Host rock analysis for the German nuclear waste disposal site-selection: review of subsurface geometries and input data for geological modelling

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Abstract

Geological modelling is essential for visualizing the subsurface and utilized, for example, in the search for national nuclear waste disposal sites. In Germany, the current work of the federal company for radioactive waste disposal (BGE) addresses the question which software and workflows are most suitable to model the different potential host rocks (claystone/shale, crystalline rocks and salt), as the input data vary in quality and quantity, with their reprocessing and integration resulting in uncertainties.

The GeoBlocks project aims at developing a modelling workflow that includes uncertainty quantification. This study represents the basis for this objective. After reviewing relevant material properties of the host rocks, the host rocks structures in the subsurface are analysed. Important here is the realization that only a specific range of geological settings and structures is considered for waste storage. As these structures can often be approximated using regular geometric bodies, the standard geometries are systematized and catalogued in an online library. This open-access collection will serve as a visual introduction when executing the targeted modelling workflow and will be used to display the variety of the host rocks geometries to geoscientists and stakeholders. In addition to the geometry-related work, the input data that is available for modelling in the site-selection is analysed. Here, the focus is on reviewing which data sources are typical for the different host rocks and how the data coverage varies among Germany. The obtained catalogue of relevant geometries serves as a basis for subsequent project-internal decisions and developments as well, for example to evaluate different geological interpolation approaches and methods to quantify uncertainties, as presented in the accompanying work of YANG ET AL. (2023B). Future work will utilize the standard geometries to create geological analogue models from which test data sets for various experimental approaches will be extracted. Furthermore, we will analyse the input data regarding uncertainties and interpreter bias.

1. Introduction

1.1. German search for a nuclear waste disposal site

The search for a disposal site for high-level radioactive waste in Germany is a highly debated topic, for which the federal company for radioactive waste disposal (Bundesgesellschaft für Endlagerung, BGE) is responsible since 2017. Starting with the entirety of Germany, the BGE firstly excluded areas unsuitable to host a waste disposal site, using exclusion criteria, minimum requirements and geoscientific consideration criteria, such as seismicity, volcanism, active fault zones or the minimum thickness and depth of the isolating host rock zone (BGE, 2020A). Since then, the BGE has been focusing on further narrowing the potential areas to the so-called “siting regions” that will be explored from the surface in the next step of the site-selection process. In the current step two of the phase one of their action plan, subsurface geological modelling is performed for the suitability assessment of the areas remaining in the process. For this purpose, the BGE is exclusively using existing data as prescribed by the federal law. However, as these data were gathered initially over a period of several decades and partly by private companies, data quality and quantity vary strongly. Time-consuming data reprocessing and data integration still lead to uncertainties, which are difficult to quantify and even more difficult to compare across potential sites. In order to analyse the various sources of uncertainty and to optimize and integrate the modelling workflow, the GeoBlocks project was initiated.

1.2. The GeoBlocks project

GeoBlocks is a collaboration of RWTH Aachen, University of Aberdeen and the Federal Institute for Geosciences and Natural Resources (BGR), funded by BGE with the main objective to establish an open-source workflow for geological modelling that includes the quantification and visualization of uncertainties, and leads the way to optimized sampling procedures. A first step is this study, presenting an effort to collect and catalogue relevant geometries of the potential host rocks for radioactive waste disposal claystone/shale, salt and crystalline rocks in the German subsurface. In addition to common geometries, the host rocks are often associated with typical input data that are analysed in this study as well. Our results are then the basis for further scientific investigations, as presented in YANG ET AL. (2023B), where the suitability of various geological interpolation methods to model different host rock geometries is reviewed.

1.3. Input data for geological modelling

The data types used for geological modelling have been classified by WELLMANN & CAUMON (2018) into surface data, geologic maps and cross sections, geophysical surveys, borehole and flow data.

The first step of the geological modelling process is to incorporate the surface data to establish the soft constraints of the geological environment. Subsequently, maps and sections are utilized to construct the structural model. If accessible, geophysical data can be employed to enhance or revise the existing geological framework. To refine the model, borehole data is used to calibrate and assign rock properties, resulting in what is referred to as a static model.

A workflow example from an area in the North German Basin is presented in Fig. 1; this area is characterized by salt structures (a). A structural model is developed using geological sections (b), and the seismic information is applied to refine the model, specifically focusing on the salt dome (c). A 3D static model is the result (d). Each step of geological modelling has uncertainties, in this research we focus on the uncertainties of the input data that are associated with the methods of data acquisition, processing and interpretation.

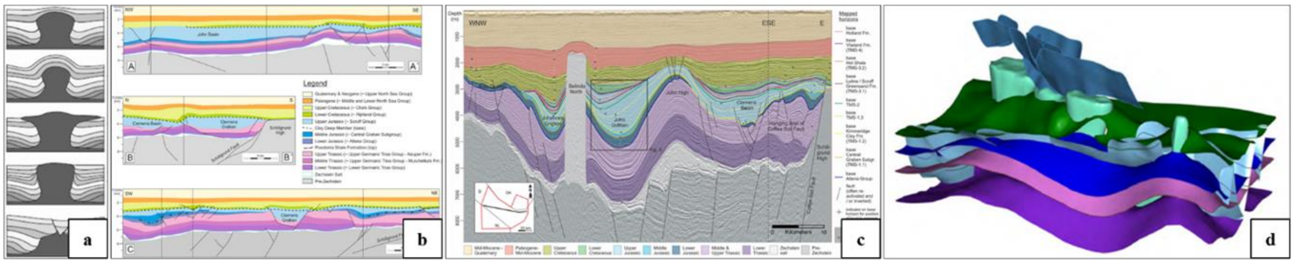

Figure 1: Geological modelling workflow, example from the North German Basin. a) Geological framework, possible salt structures are displayed after JACKSON & HUDEC (2017). b) Geological sections from the area (MÜLLER ET AL., 2020). c) Interpreted seismic section (MÜLLER ET AL., 2023). d) 3D model of the area (BGR 2022)

1.4. Spatial distribution of host rocks in the German subsurface

In the German subsurface, 90 "sub-areas" that might be suitable to host a nuclear waste disposal site were defined, encompassing 54% of the land area (BGE, 2020A; see Fig. 2). For the site-selection currently relevant claystone/shale formations can be found mostly in the northern half of Germany, as well as in Baden-Wurttemberg and Bavaria in the south. Stratiform salt structures are located in the central part of the country, while steep structures are exclusively found in the northern half of Germany. Crystalline rocks in relevant conditions are located in the south and the east of the country (BGE, 2020A).

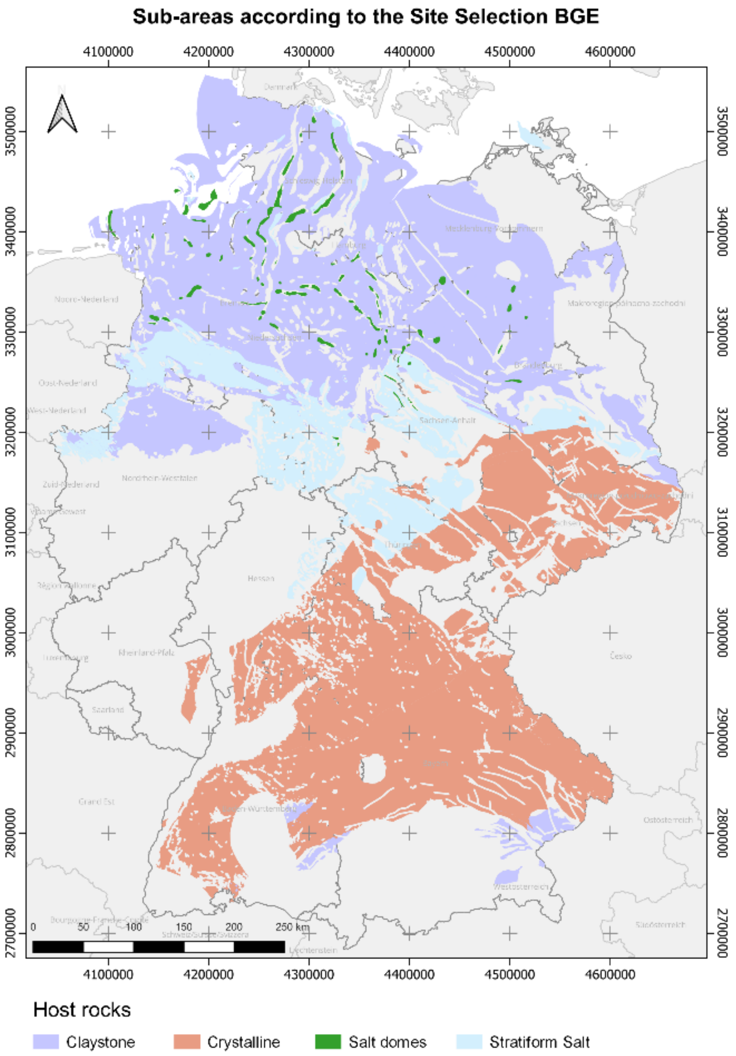

Figure 2: Distribution of the host rocks in Germany. Remade after BGE (2020A). Data set provided by BGE

1.5. Geological data in Germany

In Germany, each federal state operates its independent geological survey, while the BGR serves as the central authority at the federal level. The responsibility for the creation, collection, and archival of geological maps and sections lies with the respective state geological surveys. Seismic acquisition in Germany started 100 years ago, primarily for hydrocarbon exploration. An example of the seismic data from the North German Basin is shown in Fig. 3, illustrating various seismic display types across different decades that reflect the advancements in technology and improved resolution quality (BENSE, 2023).

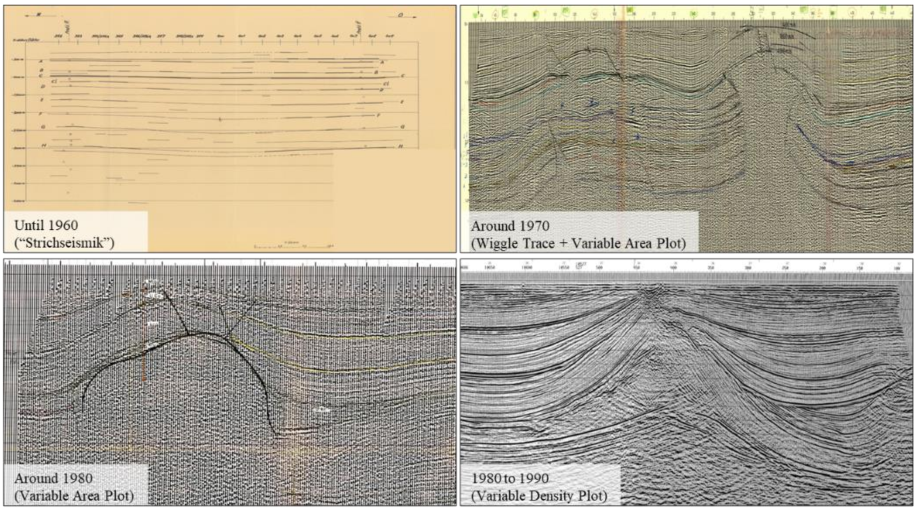

Figure 3: Example of the available seismic data from the North German Basin across several decades in various seismic display types (Bense, 2023).

The coverage of the subsurface data in Germany varies strongly between regions, as displayed in Fig. 4. On the left, the 2D and 3D seismic surveys for hydrocarbon exploration are shown; those areas are specifically the Permian Basin in northern Germany and the Upper Rhine Graben in southern Germany. In the middle, the available seismic data is classified per year. The seismic surveys have been grouped by decades; the darkest colours are the most recent data. At least 75% of the 2D seismic information displayed was acquired before the 1980s, the decade in which 3D surveys began. However, the acquisition parameters of the data do not meet the required standards for accurately assessing the suitability of an area to host a high-level radioactive waste disposal site. As a result, either the data needs to be reprocessed, or a new acquisition is necessary (SCHOLZE & DING, 2021). On the right, the well density in Germany is shown using a raster with 40x40 km cells. The wells are concentrated mostly in the north and south of the country.

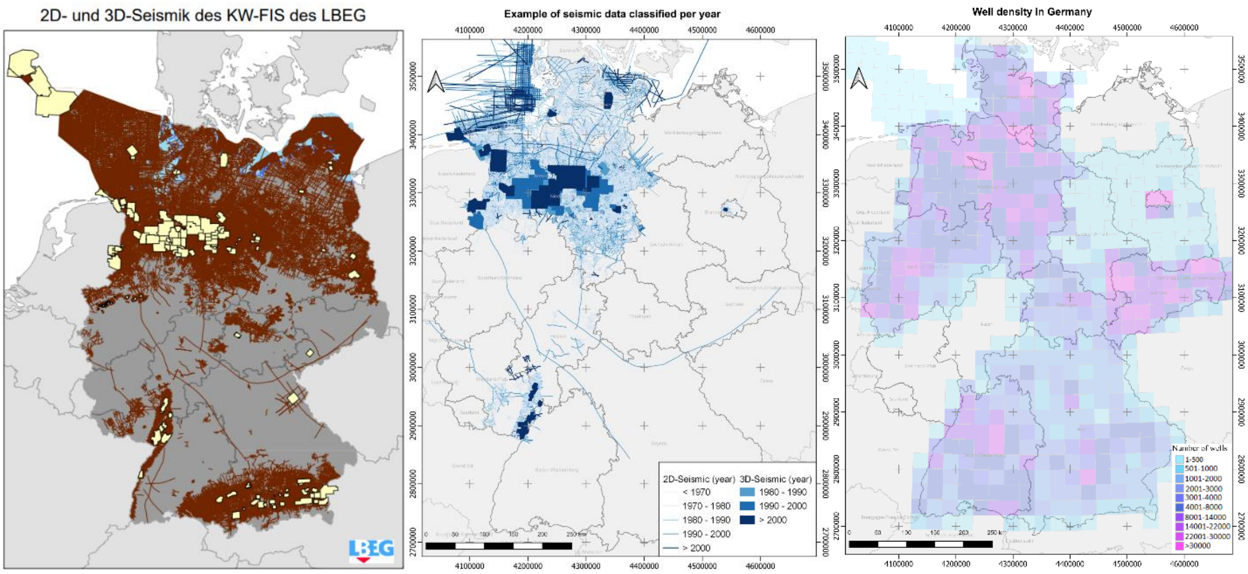

Figure 4: Coverage of seismic and well data in Germany: On the left 2D lines and 3D seismic volumes for hydrocarbon exploration are shown (Kohlenwasserstoff-Fachinformationssystem (KW-FIS) | Landesamt Für Bergbau, Energie Und Geologie, n.d.). In the middle, part of the seismic data is classified per year (LBEG, 2019). On the right, well density in Germany is represented by a raster with 40x40 km cells (GBL, 2016.)

2. Methods and results

2.1. Review of material properties and systematization of rock geometries

Realistic geological models depend on a clear definition of the rock type and the three-dimensional geometries of the potential host rocks. These parameters are shortly introduced in the following sections and the geometries are categorized in Fig. 5.

2.1.1. Claystones and shales

Claystones and shales are clastic sedimentary rocks consisting of at least 50% particles smaller than 4 µm (e.g., PICARD, 1971). They often show very low permeability, high adsorption capacity for radionuclides, low solubility and high plasticity in their unconsolidated to semi-consolidated state (BGE, 2020B). Furthermore, some clay minerals are swellable, thereby having the ability to heal fractures within the rock. However, claystones and shales have low thermal conductivity and some clay minerals are subject to mineral reactions when temperatures higher than 60°C are reached (BRACKE ET AL., 2019).
As all clastic sediments are initially deposited conformably on the underlying rocks (SELLEY, 2000), conformable layers are the most common geometry of claystone/shale deposits (see Fig. 5 upper section). However, the appearance of conformable deposits can differ greatly: mainly tilting and folding can create a wide range of geometries, varying from a "flat layer case" while maintaining the generally conformable character. In contrast, mostly folding, faulting, and erosion create unconformable geometries.

2.1.2. Salt

Salt rock in general is a potential host rock if it is mainly composed of halite (BGE, 2020C). Regarding its material properties, halite is suitable as a potential host rock due to its high thermal conductivity, low permeability, its ability to deform plastically under pressure, and its high unsupported stability. However, halite is easily dissolved by NaCl-undersaturated fluids and has a low adsorption capacity for radionuclides.

Halite is initially deposited conformably as an evaporitic sediment. Apart from the resulting undeformed, concordant, flat layer geometry, halite structures are mainly categorized according to two principles: While a supplementary subdivision from an extensional perspective, namely according to the length-to-width ratio of salt bodies, is discussed by some authors (e.g., HUDEC & JACKSON, 2011), the common classification is based on the question whether a structure is concordant in respect to its overlying rocks or intrusive (HUDEC & JACKSON, 2007; see Fig. 5 middle section). Following this systematization, salt anticlines, pillows and rollers are categorized as concordant while salt stocks, sheets and walls are intrusive bodies. BGE, however, subdivides the structures into "stratiform" and "steep" halite geometries. Here, they do not only consider flat undeformed conformable layers but also the concordant salt rollers, anticlines and pillows as stratiform, irrespective of the dip angles of the structures (BGE, 2020C). Accordingly, the intrusive salt stocks, sheets and walls are the only bodies defined as steep. Since the differences between both classifications only have a minor influence on our current work, we decided to use the common scientific systematization until the BGE elaborates on the exact geometries that they consider to be relevant in the site-selection process ("decision relevant geometries").

2.1.3. Crystalline rocks

The potential crystalline host rocks considered by the BGE are plutonic rocks and high-grade metamorphic rocks (migmatites and gneisses) (BGE, 2020D). In the German subsurface, granitoids are the most abundant crystalline rocks. In general, the crystalline rocks considered show high unsupported stability, very low solubility of the minerals present and low susceptibility to mineral reactions under high temperatures. However, under upper crustal temperature and pressure conditions, the crystalline rocks fracture brittlely (CRIDER, 2015), thereby creating possible preferential pathways to fluids and nuclide migration. Furthermore, the adsorption capacity for radionuclides is low.

For crystalline rocks, a coherent geometrical systematization of the high-grade metamorphic rocks considered by the BGE as potential host rocks, together with the structures built up by plutonic rocks, is difficult to create since the former originate from various protoliths, resulting in a variety of geometries. Orthogneisses and part of the migmatites, for example, are formed from plutonic protoliths such as granitoids and resemble the structures of these rocks. In contrast, paragneisses and the remaining migmatites result from various sedimentary sources, with their geometric shape being dependent not only on the structure of the original geological body but also heavily on the minerals present in the protolith and the existing temperature as well as pressure conditions during the metamorphosis. Overall, since most high-grade metamorphic rock bodies are bordered by plutonic rocks and/or faults, we will approximate them geometrically as irregular, discordant structures (see Fig. 5 lower section).

For plutonic rocks, the classification used in this study combines the shape of the bodies with their relationship to the overlying strata (concordance or discordance) (PHILPOTTS & AGUE, 2009; see Fig. 5 lower section). Two types of irregular, discordant structures exist that are differentiated in their size: batholiths (larger than 100 km^2) and stocks (smaller than 100 km^2). Moreover, cylindrical, discordant bodies can be found that mostly represent feeder pipes for magma ascendancy. Furthermore, two kinds of tabular geometries can be distinguished: dikes (discordant) and sills (mostly concordant). Besides, three other concordant structures exist: while laccoliths possess a roughly flat base and a convex top, lopoliths show a roughly flat top and a shallow convex base, whereas phacoliths lack flat sides as they are lensoid.

2.2. Catalogue of geometries

Applying the systematizations reviewed above, a collection of standard geometries that approximate the structures of the host rocks in the German subsurface is set up. The online repository currently developed and updated repeatedly, will be accessible at https://github.com/cgre-aachen/geoblocks-geometries. In this catalogue, we are focusing primarily on the geometric shape of the bodies, disregarding penetrating faults that might create offsets in the structures. Please note, that the library found online aims to represent only those geometrical bodies that might be of interest in the site-selection process, not the entirety of geometries that can be approximated when looking at the real structures found in the German subsurface.

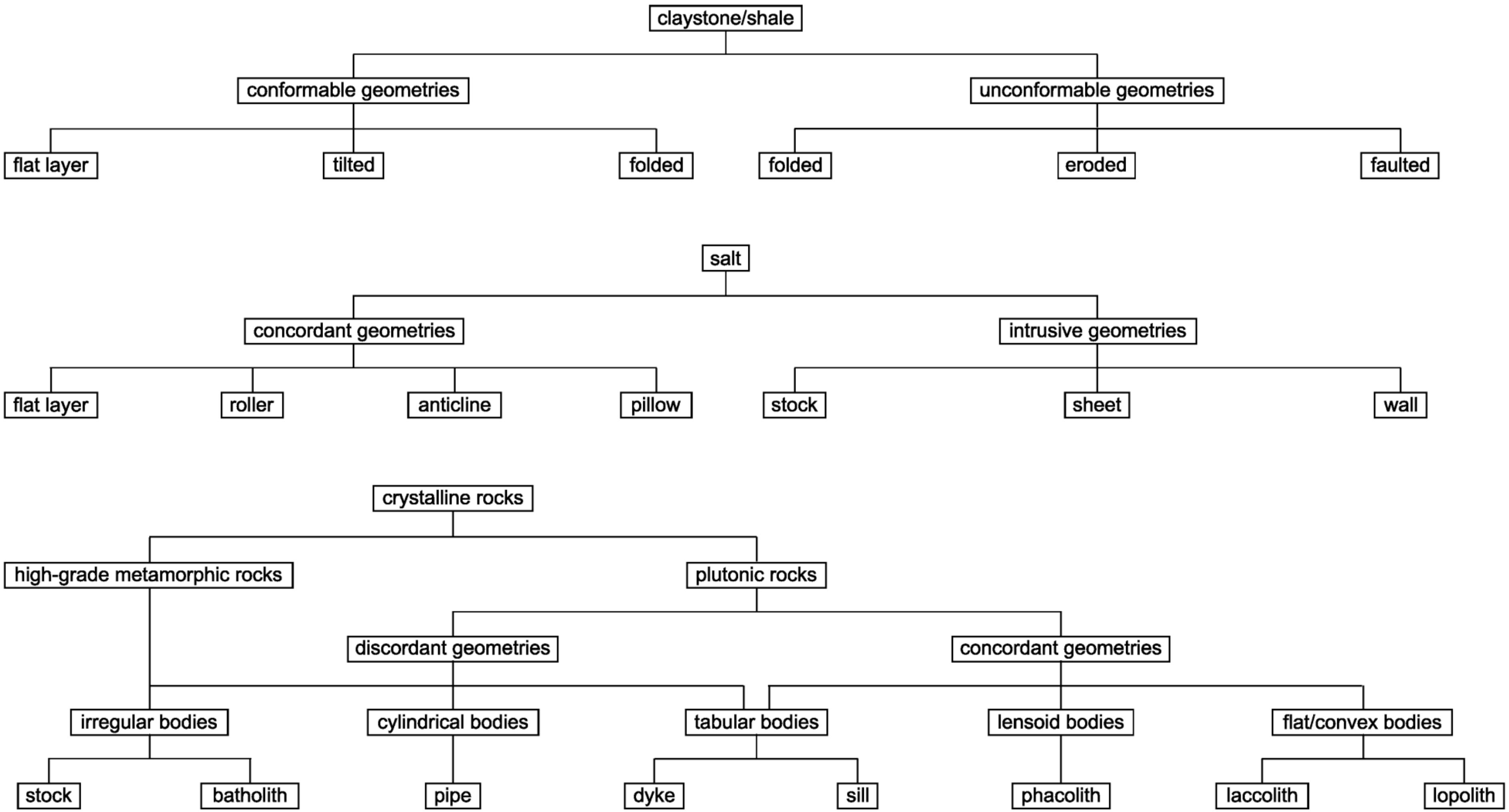

Figure 5: Systematization of the geometries that the host rocks show in the subsurface. Please find the respective references in the text

2.3. Applicability of input data

Studies offering deeper insights were identified based on the host rock. The most common types of data were selected in each category (see Table 1), providing information for geological modelling at varying resolutions. For example, calibrating gravity and magnetic surveys with well data produces a more precise delineation of crystalline rocks and steep salt structures.

Table 1: Applicability of the input data types according to the host rock.

Category	Data	Parameter for modelling	Host rocks			
			Claystone	Crystalline rocks	Steep salt	Stratiform salt
Surface data	Geological framework	Framework	•	•	•	•
	Stratigraphic data	Topology analysis			•	
	Sedimentologic data	Facies	•		•	
		Structure	•			
Geological maps and sections	Maps and sections	Structure Horizons Faults	•	•	•	•
Geophysical surveys	Seismic data	Structure Horizons Faults	•	•	•	•
	Gravity data	Structure delimitation		•	•	
	Magnetic data	Structure delimitation		•	•	
Borehole data	Well tops	Structure Contacts	•	•	•	•

3. Discussion

The aim of the GeoBlocks project, the modelling workflow that includes the visualization and quantification of uncertainties, should aid in the German site-selection process. Therefore, the workflow is specifically designed for the modelling of potential host rocks. Thus, it was essential to collect information about the data structure and the subsurface geometries of the rock types in the early stages of the project.

From a geometrical point of view, it became apparent that most of the host rocks structures in the subsurface can be approximated using a subset of geometric shapes. This resulted in the collection of typical settings in a systematic catalogue of geometries that can serve as the visual preface, since we expect the geomodelling workflow to depend on host rock and geometry to be modelled. Furthermore, an open-access collection is a convenient tool to visualize the range of three-dimensional geometries of a host rock to a broader audience, which aids in the communication of uncertainties and decisions for geoscientists and stakeholders (see ZEHNER, 2021). The decision to exclusively focus on geometries that are likely to be considered in the site-selection excludes geological bodies that usually lack the lateral or vertical extents (see BGE, 2020E) required to be a potential disposal site. Therefore, several crystalline geometries, namely pipes, dykes, sills, phacoliths, laccoliths and lopoliths are currently not considered.

Looking at the availability of input data, seismic surveys, along with well data for calibration, serve as the primary source of information for structural models. However, in Germany, there is a significant lack of seismic information coverage for crystalline rocks when comparing the distribution of host rocks in the country (Fig. 2) with the available data (Fig. 4). The majority of seismic data is concentrated in claystone and salt structures. The distribution of the well data is similar across different host rock types. Due to the availability of additional subsurface data for many salt rock and claystone sites, we will be focusing on these rock types first in the upcoming project activities. In regions lacking seismic data, primarily in the crystalline host rock, it is suggested to employ structure delineation using gravity and magnetic data, along with well data available in the area. However, it is crucial to validate their suitability for investigating depths.

The review of the input data and geometries was valuable for the second study of our project group (YANG ET AL., 2023B): Some of the geometries defined in this study were directly part of the workflow of YANG ET AL. (2023B), as they were constructed in the open-source Python package GemPy (DE LA VARGA ET AL., 2019) and used as synthetic input models for the testing process (see YANG ET AL., 2023B).

4. Outlook

This study provides the foundation for several future subprojects of GeoBlocks. Follow-up studies of YANG ET AL. (2023B), for example, will benefit from our research when integrating real data into the testing of modelling methods: When evaluating which geological interpolation methods are suitable to model the host rocks, it will be essential to know, which input data types will be primarily available and what kinds of geometries (hence, what kind of structural model) will be modelled as this will have an impact on the efficiency and overall applicability of methods. Furthermore, in the upcoming months, representative geological analogue models of the host rocks will be created, using standard geometries established in this study as well as subsurface data provided by BGE and BGR. These data sets are of good data quality as well as quantity and originate from German areas already excluded from the site-selection process. From the models, we will extract test data sets and additionally generate synthetic data sets. This will enable us to experiment with various data configurations regarding quantity and spatial heterogeneity, for example in the studies built upon the results of YANG ET AL. (2023B). Furthermore, the synthetic data sets can be used to simulate measurement errors and mistakes in data interpretation, which will be beneficial, for example, when analysing the input data regarding uncertainties and interpreter bias. Here, the focus will be on borehole data and seismic interpretations as the most abundant data sources. The aim of this work package will be to develop methods that allow us to analyse and generalise knowledge about uncertainties in measurements and interpretations as well as expert knowledge on distributions at individual data points, thereby making it applicable to a larger part of the available database.

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