Contents

IMPORTANT SOIL SAMPLE AND ANALYTICAL INFORMATION ................................................................. 3
AGGREGATE SAMPLES, SOIL DEPTH AND FRACTION SIZE ................................................................. 3
TOTAL AND PARTIAL ANALYTICAL DETERMINATIONS ........................................................................ 3
SCALE AND USE OF NORMAL BACKGROUND CONCENTRATIONS ....................................................... 6
USE OF VARIOGRAMS ............................................................................................................................ 6
NATIONAL MAP SHOWING THE DISTRIBUTION OF NICKEL IN TOPSOILS ............................................. 7
DESCRIPTIVE STATISTICS FOR NICKEL IN TOPSOIL DATA ..................................................................... 9
NICKEL Domain percentile classifications ............................................................................................... 9
DESCRIPTIVE STATISTICS COPPER TOPSOIL DATA SET ........................................................................ 10
DATA DISTRIBUTIONS ............................................................................................................................ 12
LANDSCAPE DATA USED TO DEFINE CONTAMINANT DOMAINS ...................................................... 14
SOIL PARENT MATERIAL .......................................................................................................................... 14
METALLIFEROUS MINING AND MINERALISATION .............................................................................. 15
SUMMARY OF STATISTICAL PROCEDURE TO DETERMINE NBCS ...................................................... 16
ACCESS TO DATA AND INFORMATION RESOURCES USED TO CALCULATE NBCS .............................. 19
PROJECT REPORTS AND INFORMATION .................................................................................................. 19
PRINCIPAL CONTAMINANT DATA SETS FOR ENGLAND ...................................................................... 19
SOIL PARENT MATERIAL .......................................................................................................................... 19
LAND USE DATA INCLUDING METALLIFEROUS MINING AND MINERALISATION .................................. 19
FURTHER READING ................................................................................................................................. 20
List of Figures

Figure 1: Comparison of topsoil Ni concentrations in NSI samples determined by XRFS and by ICP-AES following an aqua regia acid digest ...................................................................................................................................................... 4

Figure 2: Comparison of GEMAS topsoil Ni data by analytical method and categorised by land use type……………….. 4

Figure 3: Comparison of topsoil As concentrations in Northern Ireland (Tellus Project) by XRFS and aqua regia digest ICP-MS (excluding 2 extreme outliers)....................................................................................................................... 5

Figure 4: National map of nickel distribution in topsoils with county boundaries (using G-BASE and NSI (XRFS) results) ....................................................................................................................................................................................................... 7

Figure 5: Probability plot of topsoil Ni results categorised by domains................................................................. 12

Figure 6: Boxplot of Ni topsoil results attributed to domains ................................................................................ 12

Figure 7: Flow chart for the calculation of the NBC for a given contaminant domain................................. 16

List of Tables

Table 1: A summary of the nickel domain percentile classifications. Domain NBCs shown in bold red ................. 9

Table 2: Descriptive statistics of underlying primary data sets for Ni in all topsoils .................................................. 11

Acknowledgments

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When referring to this document the following bibliographic reference should be made:


The nickel Technical Guidance Sheet which this document supplements:

Technical Guidance Sheet (TGS) on normal levels of contaminants in English soils

Supplementary Information

Important soil sample and analytical information

Aggregate samples, soil depth and fraction size

Both the NSI (XRFS) and G-BASE data sets are derived from a soil sample that has been aggregated (composited) from a number of subsamples collected over the area of a site, rather than a single point sample. In the case of NSI this is 25 cores (subsamples) from a 20-m square (McGrath and Loveland 1992) whereas G-BASE is 5 cores, also from a 20-m square (Johnson et al. 2005; Fordyce et al. 2005). If a sample is collected as a single core, and the result is compared to the NBC, it is important to be aware that short-range variation (which can be substantial) for the single core sample will be potentially much greater than for the samples from which the NBC values are derived (Lark, 2012).

Soil samples used to calculate the Ni NBCs have been collected from the top 15 cm of the mineral soil profile (hence they are referred to as topsoils). When the sample is collected from a site covered with vegetation the surface organic layers does not form part of the sample collected. This is important for two reasons. Firstly, any recently deposited airborne particulates that have not yet migrated into the soil profile will not be sampled and secondly, surface organic material (litter), which has the capacity to fix some contaminants from atmospheric deposition, is not included as part of the sample. In urban areas the top 15 cm will reflect historical urban land uses and in rural agricultural areas, where relevant, will be within the ploughed horizon. Surveys targeting recent airborne pollution added to the soil will generally only collect from the top 2 cm of the profile in order to bias the soil results toward the airborne pollutant inputs. Such data has not been used in the NBC calculations.

Another consideration is the soil size fraction to be submitted for chemical analysis. The <2 mm fraction is widely used for soil analyses. However, other fractions are sometimes reported (e.g. <150 µm) in order to enhance some chemical contrasts and to reduce variability in the chemical results – coarser grains mean that a single “nugget” will give rise to greater variability in the analyses than will occur with a finer more homogenous material. The NBCs calculated here are exclusively based on the <2 mm soil fraction.

Total and partial analytical determinations

There are established international procedures and standards for the determination of naturally occurring elements in the Earth’s surface environment (Darnley et al. 1995). These procedures have been set up in order to develop a global database of chemical results that is compatible and of sufficient quality to be used for environmental and resource management. The analytical requirements to realise this objective includes: “The total amount of each element present is the most fundamental (and reproducible) quantity in any sample, therefore direct measurement techniques, e.g. XRFS or neutron activation analysis (NAA), or total extraction procedures should be employed as a first priority”. The British Geological Survey has been one of the leading organisations in the development of this global geochemical database. Therefore, the vast majority of systematically collected soil sample data that is available for NBC calculations for English soils are total element concentrations determined by XRFS. Other analytical techniques that do not give total element concentrations are used to determine the nature of occurrence and speciation of an element within a sample.

When using NBCs a common question will be “how should I interpret NBCs in the context of non-total analyses”? This was investigated as part of the data exploration phase of this project (Ander et al. 2012). Figure 1 shows a plot of Ni in the NSI topsoils which have been analysed by both a total (XRFS) (Rawlins et al., 2012) and partial (aqua regia followed by ICP-AES (McGrath and Loveland, 1992). There is a linear relationship between the two analytical methods with an almost 1:1 relationship. The regression equation for NSI soils is:

Regression equation for NSI soils is:
$[\text{Ni}_{\text{XRFS}}] = 0.949 + (0.878 \times [\text{Ni}_{\text{aqua regia}}])$ (n=3,956; $R^2 = 97\%$; and $P<0.05$)……Equation 1

Figure 1: Comparison of topsoil Ni concentrations in NSI samples determined by XRFS and by ICP-AES following an aqua regia acid digest.

Figure 2: Comparison of GEMAS topsoil Ni data by analytical method and categorised by land use type.
Similar comparisons of XRFS and ICP-MS analytical methods can be made with the GEMAS Project soils from England (Reimann et al., 2012) (Figure 2) and also the Tellus Project soils from Northern Ireland (Smyth, 2007) (Figure 3). Both these data sets, as might be expected, show a systematic bias towards higher Ni results when determined by XRFS. The acid digest, unlike total measurement by XRFS, will leave a quantity of trace element-bearing, residual material. This may be greatly influenced by the type of parent material on which the soil has formed. In Northern Ireland there are a large proportion of soils developed on basic rocks (basalts). There would also be expected to be an inherent, systematic bias expected between any two analytical measurement techniques.

The regression equation for the GEMAS soil data is:

\[ [\text{Ni}_{\text{XRFS}}] = 3.61 + (1.12 \times [\text{Ni}_{\text{aqua regia}}]) \quad (n=130; \quad R^2 = 89\%; \quad \text{and} \quad P<0.05) \ldots \text{Equation 2} \]

The regression equation for Tellus Project soil data is:

\[ [\text{Ni}_{\text{XRFS}}] = 8.06 + (0.961 \times [\text{Ni}_{\text{aqua regia}}]) \quad (n=6,871; \quad R^2 = 79\%; \quad \text{and} \quad P<0.05) \ldots \text{Equation 3} \]

Using equations 1, 2 and 3, a soil with 50 mg/kg Ni determined by \textit{aqua regia} followed by ICP-MS could be estimated to have a total concentration of 45, 60 and 56 mg/kg (rounded to nearest 1 mg/kg), respectively. The regression equations are therefore a tool to estimate total concentration for \textit{aqua regia}/ICP-MS determined samples, though its application must be done with an awareness of the analytical error range, particularly at higher concentrations. The differing regression equations probably reflect slight differences in the extraction procedures and the nature of the soil's underlying parent material. The large number of samples and the diverse range of underlying parent materials would probably make the Tellus soil data (equation 3) the most reliable to base total estimates on.
**Scale and use of Normal Background Concentrations**

NBCs have been determined for Ni using soils collected at a range of sampling densities, from 1 sample per 0.25 km² (G-BASE urban) through to 1 sample per 25 km² (NSI XRFS). The G-BASE urban samples provide a definition of the chemical surface environment to a much higher resolution than do the NSI (XRFS) samples. Thus G-BASE rural samples (collected at 1 per 2 km² sampling density) can show contaminant variability at a local area scale (1:50,000). When investigating a sample result in the context of a NBC, it is important to ask whether localised variability (scales at less than 1:50,000), say within the Principal Domain, has been truly captured during the determination of the NBCs. Areas characterised by the lower density NSI samples are likely to miss the relatively smaller areas of basic/ultrabasic rocks (e.g. basic dykes in northern England). Therefore, a high contaminant result should be attributed to a domain, taking account of the localised underlying parent material feature, even where this has an extent which is very discontinuous.

**Use of variograms**

The domains that are defined for a particular contaminant correspond to major sources of variation in concentrations of that contaminant in soil, such as urbanisation, mining or mineralisation. Concentrations of the contaminant vary within the domains, the procedure to define normal background concentrations (NBCs) quantifies this variation with robust statistics, from which the NBCs are computed. The spatial variation of a contaminant within a domain can be quantified by the variogram (Matheron, 1962). The variogram is a function that shows how the variation between observations of a variable at two sites depends on the distance in space between the sites. The variogram is half the mean squared difference between two observations plotted against the distance between them for all the results in a data set. Typically the variogram increases with distance until a plateau in the plot is reached at a value called the sill variance, which it reaches at a distance called the range. If the range is very short then this shows that the spatial variation is very intricate. If the range is longer then it may be feasible to map spatial variations from sample observations on a grid.
Supplementary Information

National map showing the distribution of nickel in topsoils

Figure 4: National map of nickel distribution in topsoils with county boundaries (using G-BASE and NSI (XRFS) results).
The national map of Ni distribution in topsoils (Figure 4) is shown here along with county boundaries to help with location at a regional scale. This map is given to demonstrate the variability in Ni across England and is also available to view on-line at the [BGS project web page](http://www.bgs.ac.uk). The map has been generated from G-BASE and NSI (XRFS) topsoil data using 42,133 samples. Because central and eastern England have been sampled at a much higher density (by G-BASE), resolution of information in these areas is much higher. Figure 4 has been produced in ArcGIS v9.3 using the IDW option of the Spatial Analyst tool, cell size 1000 m and search radius 5000 m (inverse square option selected). The percentile classification is based on all data and differs from the domain data sets in which results are modelled to fit a normal distribution and the effect of outliers (representing point rather than diffuse pollution) have been reduced by normalisation of the data.

The map shown in Figure 4 uses soils to represent the geochemical baseline. Other national/regional scale geochemical atlases for soils are those of McGrath and Loveland (1992) (NSI *aqua regia* data) and Rawlins *et al*. (2012) (NSI XRFS data). A preferred way of representing the geochemical baseline at a national/regional scale is to use stream sediments. The fine stream sediment in a drainage channel is representative of material washed down the drainage catchment to the sampling site in the stream and so gives a much better regional average of the chemical environment than is given by soils. The G-BASE project also collects stream sediments at a sampling density of approximately one sample per 2 km² and results for England have been presented in a series of atlases (e.g. Lake District (BGS 1992) and NE England (BGS 1996)) and these can be used to further demonstrate element variability across the surface environment of England. For the more recently sampled parts of England, the G-BASE project has also determined a large range of elements in stream waters (e.g. *Environmental Geochemical Atlas of Central and Eastern England*). Comparing the element concentrations and distributions of different sample types collected from the same locality can provide useful information about the mobility of a chemical element in that area.

A stream sediment atlas for England and Wales was also completed by Webb *et al*. (1978) (*Wolfson Geochemical Atlas*) and more recently low density sampling has produced continental scale geochemical baselines for Europe based on a number of sampling media, including stream sediments, stream waters and soils (Salminen *et al*. 2005) and the ongoing GEMAS project (Reimann *et al*. 2012). Appleton *et al*. (2008) using the BGS soil and stream sediment results and the Wolfson data, have produced national-scale estimation of potentially harmful element ambient background concentrations in topsoil using a parent material classified soils:stream-sediment relationships. These geochemical data have been used to derive geospatial data sets that identify the estimated concentrations (mg/kg) of As, Cd, Cr, Ni and Pb in soils.
Supplementary Information

Descriptive statistics for nickel in topsoil data

Nickel Domain percentile classifications

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Figure in brackets represents the number of samples used in the domain calculation

Table 1: A summary of the nickel domain percentile classifications. Domain NBCs shown in bold red. Concentrations in mg/kg. Note that as the Ultrabasic and Basic Domain NBCs are based on less than 30 samples these values have not been used.

A percentile of a data distribution (in this case the distribution of Ni in soil for a given domain) is the value of a variable below which a certain percentage of observations fall. The 95th percentile, for example, is the value below which 95% of the observations may be found, i.e. it encompasses the majority of the data. The contaminant concentrations in the soil for a given domain are a subset of the total population of all possible soil concentrations and therefore any percentile calculation will only be an approximation of the true value. The uncertainty on the percentile increases as the number of samples used to calculate it decreases. Lower and upper limits can be statistically estimated for each percentile giving a confidence interval for that...
percentile. **The Ni NBC for each domain is defined as the upper 95% confidence limit of the 95th percentile for the Ni topsoil results that fall within that domain.** A summary of domain percentiles with their upper and lower limits is given in Table 1. The domains for basic and ultrabasic rocks are shown here even though the number of samples available for their determination is below 30 (see Cave et al. 2012). These soil parent materials are known to be the cause of elevated Ni levels in soils (see the Tellus Project soils of Northern Ireland for example, Ander et al. In Press) and the NBCs can be improved as more data becomes available in England.

**Descriptive statistics copper topsoil data set**

Table 2 shows descriptive statistics for all the topsoil Ni results from the G-BASE and NSI (XRFS) data sets. The cities and towns in Table 2(c) are those that have been systematically sampled by the G-BASE project. Some of these data sets have associated reports that can be downloaded by clicking on the location place marker on the map at [http://www.bgs.ac.uk/gbase/urban.html](http://www.bgs.ac.uk/gbase/urban.html). Other data sets for other English cities may exist but they are not made publicly available and are not sampled and analysed to a nationally consistent standard.
Table 2: Descriptive statistics of underlying primary data sets for Ni in all topsoils. These are classified by various data set subgroups (total concentrations (XRFS) in mg/kg) (from Ander et al. 2012, with results cited to three significant figures).
Figure 5 and Figure 6 show the frequency distribution of results for soils over the five domains defined for Ni using the G-BASE urban and rural data sets and the NSI(XRFS) data. These plots can be used in conjunction with any new results plotted in a similar way to compare distributions with the defined domains. The box of the boxplot represents the interquartile range (Q1, Q3), with the median (Q2) as a line within the box. The
point symbol shows the mean value. The upper whisker = Q3 + 1.5(Q3-Q1); lower whisker = Q1-1.5(Q3-Q1).

Archer and Hodgson (1987) carried out a study of total and extractable trace element contents of agricultural soils (from a depth of 15 cm) in England and Wales, including Ni. “Total” Ni analyses were done by AAS following a digestion using perchloric and nitric acids. They defined the normal range for trace element contents as that between twice the log-derived standard deviation above and below the mean; approximately 95% of the data range. For 1,521 agricultural topsoils they determined a Ni median of 23.7 mg/kg and a “normal” range of 7.3-70 mg/kg.

Paterson et al. (2003) reporting on background levels of contaminants in Scottish soils report a range of Ni concentrations for mineral soils from 0.4 – 233 mg/kg with Q1, Q2 and Q3 values of 10, 17.5 and 25.7 mg/kg, respectively. These are lower than the English soils (all data - Table 2) of 16.7, 23.5 and 31.9 mg/kg (Q1, Q2 and Q3, respectively), probably reflecting the greater variety of land uses (i.e. possible anthropogenic input) associated with the English soils.
Landscape data used to define contaminant domains

Rather than seeking to define a single Ni NBC for the whole of England, the project has, through its data exploration (Ander et al. 2012), determined the most significant domains that can be defined in order to capture the most significant controls on Ni distribution in soils. For Ni five domains have been identified and these (with the exception of the Principal Domain) are related to soil forming parent materials and mineralisation. Although there is evidence of some urban areas having elevated soil Ni concentrations (see Table 2c), urbanisation and industrialisation is not considered to be as significant in contributing to the “widespread and normal” Ni concentrations as is observed for other contaminants. These domains have been defined using some key datasets within a GIS environment, namely: the BGS Soil-Parent Material Model (SPMM) (Lawley, 2009) and a revised and digitally updated version of the Ove Arup (1990) Department of the Environment (DoE) Metalliferous Mining and Mineralisation data set.

Soil parent material

The Soil-Parent Material Model1 (SPMM) has been developed by BGS, using as its basis the mapped boundaries of the national 1:50,000 superficial and bedrock geological data (DigMapGB-502), and is used within a GIS environment. Soil ‘Parent Material’ is the first recognisably geological material found beneath a soil profile, and is the lithology on which that soil has developed. Soils thus inherit many properties, including chemical composition, from this material.

In the SPMM the geological data have been combined into one layer of information which indicates the rock/sediment formation mapped as directly underlying soil. Where this is a superficial deposit (such as alluvium, glacial deposits, peat), the data set also maintains the record of the solid geological formation first encountered beneath this surface sediment; such information is of benefit where the underlying solid geology imparts chemical (or other) characteristics into the overlying superficial deposits, and thus the soil. The information, which has historically routinely been attributed to the mapped digital polygons in DigMapGB, largely comprises lithological and chronological information. Augmenting this in the SPMM is additional information on texture, mineralogy and lithology, which is attributed in a hierarchical classification system. In the context of the present study this means that a higher level of aggregated characteristics can easily be applied to soil geochemical data than is possible solely using DigMapGB, for instance, retrieving all formations which are classed as ‘ironstones’ (irrespective of their formal name) and confers benefits from using the SPMM.

The scale of mapping for the soil parent material is also relevant – 1:50,000 is the scale at which much of the systematic soil sampling has been undertaken, and gives the user a reasonable feel for the degree of uncertainty on the data. Where geographical information is provided at other common scales, such as 1:250,000 or 1:625,000, the boundaries and number of polygons are simplified and aggregated in order to provide generalised information at the national-scale. More detailed mapping, such as 1:10,000, is not available in a consistent format or as part of the SPMM data, and would imply greater certainty in sample locations and polygon boundaries than is appropriate from the data. Soil mapping is available at a national-scale (see e.g. NSRI NATMAP3) but this is not systematically mapped at 1:50,000 and would require attribution with the latest geological mapping data in order to retrieve information on key formations, and so has not been used in this study.

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1 http://www.bgs.ac.uk/products/onshore/soilPMM.html
2 http://www.bgs.ac.uk/products/digitalmaps/digmapgb_50.html
3 http://www.landis.org.uk/data/natmap.cfm
Metalliferous mining and mineralisation

The data set which has been examined in this project is that of non-ferrous Metalliferous Mineralisation and Mining database, originally produced in hard-copy by Ove Arup (1990) for DoE (Department of Environment), but which has been ‘cleaned’ and turned into a polygon layer by BGS. The data for England has been further attributed for this project by giving a name to the major ore fields allowing soil sample sites and geochemical data to be joined to the ore fields and separately analysed for typical soil concentrations. This mapping is generalised to 0.5 km grid squares, which is a suitable level of spatial resolution for this type of data. Therefore, it should be expected that not every occurrence of mineralisation/mining has been captured within this GIS layer. Where soil chemical data is encountered that is located outside a given mineralisation domain, but of a concentration expected for that contaminant within the local mineralisation domain, and lies over the parent material which is known to be affected by mineralisation in that ore field, then that high soil concentration could relate to either natural processes, or historical mining.
Summary of statistical procedure to determine NBCs

1. Can the contaminant be considered for NBC?
   - NO: No NBC determined
   - YES: Select contaminant

   2. Number of domain samples ≥ 30?
      - NO: Subset data into domains based on major factors controlling contaminant variability
      - YES: Determine skewness coefficient (SC) and octile skew (OS) and plot of data distribution

Figure 7: Flow chart for the calculation of the NBC for a given contaminant domain (OS and SC are octile skew and skewness coefficient, respectively. MAD = median absolute deviation). See text for explanation, continued overleaf.
Figure 7 continued. Flow chart for the calculation of the NBC for a given contaminant domain (OS and SC are octile skew and skewness coefficient, respectively. MAD = median absolute deviation). See text for explanation.

Figure 7 summarise the statistical procedure used to determine contaminant NBCs (see Cave et al. 2012). Part I essentially represents the data gathering and exploration phase of the project (WP1&2) in which domain...
areas are identified. Question 1 asks if the contaminant is suitable for a NBC. Asbestos and manufactured organic contaminants with no natural origin, for example, fail this question. The data exploration (Ander et al., 2011) identifies the areas (domains) where there are clearly identifiable controls on high concentrations of a specified contaminant. The contaminant data set is then subdivided into domain data sets. In question 2 a minimum of 30 results are considered necessary to determine a NBC (see Cave et al., 2012). Once the data has been subsetted into domains, then skewness testing and inspection of frequency distribution plots can be done to select the appropriate data transform and method of calculating percentiles (Parts II – IV). Question 3, the skewness test, has three possible outcomes. TEST 1 (OS > 0.2 and SC >1) is true if the data distribution is skewed and not suitable for fitting to a Gaussian model and the data need to be transformed to using either a logarithmic or Box-Cox transform. If TEST 2 (OS < 0.2 and SC <1) is true then the data are consistent with the assumption of a Gaussian distribution and the parametric percentiles are fitted based on the mean and standard deviation of the data. Finally, TEST 3 (OS < 0.2 and SC >1) means the data show a mostly symmetrical distribution but with potential outliers. Here the data are consistent with the assumption of a Gaussian distribution and the parametric percentiles are fitted using median and the median absolute deviation (MAD) in place of the mean and standard deviation as these measures are robust to outliers.
Supplementary Information

Access to data and information resources used to calculate NBCs

These resources are available from the BGS project web page and include:

- Data Exploration Reports (BGS report No. CR/11/145 and CR/012/041); Methodology Report (BGS report No. CR/12/003); Final Project Report (BGS report No. CR/12/035); Technical Guidance Sheets and supplementary information; MS Access Database summary of available data; Project Bibliography (Endnote bibliography); R code scripts used to determine NBCs; and GIS Resources served as WMS files (Domain polygons; the urbanisation index polygons defined from GLUD database; and the national contaminant interpolated image maps).

Web map services (WMS) are an industry standard protocol for serving georeferenced images across the web. They were developed and first published by the Open Geospatial Consortium (OGC) in 2000. Since this date WMS have had a steady uptake and are being increasingly used in traditional desktop based GIS, web-based GIS systems (including Google Earth), and Smartphone ‘apps’. BGS holds the data on their servers and publish it openly via the BGS project web page.

Principal contaminant data sets for England

Intellectual Property Rights for the raw soil data sets resides with the organisations responsible for those data sets. In the case of the G-BASE and NSI (XRFS) data is made freely available subject to certain licensing terms and conditions. For large data sets there will also be a data handling fee. Further information regarding access to the G-BASE and NSI (XRFS) soil data is given at the BGS project web page and enquiries should be sent to enquiries@bgs.ac.uk.

Other data sets providing information on soil chemistry are summarised in Appendix 2 of Ander et al. (2011) and this includes contact and web site links.

Soil parent material

The BGS Soil-Parent Material Model is described on a BGS web page (SPPM) and this contains information regarding further information and pricing.

Land use data including metalliferous mining and mineralisation

The Generalised Land Use Database (GLUD) Statistics for England 2005 is available for free from the Communities and Local Government website. Users interested in the detailed maps at land parcel level who hold the appropriate public sector licence to use OS MasterMap® can request to see the GLUD data at this large scale level (gis@communities.gsi.gov.uk).

The Ove Arup Mineralisation and mines data updated and modified by BGS is available from BGS subject to terms and conditions (see the BGS project web page).

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4 http://www.bgs.ac.uk/gbase/NBCDefraProject.html
5 http://www.bgs.ac.uk/products/onshore/soilPMM.html
6 http://www.communities.gov.uk/publications/planningandbuilding/generalisedlanduse
Further Reading

The following is a list of bibliographic references that provide more detailed information regarding the distribution and behaviour of nickel in the surface environment. Some of these references are referred to in this supplementary information section.


Technical Guidance Sheet (TGS) on normal levels of contaminants in English soils

Supplementary Information


Ove Arup (1990). Mining Instabililty in Britain. Unpublished reports by Ove Arup for the Department of the Environment (DoE), UK. Associated data sets modified by BGS into GIS format (see http://www.bgs.ac.uk/gbase/NBCDefraProject.html).


