Project acronym and title:

SECURe – Subsurface Evaluation of Carbon capture and storage and Unconventional risks

INTEGRATED DATA PLATFORM FOR MULTISOURCE MULTISCALE SENSOR DATA

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Disclaimer

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Public introduction

Subsurface Evaluation of CCS and Unconventional Risks (SECURe) is gathering unbiased, impartial scientific evidence for risk mitigation and monitoring for environmental protection to underpin subsurface geo-energy development. The main outputs of SECURe comprise recommendations for best practice for unconventional hydrocarbon production and geological CO2 storage. The project is funded from June 2018–May 2021.

The project is developing monitoring and mitigation strategies for the full geo-energy project lifecycle; by assessing plausible hazards and monitoring associated environmental risks. This is achieved through a program of experimental research and advanced technology development that includes demonstration at commercial and research facilities to formulate best practice. We will meet stakeholder needs; from the design of monitoring and mitigation strategies relevant to operators and regulators, to developing communication strategies to provide a greater level of understanding of the potential impacts.

The SECURe partnership comprises major research and commercial organisations from countries that host shale gas and CCS industries at different stages of operation (from permitted to closed). We are forming a durable international partnership with non-European groups, providing international access to study sites, creating links between projects and increasing our collective capability through exchange of scientific staff.

Executive report summary

The SECURe project has used, produced and analysed a vast amount of data in a wide range of formats, types. Like in many other data-intensive applications, users and researchers are accustomed to certain workflows which often do not explicitly consider other possible usages of the same data. Despite the strong effort in recent decades towards reproducible research and open and interoperable data, particularly in the geoenergy sector, many challenges are present to allow a proficient and consistent data management, storage, reuse and sharing: this includes qualitative nature of some data, lack of common formats, commercial or closed data format, while intrinsic variabilities and uncertainties present in the subsurface lead immense difficulties in distinguishing between local (reservoir-specific) and more general data. In this report, we propose a systematic way of collecting data and (meta)analyse it and apply it to the data produced within the project. This is to provide a long-lasting legacy for the project. Best practices for data integration are also discussed.

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Contents

FIGURES

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Objectives, aims and scope

The main objective of this report is to summarize and integrate data and software for subsurface carbon capture and storage and shale gas applications developed in SECURe.

These are mostly based on field data obtained in the sites of Borzecin, Sleen, Foantaine Ardente, Vroegum, and Rochasson field sites, alongside data obtained from experiments conducted in the laboratory or at the GeoEnergy Test Bed. Furthermore, SECURe produced several simulation data and software that work in symbiosis with experimental and field data.

Such collection of data is multisource, in the sense that it comprises data of different origin and format, and is multiscale, as it refers to different levels of description of a reservoir (e.g., microscopic, pore-scale, porous medium, reservoir scale, etc.). However, to exploit such a vast array of data, it is necessary to establish the criteria for their interoperability: their ability to operate in conjunction with each other. Once such criteria have been identified, the heterogeneous collection (or repository) of data can be interpreted as an integrated platform that can be employed to model and understand the process of subsurface carbon sequestration.

The report aims to disseminate a concise, integrated review of data, together with best practices for data interoperability that can be applied also to future projects.

At the end of the report, short data reports are provided for quick access and reference.

Heterogeneous data collection: metadata

The SECURe project features an impressive variety of diverse datasets. Some are generated as a result of measurements conducted in the laboratory or in the field, while others are the result of numerical simulations performed using specialised software. Others are dissemination data like publications or presentations.

Therefore, it is of primary importance to provide a common interface for describing different data and collecting them into reports. This approach roughly follows some of the principles of Object-Oriented Programming, specifically the concepts of abstraction, inheritance, and polymorphism.

Abstraction means that data reports should only expose non-technical information therefore being accessible to non-expert readers. Complex information should be common to all the reports (and therefore not repeated in every report) or available in the deliverables.

Inheritance here is interpreted as keeping the format of the reports consistent and based on a common template.

Finally, polymorphism means that all the data reports can be accessed and processed by only knowing the basic template.

Hence, a standard template for data report has been developed with the central scope of making the data accessible and usable by a wider public. Each report has to start with the following entries:

- **DATASET**: name of dataset
- **AUTHORS**: names of the data producers
- **PARTNER**: affiliation of the authors

Then data are reported by completing the following five sections:

- **Data category**: Select from the following data categories (basically any output is considered as data). A category must be entered.
    - Site data (on-site measurements and other data)
    - Simulation data (data produced by numerical simulations)
    - Research data (reports on technologies, guidelines, new methodologies)
    - Dissemination data (presentations at events and other dissemination activities)

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- **Data description and information created**: A layperson description of the data and the implications/interpretation of the data (i.e. information created). Clearly mentioning any 3rd party datasets/software if you have used these and include links. The description should answer the following questions:
    1. What does the data represent? *For example: this dataset contains results from numerical simulations of [...] using the software [...] or this dataset contains data from the site located in [...] through a campaign [...]. Assume the reader is unfamiliar with the topic.*
    2. How was the data extracted/created? *For example: this data represents the raw (unprocessed) readings from this sensor [...] or this data was obtained performing [...] on the unprocessed raw data extracted from/available at [...]*. Furthermore, any other datasets employed should be indicated: *For example: open-access CCS geological data from the repository (include link) where used in conjunction with the chemical library [...]*
    3. Is this data reusable? In which context? *For example: these data can be used as benchmark for numerical simulations, or This dataset can be employed to suggest policies and decision-making.*
    4. Is there, or will there be, a publication associated with the data? *For Example: These data have been used in the following journal articles: [...]*
    5. Eventual limitations of the data. *For example: measurements for [...] are incomplete due to [...] or unfortunately the collected data in [...] may be affected by large errors due to [...].*
- **Standards for format and content:** This is a brief but complete description of what the data looks like and their format. Also, eventual software required to visualise the data should be mentioned. *Example: Data are provided in CSV (comma separated value) format. For a detailed description of this format, please refer to https://en.wikipedia.org/wiki/Comma-separated_values. In our file [...] the three columns represent the sensor ID, the pressure, and the velocity. Each row corresponds to a different sensor (please refer to table X of deliverable Y.Z for an extensive description of the sampling campaign). These data can be imported natively into most data processors (MATLAB, Excel, etc.).*
- **Polices for stewardship and preservation:** This section should explain how data will be maintained and preserved. What policies have been/will be enacted to ensure that the data remain accessible. In the case of GitHub for example, data could be uploaded on a repository belonging to a group administered by the work package/task leaders.

  Example: Data have been uploaded to the open free repository [...] which provides free storage for data. Administrator rights have been given to [...].

- **Procedures to provide access:** This is an uncomplicated explanation of how to get the data. This section can be extremely short and where data are available online it should include a link. If the data has a Digital Object Identifier (DOI), this should be included.

  Example: Data are publicly available here: https://github.com/multiform-UoN/SECUReFOAM

Such a brief and concise method of data collection based on a simple and short template has proven to be useful also for creating a simple and effective framework of data management that each partner in the project can follow.

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Furthermore, a complete list of data produced within SECURe is available online (www.securegeoenergy.eu) with indication regarding their availability and location.

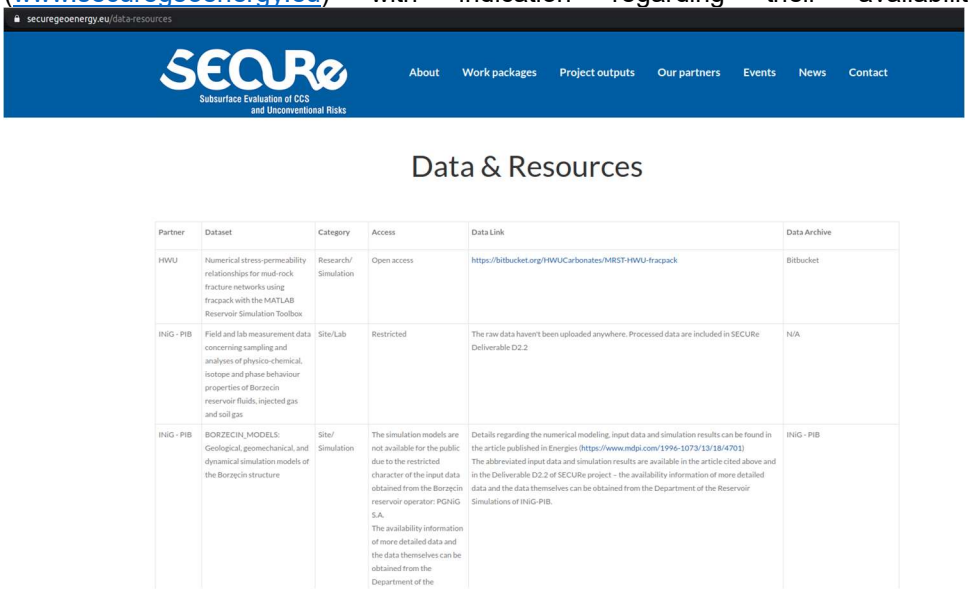

Figure 1 The data repository of the SECURe website

Data type, formats, and open data

Currently, a total of 71 dataset have been collected from SECURe.

Forty-four of these have been stored in open-access repositories or will be made available after an embargo period (for example, due to a peer-review process for a publication). The remaining data have been kept confidential (due to their commercial sensitivity) or they are available by request to the authors.

The most common formats are “Microsoft Excel-compatible” formats such as xlsx or csv. As a result, a large portion of the data is represented by numbers stored in spreadsheets. Other formats include input files for MRST, VTK for simulation output, and human readable text data. Other more qualitative data include video and image formats.

The storage platform employed includes the database of the UK Carbon Capture and Storage Research Centre UKCCSRC (26 datasets) and the GFZ archive (11 datasets). Other storage platforms include openly accessible databases like the website of the British Geological Survey (BGS) or GitHub.

Data integration: challenges and exploitation pathways

Currently, data integration remains one of the major challenges in large European Projects as many partners with significantly diverse background, scientific approach and scope are involved. Effective communication remains a significant issue when collecting data from different partners, especially in the case of large and sensitive datasets. Therefore, an effective and standardised approach to report data (similar to the one already outlined in this report), should be devised before the projects start date. However, this is seldom the case with large projects, and global data administration is still regarded as a minor issue. While the use of artificial intelligence and machine learning has drastically changed the way data is processed and has enabled integration of massive amounts of data, proper data interfaces are still required for data interoperability. Citizen science might also play a key role both as a consumer and producer of data. Amateur researchers should be able to access data in a human-readable and intuitive format, as they might not be in possession of sophisticated or expensive data processing tools. Or simply, they might not have enough time to go through complicated instructions; a circumstance that would effectively render the data inaccessible to them. On the other hand, automatic processing of data from citizen science (or even research groups), and its reduction into standard

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format, is only possible when a sufficient amount of meta-data is provided. A file called fieldData.txt with twenty columns of raw numbers would be extremely hard to process automatically when no additional information regarding the file content is given.

SECURe is not exceptional in this regard, and data interoperability is complicated by several factors, especially:

- The broad scale and significance of the data reported.
- The different perception that the partners have regarding what is significant and what is not.
- Multiple competing simulation tools (MRST, Eclipse, OpenFOAM) and specialised data visualisation and post-processing software (Paraview or ResInsight).
- Lack of a standardised approach to data format, especially considering open-source general formats like VTK against formats specific to proprietary software. Proprietary data formats are not recommended in large projects (unless the software owner is a partner) since they tend to have closed source readers that make it impossible to fully understand the logic behind them. This constitutes a significant obstacle to interoperability.

However, data can be exploited by further connection. For example, data in MS Office format can be employed to provide input to simulation software for both direct or inverse analysis. Specifically, site data combined with laboratory data can be employed in conjunction with simulation software to calibrate mathematical models for reservoirs at different scales and different physics. Furthermore, it is possible to investigate the configuration of unknown parameters or "states" (for example underground soil composition and material properties) that lead to predictions resembling the survey data. This would allow to quantify the impact of uncertainty on the predictive power of current models and suggest new paths for improvement.

Connecting different data types

As already outlined in deliverable D4.4, there are still issues regarding the actual usability of geological data, especially when crossing disciplinary barriers.

This is mostly due to the highly non-standard (or proprietary) data format used in reservoir simulations, which targets specific software like Eclipse (Schlumberger, 2020), while other opensource libraries like MRST (Industries, 2020) and OpenGeoSys (OpenGeoSys, 2020) adapt their internal algorithms to read such formats.

While there are utilities provided in the Open Porous Media that provide data conversion, these are not always maintained and, since data files from reservoir simulations do not obey a unique standard, interoperability is not always straightforward or even possible without a significant amount of dedicated work. Such problems can only be addressed if the community migrates to standard formats, with focus on connection with other data and software.

Automatic data connection requires a predefined data structure to be clearly devised before the project starts, and this was not available in SECURe. However, off-line data connection involving proper storage and documentation of a large array of data, might be even more effective for future projects outside of SECURe. This is the case when considering some of the key characteristics an automatic data connection system might have:

1. Ability of reading different data formats and perform appropriate conversions.
2. Easy to use by non-experts (non-developers)
3. Portable (can work in different architectures/operating systems).

Hence, in most circumstances an off-line data would result in easier access to the data.

Conclusions and best practices

In this report, we illustrated an approach to connect multi-source and multi-scale data to provide a platform that can be exploited in future, more advanced, studies. Specifically, we discussed the need for a standardized data interface that allows data interoperability and efficient communication between the modules of the data platform. A FAIR (Findable, Accessible, and Reusable) paradigm should be

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followed. Below, we report some recommendations for management of geological data in future European Projects:

OPEN DATA

Data should be visible and accessible both by the partners and the public. Timely data access and transparency regarding data formatting are of paramount importance to effectively deliver a platform.

OPEN FORMAT

Data formatting should be easily readable, standardised, and open. As discussed previously, closed-source data formats often contain subtleties that require full access to the original reader, which is often impossible due to licensing.

LONG-TIME AVAILABILITY

Stewardship is pivotal to ensure that datasets remain available after the project is concluded. Hence, we recommend the use of public repositories or even a unique repository for all the datasets produced within the project.

METADATA

Metadata play a key role in the collection and processing of diverse datasets. In this report, we emphasised how a brief but precise description of the data format and stewardship can drastically improve their accessibility. A precise design of appropriate metadata that can be applied to a broad range (or all of the) datasets should be discussed and agreed upon at the very beginning of every research project.

VERSIONING AND UPDATING

Data may require updates in the months or years following the end of the project. These could be in the form of rectifications or upgrades (for example, in the case of a software). Whenever newer versions are available, an appropriate link should be made available.

DATA SECURITY AND RE-USE

Repositories holding publicly available data should be secure enough to prevent deliberate (or accidental) modification or destruction of the data. Data corruption can negatively impact the reusability of the data. However, the licence should not prevent data reuse.

List of available datasets from SECURe partners

Data owners can be contacted at info@securegeoenergy.eu

OPENFOAM SOLVER FOR THE FORMAL UPSCALING OF TRANSPORT WITH SURFACE REACTIONS IN POROUS MEDIA

AUTHORS: Federico Municchi, Matteo Icardi

PARTNER: University of Nottingham

Data category

Research data

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Data description and information created

This dataset contains the source code for a computer application for the numerical upscaling of transport equations in porous media.

The code is written in C++ using the open-source finite volume library OpenFOAM (https://openfoam.org/). Examples of applications are also included.

The code was written conformally to the object-oriented philosophy employed in OpenFOAM, and can be extended to include new physics and model different systems, enabling the computation of macroscopic coefficients for a wide range of problems.

Details regarding the numerical and mathematical formulation can be found in the article published in Advances in Water Resources (https://linkinghub.elsevier.com/retrieve/pii/S0309170819308474). The code is also citable via Zenodo (https://zenodo.org/record/3736339#.YByR-lnnh_s).

As the code is based on OpenFOAM, it is subject to GNU General Public License and is distributed in the hope that it will be useful, but without any warranty; without even the implied warranty of merchantability or fitness for a particular purpose.

Standards for format and content

The code is written in C++ and therefore is composed by ascii text files. Instructions for compiling the code are provided in the README.md file, together with the detailed folder structure of the library. An application based on the MATLAB library Chebfun is also provided for benchmark. Other formats follow the standard for OpenFOAM (https://cfd.direct/openfoam/user-guide/).

Polices for stewardship and preservation

The code is uploaded on GitHub under the multiform-UoN group. Ownership and responsibility for preservation goes to the administrators Federico Municchi and Matteo Icardi. Please contact them if data becomes unavailable.

Procedures to provide access

The code is publicly available at https://github.com/multiform-UoN/porousTransportUpscalingFoam

FLUID PH AND MAJOR AND MINOR ELEMENT DATA FROM SHALE-ACIDIC FLUID INTERACTION LABORATORY EXPERIMENTS

AUTHORS: Yukun Ji, Veerle Vandeginste

PARTNER: University of Nottingham

Data category

Research data

Data description and information created

1. This dataset presents major (ICP-OES) and minor (ICP-MS) element data and fluid pH during interaction of simulated fracturing fluids with the Bowland-Hodder shale at a variety of conditions, i.e. fluid acidity (pH 1-5), temperature (25-70 C), and rock/fluid ratio (from 0.2:200 to 20:200), as well as two end member mineralogical compositions (from 618 m depth and 673 m depth).
2. The shale powders were used for X-ray diffraction (XRD) analysis to determine their mineralogical composition. During water-rock interaction, a total of 1 mL extracted fluid was used for pH analysis by using a Fisher Scientific accumet benchtop pH meter and another 1 mL extracted fluid was acidified and diluted 10 times with ultrapure HNO_3 (2%) for elemental analysis using

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inductively coupled plasma optical emission spectroscopy (ICP-OES) and inductively coupled plasma mass spectrometry (ICP-MS).

3. A wide range of fluid acid concentrations, temperatures, and rock/fluid ratios have been tested to investigate element mobilisation and to gain insight into the chemical processes that take place during hydraulic fracturing fluid-shale interaction. These data identify chemical reaction pathways of geochemical elements (including contaminants) in fracturing fluids over a range of fluid chemistries and environmental conditions, and helps to evaluate element mobilisation from shale reservoirs with differing mineralogies.
4. Details regarding the data can be found in the article published in Fuel *(https://doi.org/10.1016/j.fuel.2020.119914)*.
5. Not Applicable

Standards for format and content

Experimental data are provided in CSV (comma separated value) format. For a detailed description of this format, please refer to *https://en.wikipedia.org/wiki/Comma-separated_values*.

Polices for stewardship and preservation

Experimental data is uploaded on NERC Data Service. Ownership and responsibility for preservation goes to the administrators Yukun Ji and Veerle Vandeginste. Please contact them if data becomes unavailable.

Procedures to provide access

Experimental data are publicly available here: *https://data-search.nerc.ac.uk:443/geonetwork/srv/api/records/ac473e73-bea3-58bb-e054-002128a47908*

FIELD AND LAB MEASUREMENT DATA CONCERNING SAMPLING AND ANALYSES OF PHYSICO-CHEMICAL, ISOTOPE AND PHASE BEHAVIOUR PROPERTIES OF BORZECIN RESERVOIR FLUIDS, INJECTED GAS AND SOIL GAS

AUTHORS: Miroslaw Wojnicki, Marcin Warnecki

PARTNER: INiG - PIB (Instytut Nafty i Gazu – Państwowy Instytut Badawczy)

Data category

Site and laboratory data

Data description and information created

This data set contains all gathered data during on-site sampling campaigns and further analyses of sampled fluids from the Borzecin reservoir.

The data were created during direct measurements and studies conducted on-site (Borzęcin), including pressure, temperature, sampling depths, coordinates of sampling points as well as during laboratory studies, including PVT analyses of reservoir/injected gas, gas chromatography/mass spectrometry for analysis of reservoir, injected and soil gas chemical/isotope composition and chemical analysis of reservoir water.

Some of the data was used in simulations of the ongoing sequestration process in the Borzęcin structure performed within the SECURe project. They may be used by professionals in similar projects.

The data were published in monograph series of Scientific Works of Oil and Gas Institute – National Research Institute, titled: “Long-term sequestration process in the Borzęcin structure – observation

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evidence of the injected acid gas migration and possible leakage". It is also planned to publish the data in the *Energies* scientific journal.

Standards for format and content

The data are provided primarily in xls and csv format. These data can be processed in most data processors, including Excel.

Polices for stewardship and preservation

The raw data haven't been uploaded anywhere. Processed data are included in the Deliverable D2.2 "Report on the effects of long-term sequestration process in the Borzęcin structure – observation evidence of the injected gas migration and possible leakage" publicly available from https://www.securegeoenergy.eu/ .

FORMATION CONFINEMENT ANALYSES BASED ON AVAILABLE RESULTS OF LABORATORY GEOCHEMICAL MEASUREMENTS OF BRINE SAMPLES FOR SELECTED SITES

AUTHORS: Adam Wójcicki

PARTNER: Polish Geological Institute – National Research Institute

Data category

Research data

Data description and information created

The dataset is on analyses on formation confinement based on available results of laboratory geochemical measurements of brine samples for several field sites (shale wells, acidic gas storage within a depleted gas field and a saline aquifer structure – a possible CO_2 storage site).

The goal of these analyses was to assess the presence of relic brine within reservoirs/aquifers in question or brine exchange between reservoirs/aquifers within these sites. Results of these analyses can be used to evaluate caprock integrity for they could be indirect evidence of possible migration paths (faults, fractures) and hence possible leaks within the site currently, in the not-too-distant geological past, or no migration or fluid exchange at all (relic brine).

In case of a saline aquifer structure (a possible CO_2 storage site) available raw archive geochemical data have been collected from publications (https://www.pgi.gov.pl/oferta-inst/wydawnictwa/serie-wydawnicze/profile-otworow-pig/6105-prof-gb-otw-wiert-z-137-2012-wojszyce-ig-11a-ig-3-i-ig-4.html). In case of acidic gas storage within a depleted gas field information from unpublished archive well reports (http://geoportal.pgi.gov.pl/otwory; accessible through the National Geological Archives: https://www.pgi.gov.pl/en/services/geological-information.html) and results of brine sample monitoring carried out by INiG-PIB in the framework of WP3 of the SECURe project have been collected. In the case of the shale wells, raw archive geochemical data have been obtained from Polish Oil and Gas Company (no link can be provided).

The analyses are described in D2.5 of the SECURe project (https://securegeoenergy.eu/work-packages/wp2-risk-assessment). The methodology used in these analyses is generally based on published work presented in Hounslow (1995; https://www.routledge.com/Water-Quality-Data-Analysis-and-Interpretation/Hounslow/p/book/9780873716765) principles on degree of geochemical maturity of formation water and isolation of aquifers/reservoirs measured by total dissolved solids [TDS], Na/Cl and Cl/Br ratios.

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Regarding eventual limitations of the data the main issue is that one of the data campaigns has only one set of data collected from both before (baseline) and during exploitation/production period . In another campaign only the baseline has been collected and in a third campaign data was only collected during exploitation/production period.

Standards for format and content

The geochemical data were collated in MS Excel worksheets, so no specific formats were applied. Simple formulae were used to assess average total dissolved solids [TDS], Na/Cl and Cl/Br ratios for each of the sites in question and categorized manually according to used methodology.

Polices for stewardship and preservation

Ownership and responsibility for preservation of results of the analyses, to be uploaded to the SECURe project repository, goes to the administrator/subtask leader – Adam Wójcicki – at info@securegeoenergy.eu.

Procedures to provide access

Data – results of the analyses – are to be available at the SECURe project repository. Raw data can be accessed in the same way as they were acquired for this research by the author – see "Data description and information created".

CHARACTERIZATION OF SHALE GAS WELLS FOR WELL INTEGRITY SIMULATIONS

AUTHORS: Adam Wójcicki, Teresa Adamczak-Biały

PARTNER: Polish Geological Institute – National Research Institute

Data category

Research data

Data description and information created

The dataset contains characterization of shale gas wells for well integrity simulations. Based on raw data and other information pertaining to two shale gas wells, acquired from Polish Oil and Gas Company, input to the well integrity simulations carried out by TNO were supplied by PGI. The input consisted in elaborating generalized models of the wells and their surroundings as wells as characterization of the target formations. Well construction schemes including the production casing sizes and depths and generalized lithostratigraphy of the geological formations in question were composed. Raw data acquired from Polish Oil and Gas Company included wireline logging data (and interpretation results) together with results of laboratory measurements of drill core samples (e.g., on geomechanical properties). Regarding characterization of the target formations the most important information created were distributions of in situ stresses within particular formations in both wells, assessed on the base of results of wireline, density logging (vertical stress – based on weight of the overburden at a certain depth) and laboratory measurements of geomechanical parameters (horizontal stress – based on pressure values measured within rock sample in tri-axial chamber at reservoir conditions). Temperature values within formations in question were assessed assuming local geothermal gradient and information from POGC reports.

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As mentioned above, raw data and any other information were acquired from Polish Oil and Gas Company. Some of these data are included in unpublished archive well reports (http://geoportal.pgi.gov.pl/otwory) accessible through the National Geological Archives (https://www.pgi.gov.pl/en/services/geological-information.html) but the full set can been obtained from Polish Oil and Gas Company only (no link can be provided).

The methodology of laboratory analyses and wireline logging interpretation is included in unpublished well reports of POGC (some information is accessible through the National Geological Archives). These industrial data were used as obtained from POGC and in this research were only collated and averaged within formations/depth ranges in question.

Standards for format and content

The well data were collated in MS Excel worksheets, so no specific formats were applied. Simple formulae were used to assess average values of parameters in question.

Polices for stewardship and preservation

Ownership and responsibility for preservation of results of the analyses (input for TNO simulations), to be uploaded to the SECURe project repository, goes to the administrator/subtask leader – Adam Wójcicki – please contact him if data is or becomes unavailable at info@securegeoenergy.eu.

Procedures to provide access

Data – results of the analyses (input for TNO simulations; in D2.5 of the SECURe project – https://securegeoenergy.eu/work-packages/wp2-risk-assessment) – are to be available at the SECURe project repository. Raw data can be accessed in the same way as they were acquired for this research by the author – see "Data description and information created".

FAULTS SEALING MODELLING

AUTHORS: Kinga Bobek, Adam Wójcicki

PARTNER: Polish Geological Institute – National Research Institute

Data category

Simulation data

Data description and information created

The dataset is on evaluating the capability of large-scale natural fractures to transmit fluids through the reservoirs/aquifers. The analyses were carried out around two shale wells and, to a lesser extent, in the case of a depleted gas field – acidic gas storage. For the shale gas sites relevant data from 3-D seismic surveys together with wireline logging data were acquired from Polish Oil and Gas Company. Three-dimensional geological models in Petrel, incorporating these data were constructed for both sites (horizons and wells). A generalized geological model of a depleted gas field (acidic gas storage) was obtained from INiG-PIB (elaborated by them in D2.2 of the SECURe project on the basis of their previous projects; https://securegeoenergy.eu/work-packages/wp2-risk-assessment) and wireline logging data of archive wells within the structure were obtained from National Geological Archives

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(https://www.pgi.gov.pl/en/services/geological-information.html). Then using T7 Badley Geoscience software models of fault zones were constructed on the base of previously worked out 3D geological models, enabling the evaluation of the fault seal potential, which is determined by two components:

1. The sealing properties of the complexes juxtaposed on both sides of the fault (juxtaposition component – presented at so-called juxtaposition plots) and

2. The sealing properties of the fault zone itself (fault gauge component – which is evaluated by the shale gouge ratio [SGR] parameter – the percentage of shale or clay in the moved interval).

As mentioned above, the raw data were mostly acquired from Polish Oil and Gas Company (and a geological model of one site from INiG-PIB). Some of these data are included in unpublished archive well reports (http://geoportal.pgi.gov.pl/otwory) accessible through the National Geological Archives (https://www.pgi.gov.pl/en/services/geological-information.html) but the full set can been obtained from Polish Oil and Gas Company only (no link can be provided).

The methodology of faults sealing modelling refers specifically to the use of T7 Badley Geoscience software (http://www.badleys.co.uk/T7-overview.php; http://www.badleys.co.uk/training.php) and preparation of relevant datasets (seismic and wireline-logging data), preferably in Petrel formats, as the input to the fault sealing modelling, then characterisation of the models around wells using wireline logging data and finally elaborating fault models characterized by the percentage of shale or clay in the moved interval (https://wiki.aapg.org/Fault_seal_quantitative_prediction:_shale_smear_factor,_shale_gouge_ratio,_and_smear_gouge_ratio).

Limitations - the data quality, availability and the used software incompatibility could prevent a reliable assessment of sealing potential within the storage complex and the overburden. Preferably a 3-D seismic survey is required in order to make a reliable geological model, together with high quality wireline logging data – the more wells with such data, the better. The T7 Badley Geoscience software is optimized for clastic formations and might provide unreliable results for carbonate rocks.

Standards for format and content

The intermediate models are in Petrel format but the formats of T7 Badley Geoscience software are specific to the software and the standard usable formats for output in case of faults sealing modelling (T7 Badley Geoscience software) include graphic files (bitmaps).

Polices for stewardship and preservation

Ownership and responsibility for preservation of created information is up to PGI-NRI. However, results of faults sealing modelling are included in D2.5 and D2.6 of the SECURe project (https://securegeoenergy.eu/work-packages/wp2-risk-assessment).

Procedures to provide access

Because of the above-mentioned constraints on output format and ownership of raw data included in the intermediate Petrel models for shale gas sites (provided by Polish Oil and Gas Company) the data will not be publicly available. Raw data can be accessed in the same way as they were acquired for this research by the authors – see “Data description and information created”. The geological model of a depleted gas field – acidic gas storage was obtained from INiG-PIB and anyone interested shall contact them at info@securegeoenergy.eu.

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SEISMIC FIRST BREAKS FOR SYCZYN SEISMIC SURVEY

AUTHORS: Szymon Ostrowski, Marcin Lasocki

PARTNER: Polish Geological Institute – National Research Institute (PIG-PIB)

Data category

Site data

Data description and information created

The dataset contains condensed results of seismic refraction survey, that can be regarded as "hard data". Raw seismic data acquired in the field were analysed for occurrences of refracted waves. The time delay of the refraction wave travelling to each of the seismic sensors (geophones) used in the survey for numerous source points allow for spatial sampling of the wave field of the refracted wave, and build model of seismic velocity cross section.

Raw (field) seismic data were collected using precisely planned survey procedures. Field data were sorted, assembled and visually presented in a seismic processing software. Identification of the refracted waves were performed visually using the tendency of refracted waves to be the first waves to arrive. Time delay values were picked then manually. The results arranged in ASCII table were then exported. Model of the velocity field (seismic velocity cross-section) was computed on the basis of this tables for two lines and P (primary) and S (shear) waves for each line.

Data files Syczyn-1_P.ASC and Syczyn-1_S.ASC represents tables obtained for line Syczyn-1, wave P and wave S respectively;

Data files Syczyn-2_P.ASC and Syczyn-2_S.ASC represents tables obtained for line Syczyn-1, wave P and wave S respectively.

Each file contains 4 columns:

Record No. – sequential record identifier;

Source location – distance from the beginning of the line to the (current) source point (in meters);

Receiver location – distance from the beginning of the line to the given receiver (in meters);

First Break – delay time between emission of the wave to its arrival at the given receiver point (seconds).

The dataset is formatted in a simple table, that can be imported to other seismic software for modelling velocity field. Different computing algorithms generate slightly different velocity models, so it can be useful to have hard data for comparison.

The results gathered in the dataset might be used as a part of future scientific publication.

Standards for format and content

Dataset is composed of 4 ASCII tables (separate files). Each file contains 4 columns that can be imported to seismic software package able to compute velocity field modelling.

Polices for stewardship and preservation

The dataset will be uploaded to the open free repository belonging to a group administered by the work package 3 leader of the SECURe project. Data remain accessible according to the standard repository rules. Responsibility for the data provided goes to Szymon Ostrowski, sost@pgi.gov.pl – please contact him if needed at info@securegeoenergy.eu.

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Procedures to provide access

The data – sites location and results of field and laboratory measurements – are to be publicly available at the SECURe project repository at https://www.securegeoenergy.eu/.

GROUNDWATER GAS SAMPLING AND ANALYSIS METHOD TEST RESULTS

AUTHORS: Monika Konieczyńska, Irena Wysocka, Wojciech Wołkowicz, Tomasz Gliwicz, Adam Brodecki, Łukasz Wojcieszak

PARTNER: Polish Geological Institute – National Research Institute (PIG-PIB)

Data category

- **Research data** (new methodology testing)

Data description and information created

The dataset contains details of field collection of groundwater samples with use of different water intake devices and the measurement results of gaseous compounds (methane, ethane, carbon dioxide) obtained during analytical method validation performed in order to develop a methodology of groundwater sampling for analysis of dissolved gases.

The data represents sampling time, method details and the computed results of gas content (methane, ethane, carbon dioxide) from GC-FID (Gas chromatography with flame ionization detector), GC-MS (Gas chromatography with mass spectrometer), GC-TCD (Gas chromatography with thermal conductivity detector) measurements and $\delta^{13}C$ in methane and carbon dioxide from CRDS (Cavity Ring Down Spectroscopy). Dissolved gases were analysed with use of the headspace extraction technique.

The dataset is not intended to be used for any site characterisation. Sampling sites were chosen based on the high probability of occurrence of measurable methane content in groundwater. Furthermore, the data will be used for formal procedures to obtain methodology accreditation from the Polish Centre for Accreditation (PCA).

The developed methodology based on these data will be published in a peer review paper.

Standards for format and content

The data are provided in .xlsx (MS Excel file) format. First spreadsheet contains meta data and a detailed description of data presented in next spreadsheets. All spreadsheets have clear rows and columns descriptions.

Polices for stewardship and preservation

The dataset will be uploaded to the open free repository belonging to a group administered by the work package 3 leader of the SECURe project. Data remain accessible according to the standard repository rules. Responsibility for the data provided goes to Monika Konieczyńska, mkon@pgi.gov.pl – please contact her if needed.

Procedures to provide access

The data – results of the validation tests – are to be publicly available at the SECURe project repository at https://www.securegeoenergy.eu/.

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SOIL GAS SAMPLING AND ANALYSIS METHOD TEST RESULTS

AUTHORS: Monika Konieczyńska, Irena Wysocka, Wojciech Wołkowicz, Tomasz Gliwicz, Adam Brodecki, Łukasz Wojcieszak

PARTNER: Polish Geological Institute – National Research Institute (PIG-PIB)

Data category

- **Research data** (new methodology testing)

Data description and information created

The dataset contains details of field collection of test soil gas samples with use of Supel Inert Foil gas sampling bags and the results of methane, ethane, carbon dioxide measurements performed in order to validate a methodology of soil gas sampling and analysis.

The data represent sampling site and time details and the computed results of gas content (methane, ethane, carbon dioxide) from GC-FID (Gas chromatography with flame ionization detector), GC-MS (Gas chromatography with mass spectrometer), GC-TCD (Gas chromatography with thermal conductivity detector) measurements and direct readings of gas content (methane, carbon dioxide) and $\delta^{13}C$ from CRDS (Cavity Ring Down Spectroscopy).

The dataset is not intended to be used for any site characterisation, sampling sites were chosen based on high probability of occurrence of measurable methane content in soil gas. Furthermore, the data will be used for formal procedure to obtain the methodology accreditation from the Polish Centre for Accreditation (PCA).

The dataset might be used as a set of results of the analytical methodology in future field experimental works. However the data are related to particular soil types and beside validation/inter-comparison purpose are not reusable.

The developed methodology based on these data will be published in a peer review paper.

Standards for format and content

The data are provided in .xlsx (MS Excel file) format. First spreadsheet contains meta data and a detailed description of data presented in next spreadsheets. All spreadsheets have clear rows and columns descriptions.

Polices for stewardship and preservation

The dataset will be uploaded to the open free repository belonging to a group administered by the work package 3 leader of the SECURe project. Data remain accessible according to the standard repository rules. Responsibility for the data provided goes to Monika Konieczyńska, mkon@pgi.gov.pl – please contact her if needed.

Procedures to provide access

The data – results of the validation tests – are to be publicly available at the SECURe project repository https://www.securegeoenergy.eu/.

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POST-EXPLORATION MONITORING OF GROUNDWATER RESULTS ON POLISH SHALE GAS SITES.

AUTHORS: Monika Konieczyńska, Irena Wysocka, Wojciech Wołkowicz, Adam Brodecki, Łukasz Wojcieszak

PARTNER: Polish Geological Institute – National Research Institute (PIG-PIB)

Data category

- **Site data**

Data description and information created

The dataset contains results of field measurements (temperature, pH, conductivity, redox potential, oxygen content) of groundwater and samples collection details as well as the results of laboratory analysis of the set of dissolved and gaseous parameters performed within the environmental monitoring campaign on 3 Polish shale gas sites where exploration activities including hydraulic fracturing were conducted in 2010-2016 period.

The data represent sampling time and field measurements, the computed results of gas content - methane, ethane from GC-FID (Gas chromatography with flame ionization detector) and carbon dioxide from GC-TCD (Gas chromatography with thermal conductivity detector) measurements as well as dissolved substances determined with spectrophotometry, ion chromatography (IC), inductively coupled optical emission spectroscopy (ICP-OES) and headspace gas chromatography mass spectrometry (HS-GC-MS) methods. Dissolved gases were analysed with use of the headspace extraction technique.

The dataset is intended to be compared with the previously conducted monitoring campaigns' results for tracking possible changes in groundwater condition compared to the baseline state established prior to or at the beginning of shale gas exploration on each site. Any detected change needs to be analyse in order to establish if it is or is not caused by former drilling and hydraulic fracturing activities which effects might become observable in near surface environment after certain time due to the depth that the processes took place and specific retardation due to geological conditions.

The results gathered in the dataset will be published in future as a part of long term after-exploration site monitoring in a peer review paper.

Standards for format and content

The data are provided in .xlsx (MS Excel file) format. First spreadsheet contains meta data and a detailed description of data presented in next spreadsheets. All spreadsheets have clear rows and columns descriptions.

Polices for stewardship and preservation

The dataset will be uploaded to the open free repository belonging to a group administered by the work package 3 leader of the SECURe project. Data remain accessible according to the standard repository rules. Responsibility for the data provided goes to Monika Konieczyńska, mkon@pgi.gov.pl – please contact her if needed.

The dataset represents only a part of long-term monitoring observations and needs to be processed with other monitoring campaigns results.

Procedures to provide access

The data – sites location and results of field and laboratory measurements – are to be publicly available at the SECURe project repository at https://www.securegeoenergy.eu/.

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SLEEN FIELDSITE, HOLLAND

AUTHORS: Jurgen Foeken, Cjestmir de Boer, Tina Bech

PARTNER: TNO, GEUS

Data category

Site data (on-site measurements and other data)

Data description and information created

On December 1, 1965, an underground blowout during an exploratory drill with a catastrophic outcome occurred near Sleen, The Netherlands. During approximately 2.5 months, near-continuous leakage of large amounts of natural gas was released into the subsurface. After the blowout, the local drinking water production company installed a network of groundwater monitoring wells to monitor for possible adverse effects on groundwater quality at the blowout site. Today, more than 50 years after the blowout, the groundwater is still impaired.

Data has been correlated with previously published data by Schout et al. (2018), covering geology and well depths.

During October 2019, samples were collected from 5 groundwater wells and the following analyses were conducted:

- Gas composition (C1-C5, CO2, N_2, H_2S, Ar) and stable isotope analyses (methane $d^{13}C$ and dD, CO_2 $d^{13}C$, $d^{15}N$)
- Inorganic parameters (anions, cations, DOC, alkalinity, nitrate and ammonium)

Gas composition and stable isotope analyses were repeated on a second series of groundwater samples (3 out of the 5 wells mentioned above) collected in October 2020.

Sampling

Analysis of trace metal and major cations was conducted with inductively coupled plasma mass spectrometry (ICP-MS).

Large volume (>30L) groundwater samples with dissolved methane gas were collected in pressurised cannisters. In the laboratory, cannisters were slowly depressurised in order to allow degassing of the methane from the groundwater. Headspace methane gas was collected and transferred into all metal cannisters for methane clumped isotope analyses. Separate, small volume (~200ml) gas & water samples were collected for ach well in Isoflasks for bulk methane isotope analyses.

Natural gas composition and bulk methane and CO_2 isotope analyses were conducted on an Agilent GC with TCD detector. Carbon isotopes of methane are analysed with an Agilent 6890N GC interfaced to a Thermo Delta S IRMS. Methane isotopes are measured on an Agilent 7890A GC interfaced to a MAT 253 IRMS.

Methane clumped isotope analyses are conducted on a Thermo Scientific IRMS-253 Ultra. Main isotopologues measured on the Ultra are $^{12}CH_4^+$, $^{13}CH_4^+$, $^{12}CH_3D^+$, $^{13}CH_3D^+$, and $^{12}CH_2D_2^+$.

Publication

Data is planned to be published but is currently still in progress.

Limitations

Not relevant.

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Standards for format and content

All data is available in an Excel spreadsheet.

Polices for stewardship and preservation

Upon completion of the SECURe deliverable (March 2021), data will be uploaded to the open free repository UKCCSRC.

Procedures to provide access

Data is currently available upon request via the lead author of deliverable 4.6, but will be provided in downloadable format upon uploading to the free repository UKCCSRC.

FONTAINE ARDENTE AND ROCHASSON FIELDSITES, FRANCE

AUTHORS: Jurgen Foeken, Tanya Goldberg

PARTNER: TNO, GFZ

Data category

Site data (on-site measurements and other data)

Data description and information created

The Fontaine Ardente (FA) and Rochasson (ROC) natural gas seepage sites are located southwest (FA) and east (ROC) of Grenoble, France. For both field sites, gas is thought to originate from buried Middle Jurassic mudstones and argillaceous limestones and thought to migrate upward along small faults. At FA, the site located along a small seepage close to the river bed of a small creek. The gas seepage site at ROC is located along the flank of a thalweg and is linked to a small landslide in clayey horizons.

New methane clumped isotope data is correlated to previously published data by Gal et al (2017) and recent isotopic data acquired within SECURe deliverable 3.4.

<u>During October 2019, 5 samples were collected from the FA and ROC sites and the following analyses were conducted:</u>

- Gas composition (C1-C5, CO2, N_2, H_2S, Ar) and and stable isotope analyses (methane $d^{13}C$ and dD, CO_2 $d^{13}C$, $d^{15}N$)
- Methane clumped isotope analyses ($D^{13}CD$ and DDD)

<u>Sampling</u>

Gas sampling was performed by inserting a soil gas probe or burying an inverted funnel over an active gas vent. The gas was pumped slowly from the gas vent into 1L gas-tight glass vessels through a drying agent filled with $Mg(ClO_4)_2$. Three samples were collected in Isotubes. Both the vessel and the Isotubes were flushed with 3 volumes of gas before it was collected. Three samples were sampled directly at the main gas vents, whereas an additional two were sampled in the vicinity of the main gas vents from soil gas.

Major gas composition of the FA and ROC samples was measured on a gas chromatograph at GFZ. Carbon isotopes ($d^{13}C$) of CH_4 and CO_2 were measured on a MAT 253 GC-IRMS at GFZ.

Methane clumped isotope analyses are conducted on a Thermo Scientific IRMS-253 Ultra. Main isotopologues measured on the Ultra are $^{12}CH_4^+$, $^{13}CH_4^+$, $^{12}CH_3D^+$, $^{13}CH_3D^+$, and $^{12}CH_2D_2^+$.

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Publication

Data is planned to be published but is currently still in progress.

Limitations

Not relevant.

Standards for format and content

Excel spreadsheet.

Polices for stewardship and preservation

Access to the data is currently restricted and will be made publicly available post publication in the open free repository UKCCSRC.

Procedures to provide access

Access to the data is currently restricted and not for public dissemination.

BORZĘCIN FIELDSITE, POLAND

AUTHORS: Tanya Goldberg, Jurgen Foeken

PARTNER: GFZ, TNO

Data category

Site data (on-site measurements and other data)

Data description and information created

The Borzęcin natural gas reservoir has been producing gas since the 1970s. The natural gas reservoir is located in the Zielona Góra basin, in the Polish part of the European Permian Basin. The reservoir is within the Rotliegend sandstones and Zechstein carbonates and is capped by the Zechstein evaporites. Gas generation is proposed to be from the Carboniferous organic deposits with later migration into the Permian

In May 2019, 2 wells at the Borcezin site were sampled for methane gas analyses. The following analyses were conducted:

- Gas composition (C1-C5, CO2, N_2, H_2S, Ar) and and stable isotope analyses (methane $d^{13}C$ and dD, CO_2 $d^{13}C$, $d^{15}N$)
- Methane clumped isotope analyses ($D^{13}CD$ and DDD)

Sampling

Duplicate natural gas samples were collected from 2 wells at the Borzęcin gas reservoir. Samples are taken from gas metering lines at the surface installation and directly transferred to 1L gas-tight glass vessels at pressures of 2.26 MPa and 2.50 MPa respectively. Prior to sample collection, the vessels were flushed with reservoir gas. The sampled gas was sourced from reservoir depth of 1435m and 1419m (b.g.l.).

Major gas composition of the Borzezin samples was analysed in The Netherlands. Natural gas composition and bulk methane and CO_2 isotope analyses were conducted on an Agilent GC with TCD

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detector. Carbon isotopes of methane are analysed with an Agilent 6890N GC interfaced to a Thermo Delta S IRMS. Methane isotopes are measured on an Agilent 7890A GC interfaced to a MAT 253 IRMS.

Historic gas compositional and isotope data are available from the Oil and Gas Geochemistry Laboratory of INiG-PIB (analyses conducted on a Delta V Advantage Isotope Ratio Mass Spectrometer).

Methane clumped isotope analyses are conducted on a Thermo Scientific IRMS-253 Ultra. Main isotopologues measured on the Ultra are $^{12}CH_4^+$, $^{13}CH_4^+$, $^{12}CH_3D^+$, $^{13}CH_3D^+$, and $^{12}CH_2D_2^+$.

Publication

Data is planned to be published but is currently still in progress.

Limitations

Not relevant.

Standards for format and content

Excel spreadsheet.

Polices for stewardship and preservation

Access to the data is currently restricted and will be made publicly available post publication in the open free repository UKCCSRC.

Procedures to provide access

Access to the data is currently restricted and not for public dissemination.

GROUNDWATER CHEMISTRY DATA

AUTHORS: Rasmus Jakobsen

PARTNER: GEUS (Geological Survey of Denmark and Greenland)

Data category

Site data (on-site measurements and other data)

Simulation data (data produced by numerical simulations)

Data description and information created

This dataset contains measured data and modelling results of groundwater and associated sediment geochemistry from two sites. The Vroegum Plantation site (Denmark) was used for a CO_2 injection experiment in 2012 and the Borden site (Ontario, Canada) was used for a CH_4 injection experiment in 2015. The two sites were resampled to evaluate long term effects in 2019. The data were used to calibrate 1D reactive transport models set up in the general geochemical model PHREEQC and a 3D version of this PHAST, and the models were used for extrapolating effects. The input files for the models rather than model output is provided.

The data represent the results obtained from the measurements and the model results are obtained from the calibrated models. The calibrating of the model included data from the measurements made during and after injection from the authors of the previous studies.

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The data, if combined with the datasets from the injection experiments, could be used to develop more detailed models. They could also be used for comparing with later sampling campaigns. The data and model results as reported in Deliverable 2.4 of the SECURe project indicate that leakage events will create changes in the aquifer, but also that the effects are manageable in terms of treating the water for consumption.

Publication

The data has been used for analysis in deliverable 2.4 of the SECURe project has been produced and a journal publication is at a very early stage of preparation. Limitations

The data do not contain errors but they are by nature point samples taken at a given point in time and do not necessarily represent conditions before, after or nearby. Model results are only as good as the model representation which will always have limitations as it is a simplified and incomplete description of the system.

Standards for format and content

The measured data are given in Microsoft Excel spreadsheet files. The models are given as ASCII input text files for PHREEQC and PHAST which are both free software obtainable from USGS: https://www.usgs.gov/software/phreeqc-version-3 and https://www.usgs.gov/software/phast-a-computer-program-simulating-groundwater-flow-solute-transport-and-multicomponent .

Polices for stewardship and preservation

Data have been uploaded to the open free repository osf.io maintained by COS (Center for Open Science) access to the data will be checked by author.

Procedures to provide access

Data will be available here: *osf.io/8xvn3*

GTB ERT DATA

AUTHORS: Paul Wilkinson, Oliver Kuras, Phil Meldrum, Russell Swift, Ceri Vincent

PARTNER: British Geological Survey

Data category

Site data

Data description and information created

The data are Electrical Resistivity Tomography (ERT) measurements from the GeoEnergy Test Bed (GTB), a CO_2 injection testbed in Leicestershire, UK.

The data are collected using an array of sensors (electrodes) installed as a permanent array within six wells at the GTB. These electrodes are used in various combinations as transmitters and receivers to measure electrical properties of the rock and fluids in the subsurface that in the vicinity of the array. The electrical properties of the subsurface are influenced by the type of rock and the chemistry and saturation of the water within the rocks. The array will record changes in the ERT data which will be used to infer changes in water chemistry at the GTB. The data requires processing and interpretation before it can be used, this work is based on BGS expertise in monitoring the subsurface.

The data collection is only in its early stages as commissioning of the system is underway. Processing and interpretation is not straightforward due to a number of factors including complexity of the array.

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These data will be published after CO_2 injection has been performed at the GTB. Data publication and sharing will be in line with the GTB data access, collection and publishing agreement.

Standards for format and content

Raw data are stored in human-readable text files. Processed data are in the form of 2D or 3D time-lapse models of the subsurface geoelectrical properties in Visualization Toolkit format.

Polices for stewardship and preservation

Data will be published in BGS Open Reports and papers. Data publication will be in line with the GTB data access, collection and publishing agreement. These data will be stored in the UKCCSRC data portal (managed by BGS) in the longer term when the dataset is complete.

Procedures to provide access

To access the data, the GTB leads (Ceri Vincent BGS and Martyn Barrett UNOTT) should be contacted in the first instance to confirm which data can be shared. These data have been collected at the GTB which is a field laboratory funded by BGS, UNOTT and by Innovate UK via the Energy Research Accelerator project. The GTB has also benefitted through research projects including H2020 SECURe which have funded research using the GTB.

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