Title: Consolidated Geothermal Database UK (CGD-UK): A digital open license database for temperature and thermal conductivity in the UK.

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Abstract:

Variations in subsurface heat flow within the upper crust control the distribution of geothermal resources. Development of a robust understanding of these variations requires reliable measurements of temperature and thermal conductivity. To date, measurements of temperature and conductivity onshore the UK have been unavailable in an accessible, clearly structured digital format. Here, we rectify this problem by presenting a consolidated relational database of existing measurements. The database includes comprehensive metadata and has a consistently formatted and linked structure to enable repeatable and reliable estimation of geothermal heat flow. The database, referred to as the Consolidated Geothermal Database UK (CGD-UK), is structured as a series of comma-separated values files, with a master table providing an index of individual boreholes at which measurements have been made. CGD-UK is currently populated with data from northern England and southern Scotland for 209 locations at which temperature and/or conductivity have been measured. It also includes >30,000 data points that have been digitized using automated optical character recognition, but still require QC. CGD-UK serves as the only compressive, open-licence digital database for onshore geothermal data in the UK and provides the foundation for a single database for UK geothermal data, with a digital object identifier (DOI).

Data: The data described in this article are available at the following web link https://data.ncl.ac.uk/collections/Consolidated_Geothermal_Database_UK_CGD-UK_/6103638 with the following DOI: https://doi.org/10.25405/data.ncl.c.6103638.v1

Flow of heat within the Earth is vital in controlling processes as varied as the planetary magnetic field (Sakuraba and Roberts 2009), the movement of tectonic plates (Loyd *et al.* 2007), the distribution of geothermal and oil and gas resources (McKenzie 1978; Clauser and Villinger 1990), and the emplacement of economically valuable mineral deposits (Houseman *et al.* 1989). This heat flow has been investigated using seismic and magnetic observations, mineralogical analysis of mantle xenoliths, and computational simulations of planetary cooling (O'Reilly *et al.* 1990; Mather and Fullea 2019; Richards *et al.* 2020; Landeau *et al.* 2022). Within the Earth's crust, however, the most reliable estimates of heat flow are made using direct measurements of subsurface temperature. Such measurements have been acquired in caves, aquifers, mines, boreholes and hydrocarbon wells, and have underpinned global maps of near-surface heat flow (Pollack *et al.* 1993; Fuchs *et al.* 2021b).

Recent years have seen increasing interest in reanalysing these measurements of subsurface temperature, for two reasons. First, increases in computational resource allow estimation of heat flow using standardised methods that are far more rigorous and comprehensive than the techniques used in the past (Fuchs *et al.* 2021a). Reassessment of heat-flow values using these methods will support comparison of datasets from different geographical regions and historical periods and may provide new insights into global geophysical processes. Second, existing measurements of subsurface temperature can be used to assess the potential of geothermal energy systems that can support decarbonisation. For instance, development of a three-dimensional model of temperatures beneath the Netherlands supported a ten-fold expansion in geothermal capacity between 2010 and 2018 (*Natural Resources and Geothermal Energy in the Netherlands: Annual Review 2020* 2021).

Direct measurements of temperature beneath the UK have been recorded for at least two hundred years (Jessop 1990). These measurements show the broad pattern of variation in terrestrial heat flow, and suggest significant potential for development of geothermal energy (Gluyas *et al.* 2018). However, our understanding of this heat flow has changed little in the past 30 years, and the most commonly cited maps of subsurface temperature include numerous trends that do not reflect the crustal or tectonic structure (Busby *et al.* 2011). Reanalysis of the UK dataset may yield significantly different patterns of heat flow, and could inform development of three-dimensional, geologically realistic computational models that rigorously quantify uncertainty (Westaway and Younger 2013; Mather and Fullea 2019; Howell *et al.* 2021).

Making full use of the UK's wealth of geothermal data is, however, held up by data-access problems. Many studies do not publish their underlying data due to uncertainty surrounding legal ownership of historical records (Busby *et al.* 2011; Farr *et al.* 2021). Data from other studies, although technically non-confidential, are often unavailable to the public in any digital format and can be accessed only in hard copy at a small number of locations (Rollin 1987). Even when digital copies exist and are accessible, data are presented in a wide range of formats, few of which are computer-readable (Dickinson and Ireland 2022). By computer-readable we refer to digital files that can be directly manipulated using computer code or software packages, for example comma-separated values (CSV) files for numerical data. Lack of a digital database holds back efforts to reanalyse existing geothermal data using up-to-date computational tools and data-science techniques.

Here, we attempt to remedy these issues by presenting a digital database of publicly available UK geothermal data. This database, which we refer to as the Consolidated Geothermal Database UK (CGD-UK), combines detailed metadata with consistently formatted measurements of temperature and thermal conductivity and with standardised descriptions of lithology and stratigraphy. All data have been compiled from publicly available sources that have no restrictions on reuse. As far as we are aware, CGD-UK is the only publicly available, digitally accessible database of geothermal data for the onshore UK.

In its initial release, the database covers an area of approximately 50,000 km^2 in northern England and southern Scotland. We anticipate that the database will expand to cover all onshore regions of the UK and eventually encompass data from the UK Continental Shelf (UKCS), and hope that it will promote further sharing of not only geothermal data, but of geoscience data more widely. The database is available on Figshare under a CC BY 4.0 open licence. In this paper, we outline the history of British heat-flow measurements before describing the structure of CGD-UK and summarising the data that it contains. We then discuss how CGD-UK could be expanded and used.

2 PREVIOUS PROGRAMMES OF MEASUREMENT AND COMPILATION

2.1 Measurement

Careful measurement of underground temperature beneath the UK was first undertaken during the nineteenth century (e.g. Forbes 1846; Thomson and Binney 1868); see Prestwich, 1895, for a summary of many of these early measurements). Recognising the value of such measurements, the British Association for the Advancement of Science (BAAS) appointed a committee to investigate variations in underground temperature in a systematic way (Everett 1868). This committee, which delivered annual reports between 1868 and 1882, compiled measurements of temperature from 22 locations in the UK and 14 locations abroad (Everett *et al.* 1882). A second BAAS committee, which met between 1874 and 1882, drew together measurements of thermal conductivity from over 170 samples of a wide range of rocks (Herschel 1875, 1882; Herschel *et al.* 1877).

Using the results of these two committees, (Everett *et al.* 1882) calculated a mean geothermal gradient and a mean thermal conductivity and combined these two values to yield the first empirical estimate of geothermal heat flow. It was recognised, however, that accurate estimates of local geothermal heat flow required measurements of temperature and thermal conductivity from the same location (Anderson, 1934; Benfield, 1939; Anderson, 1940). A third BAAS committee, appointed in 1938, hoped to oversee systematic acquisition of co-located profiles of temperature and conductivity throughout the UK (Philips 1937). However, plans were disrupted by the outbreak of the Second World War, and the committee was disbanded.

During the subsequent four decades, further measurements were sporadically made at several British sites (Bullard and Niblett 1951a; Mills and Hull 1968; Bott *et al.* 1972). Prompted by increasing energy prices in the mid-1970s, the Institute of Geological Sciences (renamed the British Geological Survey, BGS, in 1984; henceforth the BGS) began to assess the potential of the UK's geothermal energy to provide heat and power (Dunham 1974; Garnish 1976a, b). Initial work focused on compiling existing measurements of temperature, which were published in a report that became known as the UK Geothermal Catalogue (Burley and Edmunds 1978); henceforth UKGC-1). Alongside the results of scientific studies, the UKGC includes measurements of temperature from oil and gas wells.

Over the following ten years, the BGS expanded the UKGC, both by sponsoring acquisition of new measurements by scientific research groups and by adding further measurements from oil and gas wells when they became available. The details of the measurement programme, which included observations of hydrogeology and geochemistry, are given in a series of 57 reports (BGS 1988; Barker *et al.* 2000). By the conclusion of the programme in 1987, a further three editions of the UKGC had been published (Burley and Gale 1982 henceforth UKGC-2; Burley *et al.* 1984 henceforth UKGC-3; Rollin 1987 henceforth UKGC-4). Between them, these editions house more than 2600 temperature measurements made at over 1150 sites (Rollin 1995) .

Few further empirical investigations of geothermal heat have been made since completion of UKGC-4. Three boreholes dedicated to researching deep (i.e. at depths > 500 m) geothermal heat have been drilled (Manning *et al.* 2007; Younger and Manning 2010; Younger *et al.* 2016), whilst temperature measurements in shallow aquifers and coal mine workings have yielded estimates of heat flow beneath Glasgow (Watson and Westaway 2020), Cardiff (Patton *et al.* 2020) and south-east England (Pike *et al.* 2013). The majority of these datasets are publicly available. Since 1987, at least 840 onshore oil and gas wells have been drilled in the UK (Ireland *et al.* 2021), and it is likely that temperatures measurements have been made in many of these wells. These measurements are housed in reports that are released to the public realm after expiration of confidentiality periods (these periods usually last three years; (Dickinson and Ireland 2022). However, the majority of these reports are not readily accessible since onshore oil and gas well data acquired after the 1960s are currently available only through commercial resellers.

The UKGC has thus remained the most complete collection of geothermal data for mainland Britain. However, it is far from an ideal resource, for two reasons. First, and most fundamentally, the UKGC does not include all the measurements that were collated during the geothermal research programme of the 1980s. For instance, although the programme acquired more than 3,000 new measurements of thermal conductivity, and compiled many more measurements from previous studies, the raw measurements are not included in the UKGC (Burley *et al.* 1984). Instead, average conductivities for different lithologies are presented (UKGC-4). For boreholes in which temperature was measured at tens or hundreds of depths, the UKGC records temperatures from only a handful of depths. Moreover, temperature data in the UKGC are presented with no quantification of their accuracy, even when the original sources provide such quantification. The lack of original measurements, and of quantification of accuracy, hinders the ability of the UKGC to support reanalysis of geothermal data using novel computational methods.

Second, the UKGC is not freely available in a computer-readable format. Scanned, digital copies of all four editions exist and are non-confidential. However, the digital copies of UKGC-1, UKGC-2 and UKGC-4 are not readily accessible. Instead, they must be purchased from the BGS or viewed in hard copy at a small number of libraries. A scanned copy of UKGC-3 is available to download (see nora.nerc.ac.uk/id/eprint/512272). However, it does not include all data presented in UKGC-1 and UKGC-2. More importantly, it is not computer readable. Anyone wishing to analyse the data must therefore spend time and effort manually copying it into computer-readable files.

Despite these problems, the UKGC is an invaluable resource in that it provides a list of the original studies and reports from which its data are compiled. To realise its full value, our initial aim is to ensure that the data and information in the UKGC are available as a computer-readable, consistently structured database with linked metadata. Subsequently, we have expanded this database by including further measurements from the UKGC's original sources and from more recent studies. Here, we outline the structure of our database, which we refer to as CGD-UK and which is currently populated with data from northern England and the Scottish Borders.

3 DATA REQUIREMENTS AND COMPILATION

3.1 Data Inclusion/Selection

Subsurface heat flow is affected by many factors, including radiogenic heat production (Strutt 1906), movement of groundwater (Smith and Chapman 1983), and changes in surface temperature (Cermak 1971) and topography (Lewis and Wang 1992) . However, heat flow on vertical length scales $\gtrsim O(10)$ m is commonly estimated to first order using measurements of only temperature and thermal conductivity (e.g. Bullard, 1939). Such estimation assumes steady-state conduction through a series of horizontal layers, with no advection or production of heat (Gallagher 1990) . These assumptions underpin most of the heat-flow estimates that have been made in the UK.

In many boreholes, only subsurface temperature, and not thermal conductivity, is measured. An approximate profile of thermal conductivity within such a borehole can be constructed from a stratigraphic or lithological log describing the units of rock within the borehole. Each unit is assigned a value of conductivity that is based on measured samples from other locations. These samples may come from a nearby borehole that penetrates the same stratigraphic units. Alternatively, samples may come from similar rocks in a range of locations, yielding an average value of thermal conductivity. Depending on the geographical coverage, this average value may correspond to a local stratigraphic unit (e.g. Millstone Grit) or to a broad lithological grouping (e.g. limestone).

To allow estimation of conductive heat flow at boreholes both with and without thermal conductivity measurements, CGD-UK includes:

(a) Measurements of temperature.
(b) Measurements of thermal conductivity.
(c) Average values of thermal conductivity for lithological and stratigraphic divisions.
(d) Stratigraphic and lithological logs.

The UKGC, and many other publications from which we have compiled data, report estimates of the local geothermal gradient and of heat flow (e.g. (Rollin 1995). We do not include these estimates in CGD-UK since they have been calculated using a variety of methods. Instead, CGD-UK provides data that allow researchers to make consistent estimates of their own. We anticipate that future releases of CGD-UK will expand to include further data that can help refine more physically complete models of subsurface heat flow (see Section 5.1).

3.2 Database Structure

CGD-UK is hosted on data.ncl.ac.uk, which is Newcastle University's data repository. This repository is maintained by FigShare and supports version control. The bulk of CGD-UK is published as a series of comma-separated values (CSV) files. A master table (**CGD-UK_overview_spreadsheet.csv**) lists all locations at which temperature and/or thermal conductivity have been measured. Many of these locations are boreholes that are listed in the BGS Single Onshore Borehole Index (SOBI; www.bgs.ac.uk/datasets/boreholes-index). These locations are referred to by their SOBI reference number, which acts as a unique identifier. Locations without a SOBI reference number are described by a unique identifier made up of the BNG grid square, easting, and northing. For instance, the borehole at Dufton (BNG grid square NY; easting 368530; northing 525030) has the unique identifier NY368530525030.

In detail, CGD-UK is housed within seven datasets, which form a single Figshare collection. Six of these datasets contain data and metadata that have been manually compiled and checked (we refer to these data as quality-controlled data):

- Dataset **CGD-UK_master_table** contains:
  - **CGD-UK_master_table.csv**: CSV file containing a master table of metadata that describe all locations with known measurements of temperature or thermal conductivity.
  - **CGD-UK_master_table_README.txt**: Text file describing the format of CGD-UK_overview_spreadsheet.csv.
- Dataset **CGD-UK_temperature_individual_measurements** contain:
  - CSV files with names of the form **XXX_temps.csv**, where XXX is the unique identifier describing each location. These files contain temperature measurements made at the corresponding locations.
  - **CGD-UK_temperature_individual_measurements_README.txt**: Text file describing the format of the data housed in the files XXX_temps.csv.
- Dataset **CGD-UK_thermal_conductivity_individual_measurements** contain:

- CSV files with names of the form **XXX_conds.csv**, where XXX is the unique identifier describing each location. These files contain thermal conductivity measurements made at the corresponding locations.
- **CGD-UK_thermal_conductivity_individual_measurements_README.txt**: Text file describing the format of the data housed in the files of the form XXX_conds.csv.

- Dataset **CGD-UK_thermal_conductivity_compilations** contain:
  - **CGD-UK_thermal_conductivity_compilations_british.xlsx**: Microsoft Excel spreadsheet containing average values of thermal conductivity for a range of British rocks.
  - **CGD-UK_thermal_conductivity_compilations_global.xlsx:** Microsoft Excel spreadsheet containing average values of thermal conductivity for a range of globally distributed rocks.
  - **CGD-UK_thermal_conductivity_compilations_README.txt**: Text file describing the form of the spreadsheets CGD-UK_thermal_conductivity_compilations_british.xlsx and CGD-UK_thermal_conductivity_compilations_global.xlsx.
- Dataset **CGD-UK_stratigraphy_lithologies** contains:
  - CSV files with names of the form **XXX_ukogl_well_tops.csv**, where XXX is the unique identifier describing each location. Each file contains stratigraphic and lithographic information from the UK Onshore Geophysical Library (UKOGL) for the corresponding locations.
  - **all_ukogl_well_tops.csv**: CSV file combining data from all files of the form XXX_ukogl_well_tops.csv.
  - **CGD-UK_stratigraphies_README.txt**: Text file describing the formats of the data housed in the file all_ukogl_well_tops.csv and in files of the form XXX_ukogl_well_tops.csv.
- Dataset **CGD-UK_sources** contain:
  - **CGD-UK_sources.xlsx**: Microsoft Excel spreadsheet providing information on the sources from which CGD-UK were compiled.
  - **CGD-UK_sources_README.txt**: Text file detailing the layout of the spreadsheet CGD-UK_sources.xlsx.

The seventh dataset contains data that have not been checked by the authors (we refer to these data as non-quality-controlled data):

- Dataset **CGD-UK_unsorted_data_tables** contain:
  - **CGD-UK_unsorted_CatalogueGeothermalData1984_Table_1.csv**: CSV file containing a copy of Table 1 of UKGC-3. This table has been read from scanned documents using automated data-recognition software. It lists selected temperature measurements and associated metadata.
  - **CGD-UK_unsorted_CatalogueGeothermalData1984_Table_2.csv**: CSV file containing a machine-read copy of Table 2 of UKGC-2. This table has been read from a scanned document using automated data-recognition software. It lists estimates of heat flow and associated metadata.
  - **CGD-UK_unsorted_CatalogueGeothermalData1984_Table_3.csv**: CSV file containing a machine-read copy of Table 3 of UKGC-3. This table has been read from a scanned document using automated data-recognition software. It lists selected geochemical measurements and associated metadata.
  - **CGD-UK_UKCS_CGG_GeothermalDatabase.csv:** CSV file containing measurements of temperature from offshore boreholes on the UK Continental Shelf. This database has been compiled and generously provided by CGG. This

currently includes temperature measurements from 2400 unique well locations on the UKCS.

Each of these seven datasets has a unique digital object identifier (DOI), which will be retained when future updates are released. With this structure, CGD-UK can be easily expanded to accommodate further datasets. For instance, in future the >30,000 lines of non-quality-controlled data can be manually checked and integrated into the six datasets of quality-controlled data as appropriate.

3.3 Quality-Controlled Data: Compilation and Summary

CGD-UK currently includes quality-controlled metadata for 209 locations within the UK, specifically within British National Grid Squares NT, NU, NY, NZ, SD, SE and TA (Figure 1). Data have been compiled from 50 reports and publications, all of which are publicly available and have no restrictions on reuse. **CGD-UK_overview_spreadsheet.csv** lists all sources of data.

Temperature records from 50 of these locations have been digitised, whilst a total of 1031 measurements of thermal conductivity from 17 locations have been digitised. During digitisation, we have taken care to trace the original sources of data and to check all of the digitised files against these original sources. Wherever possible, we include estimates of uncertainty in the measurements. Unfortunately, many of the original sources do not quantify uncertainties.

3.3.1 Temperature

Measurements of *in situ* temperature are housed in the dataset **CGD-UK_temperature_individual_measurements**. These measurements have been compiled from a range of sources (e.g., journal articles and the reports of the BGS Geothermal Programme; see the individual files for full details). In total, 180,949 temperature measurements from 50 locations have been compiled (179,216 of these measurements come from borehole NZ26SW3569 at Newcastle Science Central Deep Geothermal Borehole; see Figure 2 for a summary of the number of boreholes drilled and measurements acquired per year). Compiled measurements lie between depths of 0 m and 4170 m (all depths are reported as True Vertical Depths, TVD). The deepest measurement, which was made in borehole NZ52SW308 (Seal Sands No. 1), yielded a temperature of 104°C, which is the highest value in this compilation. As noted by previous studies, there is a very significant vertical sampling bias. Excluding data from borehole NZ26SW3569, which reaches a depth of 1790.05 m, only 40 temperature measurements come from depths greater than 1000 m, and only 14 measurements come from depths greater than 2000 m (Figure 3); (Ireland *et al.* 2021). Figures 4 and 5 present visualisations of temperature as a function of depth.

CGD-UK follows UKGC-3 in classifying temperature measurements into seven types (see Table 1 for a summary of the number of locations at which each type of measurement has been made):

- BHT (bottom-hole temperature): These measurements record temperature at a single depth within a borehole (often the greatest depth). BHT measurements are usually made during short breaks in drilling and are strongly affected by the cooling effects of mud that is circulated through the borehole during drilling. BHT measurements are commonly corrected for these cooling effects (this correction requires knowledge of the time that passes between cessation of drilling and measurement of temperature; (Goutorbe *et al.* 2007). In CGD-UK, all BHT measurements are given without correction. However, we provide where possible the time elapsed since drilling, allowing users to correct the temperatures. These currently account for 119 of the temperature records in CGD-UK

- CFM (coal field measurements): These measurements were made within specially drilled holes in coal mines, mainly in the decades between 1870 and 1930. These currently account for 10 of the temperature records in CGD-UK
- DST (drill-stem test): These measurements are made during testing of oil and gas wells in advance of the end of drilling. The test is carried out over an isolated zone within the well, and pressure and temperature are measured. These currently account for 18 of the temperature records in CGD-UK
- EQM (equilibrium measurements): Equilibrium measurements are made at least several days (or, more commonly, weeks or months) after drilling has been completed. This delay minimises the effects of drilling upon subsurface temperature and ensures that measured temperatures are as close to temperatures within the surrounding rock as possible. These currently account for 44 of the temperature records in CGD-UK
- LOG (non-equilibrium measurements over a range of depths): This category describes non-equilibrium measurements that are recorded as a temperature sensor is lowered down a borehole. Measurements are made either during or soon after drilling, and so measured temperatures depart significantly from temperatures within the undisturbed rock. Note that equilibrium measurements are often also made using vertically lowered temperature sensors – such equilibrium measurements are included in the category EQM. These currently account for 28 of the temperature records in CGD-UK
- VST (virgin strata temperature): This category refers to equilibrium temperature measurements made in coal mines and mine shafts. Similar to CFM, they were typically made within specially drilled horizontal holes in the mine workings. These account for 16 of the temperature records in CGD-UK

We emphasise that these classifications alone should not be used to judge the quality of each measurement. Instead, measurement quality should be judged using quantitative estimates of uncertainty, where they exist. 1,574 of the temperature measurements in CGD-UK include such estimates of uncertainty (Figure 3). These uncertainties lie in the range 0.01°C to 0.1°C.

3.3.2 Thermal Conductivity

The thermal conductivity of rock depends on mineralogy, porosity, depth, temperature and pressure (e.g. Brigaud and Vasseur 1989). Changes in thermal conductivity with depth are therefore most accurately determined by recovering samples of rock. Most commonly, these samples are taken from core material obtained during drilling. The thermal conductivity of samples can be measured in several different ways and the effects of *in situ* conditions can be accounted for (Banks 2012).

3.3.2.1 Direct Measurements

Direct measurements of thermal conductivity are housed in the dataset **CGD-UK_temperature_individual_measurements.** The first release of CGD-UK contains measurements made on 1,031 samples from 17 locations (see Figures 6 and 7 for histograms showing when these samples were acquired and how they are distributed by depth). Samples come from depths of 6.1 to 1828.8 m. The deepest measured sample comes from borehole NZ19SW6 (Longhorsley No. 1), which also yielded the most measurements (111) from a single location. Only 13 of the 1031 compiled measurements are presented with an estimate of uncertainty (these 13 measurements all come from (Bullard and Niblett 1951a). The estimated uncertainties lie in the range 0.04 W K^{-1} m^{-1} to 0.12 W K^{-1} m^{-1}.

3.3.2.2 Average Values

Many authors do not present values of thermal conductivity measured on individual samples, but instead report average values for different lithologies (Bott *et al.* 1972; England *et al.* 1980) . Average values for a range of rocks have been compiled by several authors, who have taken different approaches to lithological classification. CGD-UK provides data from five compilations of British rocks and ten compilations of globally distributed rocks. These data are housed in the dataset **CGD-UK_thermal_conductivity_compilations.**

3.3.3 Lithology and Stratigraphy

Lithological and stratigraphic description of borehole core is necessarily subjective, and studies have taken many different approaches. In CGD-UK, lithological and stratigraphic information is compiled from the publicly available Well Formation Tops resource, which is made available by the North Sea Transition Authority (NSTA) and which can be accessed via the UK Onshore Geophysical Library (UKOGL; see ukogl.org.uk/well-formation-tops-new-search-facility). Such information is available for 120 of the 209 boreholes, and is within the dataset named **CGD-UK_stratigraphy_lithologies**.

These stratigraphic and lithological interpretations can be combined with the average values of thermal conductivity described in Section 3.3.2 to yield estimated profiles of thermal conductivity against depth. Such profiles can provide a useful guide in the absence of direct measurements of conductivity.

3.4 Non-Quality-Controlled Data: Summary

The dataset **CGD-UK_unsorted_data_tables** include data which has not been quality controlled. It includes computer-readable copies of Tables 1, 2 and 3 of UKGC-3. These data tables have been compiled using automatic detection of data values within low resolution scanned documents, and have not been quality controlled, nor have we attempted to trace data back to the original source. The dataset also contains a database of offshore temperature measurements originally compiled by CGG, but now available through an Open Government Licence. Within this dataset

4 DISCUSSION

4.1 Data Accessibility and Availability

There is increasing recognition of the importance and value of open-access data (Mesirov 2010). While the measurements we have compiled are in the strictest sense already available, they have previously been inaccessible. Starr et al. (2015) list eight core principles of data citation, and in particular highlight that data should be identifiable by a machine, without human input. In many areas of Earth and environmental sciences there are multiple and disparate databases with overlapping but incompatible data (e.g. Hsu *et al.* 2017). Improvement of data structures and integration of databases can help support interoperability across different disciplines (Hsu *et al.* 2017).

To date, there has not been a digital open-licence dataset for UK geothermal data that allows for wide reuse (e.g. CC0 or CC-BY licence). Although there have been recent compilations of temperature data, for example for Britain's coalfields (Farr *et al.* 2021) and for the shallow temperature field (Busby *et al.* 2011), these studies do not publish their data under an open license. While the data may be considered available, they are not accessible. Accessible, open-license datasets are invaluable to maximize the potential for novel data-science techniques (Wildman and Lewis 2022).

4.2 Implications for Geothermal Energy

Geothermal resources have considerable potential to decarbonise heating in the UK (Gluyas *et al.* 2018). To date, however, exploration and exploitation of geothermal energy has been limited by numerous factors. In particular, lack of ready access to data has made it difficult to identify sites at which geothermal heat could be sustainably exploited in useful quantities (Witter *et al.* 2019a; Walker and Abesser 2022). Establishing CGD-UK as an open-licence relational database for temperature and thermal conductivity will support new exploration by improving data interoperability and by facilitating access to data that is already available without licence restrictions.

The standardised, open-access data presented in CGD-UK allow use of novel data-science methods for a comprehensive assessment of the UK's geothermal resources. These methods could be used to address questions such as:

- **Do different methods for estimating heat flow lead to different assessments of geothermal resources? How accurately can values of heat flow be estimated given uncertainties in measured datasets?** Heat flow can be estimated using a range of computational methods informed not only by measurements of temperature and thermal conductivity, but also by measurements of radiogenic heat production, by records of past climatic change, and by estimates of how topography has changed through time and space. Most estimates of UK heat flow have been made using basic deterministic calculations (e.g. Bullard and Niblett 1951b). In recent years, however, advances in computing power have encouraged development of probabilistic methods that can better quantify the uncertainties produced by combination of several datasets (e.g. Hopcroft *et al.* 2009; Mather *et al.* 2018). Systematic application of such methods to the comprehensive data in CGD-UK could better quantify the importance of different effects and the associated uncertainties. (We anticipate that CGD-UK will expand to include datasets of palaeoclimate, radiogenic heat production and topography; see Section 5.1.)
- **How well can thermal conductivity be predicted from knowledge of lithology or stratigraphy?** Previous compilations of thermal conductivity measured on samples of globally distributed rocks show that conductivities can vary widely within a single lithology (e.g. Čermák and Rybach 1982). This finding suggests that lithologically informed predictions of thermal conductivity may not be accurate. CGD-UK can be used to investigate correlations between lithology and conductivity on a more local scale. For instance, 111 measurements of thermal conductivity were made in the Longhorsley-1 borehole (reference number NZ19SW6), which penetrates five stratigraphic units (Table 2). All five units consist of interbedded sandstones, limestones, mudstones and siltstones. Variations in average conductivity between the units seem to be consistent with changes in lithology between the units — the Fell Sandstone, with the highest proportion of sandstone, has the highest conductivity, whereas the Alston Formation, with the lowest proportion of sandstone, has the lowest conductivity. However, these variations are not statistically significant given the uncertainties in each average value. Detailed statistical analysis of such measurements for hundreds of UK localities may shed light on whether there are statistically reliable relationships between stratigraphy and thermal conductivity for British rocks.
- **How significantly are UK heat-flow estimates affected by past climatic changes?** Subsurface temperatures are affected by changes in surface temperature over climatic timescales (e.g. Mareschal *et al.* 1999). In northern areas of the UK, these effects are particularly pronounced due to the presence of ice sheets during the last glacial maximum. However, the impact of palaeoclimatic changes on heat-flow estimates has been assessed using a range of methods and datasets, and so it is difficult to compare results from different studies. For instance, (e.g. Westaway and Younger 2013) reassess palaeoclimatic effects for a selected number of boreholes in England, and their results

indicate a systematic underestimation of temperatures at depth. CGD-UK provides the data needed to undertake a comprehensive, consistent reevaluation of palaeoclimatic effects at locations across the UK. Such a reevaluation may show that the UK's geothermal resource is more widespread than previously thought.

- **How well can existing measurements of subsurface temperature constrain three-dimensional models of heat flow beneath the UK?** Several studies have predicted subsurface temperatures beneath the UK by interpolating between locations at which direct measurements have been made (e.g. Busby *et al.* 2011). This approach is highly unlikely to be accurate since it does not consider geological structures that play an important role in controlling transport of heat. In future, three-dimensional inverse models of heat flow based on observed geological structure could be constrained by the measurements compiled in CGD-UK (cf. Mather *et al.* 2019).

5 FUTURE WORK AND CONCLUSIONS

5.1 Database Expansion

We anticipate that CGD-UK will encourage further digitisation and standardisation of geothermal data from across the UK. In addition to expanding the geographical coverage, the following further datasets could be added to the database:

- **Temperatures from onshore oil and gas boreholes.** Datasets from onshore oil and gas wells are released to the public realm after expiration of confidentiality periods. However, under present arrangements many of these released datasets can only be accessed through commercial resellers. In future, onshore oil and gas data may be made more readily accessible through a release mechanism similar to that used for offshore data. Such a mechanism would provide many new temperature measurements, often in the form of text within scanned documents.
- **Temperatures from offshore oil and gas boreholes.** The NSTA maintains a publicly available National Data Repository (NDR; www.nstauthority.co.uk/data-centre/national-data-repository-ndr), which currently includes records of >12,000 offshore boreholes. Many of these records contain temperature measurements. In addition, a database housing >12,000 temperature measurements from 2,400 boreholes on the UK Continental Shelf (UKCS) was published in 2017 and is available through an Open Government Licence. We have started to consolidate these data into CGD-UK.
- **Further stratigraphic interpretations.** The database currently includes only stratigraphic interpretations that are provided by the NSTA and hosted by the UKOGL. Subject to the necessary legal agreements, further interpretations could be digitised from technical reports, from journal articles, or from the BGS collection of scanned reports (https://shop.bgs.ac.uk/Shop/search?type=boreholeIndex). If CGD-UK expands to include offshore data, there exists a datasheet of offshore stratigraphic information that could be included.
- **Indirect measurements of thermal conductivity.** Where it is not possible to recover samples for direct measurement, thermal conductivities within boreholes can be estimated by measuring the time-dependent response to a carefully controlled source of heat (Banks 2012). Similar approximations of thermal conductivity can be estimated from mineralogical composition or from borehole logs of petrophysical properties (e.g. gamma ray count; (Griffiths *et al.* 1992; Fuchs *et al.* 2015).
- **Measurements of radiogenic heat production.** Generation of radioactive heat over the range of depths penetrated by a borehole can have a small but non-negligible

effect upon measured subsurface temperatures (Gallagher 1990). Consideration of this effect can be important in accurate estimation of geothermal gradients.

- **Records of surface temperature.** Previous climatic changes strongly affect present-day flow of geothermal heat, particularly in regions that were once glaciated. Inclusion of climatic datasets in CGD-UK would help standardise the calculations that are made to correct for the effect of climatic variations on estimates of heat flow.
- **Records of topography and erosion.** Geothermal heat flow is affected both by present-day topography and by changes to topography in the past (England 1978). Addition of topographic and erosional datasets to CGD-UK would make it easier for researchers to account for these effects when assessing heat flow.

Many of these data are contained in scanned documents, and we have not included them in the first release of CGD-UK due to the time taken to manually identify and digitise the data. Recent advances in detecting data within scanned text (Kasar *et al.* 2013; Gilani *et al.* 2017) raise the possibility of automatically extracting valuable information from these documents, whose pages run into the millions (Dickinson and Ireland 2022). Since 2014 a UK legal framework has existed to support widespread preservation of data from existing documents. Specifically, researchers are permitted to copy any copyright material for the purpose of non-commercial computational analysis, provided they already have the right to read the material (Participation n.d.). Under this framework, CGD-UK could be rapidly expanded by a concerted and coordinated programme of automated data detection.

5.3 Conclusions

By providing consistently structured data together with clear metadata, CGD-UK forms an invaluable resource for anyone wishing to investigate heatflow of onshore (and offshore) the UK. It builds on past efforts of data compilation by updating records to a computer-readable format. CGD-UK data are structured in a simple yet flexible format and hosted within the widely used Figshare infrastructure. This infrastructure ensures that datasets can be easily updated and maintained, including version control, whilst retaining the same digital object identifiers (DOIs). The first release of CGD-UK contains: 1) quality-controlled data that have been consistently structured and formatted; 2) non-quality-controlled data that have been converted to digital records by yet to be quality controlled.

The quality-controlled data include 235 independent measurements of temperature from 50 locations and 1,031 measurements of thermal conductivity from 17 locations. These locations, all of which are onshore, are distributed across northern England and southern Scotland. The non-quality-controlled data comprise >30,000 records. Some of these data have been digitised from tables within UKGC-3 using optical character recognition software, whilst the remainder come from a database of offshore geothermal measurements made publicly available by CGG. We anticipate that these data will be subsequently checked and added to CGD-UK's quality-controlled datasets in the future.

The comprehensive data in CGD-UK provide opportunities to standardise estimates of heat flow beneath the UK taking advantage of the application of data-science techniques to Earth sciences that have become widely available in the past decade. Standardised estimates may lead to reassessment of the UK’s geothermal resource, contributing to informing energy strategy for achieving net-zero. As far as we are aware, CGD-UK is the only compressive, open-license digital database for temperature and thermal conductivity in the UK, and therefore represents a unique resource.

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Author contributions

AD: conceptualization (lead), data curation (lead), formal analysis (lead), investigation (lead), methodology (lead), writing – original draft (supporting), writing – review and editing (supporting).

MI: conceptualization (lead), data curation (supporting), formal analysis (supporting), investigation (supporting), methodology (supporting), writing – original draft (lead), writing – review and editing (lead).

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Data availability

The database is available at data.ncl.uk (https://doi.org/10.25405/data.ncl.c.6103638.v1) and is published under a CC BY 4.0 open licence. Where data copyright belongs to NERC, data are reproduced and stored in the database in accordance with the NERC Open Research Archive (nora.nerc.ac.uk). The CGG Geothermal Database is reused, and contains public sector information licensed under the Open Government Licence v3.0. Due to the varied nature of the historical records, there may be inaccuracies in the database. Please report any inaccuracies by using the following online form https://forms.office.com/r/TK0ak3ucFu.

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TABLES

Table 1. Summary of number of locations within first release of CGD-UK at which different types of temperature measurement have been made. Column headings list different measurement types (see Section 3.31 for definitions). Row titled 'All' gives total number of locations at which each measurement type has been made. Note that more than one measurement type has been made at some locations. Row titled 'Max. depth 0 – 500 m' gives number of locations at which the deepest measurement was made at a depth of 500 m or less. Row titled 'Max. depth > 500 m' gives number of locations at which the deepest measurement was made at a depth of more than 500 m.

	BHT	EQM	LOG	DST	MWT	VST	CFM
All	117	44	28	15	2	15	10
Max. depth 0 – 500 m	13	23	6	0	0	1	5
Max. depth > 500 m	104	21	22	15	2	14	5

Table 2. Thermal conductivities for borehole NZ19SW6 (Longhorsley No. 1), grouped by stratigraphic subdivisions. k_a = arithmetic mean of measured thermal conductivities; k_h = harmonic mean of measured thermal conductivities.

Subdivision	Depth Range (m)	k_a (W m-1 °C-1)	k_h (W m-1 °C-1)
Stainmore Fm	100.00-318.52	2.916±0.714 (±1 σ)	2.785±0.515 (±1 σ)
Alston Fm	318.52-743.71	2.722±0.439 (±1 σ)	2.652±0.430 (±1 σ)
Tyne Limestone Fm	743.71-1321.0	2.979±0.502 (±1 σ)	2.906±0.438 (±1 σ)
Fell Sandstone Fm	1321.0-1632.2	3.204±0.557 (±1 σ)	3.108±0.549 (±1 σ)
Lyne Fm	1632.2-1828.8	2.804±0.447 (±1 σ)	2.739±0.410 (±1 σ)
Overall	100.00-1828.8	2.925±0.543 (±1 σ)	2.835±0.483 (±1 σ)

FIGURE CAPTIONS

Figure 1: Locations of 209 sites listed within CGD-UK (see master table **CGD-UK_overview_spreadsheet.csv**). White circles (147 sites) = temperature measurements exist but have not been digitised; conductivity measurements do not exist. White triangles (27 sites) = temperature measurements exist and are included within CGD-UK as CSV files; conductivity measurements do not exist. Yellow circles (13 sites) = temperature measurements exist but have not been digitised; conductivity measurements exist but have not been digitised. Yellow triangles (5 sites) = temperature measurements exist and are included within CGD-UK as CSV files; conductivity measurements exist but have not been digitised. Red triangles (17 sites) = temperature measurements exist and are included within CGD-UK as CSV file; conductivity measurements exist and are included within CGD-UK as CSV file.

Figure 2: Histograms displaying CGD-UK temperature data against year. (a) Histogram of cumulative number of boreholes for which measured temperatures have been digitised and included in CGD-UK. (b) Histogram of cumulative number of temperature measurements (note that 179,216 measurements from borehole NZ26SW3569 are not included; these measurements were made in 2012). Black = measurements with estimation of uncertainty; red = measurements without estimation of uncertainty.

Figure 3: Histograms of temperature measurements against depth. (a) Histogram of all temperature measurements (179,216 out of 180,949 measurements come from borehole NZ26SW3569). Note that y-axis is logarithmic; see (c) for x-axis scale. (b) Histogram of all measurements in upper 2000 m, coloured by uncertainty. Black = measurements with estimation of uncertainty; red = measurements without estimation of uncertainty. See (d) for x-axis scale. (c) Histogram of 1,733 temperature measurements from all locations apart from NZ26SW3569. Note that y-axis is logarithmic. (d) Histogram of measurements (excluding those from NZ26SW3569) in upper 2000 m, coloured by uncertainty.

Figure 4: Box plots of temperature against subsurface depth, with depth divided into increments of 200 m. (a) Box plots for all temperature measurements within CGD-UK (179,216 out of 180,949 measurements come from borehole NZ26SW3569). Grey boxes extend from the first quartile to the third quartile; black whiskers extend to maximum and minimum values; red lines denote mean temperature. (b) Box plot for 1,733 temperature measurements from all locations apart from NZ26SW3569. See (a) for y-axis scale. Figure design after Farr et al. (2020).

Figure 5: Plots of temperature against depth. (a) All measurements (179,216 out of 180,949 measurements come from borehole NZ26SW3569). (b) All measurements coloured by uncertainty. Black = measurements with estimation of uncertainty; red = measurements without estimation of uncertainty. (c) 1,733 temperature measurements from all locations apart from borehole NZ26SW3569. (d) 1,733 temperature measurements coloured by uncertainty.

Figure 6: Histograms displaying CGD-UK thermal conductivity data against year. (a) Histogram of cumulative number of boreholes in which conductivity has been measured. (b) Histogram of cumulative number of conductivity measurements. Black = measurements with estimation of uncertainty; red = measurements without estimation of uncertainty.

Figure 7: Histograms of thermal conductivity measurements against depth. (a) All measurements. (b) All measurements, coloured by uncertainty. Black = measurements with estimation of uncertainty; red = measurements without estimation of uncertainty.