



ARBEITSBERICHT NAB 24-17

Petrophysical Data and Core-Calibrated
Multimineral Interpretation

January 2024

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

Hardstrasse 73 | 5430 Wettingen | Switzerland
+41 56 437 11 11 | info@nagra.ch | nagra.ch



ARBEITSBERICHT NAB 24-17

Petrophysical Data and Core-Calibrated
Multimineral Interpretation

January 2024

J. Becker¹ & S. Marnat²

¹Nagra

²AdTerra²

KEYWORDS

Petrophysical log interpretation; core calibration; mineralogy;
porosity; workflow; methodology; stochastic approach;
multimineral; deterministic approach; uncertainties; multi-
sensor core logging

**Nagra | National Cooperative for the
Disposal of Radioactive Waste**

Hardstrasse 73 | 5430 Wettingen | Switzerland
+41 56 437 11 11 | info@nagra.ch | nagra.ch

Nagra Arbeitsberichte ("Working Reports") present the results of work in progress that have not necessarily been subject to a comprehensive review. They are intended to provide rapid dissemination of current information..

Abstract

Basic rock properties, such as mineralogy and porosity, fundamentally influence barrier integrity as they control transport properties and self-sealing, sorption and diffusion parameters. Hence, the characterisation of these parameters, next to, e.g. hydrogeological, geomechanical and geochemical parameters, is of key importance. However, standard laboratory measurements cannot easily produce continuous profiles of mineralogy or porosity since they usually have a sample spacing of several metres. Other measurements techniques, e.g. core scanning, have the potential to produce quasi-continuous profiles (as the spacing between their measurements may be limited to a few millimetres). However, as the spacing decreases, measurement time increases. In addition, these measurement techniques necessitate (almost) perfectly preserved core material. Hence, a combined approach, the so-called multiminerale interpretation, has been applied. This method is capable of combining all available data (i.e. geophysical logs, laboratory measurements and core-scanning measurements) to develop quasi-continuous profiles of borehole mineralogy and porosity.

To calculate the continuous borehole profiles at any given depth using the multiminerale interpretation approach, a mineralogical and fluid content as well as porosity are assumed (based on expert judgement and prior knowledge), and the theoretical response of the available measurements is calculated. Through local and overall error minimisation, the assumed volumes are adjusted until the errors between the calculated theoretical response and the actual measurements of the available data have been minimised and result in continuous profiles of mineralogy and porosity. This workflow obviously carries an intrinsic uncertainty with respect to interpretation. Other factors that can influence interpretation include, e.g., borehole conditions impacting the data quality of the measurements.

As previously mentioned, these interpretations result in quasi-continuous curves of mineralogy and porosity along the borehole walls. Mineralogical data include clay as well as quartz and feldspar, carbonate, halite, anhydrite, pyrite, goethite and siderite contents and their respective uncertainties. The interpretations are homogenised between the different boreholes to allow comparison of the results, both within a siting region and also across the three siting regions. This workflow has been applied to the measurements conducted in 12 boreholes (Bözberg-1-1 and Bözberg-2-1, Bachs-1-1, Stadel-2-1 and Stadel-3-1, Bülach-1-1, Marthalen-1-1, Rheinau-1-1 and Trüllikon-1-1, Benken, Riniken and Weiach-1). These are summarised here and have been detailed in a number of separate reports. However, the Benken, Riniken and Weiach-1 boreholes were drilled several decades ago and, the acquired data quality for these boreholes is therefore not on par with the very recent data acquisition in the Bözberg-1-1 and Bözberg-2-1, Bachs-1-1, Stadel-2-1 and Stadel-3-1, Bülach-1-1, Marthalen-1-1, Rheinau-1-1 and Trüllikon-1-1 boreholes.

In the more recent boreholes, the interpreted mineral data correlate very well with the respective laboratory measurements (high correlation coefficients, usually > 0.9). Several laboratory measurements of porosity exist, each using a different geophysical principle and hence each measuring a slightly different water content. Still, the correlation of laboratory and multiminerale porosity is high (> 0.8). Data trends from the laboratory mineralogy are also reproduced very well so that the continuous profiles interpreted from the geophysical logs using additional data can confidently be used for further geostatistical analyses and site characterisation.

Due to reduced data quality, correlation coefficients between interpreted multiminerale data and laboratory measurements are lower in the older Benken, Riniken and Weiach-1 boreholes. The mineralogical data from the Benken borehole, which provided the highest data quality of the older boreholes, still shows correlation coefficients of ~ 0.8 . However, correlation of porosity is much lower and ranges around 0.5. Hence, interpretation results from these boreholes should not be directly compared to the more recent boreholes and should only be qualitatively used as additional information.

Table of Contents

Abstract	I
Table of Contents	III
List of Tables.....	IV
List of Figures	IV
List of Appendices	V
1 Introduction	1
2 Input data and data preparation.....	3
2.1 Petrophysical logging data.....	5
2.2 Laboratory data.....	7
2.3 MSCL data.....	7
3 Multimineral methodology	9
3.1 Introduction	9
3.1.1 Choice of interpretation intervals	10
3.1.2 Choice of minerals and fluids	11
3.2 Multimineral interpretation runs.....	11
3.2.1 First interpretation run	12
3.2.2 Second interpretation run.....	12
4 Interpretation results.....	13
5 Summary	20
6 References.....	21

List of Tables

Tab. 1-1:	Table of references for the initial multiminerall data interpretation of the recent boreholes	2
-----------	---	---

List of Figures

Fig. 1-1:	Location of boreholes (from the recent deep borehole campaign as well as from previous campaigns) in Northern Switzerland.....	1
Fig. 2-1:	Resolution of the input data of the multiminerall interpretation. As an example, calcite (or Ca) is shown from the different measurement methods.....	4
Fig. 2-2:	Using MSCL data to complement log data or fill in gaps in the log data.....	8
Fig. 3-1:	Comparison of TOC, chlorite and smectite from the blind test dataset (prefix MM, x-axis) with laboratory measurements (y-axis) for the STA2-1, STA3-1 and BAC1-1 boreholes	12
Fig. 4-1:	Crossplots of clay mineral content measured in the laboratory (y-axis) vs. multiminerall interpretation results (x-axis) for total clay mineral content in the recent boreholes. The lower right plot is a summary including measurements from all recent boreholes	14
Fig. 4-2:	Crossplots of clay mineral content measured in the laboratory (y-axis) vs. multiminerall interpretation of clay (x-axis) for the older boreholes.....	14
Fig. 4-3:	Crossplots of laboratory measurements of clay (y-axis) vs. multiminerall interpretation results for clay (x-axis) for the Opalinus Clay in the recent boreholes. Again, the lower right plot is a summary plot included data from all recent boreholes	15
Fig. 4-4:	Crossplots of laboratory measurements of clay (y-axis) vs. multiminerall interpretation results for clay (x-axis) for the Opalinus Clay in the older boreholes.....	16
Fig. 4-5:	Crossplots of laboratory measurements of water-loss porosity using bulk wet density (y-axis) vs. multiminerall interpretation results (total porosity, PHIT, x-axis) for the recent boreholes. Lower right plot is a summary using data from all recent boreholes	16
Fig. 4-6:	Crossplots of laboratory measurements of pycnometer porosity (y-axis) vs. multiminerall interpretation results (total porosity, PHIT, X-axis) for the recent boreholes. The lower right plot is a summary using data from all recent boreholes	17
Fig. 4-7:	Crossplot of laboratory measurements of pycnometer porosity (y-axis) vs. multiminerall interpretation results (total porosity, PHIT, x-axis)	17
Fig. 4-8:	Ternary plots of the recent boreholes for clay, carbonates as well as of quartz and feldspars in the Opalinus Clay	19

List of Appendices

App. A-1	Composite plot of the borehole BOZ1-1
App. A-2	Composite plot of the borehole BOZ2-1
App. A-3	Composite plot of the borehole BAC1-1
App. A-4	Composite plot of the borehole STA2-1
App. A-5	Composite plot of the borehole STA3-1
App. A-6	Composite plot of the borehole BUL1-1
App. A-7	Composite plot of the borehole MAR1-1
App. A-8	Composite plot of the borehole RHE1-1
App. A-9	Composite plot of the borehole TRU1-1
App. A-10	Composite plot of the borehole Weiach-1
App. A-11	Composite plot of the borehole Riniken
App. A-12	Composite plot of the borehole Benken

Note: The enclosures are only included in the digital version of this report (PDF) and can be found under the paper clip symbol.

1 Introduction

For the site selection of a deep geological repository for radioactive waste in Switzerland and the subsequent site characterisation and comparison, a detailed set of geological data on the Mesozoic sedimentary sequence in the three potential siting regions is needed. This includes, next to a number of other properties, mineralogical data and porosities. This report details the steps required for data acquisition, data correction and final interpretation of the acquired data. These are used to determine continuous profiles of mineralogy and porosity using the so-called multiminerall interpretation approach, which focuses on the integration of data from different sources, in this case obtained from petrophysical borehole logs and measurements of cores and core plugs. The data were taken from three previously drilled boreholes in Benken, Riniken and Weiach-1; and from nine recently drilled boreholes in Bözberg (BOZ1-1 and BOZ2-2), Bachs (BAC1-1), Stadel (STA2-1 and STA3-1), Bülach (BUL1-1), Marthalen (MAR1-1), Rheinau (RHE1-1) and Trüllikon (TRU1-1). The location of the boreholes is given in Fig. 1-1.

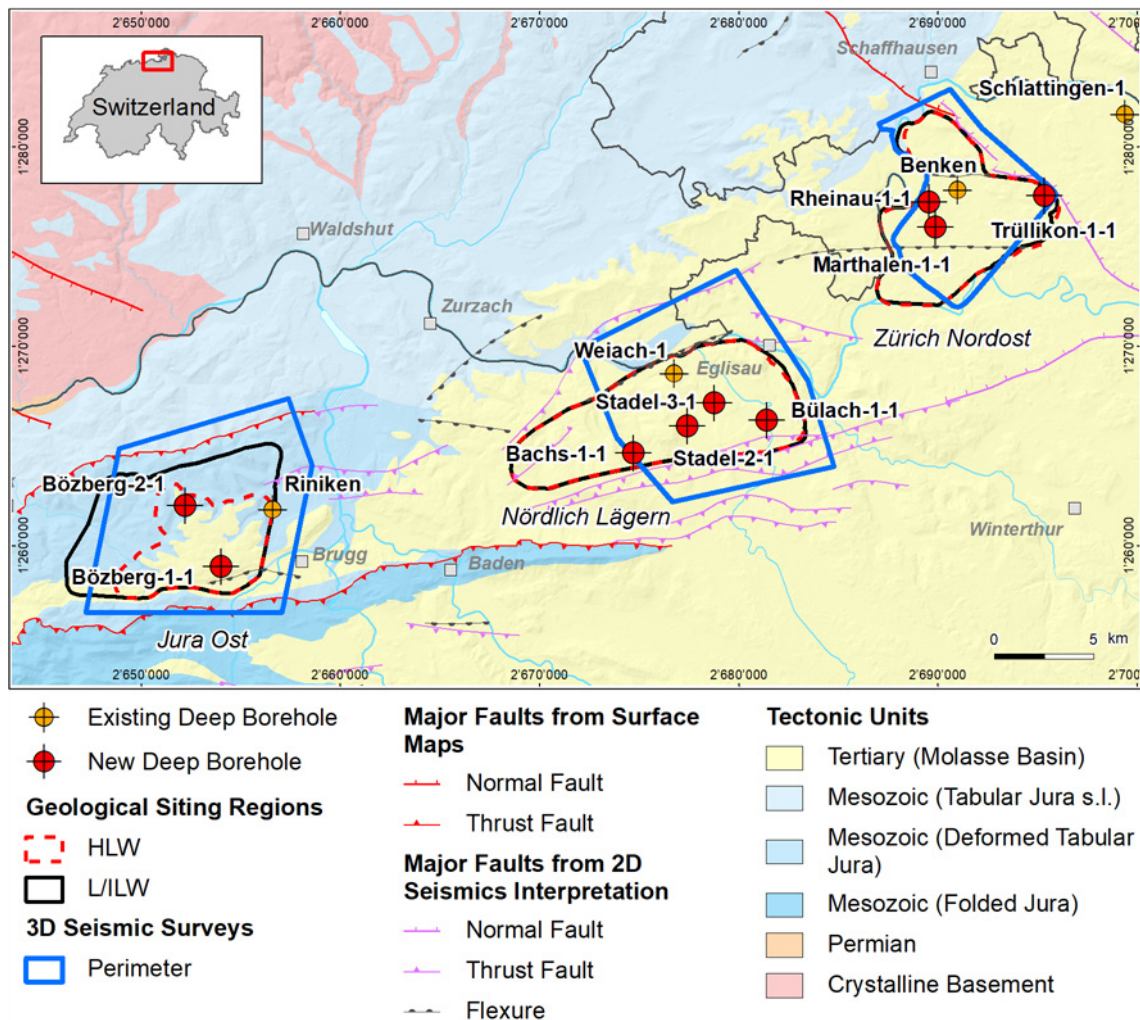


Fig. 1-1: Location of boreholes (from the recent deep borehole campaign as well as from previous campaigns) in Northern Switzerland

A first set of results detailing, e.g., the drilling process, logging operations or the first multiminerall interpretations, was published in a set of reports immediately after data from each respective borehole became available. Tab. 1-1 lists the respective reports for each of the boreholes that are important for the multiminerall interpretation. The multiminerall interpretation was repeated at the end of the drilling campaign when final data were available from all boreholes. The main differences between the initial interpretation published in Dossiers X (see Tab. 1-1) and the results presented in this report are that the interpretation was homogenised across all boreholes.

Tab. 1-1: Table of references for the initial multiminerall data interpretation of the recent boreholes

Dossier I details the drilling process, while Dossier VI reports on the petrophysical logging, Dossier VIII on lab-based rock properties and porewater geochemistry and Dossier X on the multiminerall interpretation of the respective borehole.

Borehole	Abbreviation	Reference
Bözberg-1-1	BOZ1-1	NAB 21-021 Dossier I, VI, VIII and X
Bözberg-2-1	BOZ2-1	NAB 21-022 Dossier I, VI, VIII and X
Bachs-1-1	BAC1-1	NAB 22-004 Dossier I, VI, VIII and X
Stadel-2-1	STA2-1	NAB 22-002 Dossier I, VI, VIII and X
Stadel-3-1	STA3-1	NAB 22-001 Dossier I, VI, VIII and X
Bülach-1-1	BUL1-1	NAB 20-08 Dossier I, VI, VIII and X
Marthalen-1-1	MAR1-1	NAB 21-20 Dossier I, VI, VIII and X
Trüllikon-1-1	TRU1-1	NAB 20-09 Dossier I, VI, VIII and X
Rheinau-1-1	RHE1-1	NAB 22-003 Dossier I, VI, VIII and X

This report details the petrophysical logs (see Section 2.1), lab data (see Section 2.2) and core measurements (see Section 2.3) used. The multiminerall interpretation and required harmonisation are detailed in Chapter 3. A comparison of the multiminerall interpretation with laboratory data obtained from cores is given in Chapter 4.

2 Input data and data preparation

To determine mineral content and other important geophysical parameters, petrophysical logs, laboratory measurements and multi-sensor core logging (MSCL) data were used as input data for a multiminerall interpretation. Each of these methods determines the respective parameters on a different volume of rock and with a different resolution.

Petrophysical log measurements are recorded in situ in the borehole every ~15 cm, but they integrate over a certain length (and hence volume). This integration length depends on the type of log, the logging speed and the rock type and may be as short as ~30 cm (e.g. gamma-ray logs), but can also reach several metres (e.g. deep resistivity logs). In some cases, petrophysical logs directly represent rock properties or rock mineralogy while, in other cases, they only give qualitative, indirect information. For example, a sonic log can be used to determine porosity by charting the speed of a compressional sound wave as it travels through the formation. However, results of the sonic log cannot be used to infer porosity directly as measurements have to be interpreted first.

MSCL measurements provide information comparable to that of the petrophysical logs, but they measure a different rock volume at a different resolution. The resolution of MSCL measurements can be defined by the user and is a trade-off between desired resolution and measurement time. Here, MSCL measurements were, in general, recorded every 5 cm. While petrophysical wireline logs measure the immediate surroundings of the borehole in situ, MSCL measurements are restricted to measuring the available core volume. This means that they measure a much smaller rock volume and under very different conditions, i.e. not in situ as is the case in petrophysical wireline logging.

Finally, laboratory measurements are performed on samples taken from cores, so the integration length of these measurements is determined by the sample size. In this study, laboratory measurements to determine mineralogy were performed on 15 – 25 cm long core samples that were subsequently homogenised. A subset of this homogenised powder was analysed, resulting in a maximum integration length of 25 cm. For porosity measurements, homogeneous rock samples with a volume of about 1.5 – 2 cm³ were taken from the centre of the core, so these measurements represent the most precise measurements in terms of integration length.

An example of the different resolutions from the different measurement methods is given in Fig. 2-1. However, it must be kept in mind that the different data types all integrate over different rock volumes/lengths, so the precision of the data is not necessarily determined by the number of measurement points in a certain interval.

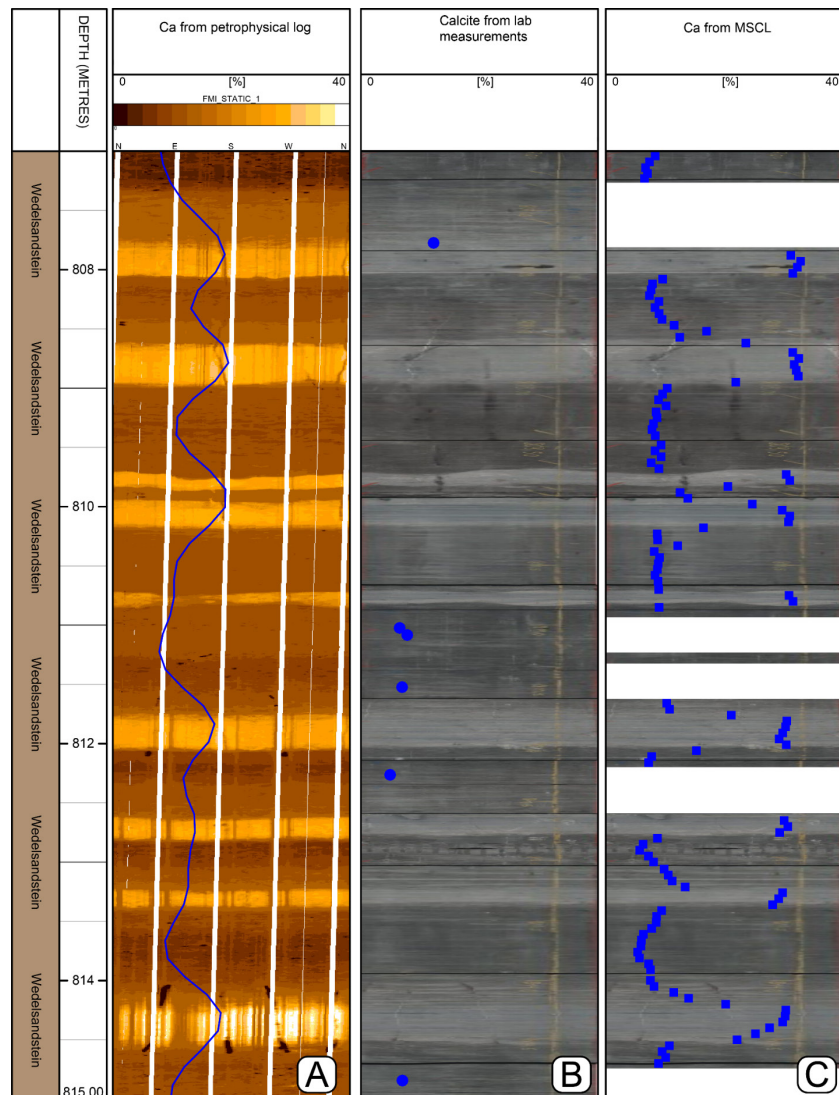


Fig. 2-1: Resolution of the input data of the multiminerall interpretation. As an example, calcite (or Ca) is shown from the different measurement methods

The background of the tracks show images (formation micro imager (A) or core photos (B) and (C)) detailing the geological layering in the shown section. Input data are available on different scales and with different spacing. Petrophysical logging produces quasi-continuous curves (A). Core samples for laboratory testing are taken immediately after the core has been retrieved and one or more measurements have been performed on homogenised sample(s) (B). These sampled intervals are no longer available for MSCL measurements (C). Hence in track C, core images from areas where laboratory samples have been taken are not shown. Only continuous measurements from the petrophysical logs and the MSCL scanner can be used to determine the thin layering. It also becomes apparent that the integration length of the petrophysical logs significantly smoothed the data, sometimes to a point that (very) thin layers can no longer be differentiated while they still clearly show in the MSCL measurements.

2.1 Petrophysical logging data

In most of the deep boreholes, a large suite of petrophysical wireline logs was acquired measuring/determining the following petrophysical parameters used in this study: borehole shape, total and spectral gamma ray, sonic velocities, resistivity, bulk density, photoelectric factor, neutron hydrogen index, elemental spectroscopy and spontaneous potential. To minimise logging time, different logging tools were combined in so-called toolstrings. The petrophysical logging tools used here were usually combined so that three logging runs using three different toolstrings were sufficient per borehole. Furthermore, the borehole was not drilled in its entirety and then logged, as this would cause stability problems. Rather, drilling was performed until a predetermined lithology (or lithological boundary) was reached and logging (along with additional measurements, e.g. hydrogeological or geomechanical measurements) was performed then. After the measurements were completed, a (steel) casing was lowered into the borehole (for stability purposes), and the next borehole section was drilled. The recent boreholes required a minimum of three such borehole sections. A more in-depth discussion of the drilling process, the measurements and applied logs can be found in Dossiers I and VI (see Tab. 1-1 for references).

Next to the petrophysical wireline logs mentioned above, additional logs are also available for some of the deep boreholes (such as the formation micro imager, FMI). These logs are mainly image logs that detail the borehole wall to allow for, e.g., a structural mapping of the borehole. They do not provide additional lithological information of direct value for the multimineral interpretation.

As stated earlier, the quality of the log data for the Benken, Riniken and Weiach-1 boreholes is very different from that of the recently drilled deep boreholes. These older boreholes were completed 20+ years ago so the logging tools at that time cannot be directly compared to the logging tools in service today (though they rely on the same principles). Therefore, while a multimineral interpretation of these boreholes has been performed, the results were only used qualitatively when making comparisons between the different boreholes.

Data preparation of the initial raw logging data is a necessary step when using petrophysical logging data for subsequent interpretations. These data were prepared in two steps (see below), with the second step depending on results from the first step.

Initial log data preparation

The first important log correction is the initial depth calibration of the different logging runs based on the first gamma ray (GR) log in the borehole. All toolstrings include a GR tool as it is a relatively robust measurement insensitive to borehole conditions (e.g. borehole breakouts). The depth measurements of the different toolstrings can therefore be harmonised by comparing the GR measurements from each toolstring and shifting the respective depths to the depth of the GR measurement from the first toolstring in hole. This harmonises the depth between the different logs.

The next correction consists of editing the first and last readings of the logs. The first reading occurs where the logging starts after tension pick-up, and the last reading occurs when the tool enters the casing in previous sections (logging is always performed from the bottom up) or when the toolstring reaches the surface. These readings have to be deleted/adjusted because they do not necessarily represent actual formation readings.

Another correction is for environmental parameters. The continuous readings of logs are, where necessary, corrected by the contractor on site according to tool statistics and environmental parameters such as borehole fluids. For example, the logs that measure the variation of natural radioactivity (GR and SGR, spectral gamma ray) are sensitive to any amount of artificially introduced K (and Th and U). To increase borehole stability, especially in lithologies with a high

clay mineral content, a high-K borehole fluid was used, hence the GR and SGR measurements had to be corrected for the increased K in the borehole fluid. This was achieved using the spectral gamma ray logs as they measure the K, Th and U content. By correcting the measured K-concentration from the SGR log with the known K-concentration in the borehole fluid, all gamma-ray logs were corrected where necessary.

Finally, the logging data have to be corrected for borehole shape and diameter since some logs are sensitive towards borehole geometry. If the borehole geometry deviates too much from the original circular shape and diameter (e.g. where borehole breakouts occurred), the log readings measure the material properties of the borehole fluid rather than those of the surrounding rocks. False readings due to large borehole breakouts were hence removed from the data.

After all these corrections were applied, a log quality control was performed based on the calliper, density correction, the neutron-computed stand-off and the density-neutron crossplot. A log quality control flag was generated, highlighting the intervals where the data quality decreases due to, e.g., borehole washouts or breakouts. This flag was later used to determine the weight required for each log in the multimineral interpretation (see Chapter 3), or to switch to an alternative bad hole model.

The initial log data preparation was performed immediately after log acquisition on a per-borehole basis to enable quick-look interpretation using the logging data. After the corrections were applied, the logs from different logging runs were combined (spliced) for each borehole into a composite log along the entire borehole (see references to Dossiers VI in Tab. 1-1).

Reconditioning of log data

Once all boreholes were completed and all logs were initially corrected, the logs were reconditioned in a second phase. This was done to harmonise the applied corrections so that borehole log data are readily comparable across all boreholes. This included checking the initial log data preparation and corrections as needed.

Additional so-called geochemical closure models for the element capture sonde (ECS) were also calculated during reconditioning. Currently available ECS tools can directly measure the dry weight of Si, Ca, Fe, S, Ti, S, H and Gd but cannot directly measure potassium (K), sodium (Na), aluminium (Al) or magnesium (Mg). Hence, the standard closure model, the so-called WALK2 model, can only determine Si, Ca, Fe, S, Ti, S, H and Gd. A different geochemical closure model, MGWALK, can also determine Mg (using additional information from other, independent logs). Mg is an important input to differentiate between calcite and dolomite from the total carbonate content. Hence, in areas with a predominantly carbonate-rich lithology, data from the MGWALK closure model were preferred over those from the WALK2 closure model. The same approach was used to determine quartz and feldspars. The Al content is of particular importance to better differentiate between these two, and it can be calculated (from Si, Ca and Fe) using the so called ALKNA closure model. Therefore, in lithologies with a high content of quartz and feldspars, the Al from the ALKNA closure model was used. Hence, in this final reconditioning step, information from different ECS closure models was combined depending on the prevailing lithology and used for all subsequent interpretations using logging data.

2.2 Laboratory data

Core data from laboratory measurements are available for the boreholes and include XRD bulk mineralogy, porosities and grain densities, amongst other parameters that are not strictly necessary for the multiminerall interpretation (see Mazurek, 2017; Waber, 2020 and references to Dossier VIII in Tab. 1-1). Measurements were performed on samples taken, on average, every 3 – 5 m. The available core data could be used to calibrate and compare several parameters, such as XRD mineralogy results, with predicted multiminerall interpretation results. Porosities were available from the core measurements in the form of measurements of water-loss porosity (105 °C) using bulk wet density, water-loss porosity (105 °C) using grain density and pycnometer porosity (see details in Waber (2020)). Pycnometer porosity is calculated from the bulk dry density of the rock and the average grain density. For this reason, the drying temperature determines how much of, e.g., the clay-bound water is included in this calculation. The water-loss porosity is the ratio of the connected, water-filled pore volume to its total volume. Thus, unconnected pores, which are included in the measurements of geophysical logs, are not accounted for. In petrophysical applications, total porosity is defined as the volume of voids divided by bulk rock volume in a volume/volume unit (v/v, equals the normally used percentage). Total porosity includes all water (or any other pore fluid) present in the rock (except crystal water) so clay-bound water and capillary-bound water are also part of the total porosity. In a fully water-saturated system, like the rocks investigated in the siting regions, the capillary-bound water is of little relevance. While still a result of petrophysical logging, the differences in the different porosity values are usually very small and can be neglected in larger-scale comparisons.

Laboratory measurements require minimal data preparation as only a depth shift of the core data compared to the log data has to be considered. Core depths are reported based on the length of the casing while the depth for petrophysical logs is measured depending on the length of the cable used to attach the logging tools. These two reported lengths usually are very close to one another but not identical. Using image logs (such as the FMI), core depths were depth-shifted to the correct logging depth based on their lithological layering and/or visible faulting in both types of data. This shift was later applied to the depths of the laboratory samples.

2.3 MSCL data

MSCL can measure various petrophysical data on cores, including bulk density, P-wave velocity, magnetic susceptibility, SGR and elemental concentration from X-ray fluorescence (XRF) at a very high resolution (here, measurements were taken on average every 5 cm). However, since the MSCL data are measured on cores with a comparatively small measurement volume (core volume), while petrophysical wireline logs are measured in a borehole with a larger measurement volume, the MSCL data must be adjusted to the wireline data before merging the two data types. This involves a quality control of the MSCL logs, a detailed depth shift with petrophysical logs used as the depth reference (in the same way as for the laboratory data, see Section 2.2), determination of a correlation between the two datasets, application of the correlation to the MSCL logs, filling in gaps or intervals with poor-quality wireline logs with MSCL data, and using the resulting mixed-origin log as input for the multiminerall interpretation (see e.g. NAB 20-08, Dossier X from the Bülach-1-1 borehole for a detailed example, see also Fig. 2-2).

MSCL data were acquired for the new boreholes only. After roughly 20 years of storage, core conditions from the older boreholes, Riniken, Weiach-1 and Benken, were found to be insufficient to perform reliable MSCL measurements.

In general, MSCL data require very little preparation after acquisition. The only really necessary step is to remove low-quality data from the dataset and the aforementioned depth shift. Low-quality data either result from poor sample quality (e.g. extensive geometry variations of the cores) or extensive cracking/fracturing of the cores.

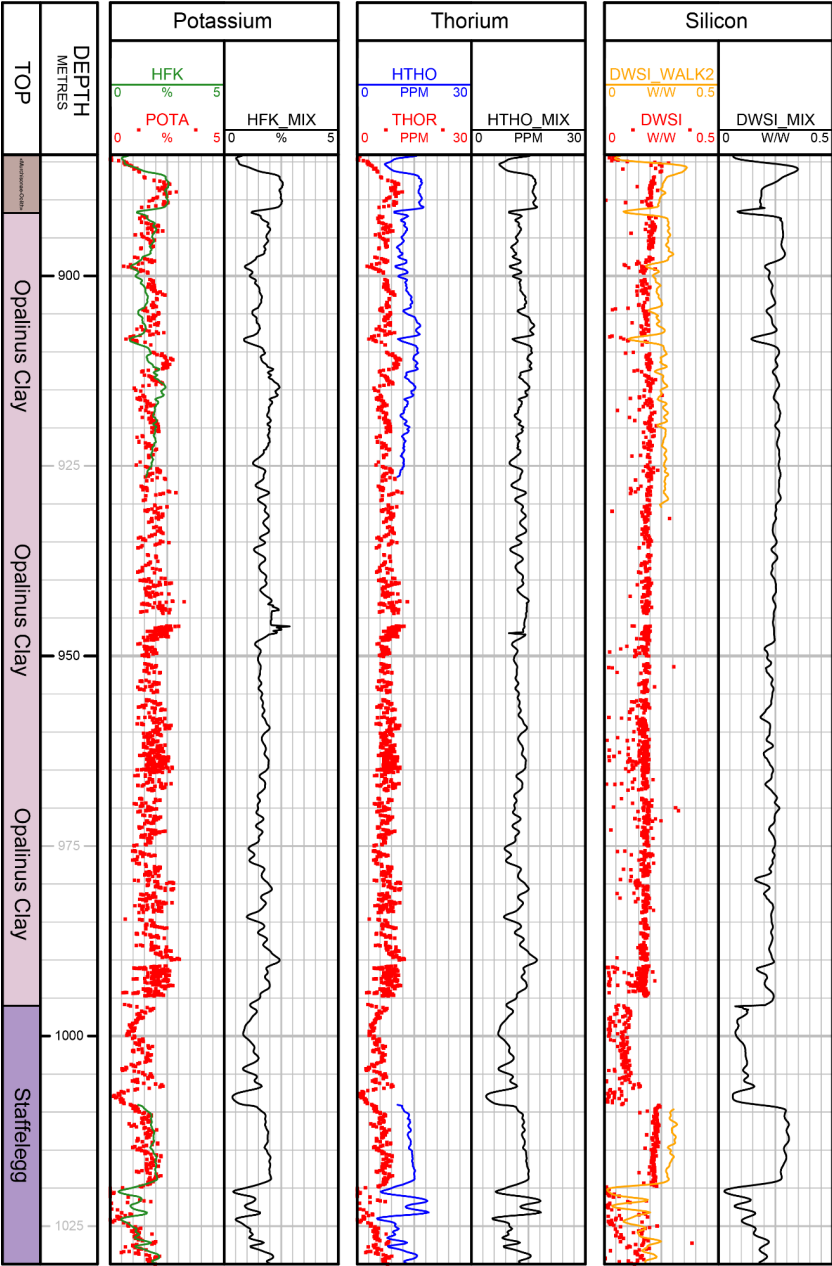


Fig. 2-2: Using MSCL data to complement log data or fill in gaps in the log data

When data gaps of the geophysical logs are encountered, or when logging data are of reduced quality due to, e.g., borehole breakouts/washouts, MSCL data can be used to complement the available data from geophysical logs. Shown here is an example of a logging gap within the Opalinus Clay. MSCL measurements (red squares) are used to complement petrophysical log measurements (green, blue and yellow curves, respectively), resulting in a continuous mixed log (black curves).

3 Multimineral methodology

3.1 Introduction

The multimineral interpretation is based on the fact that each log measurement within a borehole is determined by the mineral and fluid contents in the measured interval. If the mineral and fluid contents are known, a theoretical log response can be calculated. The reverse approach is also possible, i.e., where the petrophysical log measurements are known but the mineral and fluid contents are not. In this case, mineral and fluid contents can be assumed, and a theoretical log response can be calculated for this assumption. This theoretical log response can then be compared to the actually measured petrophysical logs and adjusted until the theoretical logs are in good agreement with the measured ones.

Linear equations are used to predict the response of most of the logging tools (e.g. bulk density, gamma ray, ECS, etc.). The general form of these equations can be written as:

$$\text{Theoretical log response} = \sum_{k=1}^n \text{Vol}_{(k)} * \text{Endpoint}(k)$$

with:

Vol_(k): fluid or mineral volume

Endpoint (k): log response of the fluid or mineral.

Endpoints are defined as the log response of a given petrophysical log for a pure fluid or mineral. For example, the endpoint of a pure calcite to a density log would be 2.71 gg/cc. Endpoints can be evaluated using readily published values, from the log responses in intervals with pure mineralogies or from calibration of log data to core measurements.

Some logs require the use of non-linear equations to calculate their theoretical log response. The equations used are described in more detail in Marnat & Becker (2021). As an example, only the equation to predict total porosity (PHIT) from the neutron hydrogen index (NHI) is given here.

The responses of neutron tools are non-linear with respect to the fluid and mineral volumes. The effect of this non-linearity can be seen in the logging operator, density-neutron charts where the matrix lines are not straight. This is due to the fact that the apparent matrix value depends on the porosity of the rock. The formulation of this equation, as implemented, is:

$$\text{PHIT} = a + b * \text{NHI} + 10^{(c + d * \text{NHI})}$$

with:

PHIT: total porosity of the rock

NHI: neutron hydrogen index

a, b, c and d: coefficients depending on the neutron tool used, coefficients are taken from a database provided by the logging contractor.

By comparing the calculated theoretical log response to the measured petrophysical logs, errors between the two can be determined and, by adjusting the assumed mineral content, minimised,

resulting in the predicted mineral and fluid contents. The generalised form to calculate the error for each log used in the interpretation is:

$$Error = \frac{Measured\ log - Predicted\ log}{Uncertainty}$$

The denominator of uncertainty here is comparable to a weight that can be assigned to the log based on its reliability. In case of borehole breakouts, for example, some of the petrophysical log readings are influenced by the increased distance to the borehole wall. Therefore, their weight, or uncertainty, for the general calculation of mineral content from data should be decreased so that the erroneous readings do not excessively influence the general prediction as it is known that these carry a high uncertainty. The decision of how much weight is given to a log is largely based on expert judgement but is aided by the quality control flag determined during quality-control procedures applied to the petrophysical logs. The error is calculated for each log, and the errors of all logs are added to determine the overall quality of the interpretation:

$$Incoherence\ function = \sum_{k=1}^{n_{log}} Error_{(k)}^2$$

with:

n_log: number of logs

To reduce the overall error even further, the interpretation has also been calibrated to core measurements. To this end, the different assumptions used in the multiminerall interpretation steps (mainly the endpoints of the interpreted minerals and fluids) were manually fine-tuned to improve the match between predicted results and core measurements where the latter are available.

The remaining error of the interpretation is represented as several parameters of which the analyses quality is arguably the most important. The QUALITY indicator refers to the multiminerall interpretation results and is a measure of the correlation between the input data and the interpretation results. It is reported in the composite plots in the appendix for each borehole. A quality index of one or below shows that the calculated accuracy of the theoretical log response is within 95% compared to the original petrophysical logs. The accuracy decreases with increasing values of the quality indicator. However, the indicator does not consider the input data per se but reports on the correlation between the input data and the results. Hence, even if the input data are of overall low quality, the interpretation may still have a high-quality indicator because the correlation between input data and interpretation result is good.

3.1.1 Choice of interpretation intervals

An important step in multiminerall interpretation is the choice of the interpretation intervals. Usually, the data are divided into a set of interpretation intervals based on borehole lithology and pore fluid content. The latter does not play an important role in the interpretation described here as no occurrences of hydrocarbons have been observed, hence the pore fluid is always water with a slightly varying salinity.

Available data quality is also an important driver in determining the interpretation intervals. Intervals with reduced data quality due to, e.g., borehole breakouts are interpreted independently from the surrounding intervals even when lithologies and fluid content do not change.

In intervals where some of the logs are of low quality, or no logging was possible at all due to the borehole quality or the casing scheme, MSCL measurements were used, if available and appropriate, to fill in the gaps or used as additional data for the missing/low-quality petrophysical logs (see previous Section 2.3).

3.1.2 Choice of minerals and fluids

Formation water is always present in the rocks. As stated earlier, no occurrences of oil or gas were observed, hence the porewater in the boreholes interpreted here is, at a given temperature and pressure, fully characterised by its salinity, which allows for computing all log responses using saline porewater as the dominant formation fluid.

The number of minerals that can be calculated in a multimineral interpretation largely depends on the availability of high-quality logs. When this is the case, and when a number of logs measure different petrophysical parameters, as is the case in this study, quartz, orthoclase, calcite, dolomite, anhydrite, halite, pyrite, goethite and siderite can be interpreted with high confidence. Additional minerals, such as different clay minerals, can also be interpreted, but the quality of the results for these minerals must be carefully considered as it may not be sufficient for quantitative use (and is hence not reported here). If the number of logs, or, in more general terms, available input data is not sufficient for a detailed multimineral interpretation, the number of modelled minerals must be decreased. In this case, e.g. quartz and feldspars or calcite, dolomite and siderite are merged to form pseudo-minerals. In the worst case, only two mineral components can be modelled, clay minerals (*sensu lato*) and matrix/cement minerals (everything but clay). While the newer boreholes usually allowed for a detailed interpretation, the older boreholes, in particular, only allow calculating a reduced number of minerals, i.e. sometimes only clay and matrix minerals.

3.2 Multimineral interpretation runs

As previously mentioned, the multimineral approach was performed twice. The first interpretation runs were performed on a per-borehole basis immediately after borehole completion. This means that, especially during the step of error minimisation (see above), the choice of, e.g., endpoints or mineral content at any given measuring point/depth is solely based on information from the interpreted borehole. Therefore, physically based material parameters of, e.g., minerals, may slightly differ in the different interpretations between each borehole. Once all boreholes were completed, a second interpretation run was performed using harmonised interpretation intervals, endpoints, etc. for all boreholes. For the second interpretation run, additional information from the reconditioned logs was also available (see Section 2.1). Hence, the second interpretation run is the more robust multimineral interpretation, and results of this second interpretation are detailed in Chapter 4.

An exception to the above are the older boreholes in Benken, Riniken and Weiach-1. These were drilled some 20+ years ago. While petrophysical logs used in these older boreholes were then state-of-the-art, they cannot be compared to what is technically possible today. Hence, the older boreholes have been interpreted independently from the recent boreholes and on a per-borehole basis. This means that each interpretation for the old boreholes uses specifically tailored interpretation intervals, endpoints, mineral content, etc., and results are only valid for a specific borehole. Therefore, since results of these interpretations are based on (slightly) different parameters, they should not be used quantitatively but rather qualitatively to compare the general trends and possibly ratios between major mineral constituents.

3.2.1 First interpretation run

As stated earlier, the first interpretation run was performed on a per-borehole basis immediately after each borehole was completed. This work is documented in Dossier X (see Tab. 1-1 for references).

3.2.2 Second interpretation run

The second interpretation run, whose results are summarised in this report (Chapter 4), was performed after completion of all boreholes. Though the general multimineral interpretation approach as outlined above was used, necessary assumptions were harmonised between all boreholes. First, whenever possible, the interpretation intervals based mainly on lithology were kept constant between the different boreholes. If borehole quality in a certain borehole interval was reduced (e.g. due to borehole breakouts), this interval was still treated separately. All other assumptions, e.g. endpoints, were kept constant between the different boreholes. In addition, the second interpretation run made use of the reconditioned logs (see Chapter 2), hence additional input information was available. Finally, three more input curves were generated using a machine-learning and clustering algorithm for smectite, chlorite and total organic content (TOC). The first interpretation run showed that, compared to laboratory data, the content of these three accessory minerals could not be accurately reproduced. In the case of TOC, this also affected the porosity estimation in the organic-rich Staffelegg formation.

To better determine these three accessory minerals, a machine-learning algorithm based on a k-nearest neighbour approach was applied and tested using blind tests. Data from four boreholes (MAR1-1, BOZ1-1, BOZ2-1 and TRU1-1) were used for the initial training of the model. The smectite, chlorite or TOC was taken from the available laboratory data, and all available petrophysical logs at the same depth as the laboratory samples were plotted. The exponentially distance-weighted average of the logs for the three minerals was applied to the blind test data from the BAC1-1, STA2-1 and STA3-1 boreholes (BUL1-1 was not used in the training or blind test dataset due to problems encountered during drilling), and the respective mineral curves for smectite, chlorite and TOC were calculated. A comparison of the calculated blind test data with laboratory data is shown in Fig. 3-1.

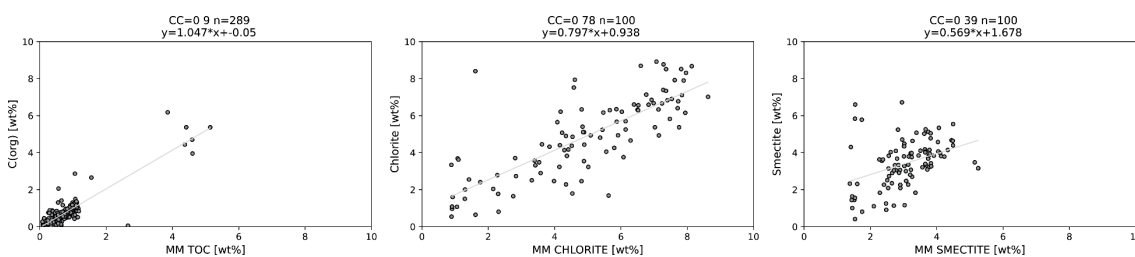


Fig. 3-1: Comparison of TOC, chlorite and smectite from the blind test dataset (prefix MM, x-axis) with laboratory measurements (y-axis) for the STA2-1, STA3-1 and BAC1-1 boreholes

For TOC and chlorite, the test and laboratory data show a very good correlation. For smectite, some dispersion can be observed, especially since possible outliers have not been filtered out, but the range of the predicted smectite content is still in good agreement with the laboratory data.

In summary, due to the inclusion of newly available data and the harmonisation across all available (new) boreholes in the second interpretation run, data quality and robustness were (much) improved and can be used quantitatively as well as qualitatively for the site characterisation or advanced interpretations.

4 Interpretation results

The results of the multiminer interpretation briefly described above are weight percentages of mineral content and fractions for porosity. These data are available in the form of continuous curves along the boreholes as long as there are enough input data (mainly petrophysical logs) to allow for a precise calculation of, e.g., mineral content. The data are presented in Appendix A in the form of composite plots. To demonstrate the quality of the correlation between laboratory measurements and multiminer interpretation results, crossplots of select data and more detailed plots of parameters within the Opalinus Clay are presented in the following. To do this, the multiminer interpretation results were interpolated and extracted at exactly the depths for which laboratory measurements were available. Hence, all figures below show multiminer interpretation results only where laboratory measurements were also available.

The important point to keep in mind is that the laboratory measurements were used to calibrate the multiminer interpretation. As a reminder, the endpoints during the multiminer interpretation were adjusted to minimise the overall error between the theoretical log response and the measured log response. This adjustment was performed to obtain a multiminer interpretation that is as close as possible to the laboratory measurements in terms of mineralogy and porosity. However, this does not mean that each laboratory measurement can be honoured exactly. The main reason for this is the natural variance of mineralogical content in the interpretation interval and the fact that laboratory measurements and petrophysical logging use very different scales, i.e., they integrate over different lengths. Hence, they measure different volumes of rock and in a different state (in situ vs. in a laboratory). However, one can reasonably assume that a good correlation between multiminer interpretation results and laboratory measurements requires a good adjustment of the necessary assumptions used in the multiminer interpretation to calculate mineralogy and porosity with reasonable confidence. This, in turn, means that the multiminer interpretation is also valid in intervals where no laboratory measurements are available for the purpose of, albeit not fully independent, quality control.

As mentioned in Section 2.2, depths from laboratory measurements and logs were determined based on different depth systems (casing length vs. cable length) and were adjusted using the very high-resolution FMI tool, which essentially maps the borehole on a mm-scale. While this results in an accurate depth for both log and laboratory measurements, the impact of a slightly erroneous depth conversion was still tested as a safety precaution by arbitrarily bulk shifting the laboratory samples by 50 cm and performing a multiminer analysis. This resulted in negligible differences of the two interpretations, mainly because the logs integrate over a certain interval.

The quality of the correlation between laboratory data and multiminer interpretation can be tested when cross plots of mineralogy from the multiminer interpretation against laboratory measurements are analysed (see Fig. 4-1 for an example of clay mineral content in the recent boreholes and Fig. 4-2 for clay mineral content in older boreholes). The correlation coefficients for all recent boreholes are high when clay mineral content is analysed. For the older boreholes, the correlation coefficients are generally lower, owing to the fact that fewer high-quality petrophysical logs were available for the multiminer interpretation. In addition, clay mineral content in the older boreholes seems to be much more variable throughout the boreholes.

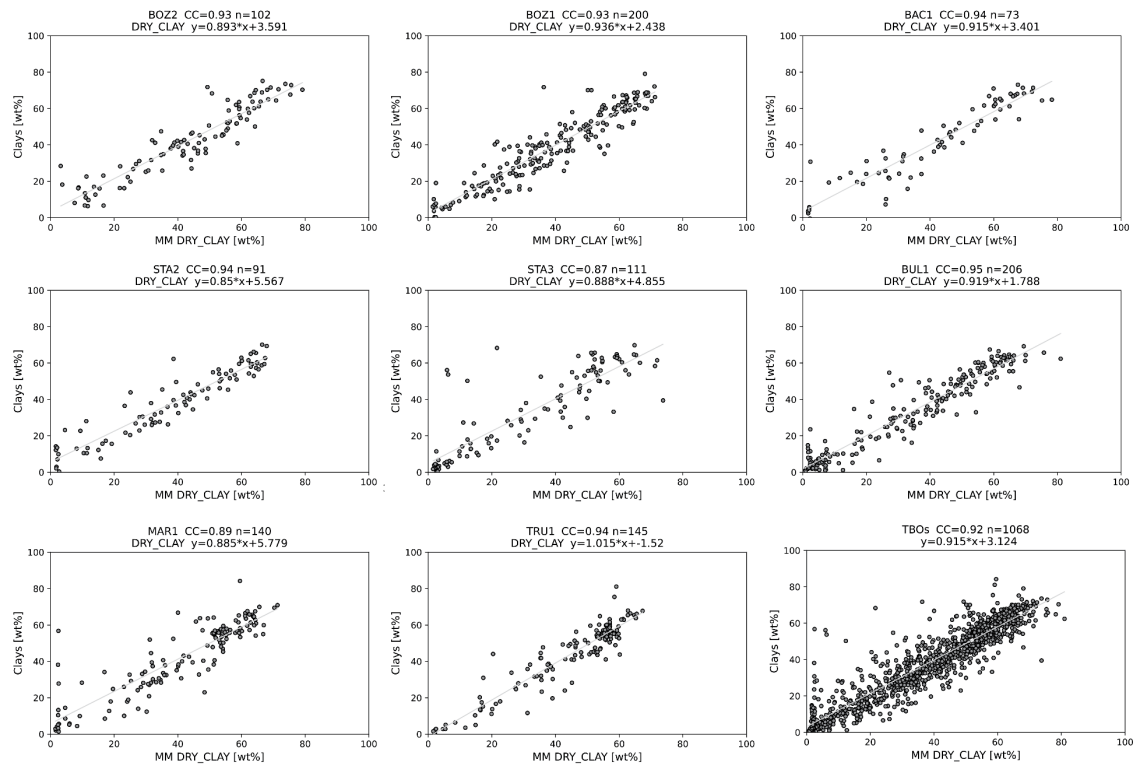


Fig. 4-1: Crossplots of clay mineral content measured in the laboratory (y-axis) vs. multiminer interpretation results (x-axis) for total clay mineral content in the recent boreholes. The lower right plot is a summary including measurements from all recent boreholes

The name of the borehole, the correlation coefficient (CC), the number of samples (n) and the equation for the linear fit are provided at the top of each crossplot. Note that no laboratory measurements were performed in Rheinau-1-1, which is why Rheinau-1-1 is not included here.

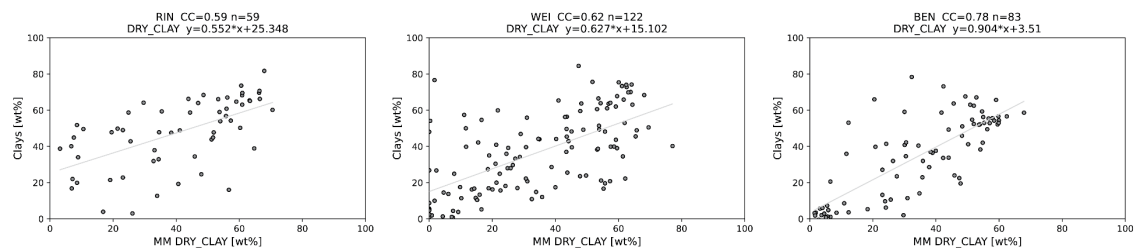


Fig. 4-2: Crossplots of clay mineral content measured in the laboratory (y-axis) vs. multiminer interpretation of clay (x-axis) for the older boreholes

The name of the borehole, the correlation coefficient (CC), the number of samples (n) and the equation for the linear fit are provided at the top of each crossplot

The same can be deduced from crossplots of clay mineral content in the Opalinus Clay only (Fig. 4-3 and Fig. 4-4). Again, the fit, and hence the correlation coefficients, are high for the recent boreholes but significantly lower for the older boreholes. For other minerals or mineral groups (quartz and carbonates), generally high correlation coefficients can be calculated (ranging between 0.8 and 0.9) for the recent boreholes. Benken also shows comparatively high correlation coefficients for quartz and carbonates while for Riniken and Weiach-1, these two mineral groups could not be calculated because logs were insufficient. This means that only clay mineral content could be determined in Riniken and Weiach-1 (mainly because a spectral gamma ray but no elemental spectroscopy log was available, i.e. all other minerals were lumped together into a single pseudo-matrix mineral).

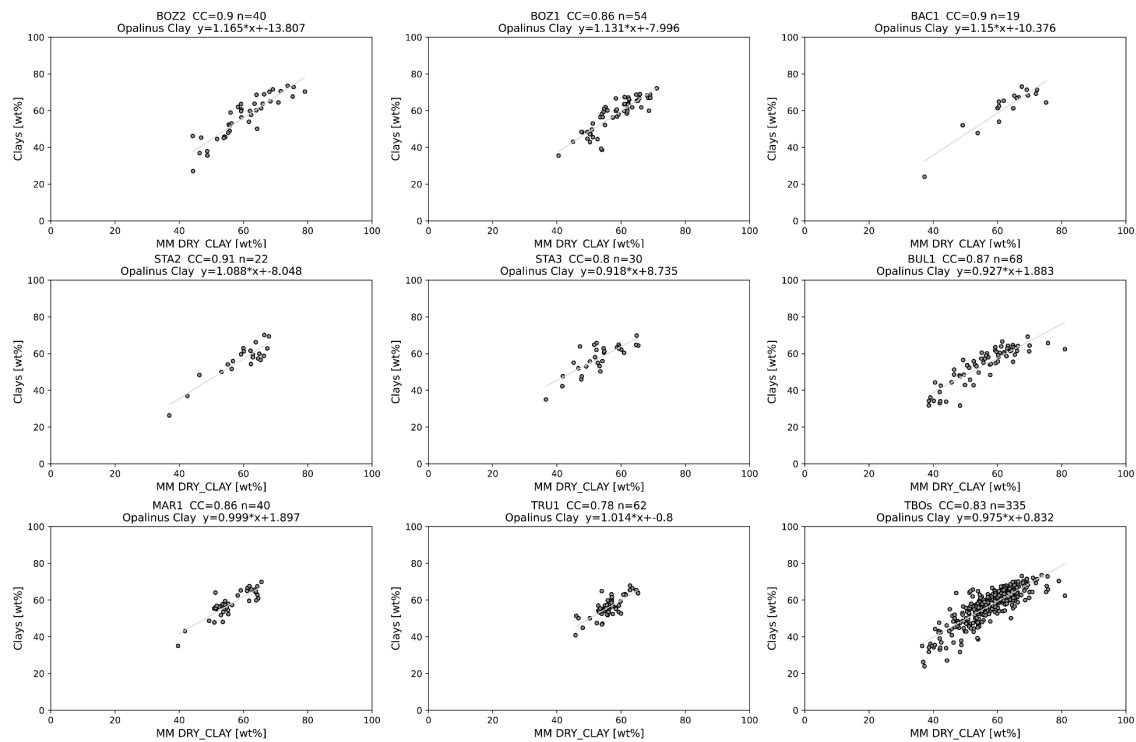


Fig. 4-3: Crossplots of laboratory measurements of clay (y-axis) vs. multiminerall interpretation results for clay (x-axis) for the Opalinus Clay in the recent boreholes. Again, the lower right plot is a summary plot included data from all recent boreholes

The name of the borehole, the correlation coefficient (CC), the number of samples (n) and the equation for the linear fit are provided at the top of each crossplot. Note that no laboratory measurements were performed in Rheinau-1-1, which is why Rheinau-1-1 is not included here.

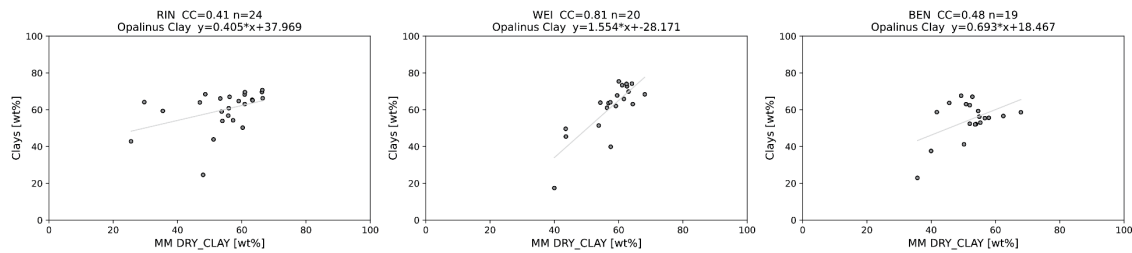


Fig. 4-4: Crossplots of laboratory measurements of clay (y-axis) vs. multiminerall interpretation results for clay (x-axis) for the Opalinus Clay in the older boreholes

The name of the borehole, the correlation coefficient (CC), the number of samples (n) and the equation for the linear fit are provided at the top of each crossplot.

In general, the same observations apply to porosity measurements as to the mineral content. As stated earlier, two different types of porosity measurements were performed in the laboratory and were used for the multiminerall interpretation: pycnometer porosity and water-loss porosity using bulk wet density. For both, the correlation between laboratory measurements and multiminerall interpretation is high for the recent boreholes (see Fig. 4-5 and Fig. 4-6).

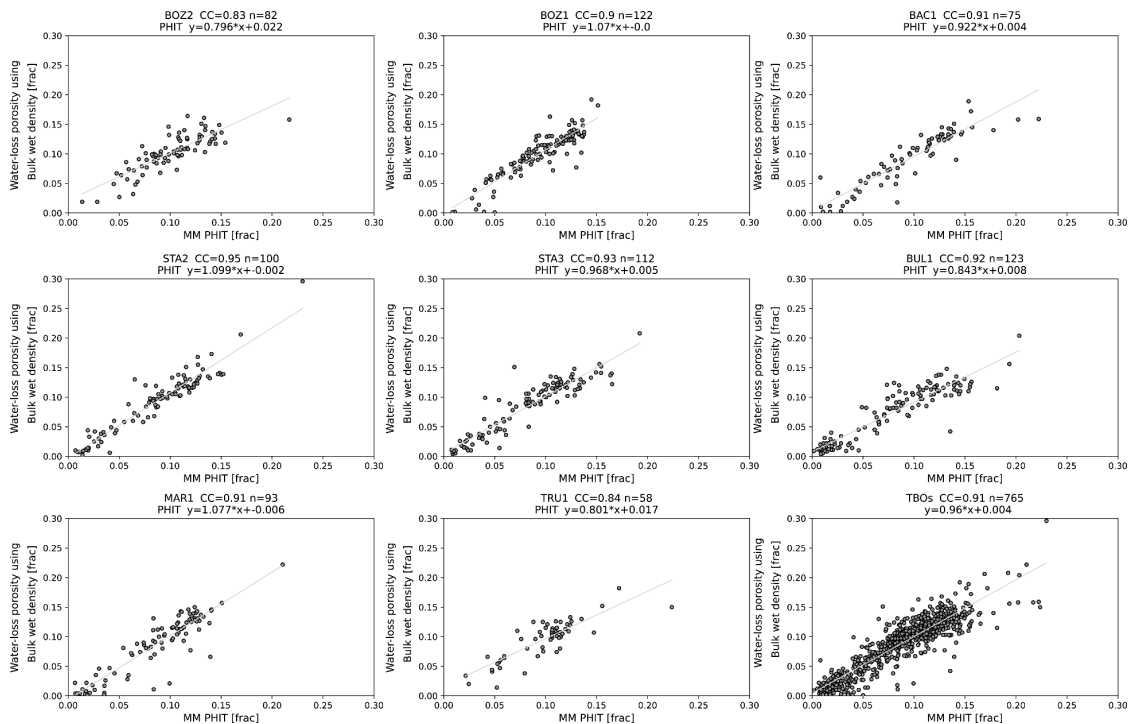


Fig. 4-5: Crossplots of laboratory measurements of water-loss porosity using bulk wet density (y-axis) vs. multiminerall interpretation results (total porosity, PHIT, x-axis) for the recent boreholes. Lower right plot is a summary using data from all recent boreholes

The name of the borehole, the correlation coefficient (CC), the number of samples (n) and the equation for the linear fit are provided at the top of each crossplot. Note that no laboratory measurements were performed in Rheinau-1-1, which is why Rheinau-1-1 is not included here.

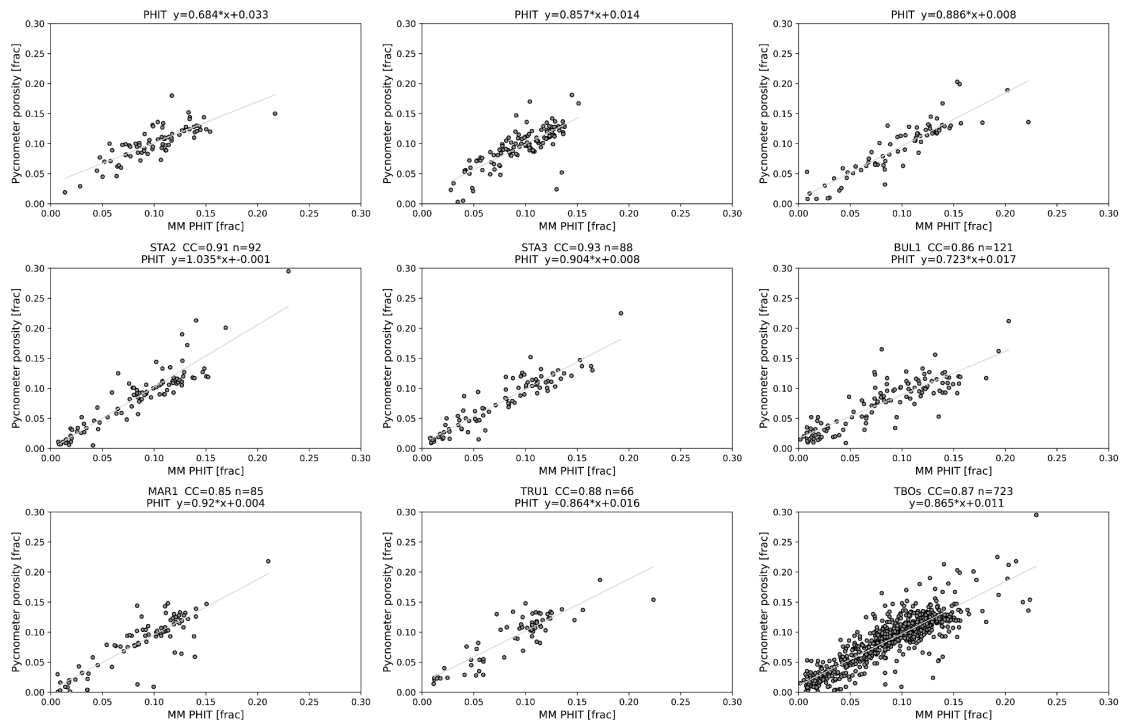


Fig. 4-6: Crossplots of laboratory measurements of pycnometer porosity (y-axis) vs. multi-mineral interpretation results (total porosity, PHIT, X-axis) for the recent boreholes. The lower right plot is a summary using data from all recent boreholes

The name of the borehole, the correlation coefficient (CC), the number of samples (n) and the equation for the linear fit are provided at the top of each crossplot. Note that no laboratory measurements were performed in Rheinau-1-1, which is why Rheinau-1-1 is not included here.

For the older boreholes, only the pycnometer porosity was measured (see Fig. 4-7). For Benken and Weiach-1, this shows only a weak correlation, mainly because the variability of the multimaterial interpretation is comparatively high and includes several outliers.

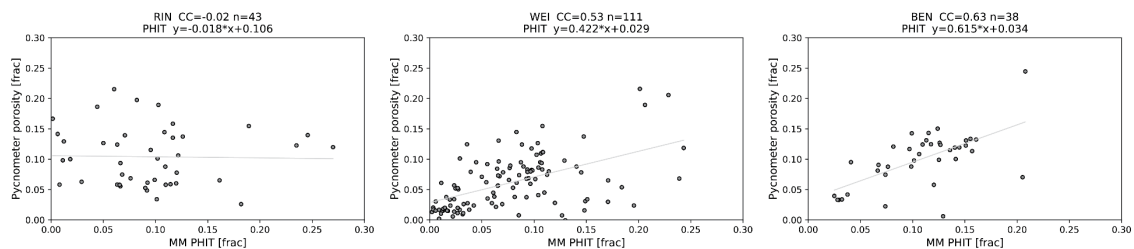


Fig. 4-7: Crossplot of laboratory measurements of pycnometer porosity (y-axis) vs. multi-mineral interpretation results (total porosity, PHIT, x-axis)

The name of the borehole, the correlation coefficient (CC), the number of samples (n) and the equation for the linear fit are provided at the top of each crossplot.

For Riniken, it is not possible to determine a correlation between the laboratory and multimineral interpretations. Both measurements show a large variance resulting in a rather random distribution of data in the laboratory/multimineral interpretation crossplot (see Fig. 4-7).

The Mesozoic sequence of the areas of interest is uniquely described by its lithology which largely reflects the mineralogical content of the different formations. Though the different boreholes generally share the same lithologies and lithostratigraphic units, there are too many different lithologies to adequately display them all here in the form of ternary plots. Hence, Fig. 4-8 only shows the ternary plots of the Opalinus Clay. Each plot includes the laboratory measurements and the results from multimineral interpretation. While the laboratory measurements are shown as distinct points, the multimineral interpretation results are displayed as contour lines which enclose a certain percentage of the multimineral interpretation results, hence the contour lines represent a sort of density map for the multimineral interpretation.

As previously shown, both measurement and interpretation are highly correlated. The differences of the mineral content in the different boreholes in the Opalinus Clay is small, and they generally show a high clay and low carbonate or quartz and feldspar content.

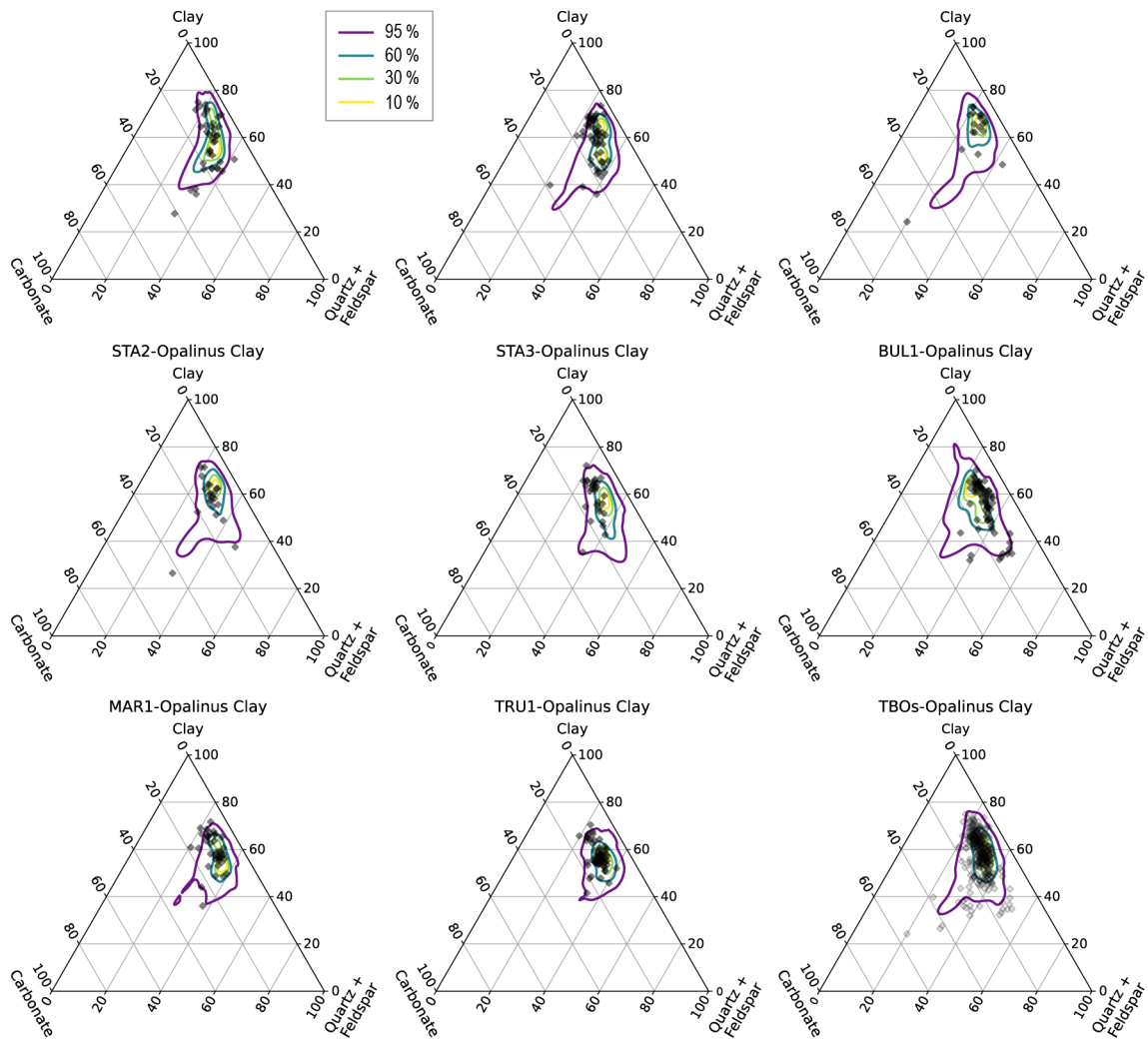


Fig. 4-8: Ternary plots of the recent boreholes for clay, carbonates as well as of quartz and feldspars in the Opalinus Clay

The squares represent mineralogical content measured in the laboratory while the density lines represent all multimaterial measurements for each borehole. The figure on the lower right combines all laboratory and multimaterial measurements of all recent boreholes. The lines enclose a certain percentage (95, 60, 30, 10) of the multimaterial interpretation results.

Due to the limited amount of petrophysical logs in the older boreholes, carbonates and quartz/feldspars could not always be interpreted using the multimaterial approach, hence no ternary plots of these boreholes are shown here.

5 Summary

The multiminerall interpretation using all available input data resulted in continuous profiles of key properties (mineralogy and porosity) for the different boreholes. For the recent boreholes, it was possible to achieve consistently high correlation coefficients with laboratory data for the main minerals, clay, carbonates as well as quartz and feldspars, mostly ranging between 0.8 and 1 in the Opalinus Clay. The same holds true for the porosity estimations. For the older boreholes Benken, Weiach-1 and Riniken, the correlations are less good. For these boreholes, the resulting property profiles should therefore be used only qualitatively.

Thanks to the harmonised approach between all the boreholes from the more recent drilling campaign, the second multiminerall interpretation run presented in this report improved the consistency and comparability of the results between these different boreholes.

6 References

- Marnat, S. & Becker, J.K. (2021): Petrophysical log analyses of deep and shallow boreholes: Methodology report. Nagra Arbeitsbericht NAB 20-30.
- Mazurek, M. (2017): Gesteinsparameter-Datenbank Nordschweiz – Version 2. Nagra Arbeitsbericht NAB 17-56.
- Nagra (Hrsg.) (2021): TBO Bülach-1-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 20-08.
- Nagra (Hrsg.) (2021): TBO Marthalen-1-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 21-20.
- Nagra (Hrsg.) (2021): TBO Trüllikon-1-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 20-09.
- Nagra (Hrsg.) (2022): TBO Bözberg-1-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 21-21.
- Nagra (Hrsg.) (2022): TBO Bözberg-2-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 21-22.
- Nagra (Hrsg.) (2022): TBO Stadel-2-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 22-02.
- Nagra (Hrsg.) (2022): TBO Stadel-3-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 22-01.
- Nagra (Hrsg.) (2022): TBO Rheinau-1-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 22-03.
- Nagra (Hrsg.) (2022): TBO Bachs-1-1: Data Report Dossier I-XI. Nagra Arbeitsbericht. NAB 22-04.
- Waber, H.N. (ed.) (2020): SGT-E3 deep drilling campaign (TBO): Experiment procedures and analytical methods at RWI, University of Bern (Version 1.0, April 2020). Nagra Arbeitsbericht NAB 20-13.