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User Guide for DiGMapPlus Engineering Properties: Sulfate and Sulfide Potential

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BRITISH GEOLOGICAL SURVEY

PRODUCT DEVELOPMENT, ENVIRONMENTAL MODELLING
PROGRAMME

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User Guide for DiGMapPlus Engineering Properties: Sulfate and Sulfide Potential

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Foreword

This report is the user's guide for the national assessment of Engineering Properties: Sulfate and Sulfide dataset. The purpose of this user guide is to provide the background, methodology developed by the British Geological Survey, and the potential applications and limitations of this GIS information.

Acknowledgements

A number of individuals in the Product Development and Engineering Geology Directorates have contributed to the project and helped compile this report. This assistance has been received at all stages of the study. In addition to the collection and processing of data, many individuals have freely given their advice, and provided the local knowledge.

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Summary

This report describes the national scale DiGMapPlus+ Engineering Properties: Sulfate and Sulfide dataset. The methods used to create the dataset have been critically assessed and its fitness for purpose determined by specialists in BGS.

This document outlines the background to why the dataset was created, its potential uses and gives a brief description of the content. Technical information regarding the GIS and how the data was created is described and advice is provided on using the dataset.

1 Introduction

The presence of sulfur in rocks and soils are, when in certain forms and in certain conditions, of importance to the engineered environment as they can give rise to aggressive ground conditions. This might be as a result of the presence of sulfate ions in slightly acid to alkali conditions that attack concrete; or formation of acid waters (such as acid mine waters) leading to chemical reactions with other minerals. Also, the formation of sulfate minerals, such as gypsum, and acid ground water combined with lime or concrete (used to stabilise the ground) can result in an increase in volume that disrupts the fabric of the ground and can produce ground heave. Much of the research has been focussed on the damage caused to concrete associated with gypsum. Other sulfate minerals such as magnesium sulfate (Epsom salts) and sodium sulfate (Glauber's salt) are more soluble and generally dissolve into the groundwater well below most engineering activities. However, these can occur at surface in spring water. Sulfate ions are also formed from the oxidation of iron sulfide, which in some forms oxidises under natural conditions to form sulfuric acid. Human disturbance of rocks and soils containing iron sulfide can increase the likelihood of the oxidation of this mineral.

This dataset provides a guide to the stratigraphic units and lithologies throughout Great Britain and their potential to form a sulfate/sulfide geohazard.

2 About the Engineering Properties: Sulfate-Sulfide dataset

2.1 BACKGROUND

The BGS Engineering Properties dataset is a series of digital map layers based on the BGS Digital Geological Map of Great Britain at the 1:50,000 scale (DiGMapGB-50, BGS, 2009). Current coverage includes England, Wales and Scotland. It characterizes Bedrock and Superficial Deposits on DiGMapGB-50 in terms of their engineering properties.

The product is a spatial model of sulfate and sulfide potential for use within a GIS. The model demonstrates the spatial distribution of 'sulfate/sulfide' on a map for Great Britain. It can be used as an indicator of the potential presence of sulfate species that might need to be taken into consideration during engineering design, ground investigation and construction in the ground. This includes the presence of slightly soluble sulfate minerals (generally gypsum) or iron sulfide that is likely to oxidise to form sulfuric acid and acidic ground condition or, after reacting with calcium carbonate, to form gypsum.

2.2 WHAT THE DATASET SHOWS

The information is a synthesis of national databases, ground investigation and other data held by BGS, based primarily on DiGMapGB-50 V6, the National Geotechnical Properties Database, journal papers and other documents, and is primarily aimed at the near surface (0 - 2 m depth), however, it could be used at greater depths where appropriate.

The Sulfate-Sulfide GIS comprises a series of layers detailing spatial distribution of geological and engineering factors directly relevant to the presence gypsum and iron pyrites that is likely to oxidise within a geological unit.

The primary datasets for the Sulfate-Sulfide GIS are:

1. The DiGMapGB-Plus dataset.

2. Geology - Sulfate-Sulfide data derived from the National Geotechnical Properties Database (Self et al. 2012) and other site investigation information, primarily exploratory borehole and pit logs, from the National Geological Records Centre (NGRC).
3. A 'look-up' dictionary that classifies the Sulfate-Sulfide component of material by its consistency and mineral composition. The Sulfate-Sulfide data is interpreted from BRE special digest 1 (BRE 2005).

The information provides national coverage for England, Scotland and Wales primarily at a scale of 1:50,000.

Please note: The 'Sulfate-Sulfide' model primarily provides information for the **uppermost 2 m** of the ground surface for all geological units distributed across Great Britain.

2.3 ABOUT SULFATES AND SULFIDES

2.3.1 Primary and secondary sulfate minerals

Primary sulfates are generally formed by the evaporation of water under arid conditions. They form as beds but can be as veins, nodules and cements when dissolved and redeposited. In the UK they are found mostly in Permian and Triassic age geological units and occasionally in Jurassic and Carboniferous rocks. Secondary sulfates are the weathering product (oxidation) of sulfide minerals, which are commonly present in grey clays, mudstones and minerals veins (Czerowko and Cripps 2006).

2.3.1.1 PRIMARY SULFATE MINERALS

The primary sulfates most commonly found in the UK are gypsum ($\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$) and anhydrite (CaSO_4). Gypsum and anhydrite are only slightly soluble. Gypsum is present where there is free groundwater, whereas anhydrite is found where there is little or no water available. The transformation from anhydrite to gypsum usually occurs within 60 to 100 m of the ground surface, however, this will depend on local circumstances and anhydrite might be present within thick gypsum seams nearer the surface. Primary gypsum is an evaporite mineral deposit in hypersaline lakes generally in hot, dry climates. Anhydrite forms during burial of gypsum where the temperature is greater than 42°C . The erosion and uplift nearer surface and the presence of water converts the anhydrite to gypsum. This occurs with a 63% increase in volume, which can result in brecciation and distortion of surrounding rock. Gypsum is found as finely disseminated crystals in pores, as a cement, as nodules or veins and as beds up to 2 m thick in the UK. In general, the cement and veins are redeposited gypsum probably by dissolution and precipitation in ground water but might also be due to the change of anhydrite to gypsum.

Other primary sulfates found in the UK include epsomite ($\text{MgSO}_4 \cdot 7\text{H}_2\text{O}$) and Glauber's salt ($\text{Na}_2\text{SO}_4 \cdot 10\text{H}_2\text{O}$), which are also found in evaporite deposits but are soluble and dissolve in groundwater at depth and are only found near surface in springs. Barytes (BaSO_4) and celestine (SrSO_4) can also be present in evaporites, are very low solubility and are not an engineering hazard.

Geological units that contain primary calcium sulfate (gypsum and anhydrite)

As these sulfate minerals are evaporite deposits they occur in geological units that are associated with sabkha environments, which is a broad plain or salt flat in an arid or semi-arid region. The geological units where gypsum is found are, therefore, associated with units deposited under these conditions. Most evaporites are found in the 'red beds' of the Permian and Triassic, however, it is also present in some deposits from the Upper Jurassic. The thicker beds have been exploited for gypsum from mines or quarries.

The Permo-Triassic gypsum can be associated with local karstic features from dissolution. This is most notable in parts of the Mercia Mudstone and Zechstein groups.

2.3.1.2 SECONDARY SULFATE MINERALS

Sulfide minerals, in themselves, are not usually a concern in civil engineering and some sulfide ores are mined for the production of metals such as copper, nickel, lead and zinc. The hazard is usually caused by the oxidation of iron sulfide (FeS), known as iron pyrites or pyrites, to form sulfuric acid and producing acid ground conditions. In geological materials that contain calcium carbonate, generally as macro- and/or micro-fossils, the acid reacts with the carbonate producing gypsum (and buffers the acidity). The gypsum remains in the ground until it is dissolved and removed by ground water. Iron pyrites is a common mineral in geological units that are formed in anoxic conditions such as stagnant water courses, estuaries and marine basins.

Geological units that contain framboidal pyrite and calcium carbonate (calcite and aragonite)

Framboidal iron sulfide is commonly found in many grey mudstones and clays of marine origin and include the Westbury, Charmouth Mudstone, Whitby Mudstone, Oxford Clay, Kimmeridge Clay, Gault, London Clay and parts of the Weald Clay formations. When unweathered they are generally grey or dark grey, indicating that the ferrous (Fe²⁺), most notably iron sulfide, makes up the iron content. Framboidal iron pyrites is disseminated within these formations and, generally, formed of octahedral crystals of less than 5 µm in area that form into spheres about 20 to 50 µm across. Because of their small size and large surface area they are much more reactive than other forms of natural iron sulfide.

Most of these marine deposits contain macro- and micro-fossils, which comprise calcium carbonate, commonly in the form of aragonite or calcite with varying, but generally small, amounts of magnesium replacing calcium. The oxidation of iron pyrites produces sulfuric acid which reacts with the calcium carbonate producing gypsum.

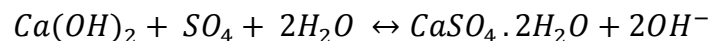
2.3.2 Mechanisms of sulfate attack on cement, concrete and lime stabilisation

Two mechanisms of sulfate attack on cement and lime based material have been recognized; the first is the conventional type and the second forms thaumasite (Czerewko & Cripps 2006).

2.3.2.1 CONVENTIONAL TYPE REACTION AND CONCRETE ATTACK

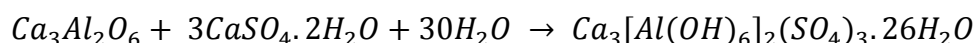
The conventional type of sulfate reaction requires sulfate ions dissolved from such minerals as gypsum or from sulfuric acid. The sulfate ion reacts with calcium hydroxide and hydrated tricalcium aluminate both present in cement. Initially, gypsum is formed from the reaction of the sulfate ion and calcium hydroxide.

Calcium hydroxide + sulfate ion + water <> gypsum + hydroxyl ion



The gypsum is precipitated in the pores. Once a pore is full of gypsum it reacts with the tricalcium aluminate in cement to produce calcium sulfoaluminate or ettringite.

Cement component + gypsum and water > calcium sulfoaluminate (ettringite)



During the reaction, the ettringite tends to form clumps and expands disrupting the fabric of the concrete. The internal stresses produced within the concrete or stabilised soil mass results in weakening of the structure. The presence of magnesium ions tends to increase the damage. If this reaction is likely to happen, as indicated by the laboratory tests identified in SD1 (BRE 2005), sulfate resisting cement, containing less Ca₃Al₂O₆, is used.

2.3.2.2 CONVENTIONAL ATTACK AND GROUND HEAVE

The precipitation of gypsum, Fe^{3+} oxides and hydroxides from pyrite-rich carbonaceous mudstones results in increases of volume and, if these materials are used to fill beneath ground bearing floor slabs, the heave produced can result in the movement of the slabs and distortion and cracking of the structure. This problem has been identified in tens of thousands of houses in Ireland and in the UK, including where material from the Coal Measures Supergroup have been used as fill for foundations, or where colliery spoil was used as hardcore (DCLG, 2008 and Taylor et al. 2013). The Westbury Formation (Hawkins and Pinches, 1987) and Whitby Mudstone Formation (DCLG, 2008) are also known to present this problem. The theoretical volume changes due to mineralogical changes are listed in Table 1.

Table 1: Theoretical expansion due to mineralogical changes (volume of dissolved components is not included (Cripps and Edwards, 1997)).

Original materials	Product mineral	Expansion (%)
Calcite	Gypsum	103
Pyrite	Gypsum	518
Pyrite and calcite	Gypsum	53
Pyrite	Jarosite	125
Illite	Alinite	160
Illite	Jarosite	38

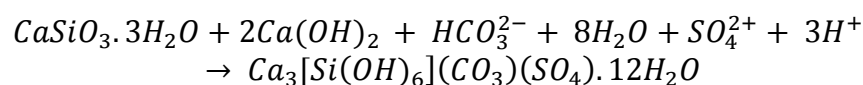
2.3.2.3 THAUMASITE TYPE REACTION AND CONCRETE ATTACK

Thaumasite causes weakening of buried structures including foundations and expensive remedial work is required to alleviate the problem. The normally strong concrete decomposes into paste. The most notable occurrences were found in bridge foundations on the M5, 30 years after construction. After the completion of the foundations, the pits formed during construction were backfilled with fresh or slightly weathered mudstone of the Charmouth Mudstone Formation. This formation is well known for containing secondary gypsum in the distinctly weathered and destructured clay. A number of important characteristics of the Charmouth Mudstone Formation and the environment were identified. At the site the fresh Charmouth Mudstone Formation contained about 1% sulfide, whereas the weathered fill was found to contain only 0.53%. Calcium carbonate, which is common in this formation, buffered sulfide oxidation reaction and the groundwater in the fill was about neutral. The construction of the fill disrupted its structure, reducing the density when compared with the *in situ* material and so water and air passed through it more easily allowing the reaction to occur.

The conditions required for thaumasite formation are high pH (>10.5) and a temperature of about 15°C. The former is common in cement, which has a proportion of high alkaline minerals.

A simplified version of the thaumasite reaction is between calcium metasilicate with calcium hydroxide, both in cement, and sulfate ions from pyrite oxidation or in the groundwater and hydrogen carbonate ions from groundwater or from the aggregate, water and hydrogen ions from an acid, most likely from the oxidation of pyrite, produces thaumasite.

Calcium metasilicate + Calcium Hydroxide + hydrogen carbonate ions + sulfate ions + hydrogen ions > Thaumasite.



2.3.2.4 OTHER REACTIONS – ACID CONDITIONS

Some deposits containing framboidal pyrites have insufficient calcium carbonate to buffer the sulfuric acid produced by oxidation of the pyrites. In these cases there is an increase in acidity until there is a reaction with a mineral, such as clay minerals and other silicates.

2.4 LEGISLATION

2.4.1 EU Soil Framework Directive

The draft EU Soil Framework Directive was introduced by the European Commission in 2006 after being proposed in an EU Thematic Strategy on Soil Protection. It seeks to harmonize and raise the level of soil protection across the EU.

The approach currently proposed would require Member States to:

- tackle degradation (erosion, loss of soil organic matter, salinisation, landslides, acidification, compaction)
- identify and remediate contaminated land
- consider soil protection/functions in national policy-making
- control loss of soil resources to development

Information from the Defra website (Feb 2011) (<http://www.defra.gov.uk/food-farm/land-manage/soil/soil-framework-directive/>) states that the UK has taken the view that the overall objective is strongly supported and that the UK already has robust domestic policies in place to protect soils. UK Ministers have called for a different approach to these issues; one which better respects the principles of subsidiarity and better regulation in order to avoid unnecessary additional administrative burdens and disproportionate costs.

Although this directive is still under development, its potential content and implications to the UK are borne in mind when creating a product such as the sulfate/sulfide dataset and its intended use in the desk study phase of UK geotechnical engineering practices. Additional consideration in creating the Engineering properties datasets is the compatibility and ease of use in line with the British Standard BS5930 (BSI 1999) and the Eurocode1997 (BSI 2007).

2.5 WHO WOULD BENEFIT FROM THE DATASET?

It is envisaged that the sulfate-sulfide layer will be of interest to a wide range of organisations concerned with development including the Highways Agency, utility companies, local authorities, developers, engineering consultants, contractors and mining.

The properties of earth materials are important in all engineering projects and the classification of the sulfate-sulfide component of a rock formation is a priority objective. An estimate of this value in any desk study exercise would provide a valuable indication and allow for more effective planning and execution of any proceeding ground investigation.

3 Technical information

3.1 HOW THE DATASET WAS CREATED

Lithological type and variability are classified in the BGS Rock Classification Scheme for each LEX-RCS code and with the geological unit origin from geological references forms the basis for identifying the likely sulfate/sulfide component.

The sulfate/sulfide GIS comprises a series of layers classifying the likely qualitative sulfate/sulfide hazard or potential.

Codes have been assessed using information in the BGS National Geotechnical Properties Database, technical reports, site investigation reports and by expert opinion. Categorisation is based on a formation level wherever possible.

The dataset is indicative for the unit within 2 m of the surface but might be applicable to greater depths.

The sulfate-sulfide dataset provides information for the **uppermost 2 metres** of ground surface of the geological units distributed across Great Britain. Further information regarding details of geological units at greater depths can be provided on request (see contact information below).

3.2 SOURCE DATASETS

The primary datasets used for the sulfate/sulfide GIS are:

1. Parent Material Map V6 dataset (Lawley, 2009);
2. Geology- sulfate/sulfide values derived from the BGS National Geotechnical Properties Database and references.
3. A 'look-up' dictionary that classifies the geological unit by its sulfate/sulfide potential or hazard.

3.3 FIELD DESCRIPTIONS

The data fields included in this dataset are described below.

General lithology (GEN_PMLITH)

This is a simplified geological description of the parent material and is derived from the original DiGMapGB-50 LEX-RCS of the mass movement, superficial, anthropogenic deposits and bedrock that make-up parent material shp file. The coding is compared with the hierarchical classification of UK rocks from the BGS Rock Classification Scheme (RCS) (<http://www.bgs.ac.uk/bgsrscs/>). In general, the aim is to provide the user with as simplified a lithological description as possible.

Sulfide class (SUL_CLSS)

The primary classifications are in Table 2 and the secondary classifications as used in the GIS are in Table 3 and are a short alpha-numeric code for GIS purposes.

Sulfide description (SUL_DESC)

The sulfate/sulfide description of the classification are in Table 2 and Table 3.

Table 2. Primary classification

Primary Class	Description
0	Sulfate/sulfide not generally present.
1	Primary calcium sulfate present.
2	Iron sulfide and calcium carbonate present. The iron sulfide will or might oxidise to form sulfuric acid and react with calcium carbonate to form secondary gypsum.
3	Units that contain sulfides that might oxidise to form acid ground conditions.
4	Mixed, contains beds with iron pyrites and calcium carbonate and beds with iron pyrites and little or no calcium carbonate.

5	Contains beds of anhydrite or gypsum, and sulfides that might oxidise and react with calcium carbonate.
6	Unknown, lithologies not known
7	Areas of mapped water – not applicable

Table 3. Secondary classification of sulfate/sulfide as used in the GIS

SUL_CLSS	SUL_DESC
0A	Sulfate or sulfide that will oxidise are not normally present.
1A	Major sulfate bed. The sulfate might be leached from the near-surface zone, the thickness depends on local conditions.
1B	Sulfate common throughout as beds, nodules and veins. The sulfate might be leached from the near-surface zone, the thickness depends on local conditions.
1C	Sulfate beds, nodules and veins are present at certain levels. The sulfate might be leached from the near-surface zone; the thickness depends on local conditions.
1D	Sulfate beds, veins and nodules are present locally at certain levels. The sulfate might be leached from the near-surface zone; the thickness depends on local conditions.
1E	Minor sulfate: in beds present locally at certain levels or as dispersed nodules. The sulfate might be leached in the near surface zone; the thickness depends on local conditions.
2A	Sulfide oxidises in weathering zone or when disturbed and reacts with calcium carbonate to form secondary gypsum.
2B	Sulfide likely to oxidise in weathering zone or when disturbed and reacts with calcium carbonate to form secondary gypsum.
2C	Sulfide might be present and oxidise in weathering zone or when disturbed and react with calcium carbonate to form secondary gypsum.
2D	Sulfide and calcium carbonate might be present, unlikely to form secondary gypsum unless reworked.
2E	Sulfide and calcium carbonate might be present, unlikely to form secondary gypsum.
3A	Sulfide likely to oxidise in weathering zone or when disturbed to form acidic conditions.
3B	Sulfide likely to oxidise when disturbed to form acidic conditions.
3C	Sulfide present locally and might oxidise when disturbed to form acidic conditions.
3D	Sulfide might be present in some beds that will only oxidise when disturbed to form acidic conditions.
3E	Sulfide might be locally present in some beds and might oxidize when disturbed to produce acidic conditions.
4A	Mixed lithologies, with beds containing sulfide, sometimes with calcium carbonate. Sulfide oxidises when weathered.
4B	Mixed lithologies, with beds containing sulfide, sometimes with calcium carbonate. Sulfate might oxidize under some conditions (e.g. reworking).
4C	Mixed lithologies, sulfide beds occasionally present sometimes with calcium carbonate. Sulfide might oxidize under some conditions (e.g. reworking).
5A	Minor sulfate and sulfide and calcium carbonate beds present locally. Sulfate might be leached in the near surface zone, depth depends on zone local conditions. Sulfide might oxidise.
5B	Contains minor beds of sulfate and sulfides that might oxidise under unusual conditions such as mining operations or reworking.
6	Sulfate/sulfide content unknown (geology unknown)
7	No hazard (water body)

Nominal Scale (NOM_SCALE)

This field describes the notional x-y spatial scale of the data. Most geological map data in the dataset is presented at a scale of 1:50,000. It is part of the metadata of the original Parent Material Map V6 dataset. The field identifies a combination of scales used to create a geological map at surface from the bedrock and superficial map sources. The available scales are shown in Table 4.

Table 4. Nominal Scale values

Field Value	Meaning
50	No superficial data is present for this sheet and bedrock data is available at 1:50,000 scale
250	No superficial data is present for this sheet and bedrock data is available at 1:250,000 scale
625_50	Superficial data is present for this sheet at a scale of 1:625,000 and Bedrock data is available at a scale of 1:50,000
50_50	Superficial data is present for this sheet at a scale of 1:50,000 and Bedrock data is available at a scale of 1:50,000
35_50	Superficial data is present for this sheet at a scale of 1:35,000 and Bedrock data is available at a scale of 1:50,000
35_250	Superficial data is present for this sheet at a scale of 1:35,000 and Bedrock data is available at a scale of 1:250,000

Two additional fields were created to contain map metadata:

UID

This is a unique object identifier based on DNF notation and arc indexing using a field calculation based on the following pseudo code: “bgsn:DPS_V6_” & FID.

VERSION

This is a layer identifier based on BGS standard practice based on the following pseudo code: “DiGMapPlus_V6”.

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: <http://geolib.bgs.ac.uk>.

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