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British Geological Survey
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User Guide Total Organic Carbon (TOC) data

Open Report OR/14/056

BRITISH GEOLOGICAL SURVEY

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

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Foreword

This report describes the Total Organic Carbon (TOC) point dataset. It contains a brief summary of the methodology and guidance on how the data can be used. The data has been critically assessed and its fitness for purpose determined by BGS Energy specialists.

The purpose of this user guide is to enable those licensing this dataset to have an appreciation of how the data set has been created and therefore better understand the potential applications and limitations that the dataset may have.

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Summary

This report describes the Total Organic Carbon point data developed by the British geological Survey (BGS). The method has been critically assessed and its fitness for purpose determined by Energy specialists in BGS and represents the best and most comprehensive data BGS currently has available.

Acknowledgements

A number of individuals in the Environmental Modelling, Energy and Informatics 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.

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.

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 Total Organic Carbon (TOC) Dataset

2.1 BACKGROUND

Great Britain has abundant shale at depth although the distribution is not well known. The BGS is investigating the location, depth and properties of the shale as well as the processes that lead to economic accumulations of gas.

BGS has produced a review dataset, based on existing published analyse. The data has been compiled as part of ongoing research of shale gas basins through the use of conventional oil and gas well data to identify potential targets; for example, total organic carbon and shale formation crops and thicknesses. This dataset represents the data gathered for this purpose and provides information on the content and variation within prospective some shale units.

Rock property characteristics, which are a function of the original depositional setting, subsequent geological history and mineralogy, are used to infer the possible presence of shale gas. A number of factors are considered in determining the quality of a source rock including:

- total organic carbon (TOC)
- net to gross organic-rich shale thicknesses
- kerogen type
- thermal maturity
- porosity and transport properties
- fracture properties

These result in the thermal decomposition of organic matter at depth and under high pressures. This process is often associated with coal, oil and gas fields and may be locally important where gasses have migrated from depth; or where there is slow release from previously deeply buried, low permeability, organic-rich rocks. It can be measured by heating a rock sample at very high temperatures in a furnace and combusting the carbon (organic matter) into carbon dioxide (CO_2). The amount of CO_2 that is released is proportional to the carbon content of the rock sample. The sample may also contain non-organic sources of carbon such as calcite or siderite and their presence must be corrected (using acid digestion) in order to determine an accurate TOC content.

The data has been derived from borehole analysis, with sampling being undertaken by the BGS Organic Geochemistry Laboratory. The analysis results are supported by expert knowledge, the dataset also underpins the conclusions published in Smith (2010).

The data reflects already processed and validated boreholes. BGS holds more data of this type and work is continuing to validate further borehole data.

The British Geological Survey has an ongoing development programme to produce datasets that inform and support research. A suite of energy related datasets are currently under development and these are complimented by existing BGS assets.

The data has been derived from publications of analyses of organic rich shale sampled from BGS (formerly IGS) boreholes (see Smith 2010).Related products:

- DiGMapGB - digital geological data bedrock and superficial at a range of scales
- Scans of onshore borehole logs for Great Britain
- Seismic locations and sections database
- Aquifer and shale maps (http://www.bgs.ac.uk/research/groundwater/shaleGas/aquifersAndShales/maps/home.html
- 3d models and cross-sections

Products under development:

- Vitrinite reflectance

2.2 WHO MIGHT REQUIRE THIS DATA?

- Hydrocarbons exploration companies
- Hydrocarbons service companies
- Central government
- Academic researchers and modellers

Total organic carbon, the amount of organic carbon in a geological formation is an indicator in exploration for shale gas/oil. Anyone involved in hydrocarbon exploration, government decision makers or academics working in the field of shale gas exploration and development may be interested in this dataset.

Extensive research is currently being carried out in this area and whilst the dataset currently encompasses a limited number of borehole locations it is expected that further boreholes will be interpreted and will continue to be added.

2.3 WHAT THE DATASET SHOWS?

The dataset shows location of boreholes where TOC analysis has been carried out. Each borehole has been sampled at a series of depths and samples have been analysed to evaluate the total organic carbon of each sample. The results of the analysis are given in the attribute table, the analysis techniques and table fields are described in the Technical Information section below.

3 Technical Information

3.1 DEFINITIONS

Total organic carbon - a measure of the dry weight per cent of organic carbon within hydrocarbon source rocks. Hydrocarbons, including natural gas (principally methane, ethane and propane), may be generated by the heating of organic carbon through burial over geological time.

S1 - the value of free oil and gas (hydrocarbons) that are volatilised from the rock sample without cracking the kerogen during the first stage of heating at 300ºC. S1 represents how many milligrams of free hydrocarbons can be thermally distilled out of one gram of the rock sample. S1 values are used to derive the Production Index (PI) and petroleum potential of a rock sample.

S2 - the value of hydrocarbons that are generated from the sample during the second programmed heating stage of pyrolysis. These result from the cracking of heavy hydrocarbons and from the thermal breakdown of kerogen. S2 represents the amount of residual hydrocarbons in milligrams per gram of rock.

The S2 value gives an indication of the potential amount of hydrocarbons that the source rock many produce if thermal maturation continues. Generally the following values apply when assessing source rock quality:

None	<2 mg/g
Poor	2 to 3 mg/g
Fair	3 to 5 mg/g
Good	5 to 10 mg/g
Very good	>10 mg/g

S2 values are used to derive the Hydrogen Index (HI), Production Index (PI) and petroleum potential of a rock sample.

Production Index (PI) - derived from the relationship between hydrocarbons generated during the first and second stages of pyrolysis. It is defined as S1/ (S1+S2). It is used to characterise the evolution of the organic matter as PI tends to gradually increase with depth in fine-grained rocks.

S3 - represents the CO_2 that is emitted from the thermal cracking of kerogen, expressed in milligrams per gram of rock. S3 values are used to derive the Oxygen Index (OI) of a rock sample.

Oxygen Index (OI) - derived from the ratio of CO_2 to TOC. It is defined as 100 x S3/TOC. The OI relates to the amount of oxygen contained in the kerogen and can be useful in tracking kerogen maturation or type.

P1 - represents the volume of bitumen (PPM) that was extracted from a sample during the older (now obsolete) analysis method of Mini-Pyrolysis.

P2 - represents the volume of pyrolysate (PPM) that was extracted from a sample during the older (now obsolete) analysis method of Mini-Pyrolysis.

Hydrogen Index (HI) - an indicator of the unoxidised hydrogen in a sample which gives an indication of kerogen maturity (MG_HC refers to milligrams of hydrocarbons – the unit in which the Hydrogen Index is reported).

High values (> 0.15) indicate good oil and gas generation potential and

Low values (< 0.15) indicate good gas generation potential.

Kerogen types can also be inferred from this index.

T_{MAX} - the temperature (ºC) at which the rock sample reaches its maximum rate of hydrocarbon generation.

3.2 ANALYSIS TECHNIQUES

Borehole samples have been analysed using one of two pyrolysis techniques. The process of thermal maturation can be simulated in the laboratory. The process involves heating a sample under controlled conditions and measuring the oil like material released from the rock. Using this technique the potential richness of immature sediments can be evaluated. Previously mini-pyrolysis and pyrolysis was used but this method has been superseded by the use of rock-eval pyrolysis.

Mini-pyrolysis and pyrolysis is an older analytical method. It is broadly similar to that of rock-eval pyrolysis with bitumen (P1) and pyrolysate (P2) the end products of the analysis, quoted in Parts per Million (PPM) the use of this analytical method has largely been replaced by the use of rock-eval pyrolyis.

Rock-eval pyrolysis is a more modern method for determining the hydrocarbons generation potential, organic type and thermal maturity of a source rock. A grounded, homogenised sample is heated in stages at set temperatures to obtain the amount of hydrocarbons (S1 and S2 peaks) and CO_2 content (S3 peak). The temperature at which S2 reaches its maximum rate of hydrocarbon generation is known as T_{max}.

3.3 FIELD DESCRIPTIONS

Table 1 Attribute table field descriptions

FIELD NAME	FIELD TYPE	DESCRIPTION
WELL_NAME	Text	Nationally registered well name in the BGS Borehole database Single Onshore Borehole Index.
REFERENCE	Text	Published reference from which the analyses values were obtained. All samples were taken from BGS boreholes
DEPTH_M	Numerical	Sample depth in metres
TOC	Numerical	Dry weight % of organic carbon -3 value in this field indicates data not available
EASTING	Numerical	Six figure National Grid reference
NORTHING	Numerical	Six figure National Grid reference
S1	Numerical	Value of free oil and gas (hydrocarbons) that are volatilised from the rock sample without cracking the kerogen during the first stage of heating at 300ºC. (mg/g) -3 value in this field indicates data not available
S2	Numerical	Volatilisation of higher carbon number hydrocarbon compounds and cracking of non-volatile organic matter, 300-600°C (mg/g) -3 value in this field indicates data not available
S3	Numerical	CO_2 trapped in 300-390°C (mg CO_2/g) -3 value in this field indicates data not available
T_{MAX}	Numerical	Temperature of maximum kerogen pyrolysate yield (S2) (°C) -3 value in this field indicates data not available
P1	Numerical	The amount of thermal bitumen released by heating a rock sample in helium up to 350°C (parts per million) -3 value in this field indicates data not available

P2	Numerical	The amount of pyrolysate released by heating a rock sample in helium from 350-550°C (parts per million) -3 value in this field indicates data not available
HI-MG-HC	Text	Hydrogen Index = yield of S2 or P2 relative to the TOC (S2/TOC or P2/TOC) (mg of hydrocarbon per g)
VERSION	Text	Version of data, updated when revisions to data take place.

3.4 CREATION OF THE DATASET

BGS borehole data was extracted from the BGS Single Onshore Borehole Index (SOBI) where TOC samples were validated with published information by a BGS Energy specialist.

3.5 DATASET HISTORY

This is the first approved BGS dataset containing Total Organic Carbon further data is to be released as it becomes available.

3.6 SCALE

The Total Organic Carbon dataset is produced as point data from a number of strategic boreholes.

Borehole locations are given to the nearest 10 metres and down borehole readings have been taken at various depths recorded in metres to two decimal places.
The boreholes are identified by an easting and northing together with field observations taken from quarries and geologically relevant outcrops.

3.7 COVERAGE

The Total Organic Carbon dataset is taken from a number of strategic boreholes around the UK, together with field samples from quarries and geologically relevant outcrops (see Figure 1).

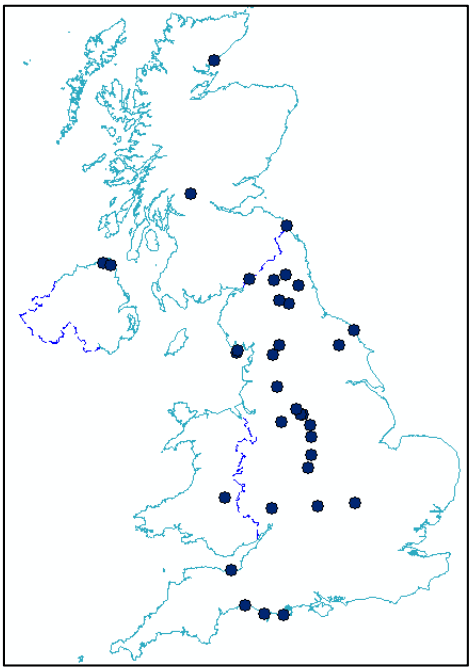

Figure 1 Sample sites included in the Total Organic Carbon dataset

Currently 36 locations are represented with a total of 572 downhole interpretations. Most boreholes include multiple interpretations from different sample depths.

3.8 DATA FORMAT

The Total Organic Carbon dataset has been created as point data and is available in a range of GIS formats, including ArcGIS (.shp) and MapInfo (.tab). More specialised formats may be available but may incur additional processing costs.

3.9 LIMITATIONS

Total Organic Carbon is based on, and limited to, an interpretation of the records in the possession of The British Geological Survey at the time the dataset was created.

A high TOC value is not necessarily an indicator of shale gas or oil potential.

The Total Organic Carbon dataset is produced as point data from a number of strategic boreholes whose location is given to the nearest 10 metres.

Where combined with field observations taken from quarries and geologically relevant outcrops the location may be more approximate.

Borehole sample readings have been taken at various depths recorded in metres to two decimal places.

4 Licensing Information

The British Geological Survey does not sell its digital mapping data to external parties. Instead, BGS grants external parties a licence to use this data, subject to certain standard terms and conditions. In general, a licence fee will be payable based on the type of data, the number of users, and the duration (years) of a licence.

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These are general comments for guidance only. A licensee of BGS's digital data is provided with full details of the basis on which individual BGS datasets licensed to them are supplied.

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