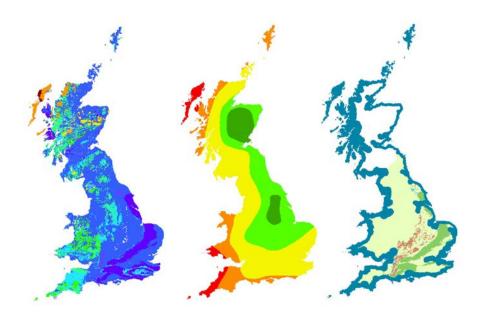


# User guide for the Biosphere Isotope Domains GB (Version 1) dataset and web portal.

NERC Isotope Geosciences Laboratory, and GeoAnalytics and Modelling Programme

Open Report OR/18/005



#### BRITISH GEOLOGICAL SURVEY

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# User guide for the Biosphere Isotope Domains GB (Version 1) dataset and web portal.

JA Evans, K Mee, CA Chenery, CE Cartwright, KA Lee, and AP Marchant

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## Foreword

This report is a user guide for the Biosphere Isotope Domains GB (V1) dataset, which includes (1) a GIS layer for strontium, sulphur and oxygen isotopes (2) datasets of strontium and sulphur isotope measurements from samples across the Great Britain - published separately and available via BGS and (3) a web portal for viewing and querying the data. A description of the data, methodology and assumptions used in the construction of the Biosphere Isotope Domains GB map is included in the associated publications for strontium (Evans, 2018) and sulphur (Chenery, 2018). The primary application of such datasets is for determining the provenance of skeletal material; although the data may also be of use in modern traceability studies of fauna and flora.

## Acknowledgements

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## 1 About the Biosphere Isotope Domains GB (V1) dataset

### 1.1 BACKGROUND

Over the last 20 years there has been a huge development in the application of isotopes as tracers for environment, diet and origin, in fauna and flora, both ancient and modern. The principle behind the use of tracers is that elements such as strontium (Sr), oxygen (O), lead (Pb), sulphur (S), carbon (C), and nitrogen (N) are incorporated into tooth enamel (Sr, O, Pb) and bone and dentine collagen (C,N,S) which preserve the life signature post burial. Since the isotope composition of the elements provides information about the environment and diet, the data can be used to constrain these factors in human and animal studies in both ancient and modern studies. However, the method is dependent on the quality of the reference dataset, and such reference data is dispersed, variable and limited in coverage. The aim of this dataset is to create a model for isotope variation across Great Britain that can be developed though time. The Biosphere Isotope Domains GB (V1) dataset and web portal, provide multi-isotope coverage, with documented uncertainties, of the isotope variations in oxygen, strontium, and sulphur. The datasets for Sr and S are available for downloading. In addition, users of the web portal can input their own sample information to determine the regions across Britain best matched to their isotope data.

### **1.2 WHO MIGHT REQUIRE THESE DATA?**

The primary users of this resource will be archaeologists using skeletal analysis to study the geographic origins, movements and diet in past people and populations. The data can also be used in modern studies of bird and fish migration, tracking sources of illegal importation of materials such as hard wood and ivory and authentication of food origins.

### **1.3 WHAT THE DATASET SHOWS?**

The Biosphere Isotope Domains GB (V1) dataset consists of 3 components:

- 1. GIS dataset showing the distribution of four domains across Britain (strontium, oxygen (groundwater), oxygen (tooth enamel) and sulphur).
- 2. An accompanying web portal for viewing and interrogating the GIS data.
- 3. Datasets for strontium and sulphur isotope values, used in deriving the strontium and sulphur domains in the map, are available as associated publications (Evans 2018 and Chenery 2018).

The Biosphere Isotope Domains GB (V1) GIS layer contains the following four isotope variables across Britain, presented as 1 km hexagon cells:

- 1. Strontium: GB has been subdivided into a number of domains based on the underlying geology and soil parent material (see Section 3.2.1), with each domain being described by their median strontium isotope value and embedded interquartile ranges.
- 2. Oxygen: the oxygen domains show isotope variations in groundwater across Great Britain, as published by Darling et al. (2003).
- 3. Oxygen isotope variations in tooth enamel given as the mean and 1SD of "local" populations as described in Evans et al. (2012).
- 4. Sulphur: the sulphur domains show isotope variation for a number of key geological units (Chalk, Jurassic Clay and Oolitic Limestone) as well as a Coastal Effects (sea spray) zone. Sulphur data are provided as median isotope values and interquartile ranges with the

exception of the Coastal Effects zone which is set at  $\delta^{34}S = 21\%$  to 8‰. (NB: There is currently no sulphur data for Scotland).

## 2 Technical Information

#### 2.1 SCALE

The dataset is represented by 1 km hexagon cells and has been derived from the BGS Geology and BGS Soil Parent Material data, both 1:50,000 in scale and therefore providing 50 m ground resolution.

#### 2.2 FIELD DESCRIPTIONS

 Table 1
 Attribute table field descriptions

FIELD	FIELD	DESCRIPTION
NAME	ТҮРЕ	
SR_DOMAIN	String (254)	Name of the strontium domain (based on geology, unit age,
	-	geography)
SR_MEDIAN	Double	Median strontium isotope value
SR_Q1	Double	First quartile strontium isotope value
SR_Q3	Double	Third quartile strontium isotope value
SR_INTERQR	Double	Interquartile range of strontium isotope values
SR_L_WHISK	Double	Lower whisker of strontium isotope value
SR_U_WHISK	Double	Upper whisker of strontium isotope value
SR_COUNT	Long integer	Number of sample measurements used in statistical analysis
SR_MIN	Double	Minimum strontium isotope value
SR_MAX	Double	Maximum strontium isotope value
SR_MEAN	Double	Mean strontium isotope value
SR_1SD	Double	Strontium isotope value to 1 standard deviation
S_DOMAIN	String (50)	Name of the sulphur domain
S_MEDIAN	Double	Median sulphur isotope value
S_Q1	Double	First quartile sulphur isotope value
S_Q3	Double	Third quartile sulphur isotope value
S_INTERQR	Double	Interquartile range of sulphur isotope values
S_L_WHISK	Double	Lower whisker of sulphur isotope value
S_U_WHISK	Double	Upper whisker of sulphur isotope value
S_COUNT	Short integer	Number of sample measurements used in statistical analysis
S_MIN	Double	Minimum sulphur isotope value
S_MAX	Double	Maximum sulphur isotope value
S_MEAN	Double	Mean sulphur isotope value
S_1SD	Double	Sulphur isotope value to 1 standard deviation
O_H2O_MIN	Double	Minimum oxygen isotope value from water samples
O_H20_MAX	Double	Maximum oxygen isotope value from water samples
O_TE_MIN	Double	Minimum oxygen isotope value from tooth enamel
O_TE_MAX	Double	Maximum oxygen isotope value from tooth enamel
VERSION	String (50)	Version number of the Biosphere Isotope Domains GB GIS dataset

## 3 Creation of the Dataset

### 3.1 ISOTOPE METHODOLOGY

#### 3.1.1 Overview

This dataset brings together the oxygen isotope groundwater map published by Darling et al. (2003), an update to the Sr isotope biosphere map, published by Evans et al. (2010), a new sulphur dataset for plants in England and Wales, and the oxygen isotope composition of human tooth enamel based on Evans et al. (2012). These four layers can be interrogated to produce a distribution map of the different isotope compositions that can be found across Britain. This is Version 1 of the dataset, which will be developed over time, as more samples are collated.

### 3.1.2 Sample types

A variety of sample types have been used in this study. They represent different aspects of the biosphere and hydrosphere and are sampled at different scales.

**Water** (Sr study). This includes river water, pond/lake water, borehole, and tap waters. River water samples provide an average value for the catchment areas of the stream/river. They can have variable isotope composition depending upon season and rainfall (Shand et al., 2007) and may introduce values into an area that are typical of the upper catchment rather than water from the immediate area of interest. Borehole water will provide an aquifer value most appropriate to wells and mineral water. Modern tap water will be the average of a large modern catchment system or possibly desalinated water in some parts of the world. Lake water will be a mixture of rainwater, river feeder system and equilibration with the lake bed.

**Groundwater (O study).** Groundwater  $\delta^{18}$ O represents a long term bulk rainfall composition and is reasonably representative of long-term rainfall across Britain. British groundwater samples were collected from shallow boreholes, local wells and pumping stations across England, Scotland, Wales and Northern Ireland (see Darling et al., 2003).

**Plants (Sr study)**. Plants provide a direct biosphere measurement. The advantages of plant samples are that they are ubiquitous and reliably geo-located. However, they only sample a small area of land and assumptions have to be made about the relationship between the isotope composition of a plant and that of fauna which consume them. In addition, they may reflect modern, rather than historic compositions. The plants collected for Sr analysis are generally collected away from agricultural land to avoid fertilizer contamination.

**Plants (S study)**. Vegetation sample sites were positioned within fields of at least 25 x 50 m at a minimum distance of 200 m from railways and major roads, and at least 100 m from high power electricity cables, to avoid anthropogenic contamination. Samples were composed of mixed grassland species dominated by grasses for the Geochemical Mapping of Agricultural Soils of Europe project (GEMAS) and grass/mainly mixed herbaceous plants for the remainder.

**Archaeological dentine/bone (Sr study)**. This material has the advantage that, when buried, it will equilibrate with strontium in groundwater close to the time of burial (Trueman et al., 2004) and thus provides a method for looking at the strontium isotope composition of diagenetic fluids from the past and provides a comparison with modern data. It is commonly used as a reference sample for the local burial environment for provenance studies based on tooth enamel and hence a number of dentine or bone analyses have been accumulated though time.

### 3.2 GIS METHODOLOGY

#### 3.2.1 Strontium isotope domains

The Sr isotope domains were created by first dividing Great Britain into 5 broad geological groups: clay, igneous, limestone, sandstone and organic material. These were then subdivided into 56 domains based on geology, age and geography. Geological and age groupings were derived from the BGS Geology GB (Version 8) and the BGS Parent Material GB (Version 6) datasets, whilst their Sr isotope ranges were derived from ~ 900 samples from plants, water and bones (Figure 1), as well as theoretical interpolations. Some geological units, such as many of the smaller igneous intrusions in Wales, Scotland and the English Lake District, could not be assigned to strontium isotope domains and therefore have no associated strontium data. These areas are represented by values of -999 in the following fields of the attribute table: SR\_MEDIAN, SR\_Q1, SR\_Q3, SR\_INTERQR, SR\_L\_WHISK, SR\_U\_WHISK, SR\_COUNT, SR\_MIN, SR\_MAX, SR\_MEAN and SR\_1SD. The full strontium isotope dataset is available to download from the BGS website (Evans, 2018).



Figure 1 Distribution of samples collected across Great Britain used in defining Sr isotope domains.

Once the domains were determined, the map of Great Britain was divided into 1 km hexagons, (each hexagon side length being 1 km). Each hexagon was assigned strontium values based on the domain that covered the largest area of that cell. Table 1 lists the attributes attached to each cell. Figure 2 shows the 57 different domains used for attributing strontium isotope values across Britain.

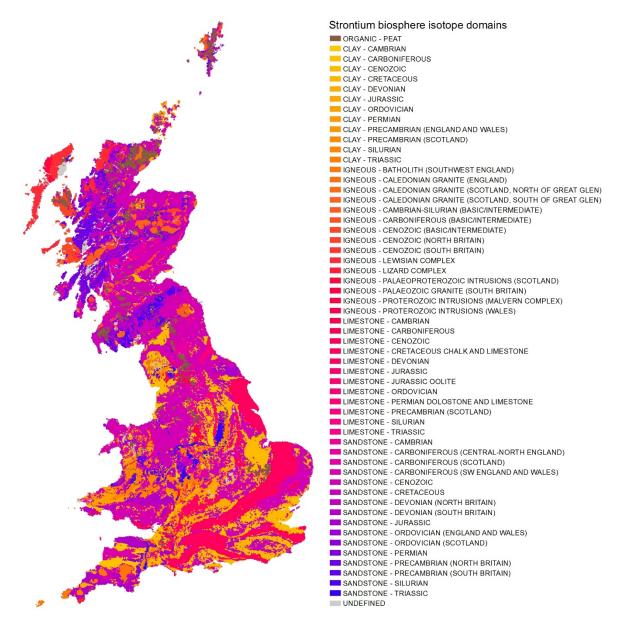
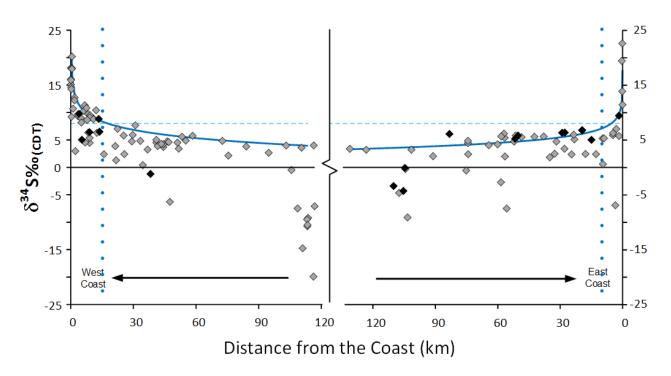


Figure 2<sup>87</sup>Sr/<sup>86</sup>Sr isotope domains.

#### 3.2.2 Sulphur isotope domains

The sulphur isotope domains comprises five domains: three that have sufficient data to characterize them individually based on geology (Jurassic Clay, Jurassic Oolitic Limestone and Chalk); one based on the effects of sea spray (Coastal Effects) and a final domain for all other regions of England and Wales (Other Geological Substrates, England and Wales). The geological domains are derived from the strontium isotope domains. A buffer zone around the GB coastline was used to create the 'Coastal Effects' domain (sea spray), which typically has higher sulphur isotope values than the other domains and is allocated the range  $\delta^{34}S = 21\%$  to 8‰. The Coastal Effects domain refers to the region inland from the coastline that is regularly affected by spray from the sea, either directly or incorporated in rain. Figure 3 illustrates a cut off value of 8‰ (horizontal dashed line) to be taken as the lower limit of costal influence. This influence occurs up to 15 km in from the west coast and 10 km in from the east coast (vertical dotted lines).



**Figure 3** The change in  $\delta^{34}$ S (VCDT) values in plants over distance from the coast.

The final sulphur isotope domain, 'Other Geologic Substrates England & Wales', is a composite of the remaining data from England and Wales. NB: There are currently no data for Scotland except in the Costal Effects zone. These hexagons are represented by values of -999 in the following fields of the attribute table: S\_MEDIAN, S\_Q1, S\_Q3, S\_INTERQR, S\_L\_WHISK, S\_U\_WHISK, S\_COUNT, S\_MIN, S\_MAX, S\_MEAN and S\_1SD. Figure 4 shows the distribution of the sulphur isotope domains across Britain.

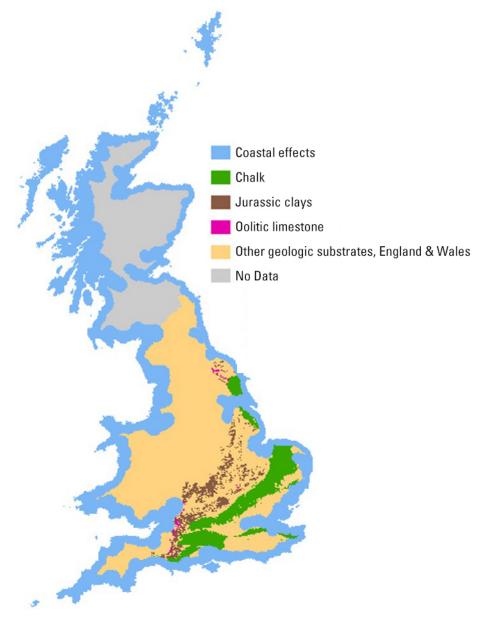
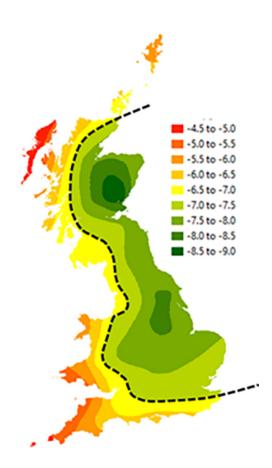


Figure 4 Distribution of sulphur isotope domains across Great Britain.

#### 3.2.3 Oxygen isotope domains

The oxygen isotope domains comprise two components: data derived from ground water samples  $\delta^{18}O_{drinking water} \%$  (VSMOW) and data derived from the measurement  $\delta^{18}O_{phos} \%$  (VSMOW) in human tooth enamel. The groundwater data were first published by Darling et al. (2003) as a series of contours across Britain reflecting specific ranges of oxygen isotope values (Figure 5).



**Figure 5**  $\delta^{18}O_{drinking water} \%$  (VSMOW) contours derived from the analysis of groundwater samples across Britain (after Darling et al., 2003).

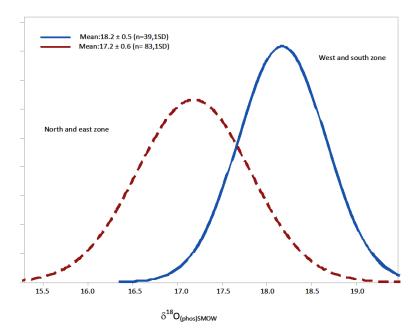


Figure 6 The datasets for the  $\delta^{18}O_{phos}$ % (VSMOW) human enamel which characterize the twofold subdivision of Great Britain.

Fractionation of oxygen isotope occurs when water is ingested and this is why there is a significant difference in the isotope composition between the measured groundwater and the tooth enamel

values Levinson et al. (1987). The boundary in the tooth enamel dataset is taken as the -7.0‰ groundwater contour, with values of 16.6‰ to 17.9‰ to the east of -7.0 contour and values of 17.7‰ to 18.8‰ to the south and west of the contour (Figure 6). For further details of these data see Evans et al. (2012).

#### 3.3 USING THE WEB PORTAL

The webpage that hosts this site is:

http://www.bgs.ac.uk/sciencefacilities/laboratories/geochemistry/gtf/environmentalTracers.html.

And should be referenced as:

J.A. Evans, C.A. Chenery, K. Mee, C.E. Cartwright, K A. Lee, A.P. Marchant, and L. Hannaford (2018): Biosphere Isotope Domains GB (V1): Interactive Website. British Geological Survey. (Interactive Resource). <u>https://doi.org/10.5285/3b141dce-76fc-4c54-96fa-c232e98010ea</u>

The Biosphere Isotope Domains can be interrogated by typing a value (or values) into the appropriate query boxes. The query will highlight in orange on the map all the areas of GB in which fall within the designated statistical ranges. The highlighted areas therefore represent regions which cannot be excluded as a source/match for the interrogation.

The results can be download by generating a report within the webpage.

#### 3.4 DATASET HISTORY

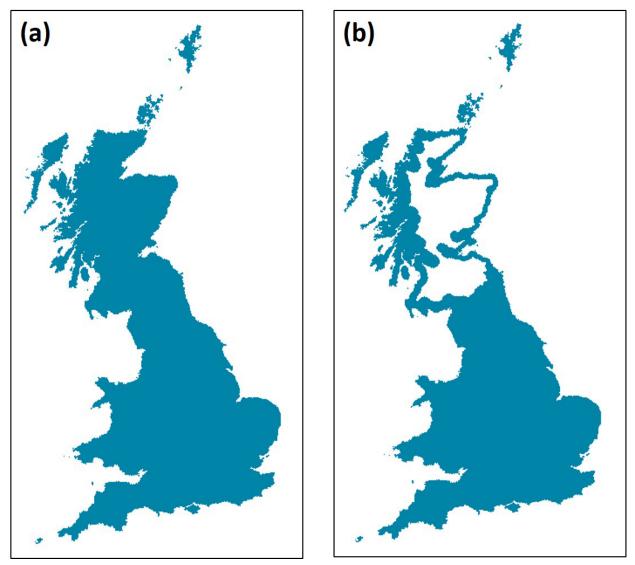
This is Version 1 of the Biosphere Isotope Domains GB dataset.

- Much of the strontium data were published in Evans et al. (2010) but this has been added to considerably from both published and unpublished datasets, as well as data from the NERC Isotope Geosciences Laboratory (NIGL).
- Groundwater oxygen isotope data is from Darling et al. (2003).
- Human tooth enamel data is from Evans et al. 2012.
- Plant sulphur isotope data from a new dataset produced by NIGL.

#### 3.5 COVERAGE

The Biosphere Isotope Domains GB (V1) dataset covers all of Great Britain, including the Shetland Islands, Orkney Islands, Outer Hebrides, Isles of Scilly and the Isle of Wight. It does not currently extend to Northern Ireland.

Strontium and oxygen isotope coverage is for all of Great Britain but coverage is inconsistent and variable. The sulphur domains cover England and Wales only; inland Scotland has no coverage, however the Coastal Effects domain has been extrapolated into Scotland (Figure 7).



**Figure 7** The coverage of the Biosphere Isotope Domains (V1) dataset: (a) coverage of the strontium and oxygen domains; (b) coverage of the sulphur domains (no coverage in Scotland except for the Coastal Effects domain).

### 3.6 DATA FORMAT

The Biosphere Isotope Domains GB (V1) dataset has been created as vector polygons and are available in ESRI ArcGIS (.shp) format. More specialised formats may be available upon request. The strontium and sulphur isotope data that underpin this dataset are also available as separate spread sheets from the BGS.

### 3.7 LIMITATIONS

There are a number of limitations that should be taken into account when using the Biosphere Isotope Domains GB (V1) dataset.

### 3.7.1 Data density and statistical reliability

• The strontium domains that have been constructed have variable numbers of samples with which to define their statistical characteristics. Some of the large datasets e.g. Chalk (n=85) and Jurassic Clay (n=100) can be viewed as statistically robust, whereas others display a large range of values over a limited number of samples, such as the Southwest England Batholith (n=2).

- Areas for which there are no data have been extrapolated using comparable datasets. For example, there are no data from sediments in the Lake District: all of these lithologies are defined by Welsh data from comparable lithologies.
- Where Count is given as 0, there are no measured data and the values have been estimated. These domains include:
  - Igneous Caledonian Granite (England)
  - o Igneous Palaeozoic Granite (South Britain)
  - o Igneous Paleoproterozoic Intrusions (Scotland)
  - o Igneous Proterozoic Intrusions (Wales)
  - Several carbonate domains for these examples, average strontium isotope values have been derived from seawater curves from McArthur et al. (2001) and an interquartile range of +/- 0.001 has been assigned.
- All of the strontium domains represent a mixture between <sup>87</sup>Sr/<sup>86</sup>Sr originating from soils with a variable contribution from rainwater and therefore it is expected that the extent of rainfall and water logging will affect the bioavailable values. Some sense of this variation can be derived from comparison of the upper quartile map, which tends towards the more geologically dominant biosphere values and the lower quartile map, which will reflect a greater rainwater contribution of strontium with a value of 0.7092 (McArthur et al., 2001).
- Sulphur isotope data are only available for England and Wales.
- The Coastal Effects domain is the extent that sea spray and sulphur rainout are likely to affect plant  $\delta^{34}S$ .
- The upper limit for the Coastal Effects domain is defined as the  $\delta^{34}$ S value of seawater (21.0 ± 0.2‰ VCDT.
- The lower limit for the Coastal Effects domain is fixed at 8.0%VCDT and was determined as a major inflection point in Probability and Kernel Density plots of all the vegetation  $\delta^{34}$ S data.
- The sea spray aerosol  $\delta^{34}$ S contribution to the Coastal Effects domain diminishes rapidly the further away from the coast one goes. As a result of prevailing wind directions and the topography, not all coastal areas will be affected in the same way, usually due to the rain shadow effect.
- The physical extent of the Coastal Effects domain is defined as the area up to 15 km inland from the west coast and 10 km inland from the east coast, see Figure 3.
- $\delta^{34}$ S values >15.0‰ VCDT analysed in this study, only occur in samples collected within the tidal zone.
- Areas where the substrate is permanently or intermittently waterlogged or is poorly draining (such as clay substrates) tend to have low  $\delta^{34}S$  values (<0.0‰) due to the effects of sulphur reducing bacteria. These areas include marshes, bogs and fluvial settings, and can be found along the coast as well as inland. Where reducing conditions exist within the Coastal Effects domain, the sea spray effect will have a less obvious impact on the  $\delta^{34}S$

values. In areas where the substrate is porous/freely draining, the sea spray sulphur aerosol effect will also be negligible as the residence time in the soil will be very short.

## 4 Licensing Information

To encourage the use and re-use of this data we have made it available under the Open Government Licence (<u>www.nationalarchives.gov.uk/doc/open-government-licence/version/3/</u>), subject to the following acknowledgement accompanying the reproduced BGS materials: "Contains British Geological Survey materials ©UKRI [2018]".

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### 4.1 **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 (<u>www.bgs.ac.uk/Opengeoscience</u>) for more information and for a full listing of datasets and services available under this service.

# Glossary

### 4.2 **DEFINITIONS**

Biosphere	The regions of the surface and atmosphere of the earth or another planet occupied by living organisms.
Count	The number of sample values used to define a category within an isotope domain.
Domain	Refers to the 3 different elements (Sr, O, S) and their isotope variations described in this dataset.
Hexagon	The shape of the cells in the map representing the isotope domains data.
Hydrosphere	Refers to atmospheric water (precipitation), surface and groundwater.
Interquartile range	Is a measure of statistical dispersion, being equal to the difference between 75th and 25th percentiles centred around the median of the sample, excluding statistical outliers.
Isotope	Each of two or more forms of the same element that contain equal numbers of protons but different numbers of neutrons in their nuclei, and hence differ in relative atomic mass but not in chemical properties; in particular, a radioactive form of an element.
Lower whisker	Represent the lower 25% of the data set around the median value, excluding statistical outliers.
Median*	Denoting or relating to a value or quantity lying at the midpoint of a frequency distribution of observed values or quantities, such that there is an equal probability of falling above or below it.
Maximum value	The highest value in a data set.
Mean*	The central value of a discrete set of numbers: specifically, the sum of the values divided by the number of values.
Minimum value	The lowest value in a data set.
Coastal Effects zone	The zone around the coast effected by precipitation containing dissolved S and Sr from sea spray aerosol with isotopic values comparable to marine values.
Soil parent material	A geological deposit over, and within which, a soil develops. Typically, the parent material is the first recognisably geological deposit encountered when excavating beneath the soil and represents the very-near-surface geology (see Lawley, 2011).
Statistical uncertainty	The margin of error of a measurement, when explicitly stated, and is given by a range of values likely to enclose the true value.
Subdomain	The subdivision of the isotope domain layers, based on geology (including soil parent material), age of deposit and geography, into zones of similar isotopic ranges.
Upper whisker	Represent the upper 25% of the data set around the median value.
1 Standard deviation (1SD)	A measure, for a set of data, of the spread from its mean. It is calculated as $\sqrt{\sum \frac{(x-\bar{x})^2}{n-1}}$ or the square root of variance by determining the variation between each data point relative to the mean.
1 <sup>st</sup> Quartile (Q1*)	The lower half of the interquartile range representing the upper 25 to 50% of the data set, excluding statistical outliers.
3 <sup>rd</sup> Quartile (Q3*)	The upper half of the interquartile range representing the upper 50 to 75% of the data set, excluding statistical outliers.

\*Calculated using Excel functions.

## References

British Geological Survey holds some 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>https://envirolib.apps.nerc.ac.uk/olibcgi</u>.

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