Example variogram of K₂O concentrations in UK stream sediments.

3.5 COVERAGE

This dataset covers the main landmasses of the United Kingdom; England, Scotland, Wales and Northern Ireland but excludes London.



Spatial coverage of the dataset



Stream sediment sample site locations

For the purposes of creating the grids, data from Northern Ireland have been re-projected into the British National Grid co-ordinate system.

The sample site data for G-BASE and TellusNI are available on request from BGS, and are provided in British National Grid or Irish National Grid coordinates as relevant. Further details can be found on the BGS website (<http://www.bgs.ac.uk/gbase/sampling.html>).

Baseline stream sediment data are not presented for the area within the boundary of the Greater London Authority as no surface drainage sampling was carried out in this area. The surface geochemistry of London is visualised by the British Geological Survey's London Earth Project. <http://www.bgs.ac.uk/gbase/londonearth.html>

3.6 DATA FORMAT

The BGS_SedGC_500m dataset has been created as a series of ASCII raster grids. More specialised formats may be available but may incur additional processing costs.

The data may also be downloaded as high resolution PNG images of single element geochemical maps. These maps have been prepared as both colour classified and histogram equalised continuous images for each of the 18 elements presented. (See Appendix 2).

3.7 LIMITATIONS

There are limitations to consider when using the BGS_SedGC_500m grids.

- Each map consists only of predictions generated by a geostatistical model and does not display absolute measurements.
- The grids provide a reasonable approximation of reality that is correct 'on average' but are not immune to error, particularly at fine scales due to the coarse sampling density.
- Grid size is set at 500m x 500m. Data should not be used beyond this scale.
- Data is based on and limited to an interpretation of the G-BASE and Tellus NI records in the possession of British Geological Survey and Geological Survey of Northern Ireland at the time the interpretation was carried out.
- The grids were created by cropping a regular grid to the UK coastline according to whether or not the centre of each grid cell lies on or off land. As a result of this process not all grid cells are contiguous with one-another, for example single offshore cells are present where their cell centre overlies a small land mass, and inland cells may be omitted in situations where the cell centre overlies water.
- Stream sediment sample density is variable over the land surface of the UK. Fewer samples were collected over areas underlain by chalk for example, where surface drainage is less well developed and many streams are ephemeral in their nature. This may result in no interpolated concentration within individual cells.
- This dataset utilises only analytical data derived from the analysis of stream sediment material. Baseline shallow soil data for England will be visualised in a future BGS data product release.

4 Licensing Information

To encourage the use and re-use of this data we have made it available under the Open Government Licence (www.nationalarchives.gov.uk/doc/open-government-licence/version/3/), subject to the following acknowledgement accompanying the reproduced BGS materials: "Contains British Geological Survey and Geological Survey of Northern Ireland materials ©NERC [2016]".

The Open Government Licence is a simple and straightforward licence that allows anyone - businesses, individuals, charities and community groups - to re-use public sector information without having to pay or get permission.

OPENGEOSCIENCE

This dataset falls under BGS' OpenGeoscience portfolio of datasets and services. OpenGeoscience provides a wide range of freely available geoscience information allowing you to view maps, download data, scans, photos and other information. The services available under OpenGeoscience include:

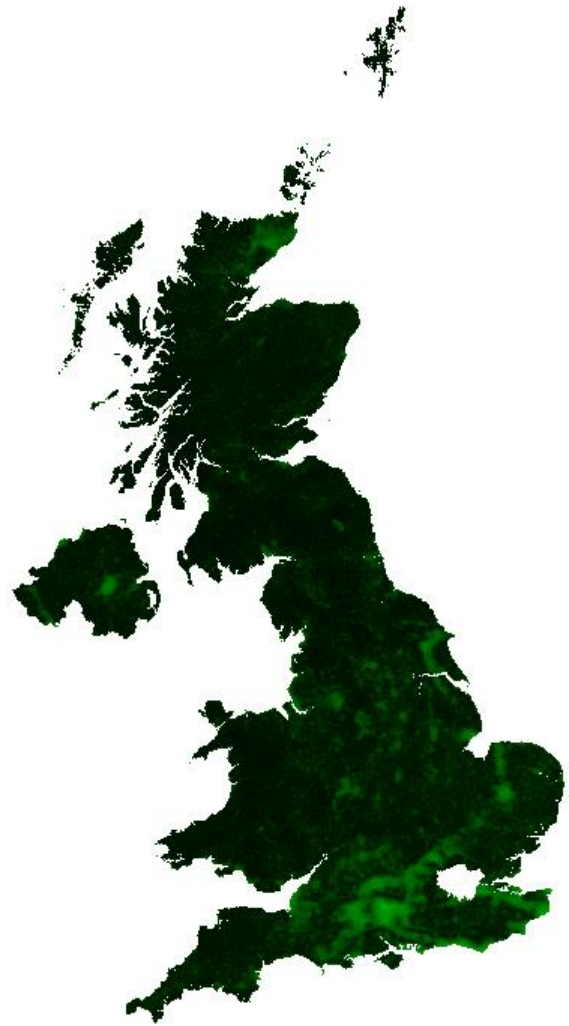
- Map viewers
- Apps
- Downloadable data
- Web services
- Photos and images
- Publications
- Scanned records
- Collections

Please refer to OpenGeoscience (www.bgs.ac.uk/Opengeoscience) for more information and for a full listing of datasets and services available under this service.

Appendix 1



K₂O concentration map on a linear red colour scale (brighter = greater).



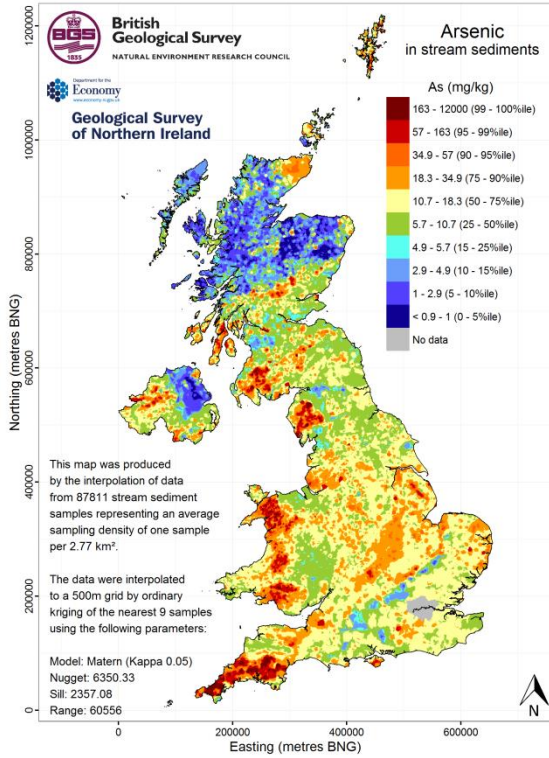
K₂O standard deviation / prediction uncertainty map on a linear green colour scale (brighter = greater).



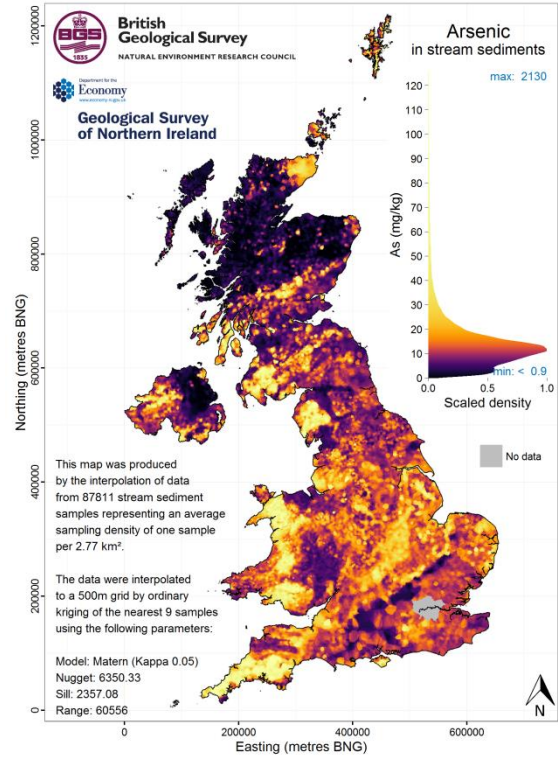
Two-channel K_2O map with concentration in red and standard deviation / uncertainty in green (brighter = greater, both linear).

Appendix 2

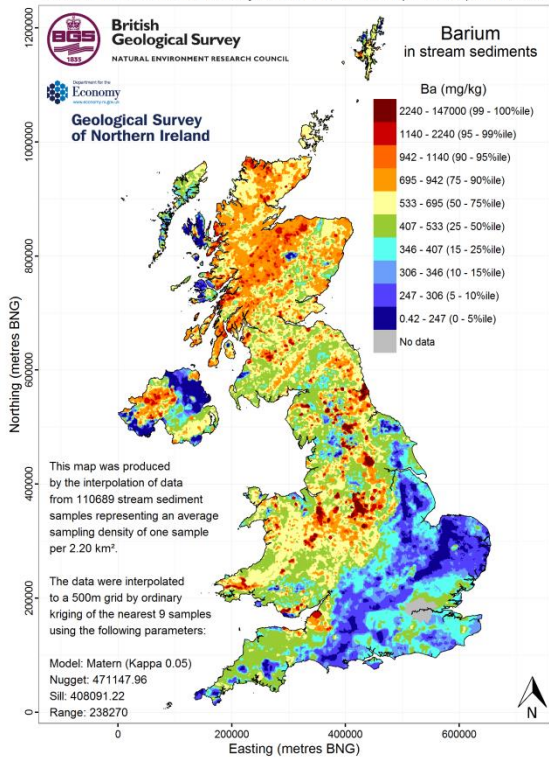
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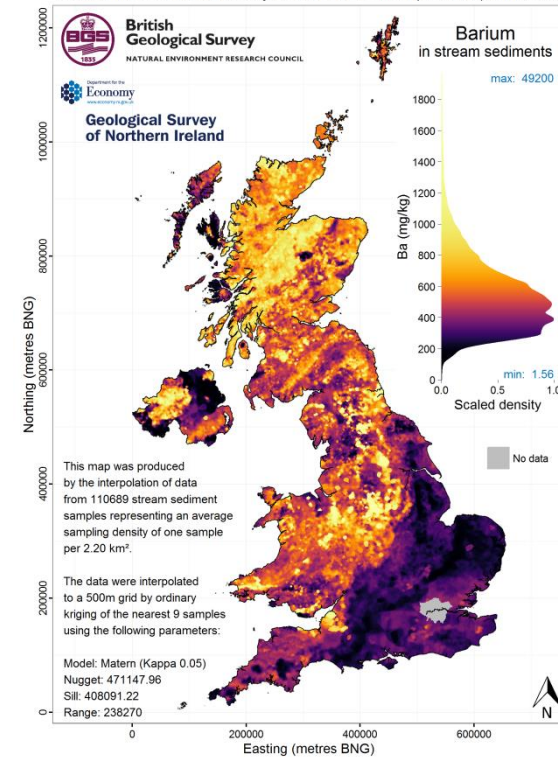
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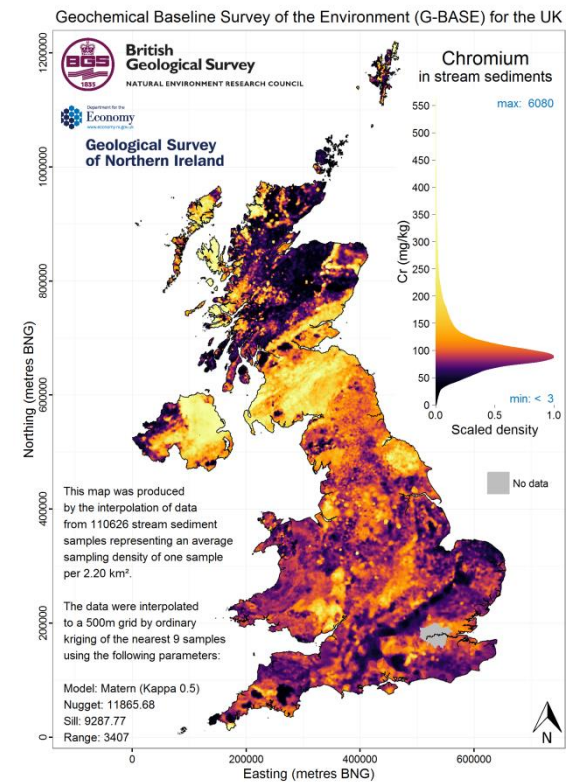
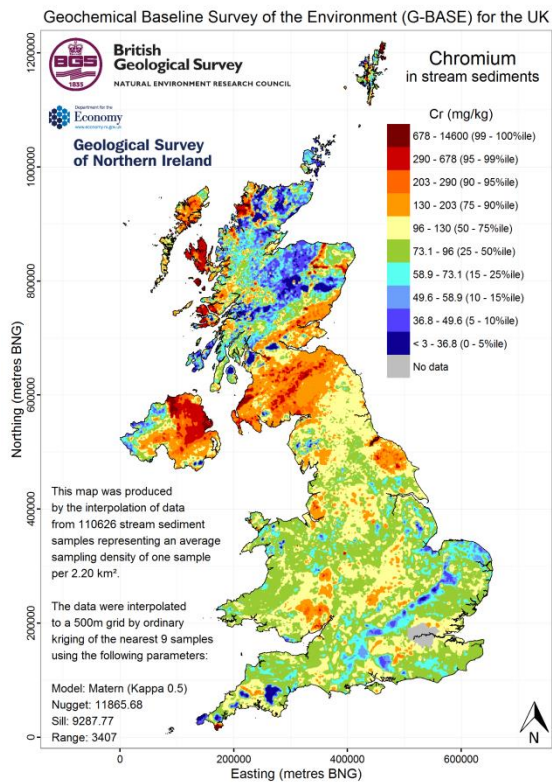
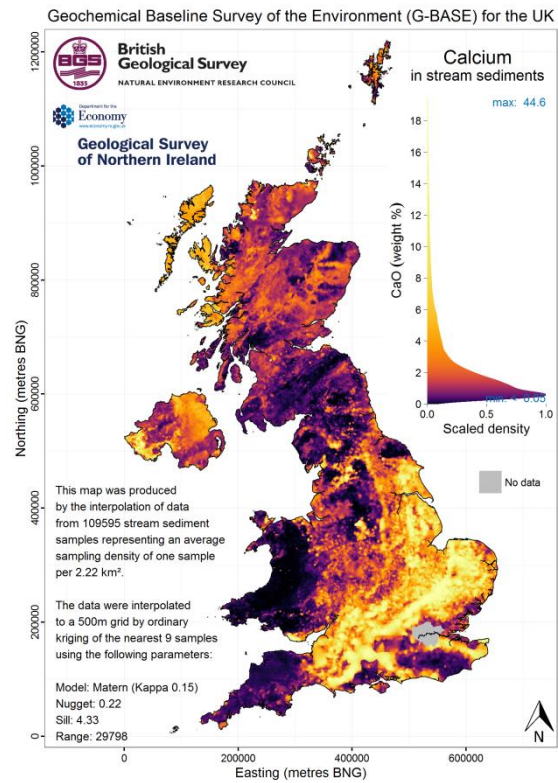
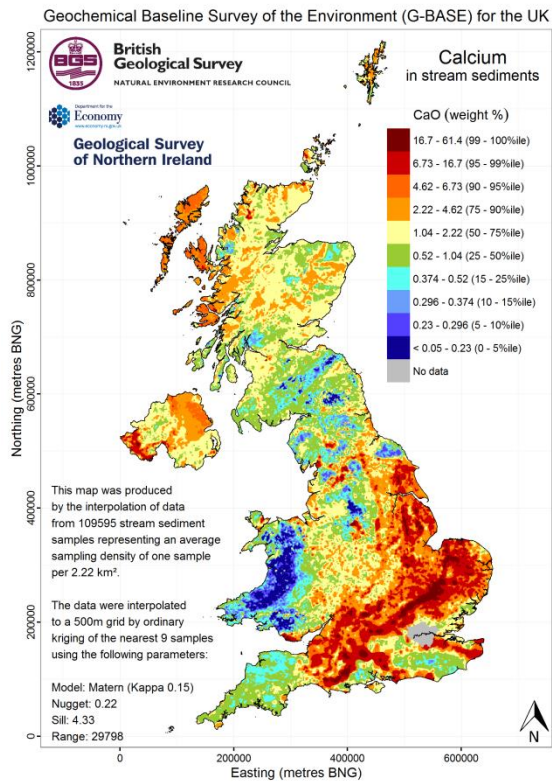


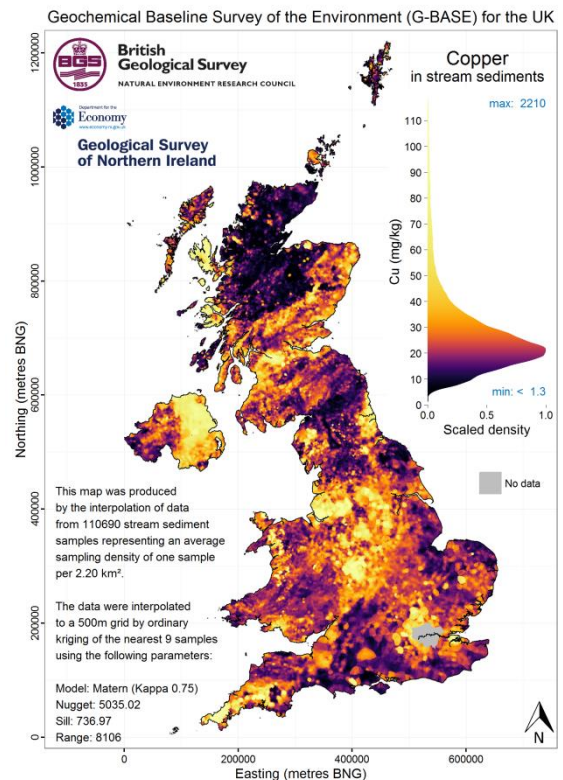
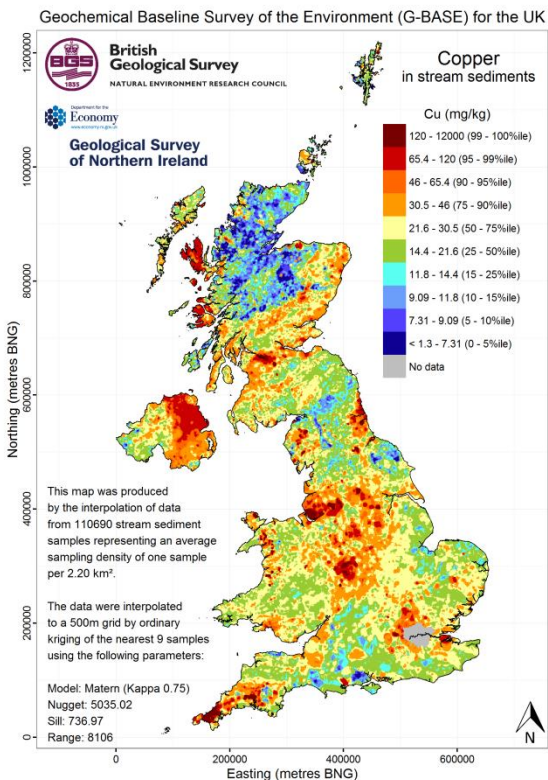
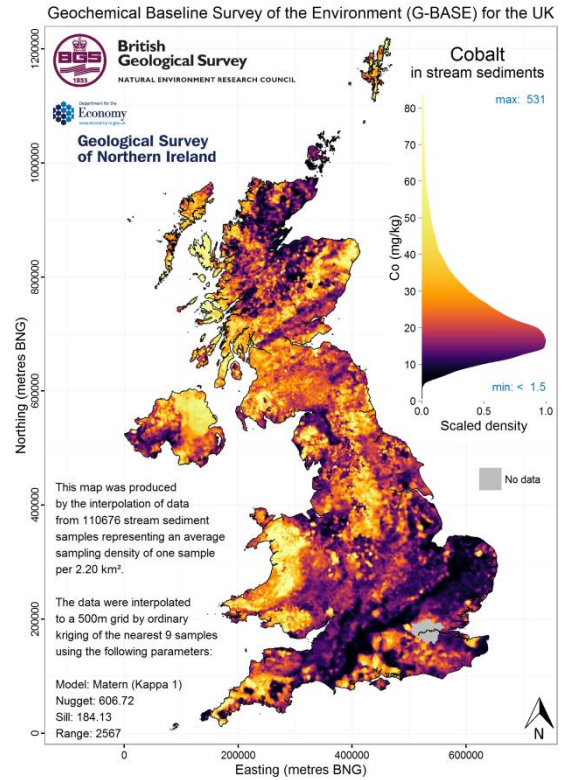
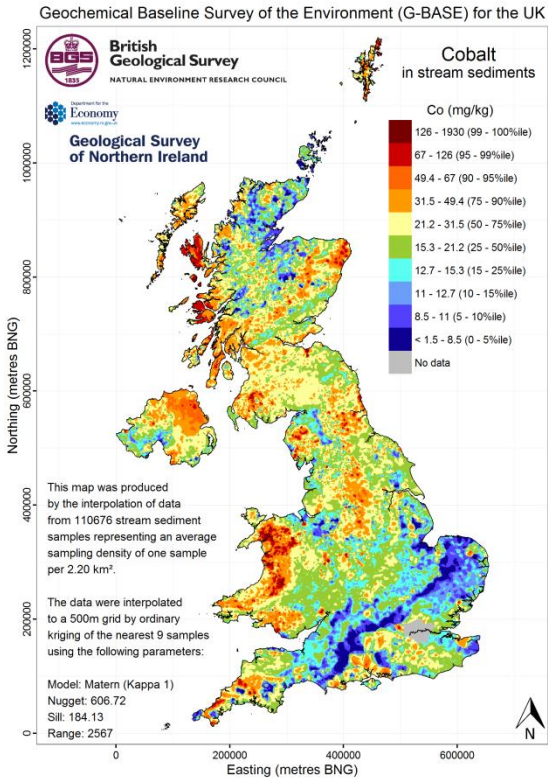
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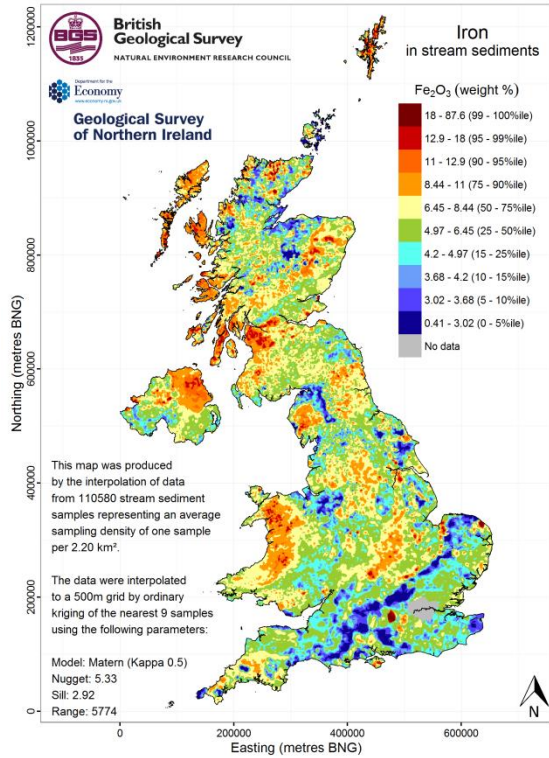
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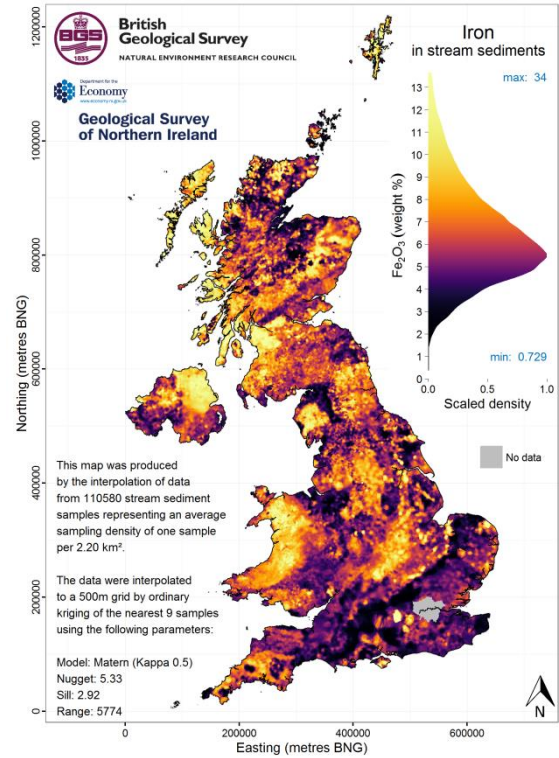




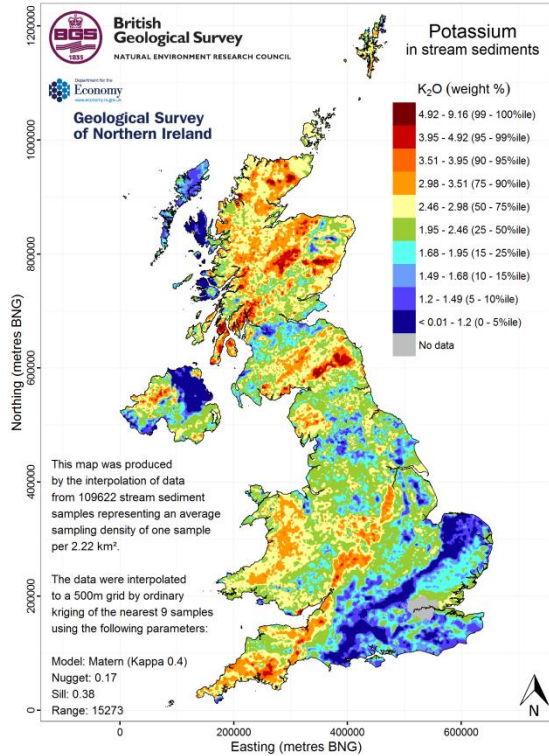
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