

Arbeitsbericht NAB 19-44

**Multi-scale Petrographic and
Structural Characterisation
of the Opalinus Clay**

February 2020

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

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Multi-scale Petrographic and Structural Characterisation of the Opalinus Clay

February 2020

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1 Introduction

The Opalinus Clay in Northern Switzerland has been the target of numerous geoscientific studies over the last 4 decades, pertaining to its geological-mineralogical, geochemical, hydrogeological and mechanical properties. While some studies have been performed in quarries and tunnels (e.g. Wetzel & Allia 2000, 2003, Gautschi 2001), most of the information originates from cored boreholes. In the 1980ies, the Opalinus Clay was penetrated by boreholes Beznau-1984 (Nagra 1984), Riniken-1 (Matter et al. 1987), Weiach-1 (Matter et al. 1988a) and Schafisheim (Matter et al. 1988b) and was subjected to a geological-mineralogical characterisation. Since the mid-1990ies, multi-disciplinary investigations in the Mont Terri Underground Laboratory boosted the state of knowledge on the formation (overviews in Thury & Bossart 1999, Bossart & Thury 2007, Bossart 2017). Core materials from and downhole measurements in the Benken borehole (drilled in 1998 – 1999; Nagra 2001) provided the opportunity to widen the scope of the investigations and to focus on mechanical and geochemical issues, including the pioneering work pertaining to the characterisation of pore-water composition (Gimmi & Waber 2004, Gimmi et al. 2007). To a substantial degree, the milestone report underlying the demonstration of disposal feasibility in the Opalinus Clay (Nagra 2002) was based on data and insights obtained from the Benken borehole. More recently, core materials from the deep geothermal borehole at Schlattingen (drilled 2010 – 2011; Wersin et al. 2013) were used for further characterisation, including several innovative techniques. The data set was further augmented by information obtained from numerous shallow geothermal boreholes, where, in the absence of core materials, geophysical logs provided valuable information (e.g. Albert et al. 2012b, Bläsi et al. 2014a). Last, the cored geothermal borehole at Lausen was used to characterise the Opalinus Clay at shallow levels (Mazurek et al. 2017a).

The purpose of this report is to integrate the information on the geological, mineralogical, petrophysical and structural characteristics of the Opalinus Clay and to highlight the progress since Nagra (2002) pertaining to the function of the Opalinus Clay as a barrier to solute transport. Mechanical aspects are not a topic of this report. Similarly, the composition of pore water and its spatial variability are out of scope but are the focus of a companion report (Wersin et al. 2020).

The relevant characteristics of the Opalinus Clay relate to features and processes on a wide range of scales between tens of kilometres (lateral variability in the region of interest, large-scale structures) to the pore scale (~ 1 nm), spanning a length-scale range of about 13 orders of magnitude. Different chapters of this report pertain to different scales:

- Chapter 2 explores the lithological characteristics of the Opalinus Clay and their variability in the vertical (scale of tens of metres) and lateral (scale of tens of kilometres) dimensions. Sub-units within the Opalinus Clay are defined and correlated laterally between observation points to the degree possible.
- Chapter 3 synthesises the available information on diagenesis and, in particular, on diagenetic mineralisation. This includes the effects of early diagenesis that occurred in the uppermost tens of metres below the surface of the unconsolidated sediment, effects of burial diagenesis at elevated pressure and temperature, and finally tectonic effects leading to vein mineralisations.
- Chapter 4 deals with the micro- and nanoscale structure of the Opalinus Clay and is mainly based on the results of innovative tools, such as SEM and TEM tomography of samples prepared using ion-polishing techniques.

- Chapter 5 addresses macroscopic structural features, such as faults and joints. The degree of tectonic overprint varies substantially in the investigation area, given the fact that the Opalinus Clay occurs in different tectonic units (Molasse Basin, Tabular Jura, Jura fold-and-thrust belt).
- Finally, an attempt is made in Chapter 6 to synthesise all multi-scale information, in particular to provide a suite of illustrations that highlight the main features on all scales.

2 Large-scale lithological subdivision of the Opalinus Clay

The objective of this chapter is to characterise lithological heterogeneities within the Opalinus Clay in the vertical and lateral dimensions and to correlate these regionally to the extent possible. The focus and main application of the study is on the characterisation of the host rock as a barrier for solute transport. To this end, the main investigation tools included lithostratigraphic information from the literature, the study of core photographs and data from geophysical borehole logs converted to logs of clay-mineral content (termed "clay-mineral logs" in the following). Biostratigraphic methods were not applied, and there was no ambition to investigate the genetic aspects of deposition, or the definition of time lines as a basis for lateral correlations.

For the sake of brevity, terms like "clay-rich" or "clay-poor" are used in the following. These terms are used in the mineralogical sense, i.e. they refer to the content of fine-grained sheet-silicate minerals and not just to grain size. The correct (but longer) term would be "rich/poor in clay minerals".

2.1 Data base

Most information about the Opalinus Clay originates from boreholes in the form of core materials, geophysical logs and additional borehole measurements. A substantial number of boreholes penetrating the Opalinus Clay were drilled in the area of investigation (Tab. 2-1, Fig. 2-1). Apart from waste disposal, the main targets of the boreholes included hydrocarbon exploration and the installation of shallow geothermal probes. The depth at which the Opalinus Clay was encountered varies from 0 (eroded top) to > 2'000 m in the southeastern, deeper part of the Molasse Basin (e.g. Triemli, Lindau-1). In some boreholes, only a part of the Opalinus Clay has been penetrated, either due to surficial erosion (i.e. top missing), limited borehole depth (i.e. base missing), or tectonic effects. The following boreholes listed in Tab. 2-1 were not considered for the study:

- Baden Münzlishausenerstrasse (strongly tectonised, repetition)
- Bözberg SB-1/13 (tectonised, no geophysical logs)
- Hemmental-1 (incomplete profile, more complete information for adjacent borehole Hemmental-2)
- Tegerfelden-1 (incomplete profile, more complete information for adjacent borehole Tegerfelden-2)
- Wölflinswil-1 (incomplete profile, more complete information for adjacent borehole Wölflinswil-2).

Further, only partial information is available for some boreholes, so these are used for specific aspects only:

- Basel-1 (limited information)
- Beznau-1984 (incomplete profile, no geophysical logs)
- Meersburg-1 (limited information, no suited and accessible geophysical logs; samples from the confining units were used for diagenetic studies in Chapter 3).

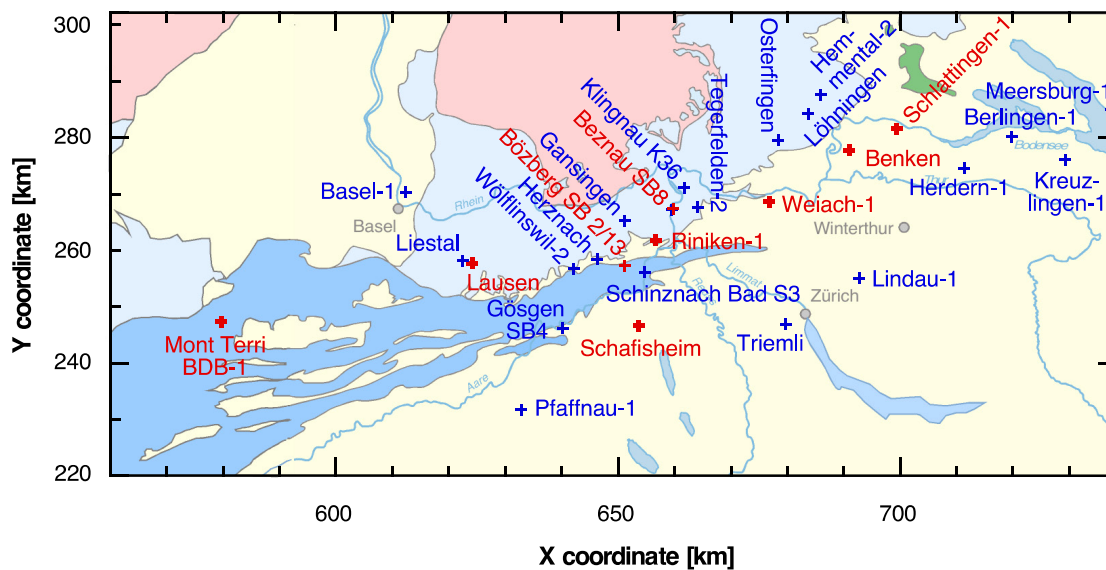


Fig. 2-1: Localities of the studied boreholes

Boreholes in which the Opalinus Clay was cored are shown in red, percussion boreholes in blue. Simplified tectonic map in the background (yellow: Cenozoic [Molasse Basin and Upper Rhine Graben]; light blue: Tabular Jura; dark blue: Jura fold-and-thrust belt; pink: Crystalline basement [Black Forest, Vosges]; green: Hegau volcanics)

Tab. 2-1: Boreholes penetrating the Opalinus Clay in the area of investigation
Numbers in italics indicate eroded top of the Opalinus Clay or base not reached by the borehole. n.d. = no data

		Stratigraphy					Geophysical logs		Coordinates			
Borehole	Abbreviation	Opalinus Clay cored	Top Opalinus Clay [m b.g.]	Base Opalinus Clay [m b.g.]	Thickness [m]	Reference	Calibrated clay-mineral log	Reference	X [km]	Y [km]	Elevation [m a.s.l.]	Reference
Baden Münzlishausenerstr.	BDM	No	12/118	> 97.5/135.5	n.d. (tectonised)	Bläsi et al. (2012)	No	Albert & Willenberg (2014)	663.580	258.600	538	Bläsi et al. (2012)
Basel-1	BS1	No	928	1'075	147	Ladner et al. (2008)	No	Geopower Basel AG (unpubl.)	611.810	270.536	250	Geoexplorers (2009)
Benken	BEN	Yes	539.7	652.04	112.34	Nagra (2001), Bläsi et al. (2013)	Yes	Albert & Willenberg (2014)	690.989	277.843	404	Bläsi et al. (2013)
Berlingen-1	BER	No	1'909.85	2'016	106.15	Bläsi (1995)	No	Albert & Willenberg (2014)	719.685	280.195	593	Bläsi et al. (2013)
Beznau-1984	BZ1	Yes	< 20.3	65.7	n.d. (top eroded)	Nagra (1984)	No log		659.491	267.242	325.8	Nagra (1984)
Beznau SB8	BZ2	No	< 22	63	n.d. (top eroded)	Albert & Willenberg (2014)	No	Albert & Willenberg (2014)	659.725	267.430	421	Roth & Gübeli (2009)
Bözberg SB 1/13	BO1	Yes	198.85	252	n.d. (tectonised)	Bläsi & Feist-Burkhardt (2020)	No log		651.809	256.627	520.61	Bläsi & Feist-Burkhardt (2020)
Bözberg SB 2/13	BO2	Yes	52.43	94.24	n.d. (tectonised)	Bläsi & Feist-Burkhardt (2020)	No	Albert & Willenberg (2014)	651.093	257.350	705.1	Bläsi & Feist-Burkhardt (2020)
Gansingen-Galten	GAN	No	< 18	56.5	n.d. (top eroded)	Bläsi et al. (2014a)	No	Albert & Willenberg (2014)	651.170	265.285	485	Bläsi et al. (2014a)
Gösgen SB4	GOS	No	498	588	90	Bläsi et al. (2014b)	No	Albert & Willenberg (2014)	640.194	246.243	381	Bläsi et al. (2014b)
Hemmental-1	HM1	No	160	> 200	126 (based on HM2)	Bläsi et al. (2013)	No	Albert & Willenberg (2014)	686.210	287.465	569	Bläsi et al. (2013)
Hemmental-2	HM2	No	151	277	126	Bläsi et al. (2014a)	No	Albert & Willenberg (2014)	685.865	287.612	578	Bläsi et al. (2014a)
Herdern-1	HER	No	1'726.85	1'848	121.15	Bläsi (1995) (base), Bläsi et al. (2013) (top)	No	Albert & Willenberg (2014)	711.308	274.597	527	Bläsi et al. (2013)
Herznach	HZN	No	209	> 226	124 (based on WO2)	Bläsi et al. (2014a)	No log		646.353	258.417	434	Bläsi et al. (2014a)
Klingnau K 36	KLI	No	62	171	109	Albert & Willenberg (2014)	No	Albert & Willenberg (2014)	661.593	271.161	505	Naef & Deplazes (2016)
Kreuzlingen-1	KRE	No	2'173.25	2270	96.75	Bläsi (1995)	No	Albert & Willenberg (2014)	729.201	276.169	539	Bläsi et al. (2013)
Lausen	LAU	Yes	< 6.2	71.34	n.d. (top eroded)	Vogt et al. (2016)	Yes	Vogt et al. (2016)	624.157	257.719	345	Vogt et al. (2016)
Liestal	LST	No	43	166	123	Bläsi & Ibele (2019)	No	Bläsi & Ibele (2019)	622.368	258.224	380	Bläsi & Ibele (2019)
Lindau-1	LIN	No	2'037.5	2117	79.5	Büchi et al. (1965)	No	Albert & Willenberg (2014)	692.815	255.098	516	Bläsi et al. (2013)
Löhningen	LOH	No	69	> 170	126 (based on HM2)	Albert et al. (2012b)	No	Albert & Willenberg (2014)	683.669	284.274	494	Albert et al. (2012b)
Meersburg-1	MEE	No	ca.2'058	2'165	ca. 107	Bläsi (1995)	No suited and accessible logs		738.558	285.036	497	Nusch et al. (2013)
Mont Terri BDB-1	MT	Yes	106.25	236.8	130.55	Hostettler et al. (2017)	Yes	Reisdorf et al. (2016)	579.515	247.412	512	Hostettler et al. (2017)
Osterfingen	OST	No	< 30	112	n.d. (top eroded)	Albert et al. (2012b)	No	Albert & Willenberg (2014)	678.400	279.555	427	Albert et al. (2012b)
Pfaffnau-1	PFA	No	1'250	1'363	113	Büchi et al. (1965)	No	Albert & Willenberg (2014)	632.708	231.789	500	Sachs & Schneider (2012)
Riniken-1	RIN	Yes	331.14	450.93	119.79	Matter et al. (1987)	Yes	Albert & Willenberg (2014)	656.604	261.800	385	Bläsi et al. (2013)
Schafisheim	SHA	Yes	1'000.65	1'079.95	79.3	Matter et al. (1988b)	Yes	Albert & Willenberg (2014)	653.620	246.760	421	Bläsi et al. (2013)
Schinznach Bad S3	SNZ	No	8	150	142	Albert & Willenberg (2014)	No	Albert & Willenberg (2014)	654.770	256.187	345	Naef & Deplazes (2016)
Schlattingen-1	SLA	Yes	831.4	949.7	118.3	Albert et al. (2012a)	Yes	Albert & Willenberg (2014)	699.380	281.630	417	Bläsi et al. (2013)
Sonnengarten/ Triemli	TRI	No	2'048	2'132	84	ewz (2014)	No	Albert & Willenberg (2014)	679.670	246.890	450.5	Bläsi et al. (2013)
Tegerfelden-1	TG1	No	130	> 200	109 (based on KLI)	Bläsi et al. (2014a)	No	Albert & Willenberg (2014)	663.906	268.059	367	Bläsi et al. (2014a)
Tegerfelden-2	TG2	No	148	> 250	109 (based on KLI)	Bläsi et al. (2014a)	No	Albert & Willenberg (2014)	664.015	267.750	367	Bläsi et al. (2014a)
Weiach-1	WEI	Yes	554.5	666	111.5	Matter et al. (1988a)	Yes	Albert & Willenberg (2014)	676.744	268.618	369	Bläsi et al. (2013)
Wölflinswil-1	WO1	No	152	> 260	124 (based on WO2)	Bläsi et al. (2014a)	No	Albert & Willenberg (2014)	642.170	257.066	442	Bläsi et al. (2014a)
Wölflinswil-2	WO2	No	157	281	124	Bläsi et al. (2014a)	No	Albert & Willenberg (2014)	642.124	256.826	438	Bläsi et al. (2014a)

2.2 Methodology

2.2.1 General

The work was mainly based on data obtained from boreholes Mont Terri BDB-1, Lausen, Schafisheim, Riniken-1, Weiach-1, Benken and Schlattingen-1. For these locations, drillcores and drillcore photographs are available, together with detailed lithostratigraphic descriptions and geological logs, as well as geophysical logs. These boreholes cover the entire area of investigation from the Jura fold-and-thrust belt in northwestern Switzerland to the eastern Molasse Basin. Data from numerous percussion-drilled boreholes for which only cuttings and geophysical logs are available were used as additional sources of information in a second step.

The following workflow was adopted:

- Compile information from existing descriptions of the cored boreholes pertinent to lithostratigraphy.
- Examine core photographs and identify features that may be used for a lithological subdivision.
- Compile a data base of discrete small-scale heterogeneities (calcareous beds/nodules, silty beds, septaria, etc.) on the basis of existing core descriptions, lithostratigraphic profiles and core photographs.
- For the cored boreholes, compile geophysical logs re-calculated to clay-mineral contents.
- Define and describe sub-units within the Opalinus Clay.
- Attempt to correlate sub-units between cored boreholes, using lithostratigraphic and geophysical characteristics.
- Compile lithostratigraphic information from existing descriptions of cuttings derived from percussion boreholes.
- For the percussion boreholes, compile geophysical logs re-calculated to clay-mineral contents. Note that no borehole-specific calibrations by mineralogical laboratory data are available, so absolute comparisons among boreholes are difficult, whereas the relative trends nevertheless yield useful information.
- Identify discrete marker horizons in geophysical logs of all boreholes.
- Use lithostratigraphic and geophysical information from percussion boreholes in combination with identified marker horizons to refine the definition of sub-units and their lateral correlation within the Opalinus Clay.

2.2.2 Lithostratigraphic information

In the frame of the various core-drilling campaigns, lithological descriptions were provided by the responsible stratigraphers on the basis of visual core logging. The results were documented in the stratigraphy sections and lithostratigraphic profiles of the respective borehole reports. Given the fact that the drilling campaigns were realised over a time period of several decades, the information is partially heterogeneous, with different degrees of detail. In order to maintain internal consistency, core photographs (available for all cored boreholes listed in Tab. 2-1 except for Beznau-1984) were revisited. Macroscopic features were logged, including general colour, presence of calcareous beds/nodules, zones with silty lenses and/or with siderite lenses/concretions. These data provided an internally consistent and somewhat adapted subdivision. However, the information on macroscopic rock texture is not directly comparable to that obtained from mineralogical analyses of specific samples, given the fact that the same minerals occurring in the identified heterogeneities (i.e. quartz, calcite and siderite) may also occur as disseminated phases in the clay-rich rock matrix, whose composition cannot be constrained by macroscopic inspection alone.

Lithological and stratigraphic descriptions with variable degrees of detail are also available for percussion-drilled holes. In some cases, lithostratigraphic information can be obtained from these, such as the identification of zones for which a higher silt content was reported.

2.2.3 Information from geophysical borehole logs

In a next step, geophysical borehole logs (most often sonic velocity, total gamma ray and resistivity) were considered. These were re-calculated to equivalent clay-mineral contents by Albert & Willenberg (2014) on the basis of borehole-specific empirical correlations. In cases where mineralogical laboratory measurements were available, these correlations were calibrated and hence the resulting clay-mineral contents can be considered as well constrained. In the absence of laboratory data, correlation functions from other boreholes were used for re-calculation. In these cases, the clay-mineral logs can be used in relative terms (for instance for the identification of specific marker horizons or relative trends in the log patterns), while the absolute values are more uncertain. Tab. 2-1 documents for which boreholes a calibration was performed.

The quality of the logs depends on borehole quality and the workflow used for logging, which both vary within and among boreholes. Criteria used for the identification included caliper logs and the heterogeneity of clay-mineral contents obtained from individual geophysical logs (sonic, resistivity, gamma-ray), expressed by the standard deviation. As an example, Fig. 2-2 shows that both criteria indicate a limited log quality in the lowermost 24 m of the Opalinus Clay at Benken. Limited log quality was also identified for the lower part of the Opalinus Clay at Schafisheim, as well as for the entire Opalinus Clay in Schlattingen-1. Log quality in all other boreholes is good to the degree this can be judged.

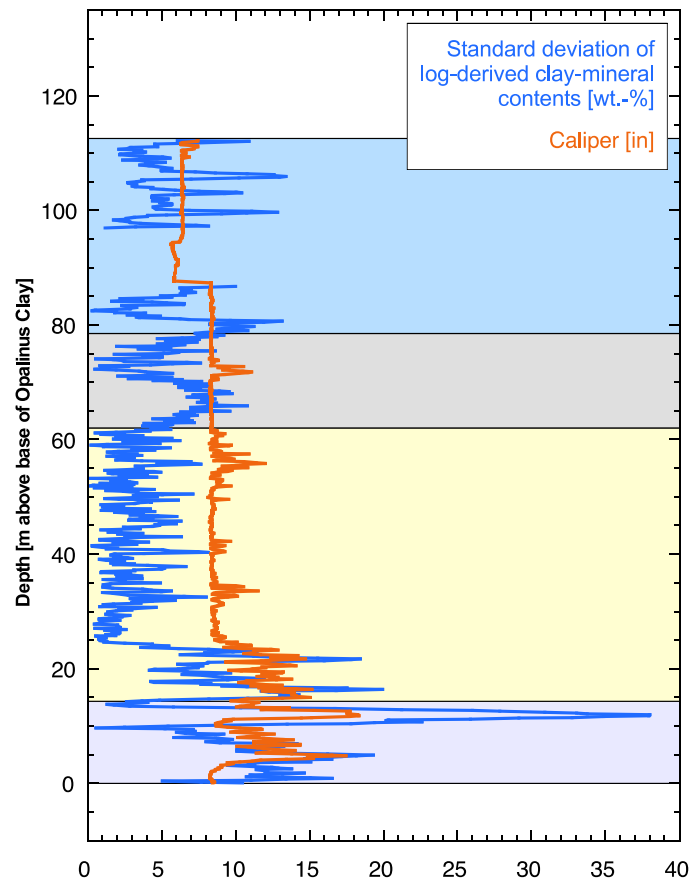


Fig. 2-2: Caliper of the Benken borehole (orange) and standard deviation of clay-mineral contents calculated from sonic, resistivity and gamma-ray logs (blue)

Background colours indicate lithological sub-units, see legend to Fig. 2-8.

2.2.4 Discrete heterogeneities

For boreholes with core material, a data base of discrete lithological heterogeneities, typically comprising calcareous beds with thicknesses of one to a few dm, septaria or zones with silty lenses, was prepared on the basis of detailed stratigraphic logs, stratigraphic core descriptions and by inspection of core photographs. The latter provided information on specific heterogeneities that in several cases were not mentioned in the original core descriptions. In general, the heterogeneities correlate with discrete excursions towards low clay-mineral contents in geophysical logs.

2.2.5 Marker horizons in geophysical logs

A number of negative or, more rarely, positive excursions of clay-mineral contents can be identified in the geophysical logs. In sections with limited quality of geophysical logs (e.g. whole section of Schlattingen-1), several spikes cannot be correlated with geological evidence and are considered to be artefacts due to borehole caliper variations or other methodological issues.

Negative excursions mostly correlate with calcareous beds or silty zones, whereas positive excursions may be correlated with dark, homogeneous, clay-rich sections. Given the small size of discrete heterogeneities within the Opalinus Clay, such as calcareous beds and nodules, the original, unsmoothed logs were used, while the common practice to work with smoothed logs generated by averaging over certain interval lengths may obliterate them.

2.2.6 Mineralogical data from laboratory measurements used for log calibration

About 10 – 30 mineralogical analyses are available for the Opalinus Clay in most of the cored boreholes, and these data were used to calibrate the geophysical logs in terms of clay-mineral content. The laboratory analyses refer to small rock volumes (typically a few hundreds of g). Because only 2 – 5 analyses are available per sub-unit and borehole, the laboratory data alone are not a sufficient basis for a subdivision of the Opalinus Clay, in particular in the more heterogeneous sub-units.

2.3 Results and discussion

On the terminology of clastic sedimentary rocks

There is no single universally accepted scheme of nomenclature for clastic sedimentary rocks, and classifications relating to particle size and/or mineralogical composition exist. Frequently used schemes, such as those of Potter et al. (1980) and Stow (1981), define indurated rocks with 33 – 65 % of particles with a radius $< 2 \mu\text{m}$ as "mudstone" and those with $\geq 66 \%$ particles $< 2 \mu\text{m}$ as "claystone". According to this definition, the Opalinus Clay is essentially a mudstone, with a smaller part corresponding to a claystone.

An alternative nomenclature has been developed by Füchtbauer (1988), originally in German. It has been adapted and translated into English by Naef et al. (2019). In particular, the grain sizes were correlated with minerals ("Sand" was replaced by "quartz + feldspars", and "Ton = clay" was replaced by "clay minerals"). The advantage of a mineralogical classification is its direct applicability in conjunction with instrumental determinations of the mineralogical composition by point counting or X-ray diffraction. For the Meso- and Cenozoic sedimentary sequence of Northern Switzerland, the correlation of grain size and mineralogy works well in practice, but this may not be the case for other areas, e.g. when substantial amounts of quartz occur in the clay grain-size fraction.

As shown in Fig. 2-3, the field typical for the Opalinus Clay in Northern Switzerland spreads over 5 groups of lithological terms in Füchtbauer's adapted triangle. On the other hand, the term "mudstone" does not appear in this scheme, and it is also not currently used in the frame of Nagra's investigations. However, it is used in this report as a translation for the field name "Tonstein", which is frequently used in existing lithostratigraphic profiles. Finally, note that the lithological and mineralogical characterisation refers to typical sample sizes of $1 - 2 \text{ dm}^3$.

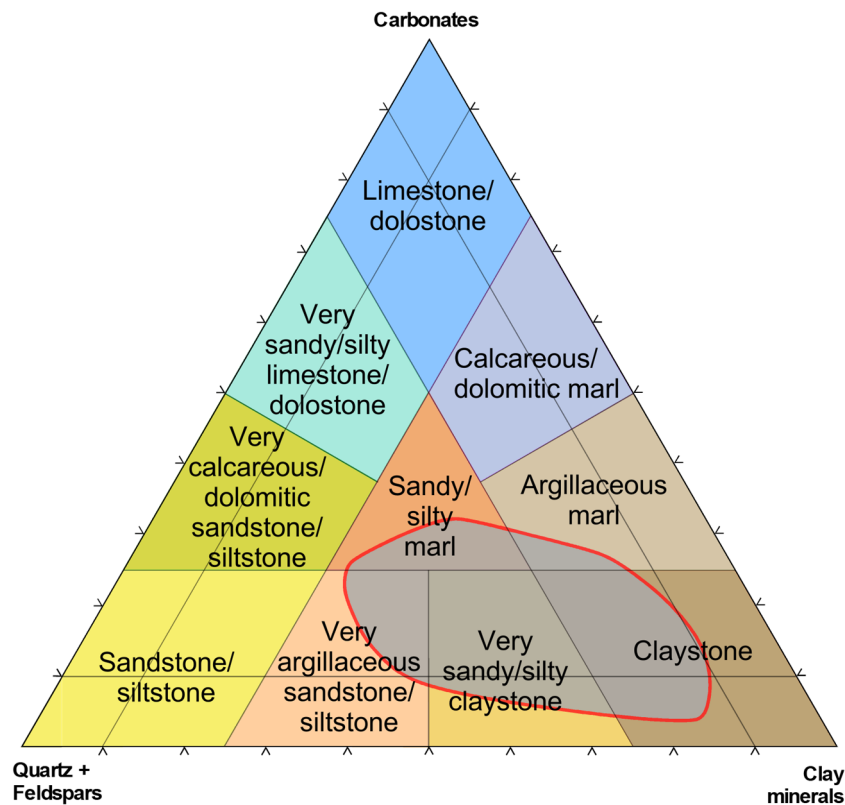


Fig. 2-3: Nomenclature of clastic sedimentary rocks based on Füchtbauer (1988)

Adapted by Naef et al. (2019). Grey field indicates the range of mineralogical compositions of the Opalinus Clay, excluding some outliers and the carbonate-rich silty and lower silty sub-units at Mont Terri because these do not occur in Northern Switzerland.

2.3.1 Lithological sub-units in the Opalinus Clay

The left side of Tab. 2-2 shows the subdivision of the Opalinus Clay in cored boreholes according to the original reports (references are given in Tab. 2-1). Based core photographs, the original data were placed in a uniform classification scheme, which allows the distinction of 6 lithostratigraphic sub-units:

- mudstone¹, clay-rich, homogeneous², dark (Fig. 2-4a)
- mudstone with some sandy lenses ± with nodular calcareous beds (Fig. 2-4b,c)
- mudstone with frequent sandy lenses (Fig. 2-4d)
- mudstone with siderite lenses/concretions (Fig. 2-4e)
- mudstone with sandy lenses and siderite lenses/concretions (Fig. 2-4f)
- carbonate-rich sandy facies (Fig. 2-4g)

¹ "Mudstone" stands for the German term "Tonstein" used in the original reports.

² The term "homogeneous" implies a limited degree of variability of relevant scalar rock characteristics, such as mineralogy or water content, when compared to other sub-units. However, it carries no implications pertinent to the degree of anisotropy of the fabric and of mechanical and solute-transport parameters.

These sub-units are highlighted by colour codes in the central part of Tab. 2-2. Thus, the main criteria to distinguish the sub-units are the presence of silty lenses (a depositional feature) and the presence of siderite lenses/concretions (an early diagenetic feature).

In a second step, the literature-based subdivision was further elaborated according to the following criteria (summarised in Tab. 2-3):

- The presence of siderite concretions was considered as a secondary criterion, given the fact that its presence refers to a post-depositional diagenetic process. It also turned out not to be a suitable criterion for lateral correlations except possibly in the Northeastern part of the investigation area. Note that siderite occurs at all investigated sites and in all sub-units (see Tab. 2-6 and 2-7 below), either as concretions and/or disseminated in the rock matrix (see Section 3.3.3).
- Discrete heterogeneities, in particular silty calcareous beds and nodules, are present in the uppermost part of the Opalinus Clay in several boreholes. The identified discrete heterogeneities (Tab. 2-4) are also well expressed as excursions in geophysical logs. The presence of the heterogeneities is the criterion to define the "*Subunit with silty calcareous beds*". An example is illustrated in Fig. 2-5b.
- Frequent lenses, typically a few centimetres wide and several millimeters thick, consist of silt (mainly quartz) and calcite cement and result in a flaser structure (example in Fig. 2-5c). The content of quartz ($\pm$ feldspars) in the bulk rock is markedly higher. This sub-unit reflects an enhanced water energy during deposition and is termed "*Silty*".
- Mostly at the base of the Opalinus Clay, a dark, homogeneous, clay-rich sub-unit can be distinguished and is termed "*Clay-rich*" (Fig. 2-5a).
- Exclusively at Mont Terri, a 4-m thick zone with particularly high carbonate and quartz contents was identified below the centre of the formation, and it has a strong expression in geophysical logs. This sub-unit is termed "*Carbonate-rich silty*" (Fig. 2-5e). It has no analogues in any of the boreholes further to the east.
- All remaining sections of the Opalinus Clay that are devoid of marked characteristics allowing the distinction of the sub-units outlined above are allocated to the "*Mixed clay-silt-carbonate sub-unit*" (Fig. 2-5d).
- The majority (but not all) of the original literature uses the term "sandy" to characterise lithologies with a higher content of quartz and feldspars. However, in most cases the grain size remains $< 63 \mu\text{m}$ and so refers to silt and not sand. Bearing in mind that exceptions exist, the term "silty" is used for the new subdivision because of the quantitative dominance of silt-size quartz. A further elaboration of this topic is beyond the scope of this report.

The resulting scheme of sub-units is shown in the right part Tab. 2-2. In most cases, the depth ranges but not the names of the new sub-units correspond exactly to those in the literature³. The few occurring deviations are commented in Tab. 2-2.

³ Note that while the term "Carbonate-rich silty sub-unit" is more accurate, it was decided by the Mont Terri Project team to maintain the term "Carbonate-rich sandy facies" for the corresponding sub-unit at Mont Terri, in order to maintain consistency with the existing literature in the frame of the Mont Terri Project.

The subdivision based on core data is consistent with the information obtained from geophysical logs (Fig. 2-8 below). However, the latter alone are an insufficient basis for a fully independent subdivision of the Opalinus Clay, given the fact that most logs yield clay-mineral contents but do not provide information on the ratio of quartz to carbonates, and they are also insensitive to rock texture. The limitations in the potential of geophysical logs as tools to subdivide the Opalinus Clay are in contrast with the experience for the Effingen Member, where geophysical logs provided an excellent basis for the subdivision (Deplazes et al. 2013). The Effingen Member essentially consists of a binary mixture of carbonate and clay minerals, which are well represented by geophysical logs, whereas textural aspects are less relevant. In addition, the lithological variability of the Opalinus Clay is low in comparison with the Effingen Member.

Tab. 2-2: Subdivision of the Opalinus Clay in cored boreholes of Northern Switzerland based on literature (left) and updated subdivision (right)

Colour codes to original subdivision:

Mudstone with some sandy lenses ± with nodular calcareous beds
Mudstone with frequent sandy lenses
Mudstone with siderite lenses/concretions
Mudstone with sandy lenses and siderite lenses/concretions
Carbonate-rich sandy facies
Mudstone, clay-rich, dark

Colour codes to updated subdivision:

Sub-unit with silty calcareous beds
Silty sub-unit
Mixed clay-silt-carbonate sub-unit
Carbonate-rich silty sub-unit
Clay-rich sub-unit

Borehole	Top [m b.g.]	Base [m b.g.]	Top [m above base of Opalinus Clay]	Base [m above base of Opalinus Clay]	Sub-unit description based on original reports		Updated sub-unit description	
Mont Terri BDB-1	106.25	137.73	130.55	99.07	1	Sandy facies 2	Silty	
	137.73	173.70	99.07	63.10	2	Shaly facies 2	Mixed clay-silt-carbonate	Clay-mineral contents based on geophysical logging/lab data (mean = 52/56 wt.-%) are lower than in the Shaly facies 1 (57 / 61 wt.-%)
	173.70	186.35	63.10	50.45	3	Sandy facies 1	Silty	
	186.35	190.40	50.45	46.40	4	Carbonate-rich sandy facies	Carbonate-rich silty	
	190.40	236.80	46.40	0.00	5	Shaly facies 1	Clay-rich	
Lausen	6.22	18.00	65.12	53.34	1	Mudstone, gray, silty	Mixed clay-silt-carbonate	
	18.00	31.00	53.34	40.34	2	Mudstone, silty, calcareous, with some siderite lenses		
	31.00	62.00	40.34	9.34	3	Mudstone, silty, calcareous, with silty laminae	Silty	
	62.00	65.02	9.34	6.32	4	Mudstone, silty, calcareous	Clay-rich	
	65.02	71.34	6.32	0.00	5	Mudstone, silty, calcareous, with shell fragments		
Schafisheim	1'000.65	1004.50	79.30	75.45	1	Mudstone with sandy marls	Silty	Abundant silty lenses
	1'004.50	1006.60	75.45	73.35			Mixed clay-silt-carbonate	Few silty lenses
	1'006.60	1023.90	73.35	56.05	2	Mudstone with sandstone and yellowish carbonate lenses		

Tab. 2-2: Cont.

Borehole	Top [m b.g.]	Base [m b.g.]	Top [m above base of Opalinus Clay]	Base [m above base of Opalinus Clay]	Sub-unit description based on original reports		Updated sub-unit description	
Schafisheim	1'023.90	1046.14	56.05	33.81	3	Mudstone with yellowish carbonate lenses		
	1'046.14	1079.95	33.81	0.00	4	Sand-poor, fossil-rich mudstone	Clay-rich	
Riniken-1	331.14	340.05	119.79	110.88	1	Mudstone with sandy marls	With silty calcareous beds	With limited silty, flaser- like lenses
	340.05	360.26	110.88	90.67	2	Mudstone with nodular calcareous beds and little sand		
	360.26	384.08	90.67	66.85	3	Mudstone with numerous sandstone lenses	Silty	
	384.08	396.48	66.85	54.45	4	Well-bedded, weakly bioturbated, dark mudstone	Mixed clay- silt-carbonate	
	396.48	423.60	54.45	27.33	5	Sand-poor mudstone with yellowish carbonate lenses		
	423.60	450.93	27.33	0.00	6	Sand-poor, fossil-rich mudstone	Clay-rich	
Weiach-1	554.50	563.40	111.17	102.27	1	Mudstone with sandy marls	With silty calcareous beds	Few silty, flaser-like lenses
	563.40	584.25	102.27	81.42	2	Mudstone with nodular calcareous beds and little sand		
	584.25	600.93	81.42	64.74	3	Mudstone with numerous sandstone lenses	Silty	
	600.93	650.02	64.74	15.65	4	Sand-poor mudstone with yellowish carbonate lenses	Mixed clay- silt-carbonate	
	650.02	665.67	15.65	0.00	5	Sand-poor, fossil-rich mudstone	Clay-rich	
Benken	539.70	558.52	112.34	93.52	0 ¹	Mudstone with sandstone lenses and siderite concretions	With silty calcareous beds	
	558.52	571.03	93.52	81.01	1	Mudstone with sandstone lenses and siderite concretions		
	571.03	574.00	81.01	78.04	2	Mudstone with numerous sandstone lenses		
	574.00	590.11	78.04	61.93			Silty	
	590.11	629.80	61.93	22.24	3	Mudstone with few sandstone lenses	Mixed clay- silt-carbonate	
	629.80	637.80	22.24	14.24	4	Mudstone with siderite concretions		
	637.80	652.04	14.24	0.00	5	Mudstone	Clay-rich	
Schlattingen-1	831.40	866.55	118.30	83.15	1	Mudstone with sandstone lenses and siderite concretions	With silty calcareous beds	
	866.55	872.70	83.15	77.00	2	Mudstone with numerous sandstone lenses	Silty	Abundant silty lenses
	872.70	879.70	77.00	70.00			Mixed clay- silt-carbonate	Few silty lenses
	879.70	905.50	70.00	44.20	3	Mudstone with few sandstone lenses		
	905.50	933.80	44.20	15.90	4	Mudstone with siderite concretions		Lighter colour
	933.80	949.70 ³	15.90	0.00			Clay-rich	Darker colour

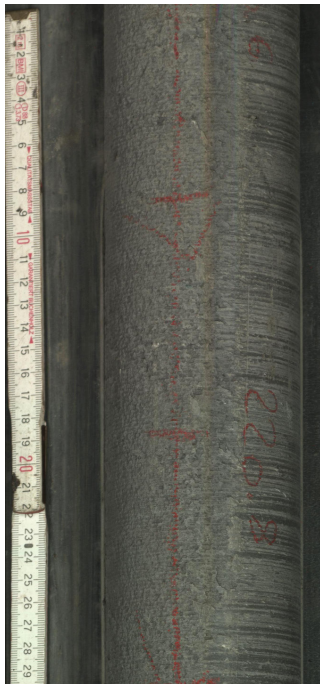
¹ Sub-unit 0 in Benken refers to the section that was originally termed "Murchisonae-Schichten" by Nagra (2001)

² The base of the sub-unit with silty calcareous beds at Benken was originally defined at 571.03 m. However, a substantial part of the core material between 571.03 and 574.30 m was sampled early on site and so was not available for lithostratigraphic studies. On the other hand, abundances of clay minerals, carbonates and quartz were derived from the ECS log by Albert (2001) and Nagra (2001), showing 2 major carbonate peaks in the depth interval 571.5 – 573.5 m, while quartz contents do not show any excursions. Due to these pronounced peaks and the absence of increased quartz content, the boundary was shifted to a depth of 574 m

³ The exact depth of the base of the Opalinus Clay at Schlattingen-1 is subject to ongoing discussions among experts in lithostratigraphy

Tab. 2-3: Criteria for the updated definition of sub-units and correlation with the subdivision in the original literature

Sub-units defined in the original literature	Criteria for updated definition	Updated sub-units
Mudstone with nodular calcareous beds, mudstone with sandstone lenses (or similar)	Presence of silty calcareous beds, therefore heterogeneous on a metre scale; widely variable clay-mineral contents in geophysical logs	Sub-unit with silty calcareous beds
Mudstone with silty laminae, mudstone with sandstone lenses (or similar); sandy facies (Mont Terri)	Flaser structure with quartz-rich lenses, heterogeneous rock on a scale of millimetres to centimetres	Silty sub-unit
Mudstone (with various attributes)	Dark rock, homogeneous, often high clay-mineral contents in geophysical logs	Clay-rich sub-unit
Carbonate-rich sandy	Anomalously calcite- and quartz-rich, major negative excursion of clay-mineral content in geophysical logs	Carbonate-rich silty sub-unit
Various	Absence of criteria used to define the sub-units above	Mixed clay-silt-carbonate sub-unit



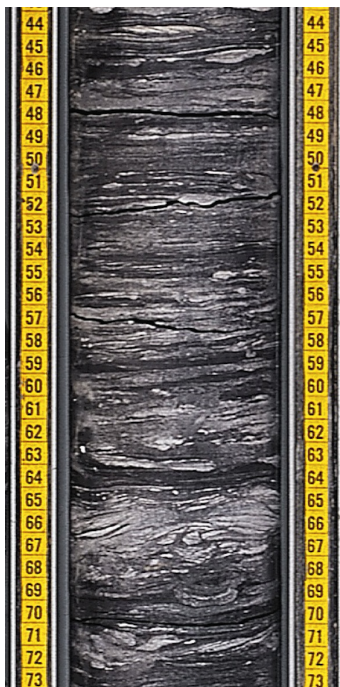
a. Mudstone, clay-rich, homogeneous, dark (MT BDB-1 220.74)



b. Mudstone with some sandy lenses (BEN 620.14)



c. Mudstone with nodular calcareous bed (RIN 360.00)



d. Mudstone with frequent sandy lenses (BEN 582.83)

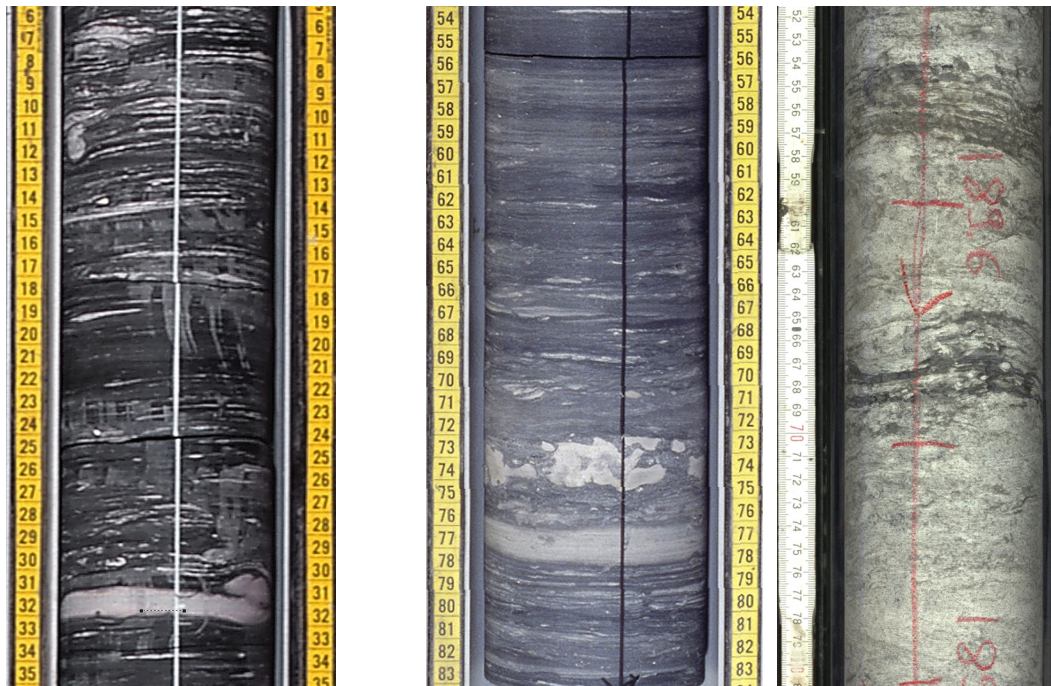


e. Mudstone with siderite lenses/concretions (left: BEN 630.67; right: WEI 622.45)



Fig. 2-4: Illustrations of sub-units within the Opalinus Clay according to the subdivision and nomenclature in the original reports

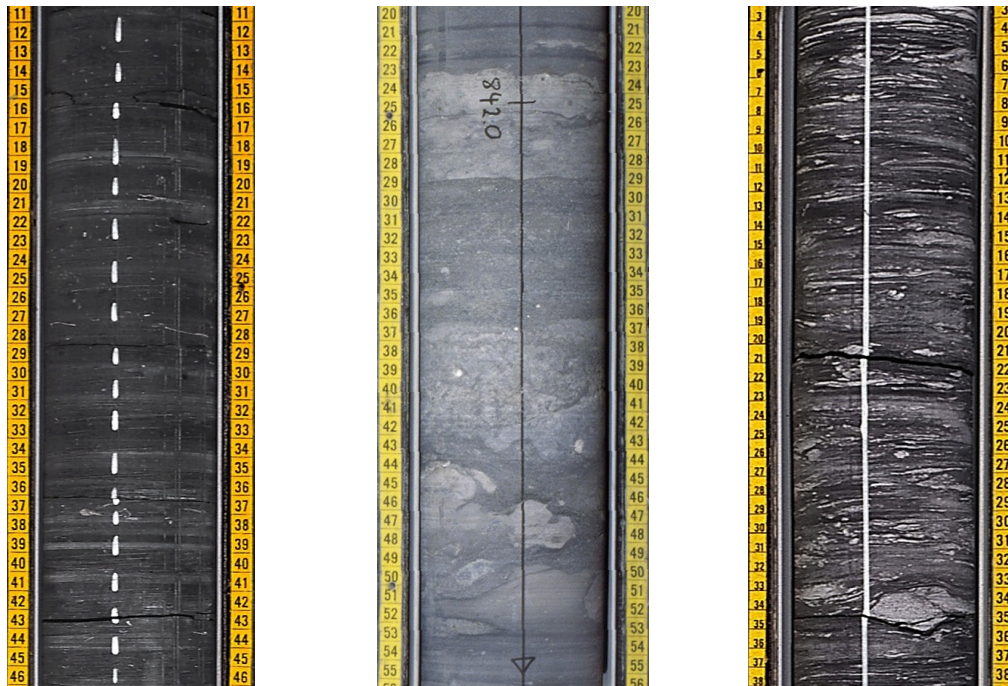
The indicated depths refer to the centre of the pictures.



f. Mudstone with silty lenses and siderite lenses/concretions
(left: BEN 568.30; right: SLA 855.27)

g. Carbonate-rich sandy facies
(MT BDB-1 189.70)

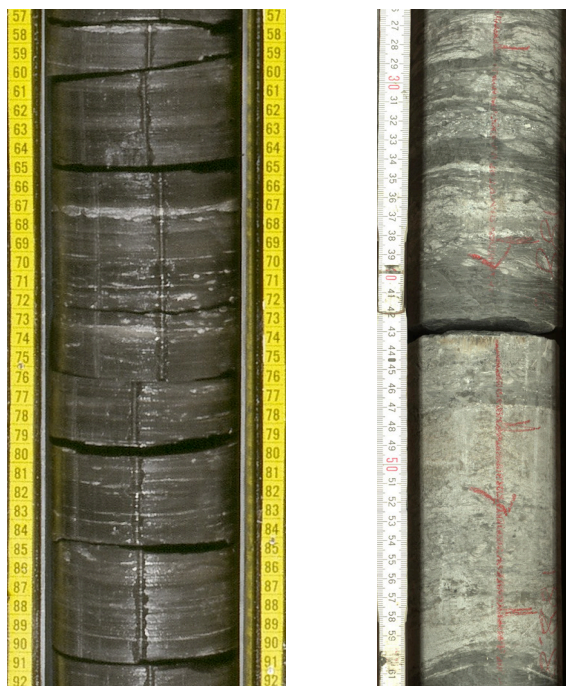
Fig. 2-4: Cont.



a. Clay-rich sub-unit
(BEN 643.22)

b. Sub-unit with silty calcareous beds
(SLA 842.13)

c. Silty sub-unit
(BEN 586.71)



d. Mixed clay-silt-carbonate sub-unit
(RIN 399.36)

e. Carbonate-rich silty sub-unit
(MT BDB-1 188.68)

Fig. 2-5: Illustrations of sub-units within the Opalinus Clay according to the new subdivision

The indicated depths refer to the centre of the pictures.

2.3.2 Discrete heterogeneities

The most conspicuous heterogeneities, in particular calcareous beds or nodule-rich strata with typical thicknesses of 10 – 60 cm, were compiled from the original reports and geological logs. Another type of heterogeneity with thicknesses of up to several metres is related to silty beds with a typical flaser texture. Apart from the heterogeneities and their characteristics documented in the literature, a number of additional features were identified on core photographs. No strict threshold value was applied for the minimum thickness of the heterogeneities. All features > 10 cm thick were mapped, augmented by some thinner features with a marked lithological contrast to the embedding rock, while other features thinner than 10 cm exhibiting less strongly expressed lithological differences were not considered. All discrete heterogeneities identified in the Opalinus Clay of cored boreholes are listed in Tab. 2-4, together with short descriptions and a simplified classification. It is evident that calcareous beds or nodule-rich strata are more abundant in the eastern part of the investigation area (Schlattingen-1 to Riniken-1), whereas they are less common further to the west.

Considering the available literature information, the observed heterogeneities can be grouped into 3 types of carbonate-rich and 1 type of silt-rich features:

1. Wetzel & Allia (2000) identified *calcareous hiatus beds* (their type 1) at various stratigraphic levels in the Opalinus Clay of Northern Switzerland. These beds formed in response to an interruption of sediment input and, therefore, over an extended exposure time of the near-surface sediments to early diagenetic processes, in particular those related to the growth of carbonate nodules and septaria in the sulphate reduction zone. In general, these horizons cannot be correlated among different sites and therefore supposedly represent local features with lateral extents in the range of kilometres. The local occurrence is taken as an argument to conclude that these hiatus beds are related to the synsedimentary tectonic evolution in a structured basin rather than to a sea-level change that would lead to hiatus beds of regional extent.
2. *Beds enriched in bioclasts and nodules* (hiatus beds type 2, 3, 4 of Wetzel & Allia 2000) formed on topographic swells during phases of enhanced hydraulic energy and resulted in the development of a sedimentary hiatus accentuated by carbonates while the fine fraction was washed out. Such processes are suggested to be typical of local temporary elevations. The aerial extent and the timing of development and disappearance of such local swells are not known. In many instances, a tendency of decreasing clay-mineral content is observed below the excursion in geophysical logs when approaching the peak value of the heterogeneity, in particular in the sonic log. Consequently, the enrichment in carbonate marks the final phase during which progressively less clay minerals were deposited. In some instances, already formed concretions were exhumed (indicated by borings and encrustations) and incorporated into such carbonate beds⁴. A detailed look into the shape of the peaks in geophysical logs indicates that some but not all excursions in the borehole profiles considered here are asymmetric, with a less steep gradient below the peak value, suggesting the presence of this type of heterogeneity (example in Fig. 2-6).
3. The erosion of crinoid populations on topographic swells during storm events may lead to transport of biodebris and the deposition of *beds enriched in bioclasts at deeper levels with a lower hydraulic energy*. In northwestern Switzerland, such tempestites rich in echinoderm debris are known from the Staffelegg Fm., the Klingnau Fm. and the Wildeggen Fm. but not from the Opalinus Clay in the investigation area. However, such beds were

⁴ According to Wetzel (pers. comm., February 2019), such beds and nodules were observed in outcrops and clay pits in the Opalinus Clay from the southern Upper Rhine Graben (Germany) and in the clay pits at Frick and Böttstein.

described by Sieverts-Doreck (1964, 1983) from the Opalinus Clay in southwestern Germany. Consequently, their presence in the investigation area may be expected. In contrast to heterogeneities of type 2, this type is not related to a lower clay-mineral content below the calcareous bed, and so symmetric excursions in geophysical logs are likely.

4. *Silty beds or zones with a lamellar flaser texture* (illustrated in Fig. 2-4d and 2-5c), sometimes with ripples, reflect storm events and deposition close to or above the storm-wave base at 20 – 30 m water depth (Allia 1996, Wetzel & Allia 2000, 2003). In geophysical logs, they are identified as relatively broad peaks or regions of lower clay-mineral content. With the exception of the lower silty sub-unit at Mont Terri, clay-mineral contents nevertheless remain higher than 40 % (see Fig. 2-8 below). While the majority of the silty heterogeneities are 2 m thick at most, some of them are substantially thicker and define broad silty zones.

According to the available information from the core profiles in the investigation area, calcareous and silty heterogeneities can be easily distinguished. On the other hand, the information pertinent to the various genetic types of the calcareous heterogeneities is limited and would require targeted studies that are not available at this stage. However, when it comes to the characterisation of the Opalinus Clay from the perspective of its barrier function to solute transport, the genetic information is not considered to be critical, given the fact that there is no evidence that these features could represent preferential pathways for fluid flow.

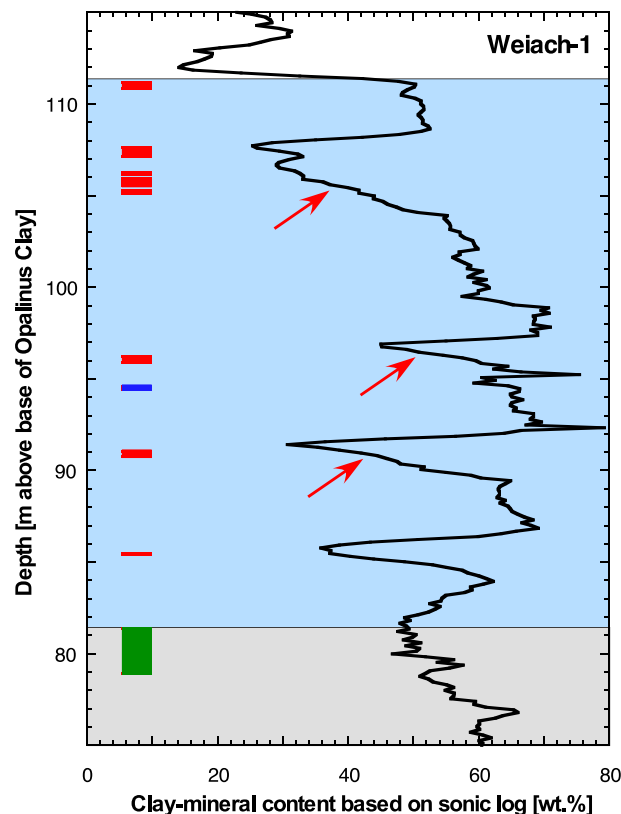


Fig. 2-6: Clay-mineral content obtained from the sonic log in the sub-unit with silty calcareous beds (blue background) at Weiach-1

Red arrows indicate asymmetric peaks related to calcareous heterogeneities. Location of heterogeneities according to core logging shown to the left (red = calcareous bed/nodule, blue = septaria, green = silty bed).

Independently of the geological information, heterogeneities were also constrained by negative excursions in geophysical logs. Unsmoothed sonic, resistivity and gamma-ray logs (recalculated to clay-mineral contents) were studied individually, as well as the median clay-mineral content based on the combination of these logs. For Schlattingen-1, only the gamma-ray log was used because the quality of the other logs was not sufficient for interpretation. The results are shown on the right side of Tab. 2-4:

- Out of the 44 heterogeneities obtained from geological information, 38 were readily identified as negative excursions in the median of the clay-mineral logs. The interval WEI 559.39 – 560.52 m contains 4 adjacent heterogeneities, which could not be resolved individually in the geophysical logs due to limitations in the spatial resolution and so yielded one single peak. Further, two thin heterogeneities (0.15 – 0.17 m thick) were identified in one single log but not in the median log. It is concluded that geophysical logs identify most lithological heterogeneities and so can be used to map calcareous and silty beds in boreholes without core.
- However, in 12 cases the median clay-mineral logs yielded negative excursions that could not be correlated with a geological feature, i.e. the logs tend to over-predict heterogeneities. At Benken, some of these "false alarms" originate from zones with enhanced borehole caliper, while in other cases there are no evident issues with borehole quality.

The thickness distributions of the discrete calcareous heterogeneities and silty zones are illustrated in Fig. 2-7. With the exception of a 1 m thick bed in the carbonate-rich silty sub-unit at Mont Terri, all calcareous heterogeneities are < 0.7 m thick. Zones rich in silty laminae may be substantially thicker, with an exceptionally high value of 12.65 m for the silty sub-unit at Mont Terri, which represents an anomaly as a whole.

Tab. 2-4: Compilation of discrete heterogeneities within the Opalinus Clay in cored boreholes

Negative excursions in clay-mineral contents observed in specific geophysical logs and in the calculated median are shown on the right side. C-s = Carbonate-rich silty; n.d. = no data.

Borehole	Sub-unit	Top [m below surface]	Base [m below surface]	Mean depth [m above base of Opalinus Clay]	Thickness [m]	Geological data		Geophysical data			
						Description	Type	Peak Sonic	Peak Resistivity	Peak Gamma ray	Peak Median
Mont Terri BDB-1	Silty	110.45	110.60	126.28	0.15	Calcareous bed	Calcareous	n.d.		x	
		114.10	115.50	122.00	1.40	Rich in silty laminae	Silty	n.d.	x	x	x
	Silty	173.70	186.35	56.78	12.65	Rich in silty laminae	Silty	n.d.	x	x	x
	C-s	188.65	188.85	48.05	0.20	Silty/calcareous bed	Calcareous	n.d.	x	x	x
	C-s	189.45	190.45	46.85	1.00	Silty/calcareous bed	Calcareous	n.d.	x	x	x
LAU	Clay-rich	65.02	65.08	6.29	0.06	Calcareous bed (firmground)	Calcareous	x	x		x
Schafisheim	Silty	1000.65	1'000.75	79.25	0.05	Calcareous bed	Calcareous	x	x	x	x
		1002.63	1'002.71	77.28	0.08	2 calcareous beds	Calcareous	x	x	x	x
		1008.68	1'008.78	71.22	0.05	Calcareous bed	Calcareous	x	x		x
		1015.90	1'016.40	63.80	0.50	Rich in silty laminae	Silty	x	x		x

Tab. 2-4: Cont.

Borehole	Sub-unit	Top [m below surface]	Base [m below surface]	Mean depth [m above base of Opalinus Clay]	Thickness [m]	Geological data		Geophysical data			
						Description	Type	Peak Sonic	Peak Resistivity	Peak Gamma ray	Peak Median
Rimiken-1	Silty	331.14	331.42	119.65	0.28	Nodular calcareous bed	Calcareous	x	x	x	x
	With silty calcareous beds	345.38	345.61	105.44	0.23	Calcareous bed	Calcareous	x	x	x	x
		353.42	353.62	97.41	0.20	Nodular calcareous bed with siderite	Calcareous	x	x	x	x
		356.18	356.52	94.58	0.34	Calcareous bed	Calcareous	x	x	x	x
		359.64	360.26	90.98	0.62	3 calcareous beds	Calcareous	x	x	x	x
	Silty	369.43	371.18	80.63	1.75	Rich in silty laminae	Silty	x	x		x
		374.78	374.85	76.12	0.07	Calcareous bed	Calcareous	x	x		x
	Mixed clay-silt-carbonate	396.48	396.69	54.35	0.21	Lowermost calcareous bed, equivalent of WEI 618.02	Calcareous	x	x	x	x
Weiach-1	With silty calcareous beds	554.50	554.80	111.02	0.30	Calcareous bed	Calcareous	x	x	x	x
		558.23	558.73	107.38	0.50	3 marly to Calcareous beds	Calcareous	x	x	x	x
		559.39	559.53	106.21	0.14	Calcareous bed	Calcareous	x	x	x	x
		559.71	559.82	105.91	0.11	Calcareous bed	Calcareous				
		560.01	560.14	105.60	0.13	Calcareous bed	Calcareous				
		560.38	560.52	105.22	0.14	Calcareous bed	Calcareous				
		569.46	569.75	96.06	0.29	Calcareous nodules, phosphoritic	Calcareous	x	x	x	x
		571.40	571.57	94.51	0.17	Septaria	Septaria			x	
		574.60	574.91	90.92	0.31	2 calcareous beds with siderite	Calcareous	x	x	x	x
		580.20	580.26	85.44	0.06	Calcareous bed	Calcareous	x	x	x	x
	Silty	584.25	586.71	80.19	2.46	Rich in silty laminae	Silty	x	x		x
		596.10	597.80	68.72	1.70	Rich in silty laminae	Silty	x	x		x
	Mixed clay-silt-carbonate	617.96	618.08	47.65	0.12	Lowermost calcareous bed, equivalent of RIN 396.59	Calcareous	x	x	x	x
Benken	With silty calcareous beds	545.90	546.35	105.92	0.45	Slightly more calcareous zone	Calcareous	x	x	x	x
		549.18	549.26	102.82	0.08	Nodular calcareous bed (Comptum-Bank?)	Calcareous	x	x	x	x
		552.47	552.85	99.38	0.38	2 biotrititic calcareous beds	Calcareous	x	x	x	x
		558.52	558.98	93.29	0.46	Nodular calcareous bed	Calcareous	n.d.	n.d.		
		571.50	572.11	80.24	0.61	Calcareous zone ¹	Calcareous			x	x
		573.02	573.48	78.79	0.46	Calcareous zone ¹	Calcareous	x	x	x	x
	Silty	582.00	587.00	67.54	5.00	Rich in silty laminae	Silty	x	x		x
	Schlattingen-1	834.50	834.70	115.10	0.20	Calcareous bed	Calcareous	n.d.	n.d.	x	n.d.
		838.80	838.95	110.83	0.15	Septaria	Septaria	n.d.	n.d.	x	n.d.
		841.98	842.27	107.58	0.29	Calcareous bed	Calcareous	n.d.	n.d.	x	n.d.
		849.37	849.48	100.28	0.11	Calcareous/silty bed	Calcareous	n.d.	n.d.	x	n.d.
		852.73	852.95	96.86	0.22	Calcareous bed	Calcareous	n.d.	n.d.	x	n.d.
		858.25	858.32	91.42	0.07	Calcareous bed	Calcareous	n.d.	n.d.	x	n.d.

¹ No core photographs are available for the heterogeneities at 571.50 – 572.11 and 573.02 – 573.48 m in Benken. The evaluation of the ECS borehole log by Albert (2001) indicates that these heterogeneities are due to enhanced carbonate contents

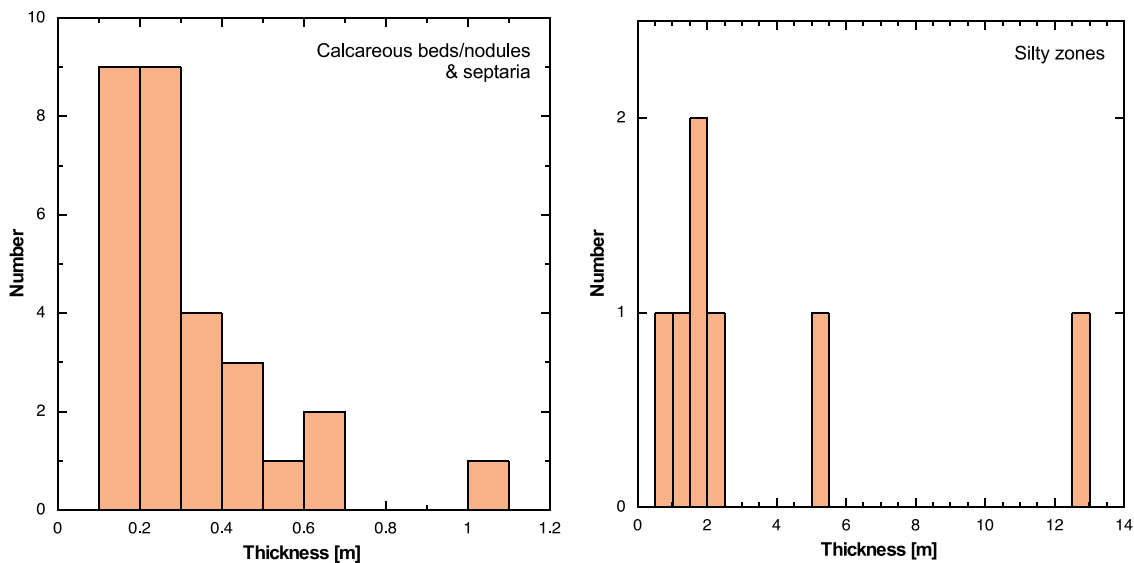


Fig. 2-7: Thickness distribution of heterogeneities within the Opalinus Clay

The left histogram is cut off at 0.1 m, as thinner features were not logged systematically.

2.3.3 Lateral correlations among cored boreholes

The full information on the cored boreholes, including lithological sub-units, discrete heterogeneities and geophysical clay-content logs is illustrated in Fig. 2-8. On the basis of this information, a lithological correlation among the seven cored boreholes was performed and is illustrated in Fig. 2-9. In Fig. 2-8, sections with limited quality of the geophysical logs are shown in grey. The logs refer to the median clay-mineral content obtained from the individual geophysical logs, except for Schlattigen-1 where only the gamma-ray log was used.

In detail, the following features can be identified (see also Fig. 2-8 and 2-9):

- The profiles of boreholes Weiach-1 and Riniken-1 are remarkably similar, in spite of the distance of 21 km. The lithostratigraphic sub-units are largely analogous, as are the clay-mineral logs. Even the location of thin calcareous beds or concretions shows analogies. Overall, the Opalinus Clay in the two boreholes is characterised by clay-mineral contents that decrease from base to top and by discrete heterogeneities that are absent in the lower part but become more frequent in the upper sub-units.
- Towards the east, the geophysical-logging-based clay-mineral profile at Benken shows conspicuous similarities to that of Weiach-1: A clay-rich basal sub-unit is seen at both locations. In the upper part of the profiles, the sub-unit with abundant silty calcareous beds and/or nodules overlies a silty sub-unit with a characteristic flaser structure. Clay-mineral contents at Benken are markedly lower than in Weiach-1, in particular in the lower half of the profile.
- The same general subdivision of the profile as in Benken can also be recognised in the Schlattigen-1 profile. As in the other boreholes, calcareous beds occur only in the uppermost sub-unit.

- At Schafisheim, towards the southwest of Riniken-1, the formation thickness drops from 120 to 80 m. On the basis of the macroscopic lithostratigraphic evaluation, a clay-rich sub-unit at the base can be identified. However, it is not clearly seen in the clay-mineral log, which is of limited quality in this sub-unit. A thin silty sub-unit occurs at the top, whereas the sub-unit with silty calcareous beds that is present in all boreholes to the northeast is missing. Apart from the clay-rich base, correlations towards the northeast are uncertain.
- At Lausen, a well-expressed clay-rich basal sub-unit is identified. It can probably be correlated with that seen in all other boreholes. The presence of a silty sub-unit that directly overlies the clay-rich base of the Opalinus Clay is a feature that is not seen in any other borehole further to the east.
- At Mont Terri, the basal clay-rich sub-unit is thicker than at Lausen. It is overlain by 4 m of the carbonate-rich silty sub-unit ("carbonate-rich sandy facies" of Bossart et al. 2017). This sub-unit is characterised by a substantial drop of the clay-mineral contents below 40 wt.-% and even to 10 wt.-% in individual beds.
- The carbonate-rich silty sub-unit is unique to Mont Terri and has no analogues further east. According to Ohmert & Rolf (1994) and in particular the detailed stratigraphic work of Contini (1970) in the French Jura, the Aalenian becomes thinner and more calcareous towards the west. The time of deposition of the Opalinus Clay covering the Aalensis and Opalinum zones at Mont Terri corresponds to the deposition of the Marnes d'Aresches (Toarcian) and the Calcaires sableux d'Aresches (Aalenian) in eastern France. Near Belfort, about 35 km northwest of Mont Terri, the whole Aalenian is 18 – 24 m thick and consists of sandy limestones with some intercalated marls. Contini (1970) explicitly mentioned the Calcaires sableux d'Aresches at Mont Terri and stated that this unit is the equivalent of what is called the Opalinus Clay in Switzerland. It is thus evident that the Mont Terri area is close to a major facies boundary in the late Toarcian and Aalenian, with the carbonate-rich silty sub-unit as the easternmost extension of the calcareous facies in France. Lauper et al. (2018) suggested local topographic highs slightly above the storm-wave base as the source of bioclastic material ("carbonate factory"), which was transported to adjacent depocentres during storm events.
- The carbonate-rich silty sub-unit at Mont Terri is overlain by the lower silty sub-unit, which can possibly be correlated with that identified at Lausen and the percussion borehole at Liestal (see below). However, at Mont Terri this sub-unit is poorer in clay minerals and richer in quartz and carbonates than its analogue at Lausen or any other occurrence of silty sub-units throughout the investigation area. The geophysical logs shown in Fig. 2-8 illustrate that the negative excursion of the clay-mineral content is much more substantial at Mont Terri in comparison to Lausen. Mineralogical data shown in Fig. 2-18 below also confirm the unique composition of this sub-unit at Mont Terri. Also note that the upper silty sub-unit at the top of the Opalinus Clay at Mont Terri is richer in clay minerals (Fig. 2-9) and lithologically comparable with other silty sub-units in the investigation area.

In summary, the following major conclusions can be drawn:

- A clay-rich basal sub-unit can be identified across the entire investigation area.
- The sub-unit with silty calcareous beds in the upper part of the profile is well correlatable between the profiles of Riniken-1, Weiach-1, Benken and Schlattingen-1 but is absent further to the west.
- A silty sub-unit underlying the sub-unit with silty calcareous beds can also be correlated between these boreholes. Its potential continuation to the west is not constrained.

- The lower silty sub-unit at Mont Terri probably has analogues in Lausen and Liestal but not in any of the boreholes further to the east. At Mont Terri, it is richer in quartz and carbonates in comparison to the other locations, indicative of a lateral facies change.
- Sub-units can be well correlated among the eastern boreholes (Riniken-1 – Weiach-1 – Benken – Schlattingen-1) on the one hand and among Mont Terri and Lausen on the other hand. The Schafisheim profile, with a thickness of the Opalinus Clay of only 80 m, marks a boundary across which the correlation of lithologic sub-units becomes difficult or impossible. West of Mont Terri, the Opalinus Clay evolves towards more calcareous lithologies.

2.3.4 Lithostratigraphic information obtained from percussion-drilled boreholes

Even in the absence of core material, some lithostratigraphic information can be obtained by the study of cuttings. Based on the original reports (references are given in Tab. 2-1), specific sub-units can be identified in some cases, in particular the sub-unit with silty calcareous beds or the silty sub-units. Clearly, the definition of sub-units without core is less certain and over-interpretation needs to be avoided.

In Fig. 2-11 and 2-12, the profiles of the percussion-drilled boreholes are shown together with those of the cored boreholes along a northern and a southern profile line (as shown in Fig. 2-10). The additional lithostratigraphic information provided by the percussion holes includes:

- The sub-unit with silty calcareous beds can be identified in boreholes Hemmental-2, Tegerfelden-2, Lindau-1, Bözberg SB 2/13 and Wölflinswil-2. Consequently, it extends far to the north (Hemmental-2) and south (Lindau-1) in the eastern part of the investigation area. It is also identified west of Riniken-1 (Bözberg SB 2/13, Wölflinswil-2), even though in reduced thickness.
- A silty sub-unit underlies the sub-unit with silty calcareous beds in borehole Lindau-1, which is analogous to all cored boreholes east of Schafisheim.
- The profile of the borehole at Liestal is consistent with the findings of the nearby cored borehole at Lausen. It confirms the presence of a second silty sub-unit at the top of the Opalinus Clay, as identified at Mont Terri.

Some additional information can be obtained from the deep geothermal borehole Basel-1 (Ladner et al. 2008), which is in an intermediate position between Lausen and Mont Terri. The gamma-ray log of the section containing the Opalinus Clay is shown in Fig. 2-13 (unpublished data from Geopower Basel AG, not converted into clay-mineral contents). It is remarkable that 5 major negative excursions are identified in the uppermost 22 m, while only smaller excursions can be seen at deeper levels. Such excursions are typical of the sub-unit with silty calcareous beds. Interestingly, slightly lower gamma-ray values are obtained at the base of the Opalinus Clay, suggesting somewhat lower clay-mineral contents. Note that this feature is not observed in the nearby borehole Otterbach-2 (Häring 2001, 2002). Based on the study of cuttings, Häring (2001) reports decreasing carbonate contents with depth in this borehole.

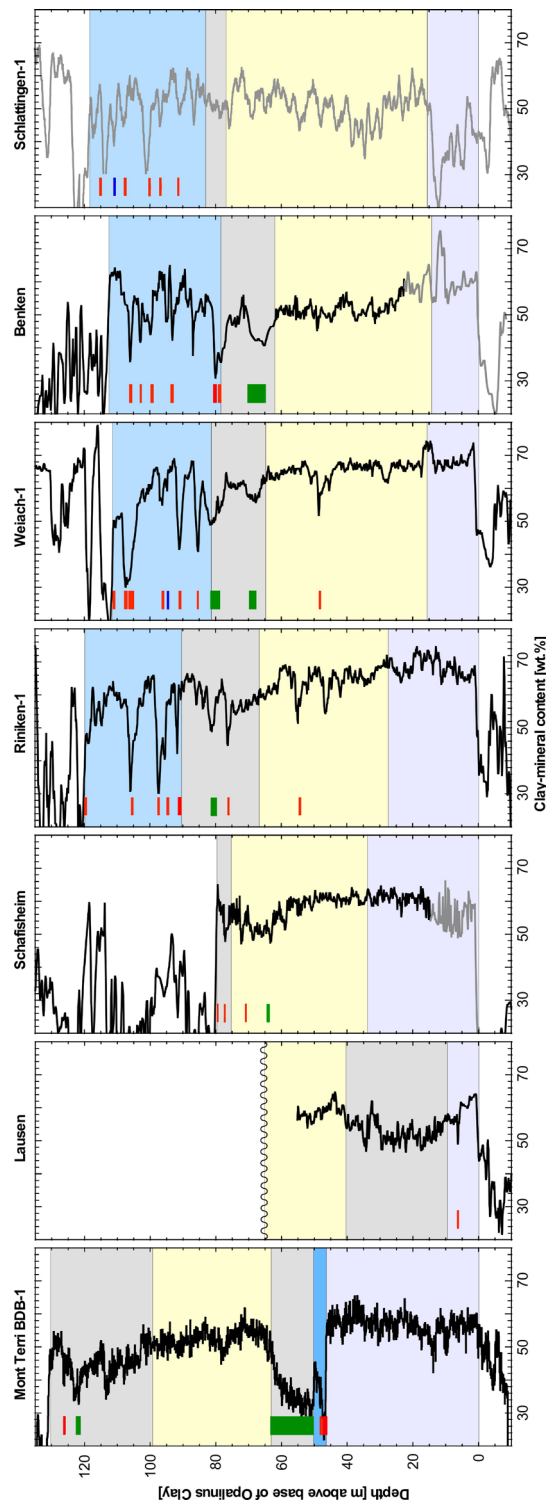


Fig. 2-8: Combined profiles of cored boreholes

Lithological sub-units: Grey = *Silty*; light blue = *With silty calcareous beds*; blue = *Carbonate-rich silty*; purple = *Clay-rich*; yellow = *Mixed clay-silt-carbonate*. Black curves indicate the median clay-mineral content calculated from geophysical logs (grey lines: limited log quality; Schlattigen-1: clay-mineral log based on gamma-ray log only). Red bars = calcareous beds/nodules; green bars = silty zones; blue bars = septaria. Sinuous line marks an erosion surface.

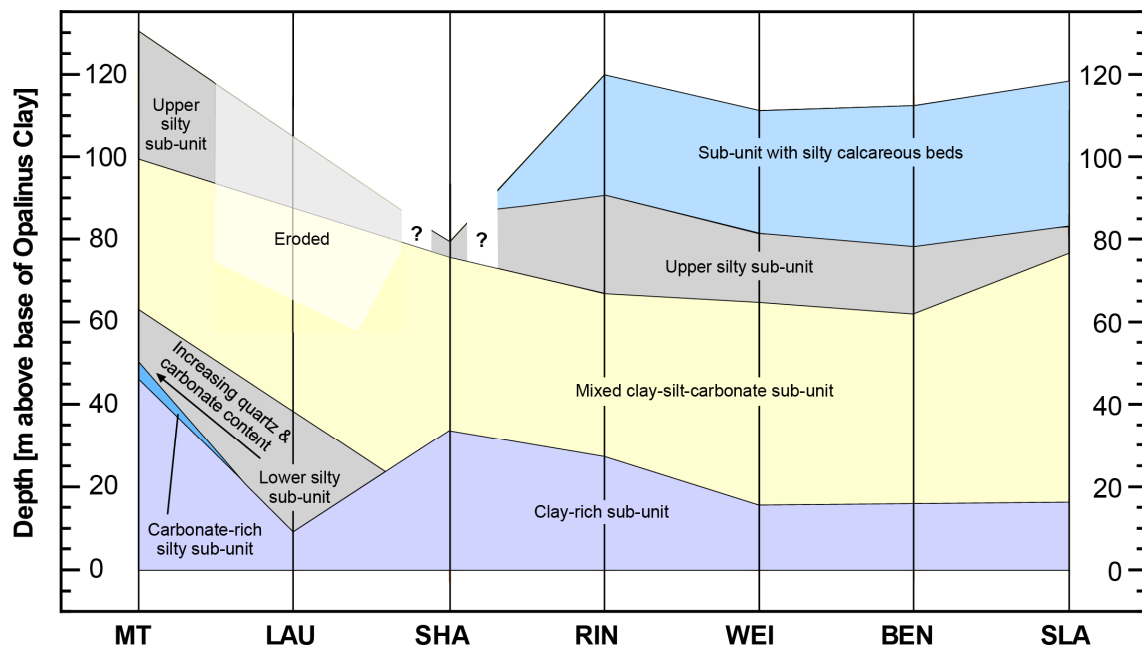


Fig. 2-9: Lateral correlation of lithological sub-units in the Opalinus Clay in cored boreholes

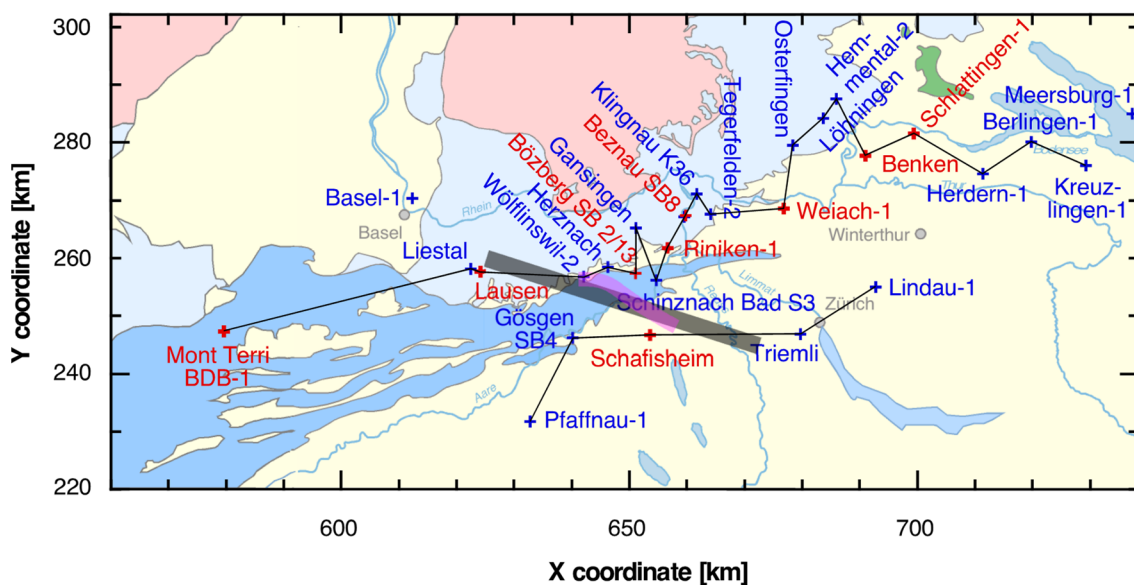


Fig. 2-10: Regional map view with the traces of profiles shown in Fig. 2-11 and 2-12

Thick grey bar separates the western and eastern realms of the Opalinus Clay (see text).
Thick purple bar separates facies realms in the underlying Lower Jurassic (based on Kiefer et al. 2015).

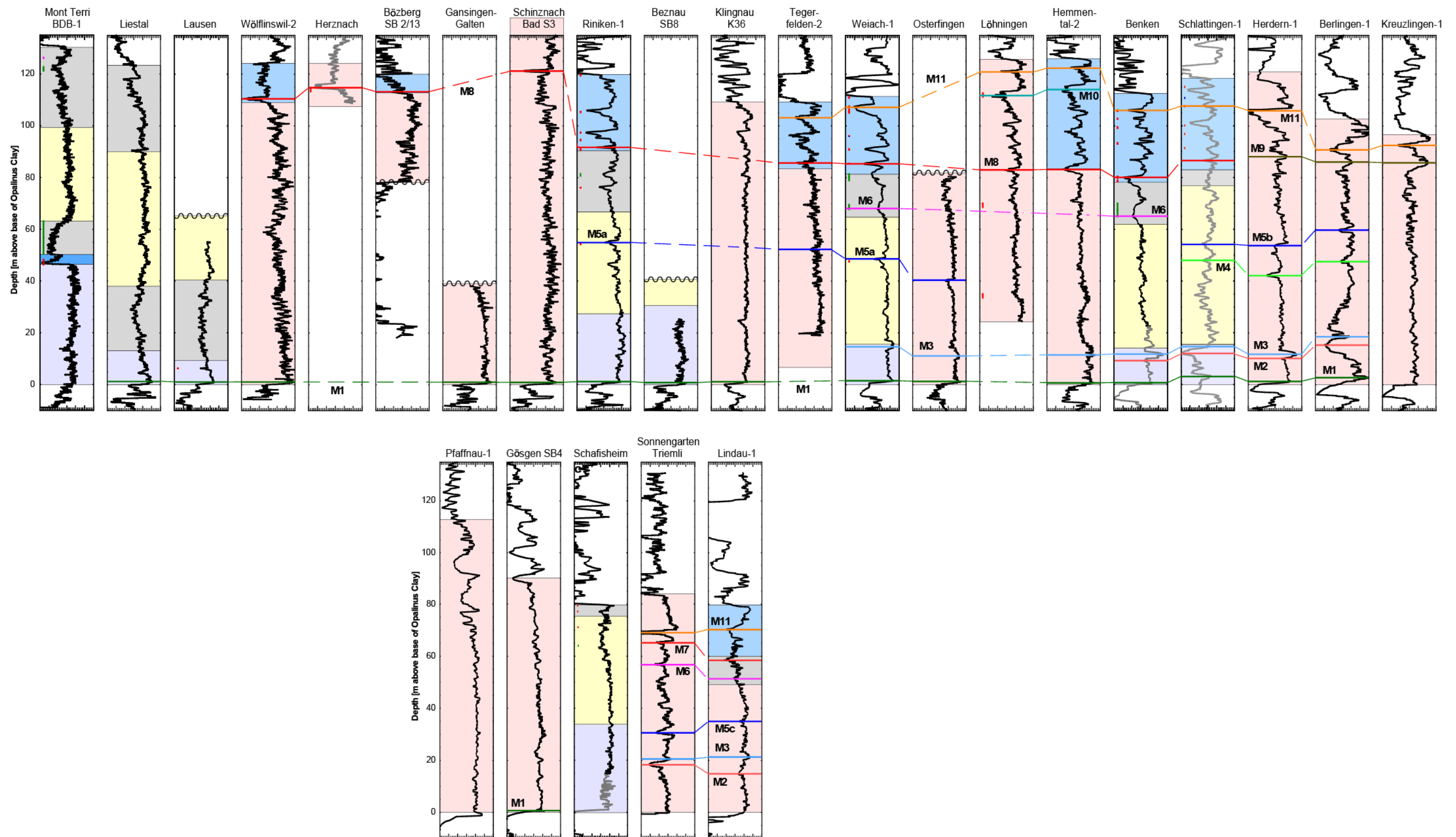


Fig. 2-11: Lithological profiles of all available boreholes and correlation of marker horizons M1–M11 in geophysical logs: northern part

See Section 2.3.6 below for a discussion of the marker horizons. Legend for colour codes is given in Fig. 2-8. Pink background colour means "definition of sub-units not possible due to absence of data". Sinuous line indicates eroded surface or tectonic contact. Range shown for clay-mineral contents is 20 – 80 wt.-%.

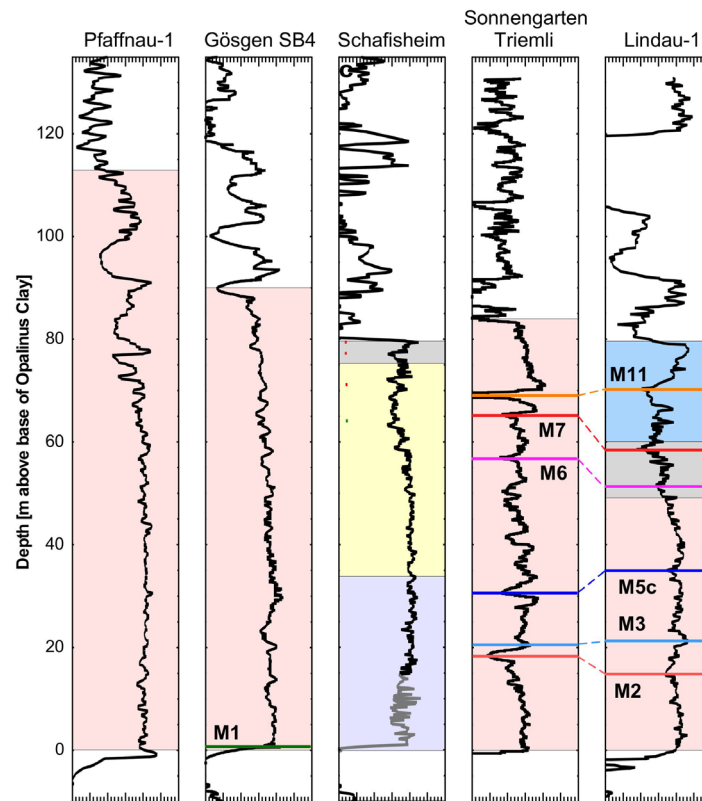


Fig. 2-12: Lithological profiles of all available boreholes and correlation of marker horizons M1–M11 in geophysical logs: southern part

See Section 2.3.6 below for a discussion of the marker horizons. Legend for colour codes is given in Fig. 2-8. Pink background colour means "definition of sub-units not possible". Range shown for clay-mineral contents is 20 – 80 wt.-%.

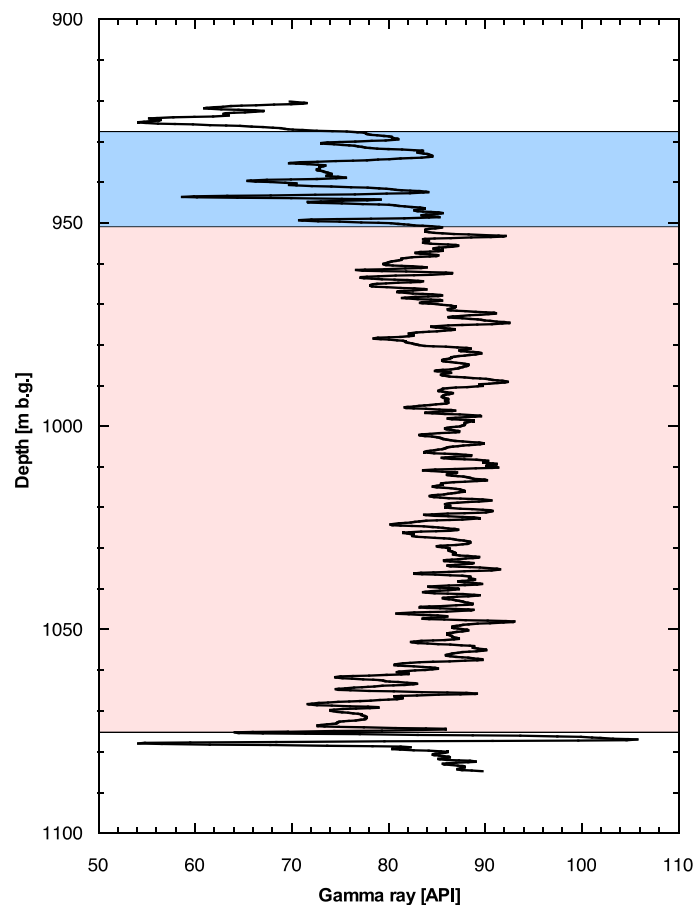


Fig. 2-13: Gamma-ray profile across the Opalinus Clay in the Basel-1 borehole

Based on unpublished data of Geopower Basel AG. Because of the heterogeneous nature of the gamma-ray log in the uppermost part of the Opalinus Clay, this zone is tentatively allocated to the sub-unit with silty calcareous beds (light blue). Pink background colour means "definition of sub-units not possible".

2.3.5 Lateral variability of the Opalinus Clay on a regional scale

By means of lithostratigraphic and geophysical criteria summarised in Fig. 2-11 and 2-12, the area of investigation can be differentiated into two realms separated by a WNW-ESE-trending zone bounded by Lausen and Wölflinswil-2 in the northwest and Schafisheim and Triemli in the southeast (as shown in Fig. 2-10). In the realm northeast of this zone, the characteristic sub-unit with silty calcareous beds occurs in the upper part of the Opalinus Clay. Note that the gamma-ray log of the Basel-1 borehole (Fig. 2-13) resembles those of the Northeastern realm, in particular the heterogeneous uppermost part that is typical of the sub-unit with silty calcareous beds, whereas it has little in common with that of Mont Terri. In the area Mont Terri-Liestal-Laussen, a silty sub-unit in the lower part of the Opalinus Clay occurs that is not found in the east.

It is worth noting that the zone shown in Fig. 2-10 also separates two depocentres within the Opalinus Clay as defined in the isopach map of Allia (1996) and Wetzel & Allia (2003), as it located in a region of low thickness. Allia (1996) discussed the potential effects of basement

structures on subsidence rates during the deposition of the Opalinus Clay and, therefore, on formation thickness. Remarkably, the WNW-ESE separation zone shown in Fig. 2-10 lies parallel to several known basement structures, such as the Eggberg and Vorwald faults in the southern Black Forest. Furthermore, Wetzel & Allia (2003) and Wetzel & Meyer (2006) provided data on palaeo-current directions. To the northeast of the separation zone, these are consistently oriented towards E-NE, while they are heterogeneous on the southwestern side of the zone. Thus, the independently obtained data documented in the literature support the distinction of two realms in which the internal subdivision of the Opalinus Clay differs.

Kiefer et al. (2015) distinguished different facies realms in the Staffelegg Formation, which underlies the Opalinus Clay. The purple zone shown in Fig. 2-10 separates a calcareous-sandy facies in the southwest from a clay-rich facies in the northeast. It is remarkable that this separation zone coincides with that between the Northeastern and southwestern realms in the Opalinus Clay. Apparently, it has had a significance over an extended period of time.

2.3.6 Identification and correlation of marker horizons in geophysical logs

In the clay-mineral logs illustrated in Fig. 2-11 and 2-12, several marker horizons characterised by distinct positive or negative excursions are evident. They correspond to calcareous beds/nodules, silty beds or beds particularly rich in clay minerals. An attempt was made to correlate these excursions among boreholes. This correlation did not consider biostratigraphic evidence and genetic information that may have been obtained by detailed lithostratigraphic studies of the marker horizons (e.g. the distinction of calcareous beds originating from different processes; see Section 2.3.2 for details). It does not have the ambition to represent markers that relate to any synchronous geological event or process. Further, the correlation is in some cases non-unique. In spite of all these provisos, the resulting pattern is plausible and further supports the lithological subdivision of Section 2.3.3.

Discrete heterogeneities are frequent, and they often appear to be correlatable between boreholes in the eastern part of the investigation area. In contrast, boreholes southwest of Riniken-1 show only few such marker horizons, and correlations among boreholes are feasible only in a few cases. Marker horizons are particularly frequent in the sub-unit with silty calcareous beds, i.e. in the uppermost part of the Opalinus Clay. Two of these marker horizons (M8 and M11) appear to be of regional extent, while several other markers (all of which are negative excursions correlating with calcareous beds) are not correlatable to any degree of certainty. Therefore, the lateral extent of such heterogeneities is less than the spacing of the studied boreholes.

The marker horizons and their lateral correlations are illustrated in Fig. 2-11 and 2-12. In total, 11 horizons were mapped, 6 out of which are of regional extent. Fig. 2-14 shows the occurrence of the regional markers in map view. While in many cases the lateral correlation is straightforward, uncertainties and ambiguities exist in several other cases. A more detailed description of the most important marker horizons, including uncertainties, is provided in Tab. 2-5.

Tab. 2-5: Characterisation of the most prominent marker horizons identified in geophysical logs

ID	Sign	Amplitude	Lithostratigraphy	Description
M11	-	High	Calcareous bed	Uppermost strong negative excursion in the sub-unit with silty calcareous beds. Corresponds to one of the uppermost calcareous beds (evidence from Benken and Weiach-1). In boreholes with several negative excursions within the sub-unit with silty calcareous beds, it is not always clear to which one the correlation should be made. Peak correlations with Lindau-1 and Triemli are uncertain.
M8	-	High	Calcareous bed	Prominent negative excursion slightly above or at the base of the sub-unit with silty calcareous beds. Corresponds to a calcareous bed or nodular horizon (evidence from Benken, Weiach-1 and Riniken-1). Widespread occurrence along the northern rim of the Molasse Basin. Peaks in Herznach and Schinznach Bad S3 allocated to this marker could also represent one of the overlying calcareous beds.
M6	-	Low-medium	Silty zone	Relatively broad peak within the silty sub-unit of Benken and Weiach-1. Correlations with peaks in Triemli and Lindau-1 are uncertain.
M5a–c	-	Low-medium	Calcareous bed	Clearly seen in Riniken-1 and Weiach-1 (labelled M5a in Fig. 2-11), where this marker correlates with the lowermost calcareous bed in the Opalinus Clay. Not correlatable west of Riniken-1. Correlations with boreholes to the east (M5b in Fig. 2-11) and southeast (M5c in Fig. 2-12) are uncertain.
M3	+	Medium	Clay-rich zone	Positive excursion at or slightly below the top of the basal clay-rich sub-unit. Present in most boreholes of the eastern part of the investigation area (Weiach-1–Berlingen-1), missing to the west. This marker may be taken as a proxy for the top of the basal clay-rich sub-unit. Presumably correlates with a particularly clay-rich zone (evidence from Benken).
M1	+	Low-medium	Clay-rich zone	Positive excursion a few m above the base of the Opalinus Clay. Probably corresponds to a particularly clay-rich bed (evidence from Riniken-1, Lausen). Largest peak in Berlingen-1, but more or less clearly seen throughout the northern part of the investigation area.

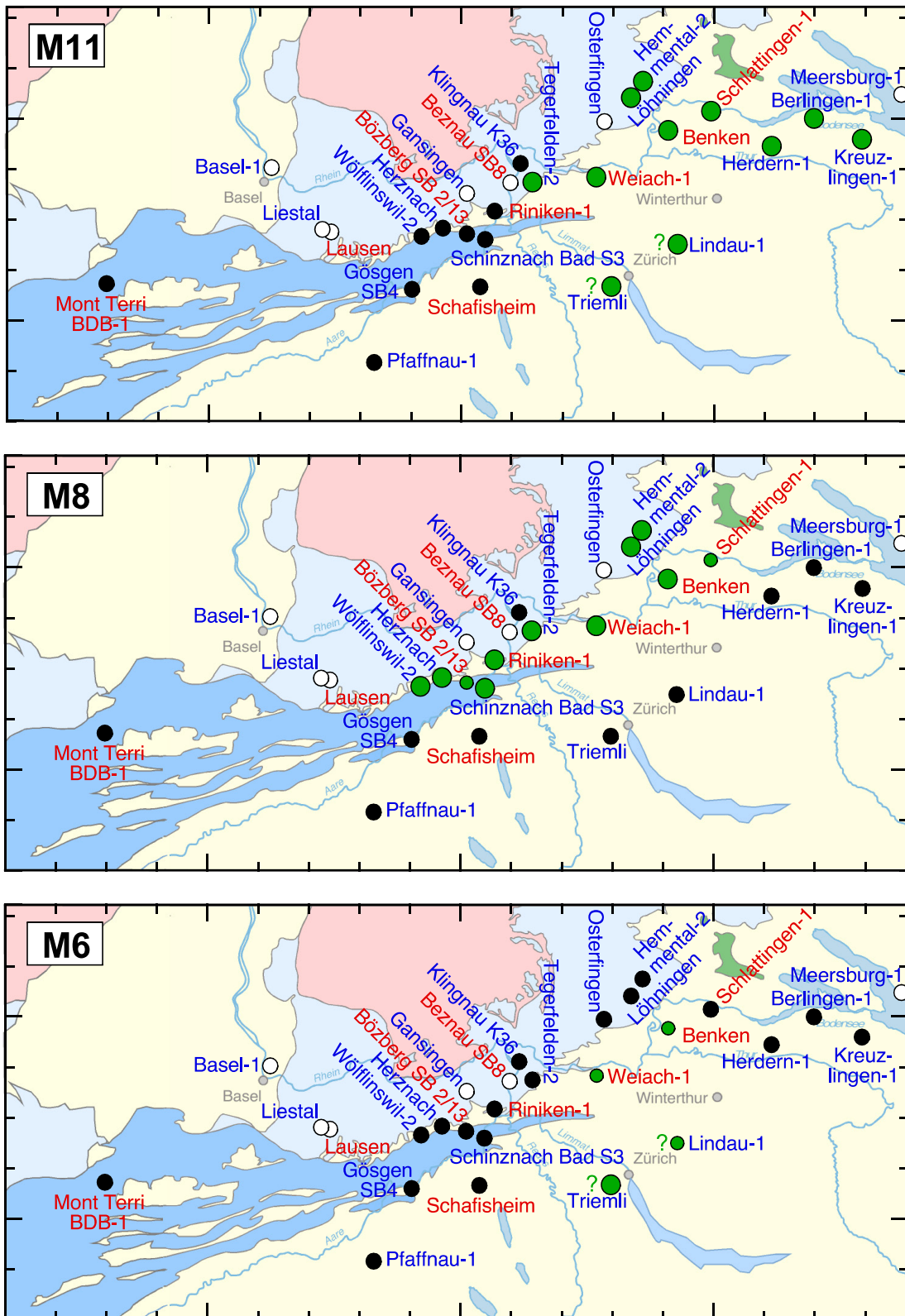


Fig. 2-14: Lateral extent of the prominent marker horizons recognised in geophysical logs

Large green circle: Marker horizon present with high amplitude; small green circle: marker horizon present with low amplitude; black circle: marker horizon not present; white circle: no information

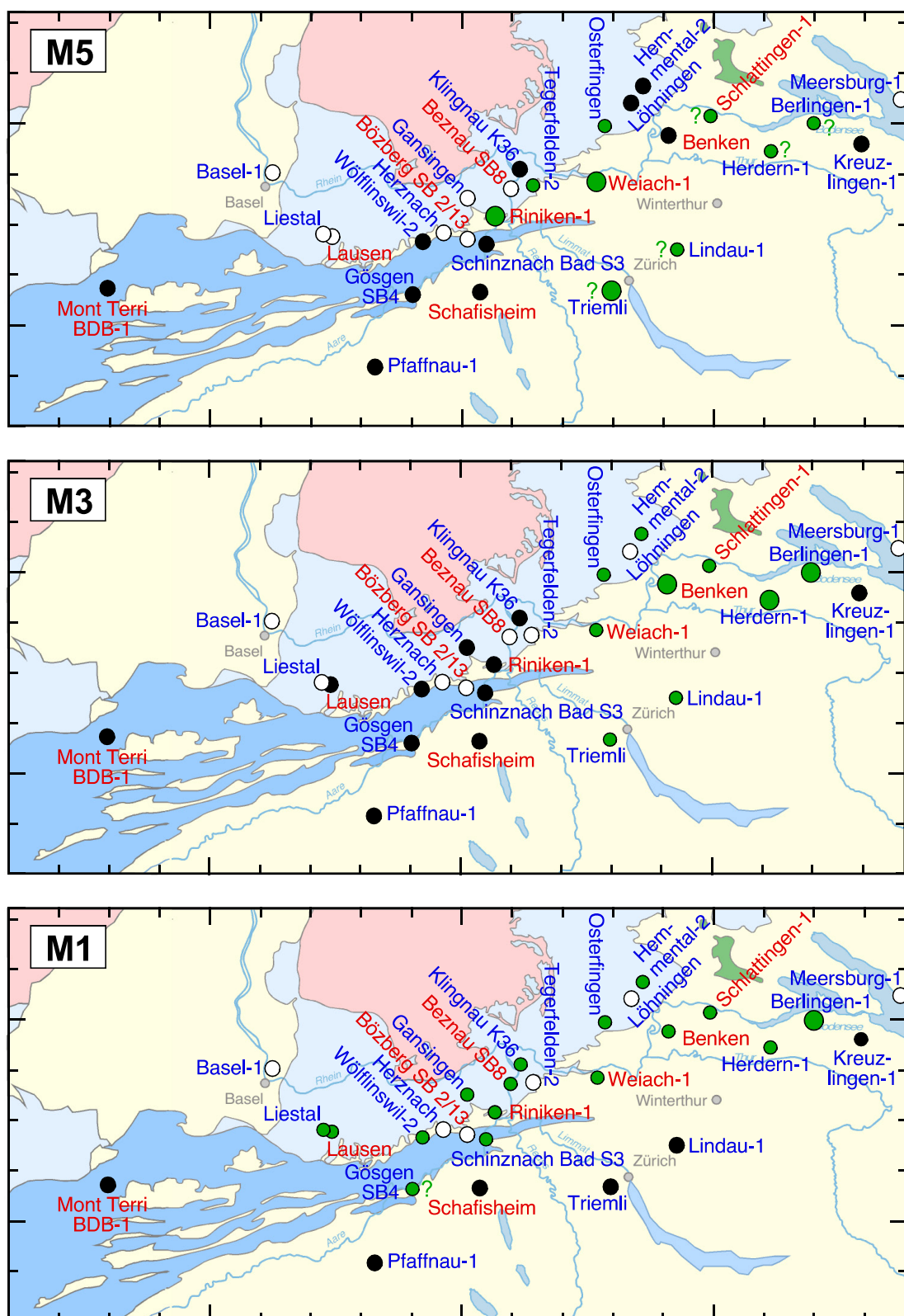


Fig. 2-14: Cont.

2.3.7 **Summary: Large-scale subdivision of the Opalinus Clay in the vertical and lateral dimensions**

- Within the investigation area, the Opalinus Clay can be subdivided into a number of lithostratigraphic sub-units in the vertical dimension (Fig. 2-8, 2-9):
 6. sub-unit with silty calcareous beds (only in the central and eastern part of the investigation area)
 5. upper silty sub-unit (occurring throughout the investigation area)
 4. mixed clay-silt-carbonate sub-unit (occurring throughout the investigation area)
 3. lower silty sub-unit (only present in the west: Mont Terri, Liestal, Lausen)
 2. carbonate-rich silty sub-unit (only in the extreme west: Mont Terri area)
 1. clay-rich sub-unit (occurring throughout the investigation area).
- In the southern boreholes closer to the Alpine front (Gösgen SB4, Schafisheim, Triemli and Lindau-1), the Opalinus Clay is less thick than in the more distal boreholes. With the exception of Pfaffnau-1, formation thickness is below 90 m. This decrease in thickness cannot be explained by the slightly higher degree of compaction alone but represents a primary feature related to paleogeography, considering that the basin margin is located in the south.
- A WNW-ESE-trending zone bounded by Lausen and Wölflinswil-2 in the northwest and Schafisheim and Triemli in the southeast separates two depositional realms of the Opalinus Clay. This zone also coincides with a low formation thickness and separates domains characterised by different palaeo-current directions. A zone at the same location also separates different depositional facies in the underlying Staffelegg Formation.
- Geophysical logs yield several discrete excursions in the Northeastern realm, mostly corresponding to calcareous beds or silty layers. Many of them are correlatable between boreholes, including those located in the southeast (Triemli, Lindau-1). The southwestern realm is essentially devoid of correlatable discontinuities in geophysical logs.

2.3.8 **Sedimentary facies on scales of centimetres to metres**

Outcrop- and drillcore-scale investigations of the Opalinus Clay have been presented in Nagra (2002). Since then, a number of studies have been undertaken at Mont Terri to describe the lithological variability and the geometric features of different depositional facies on scales of centimetres to metres. Some of the applied methods, such as the mapping of cores and outcrops by hyperspectral imaging, are still under development (e.g. Malinverni et al. 2014, Kurz et al. 2015). Here, two examples of small-scale geological mapping campaigns that pertain to the characterisation of small-scale lithological variability are presented. It is necessary to note that both studies mostly focussed on the lower silty sub-unit and the carbonate-rich silty sub-unit, both of which are unique to Mont Terri and do not occur farther to the east. In that sense, the conclusions from these studies need to be interpreted with caution, and the transferability of the information to other sites is limited.

Müller & Jäggi (2012) mapped the TT niche in the lower silty sub-unit at Mont Terri on a scale of 1:5 and distinguished three subfacies: "claystone", "silty claystone" and "limestone". Note that these are field names that have not been checked by quantitative mineralogical analyses

(therefore the quotation marks). The resulting maps are shown in Fig. 2-15. On the outcrop scale, a conspicuous layering normal to the bedding plane was observed, with laterally continuous lithologies. All subfacies contain silty lenses that are isolated, fully embedded bodies, with lateral extents in the range 1 – 20 cm.

- Subfacies "claystone" consists of dark laminated claystone that embeds silty lenses up to 4 cm thick, with a lateral extent of up to 20 cm (Fig. 2-15a).
- Subfacies "limestone" is dominated by bioclasts but also contains silty lenses (same dimensions as in the "claystone") and thin clay-rich, only partially continuous horizons (Fig. 2-15b).
- Subfacies "silty claystone" quantitatively dominates in the TT niche. It has a higher proportion of disseminated quartz than the other subfacies, in addition to frequent silty lenses. Dark, clay-rich intercalations with thicknesses in the range of cm are laterally continuous on the outcrop scale (Fig. 2-15c).

In a related study, Lauper et al. (2018) mapped drillcore BDM-B2, which penetrated parts of the clay-rich, the carbonate-rich silty and the lower silty sub-units at Mont Terri. Five subfacies were defined and are illustrated in Fig. 2-16:

- SF1 – Argillaceous subfacies: Dark, fine-grained mudstone, with cm-thick carbonate nodules as the only marked heterogeneities. Bioturbation is very weak.
- SF2 – Laminated subfacies: On a scale of millimetres to centimetres, alternation of clay-rich and quartz-rich or bioclastic beds. The silty to fine sandy quartz-rich/bioclastic laminae are continuous or lenticular, and bioturbation is weak.
- SF3 – Lenticular subfacies: Quartz-rich/bioclastic material (silt to fine sand) occurs in lenses rather than in laminae, and clay-mineral content is lower in comparison to SF2. This subfacies has high quartz content (20 – 40 %) and is moderately affected by bioturbation.
- SF4 – Sandy subfacies: Mineralogically similar to SF3 but with a somewhat higher carbonate content (bioclasts). The main difference is the strong bioturbation that homogenises the fabric on the mm-cm scale.
- SF5 – Bioclastic subfacies: Due to intense bioturbation, the fabric is homogenised and dominated by bioclasts (> 50 %), with a lower clay-mineral content than in the other subfacies.

Overall, the colour of the rocks becomes lighter from SF1 to SF5, reflecting decreasing clay-mineral contents. Bioturbation becomes progressively more intense from SF1 to SF5, with effects on the fabric on the mm-cm scale.

The occurrence of the subfacies in the 3 sub-units of the Opalinus Clay penetrated by the borehole is shown in Fig. 2-17. The clay-rich sub-unit consists exclusively of the argillaceous subfacies (SF1). The carbonate-rich silty facies is dominated by bioclastic beds (SF5), with subordinate beds of SF2 and SF4. The silty sub-unit is dominated by the lenticular subfacies SF3, with minor beds of SF2 and SF4.

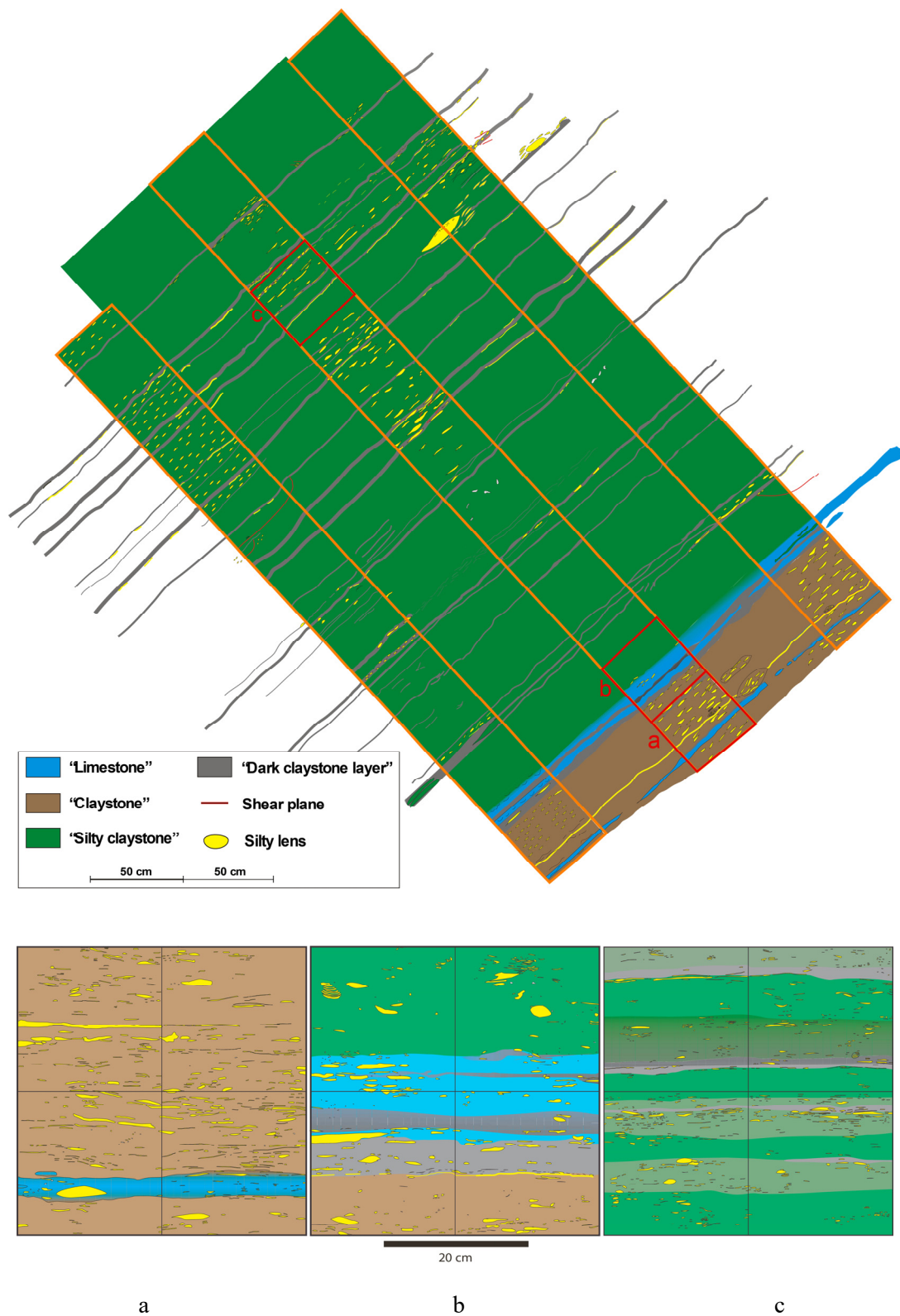


Fig. 2-15: Map of subfacies in the TT niche at Mont Terri (vertical wall)

Orange rectangles in the upper illustration indicate profiles mapped in detail, red squares show the position of enlarged maps shown in the lower illustrations. Adapted from Müller & Jäggi (2012).

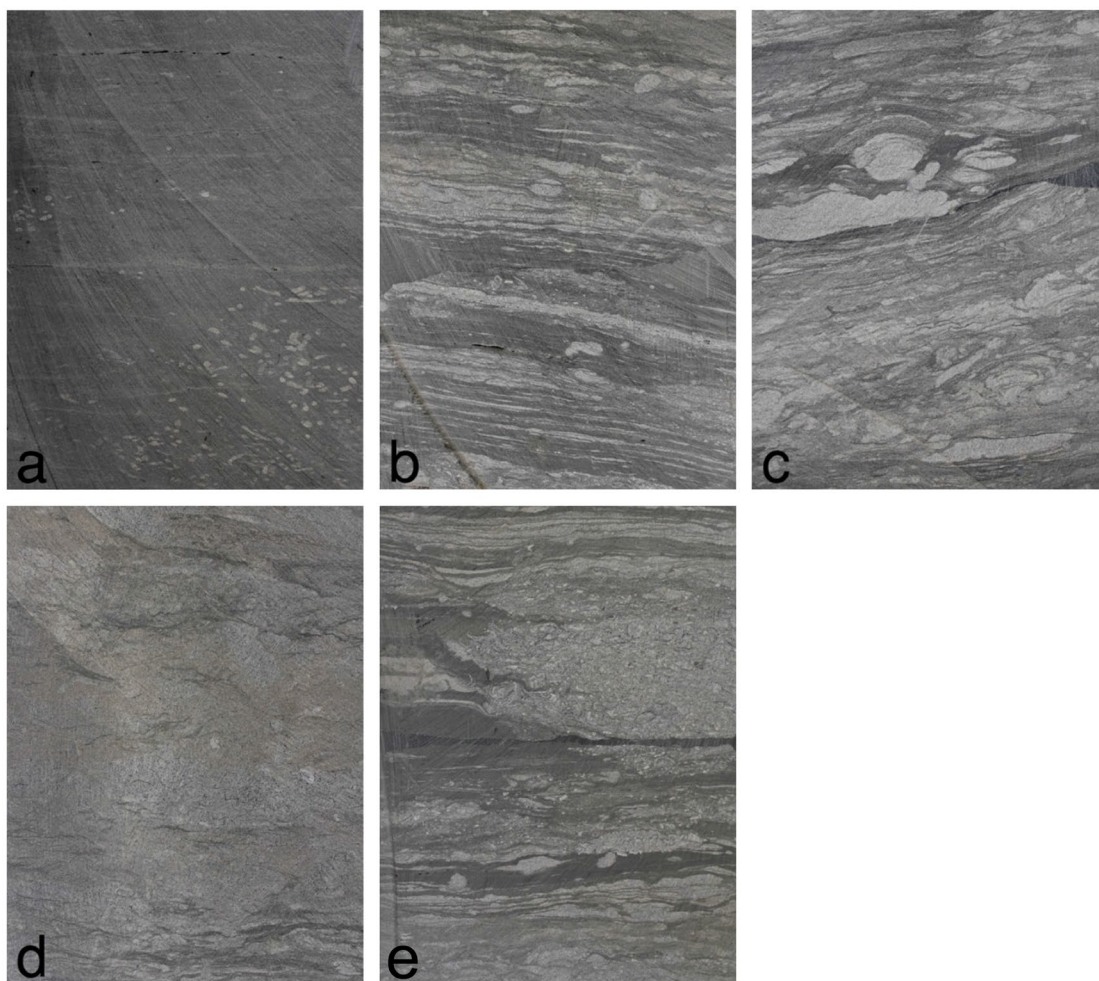


Fig. 2-16: Subfacies of the Opalinus Clay in borehole BDM-B2 at Mont Terri on the centimetre scale

- a. SF1 – Argillaceous subfacies
- b. SF2 – Laminated subfacies
- c. SF3 – Lenticular subfacies
- d. SF4 – Sandy subfacies
- e. SF5 – Bioclastic subfacies (top) and SF2 – Laminated subfacies (bottom)

Adapted from Lauper et al. (2018). Width of each photo is 7 cm

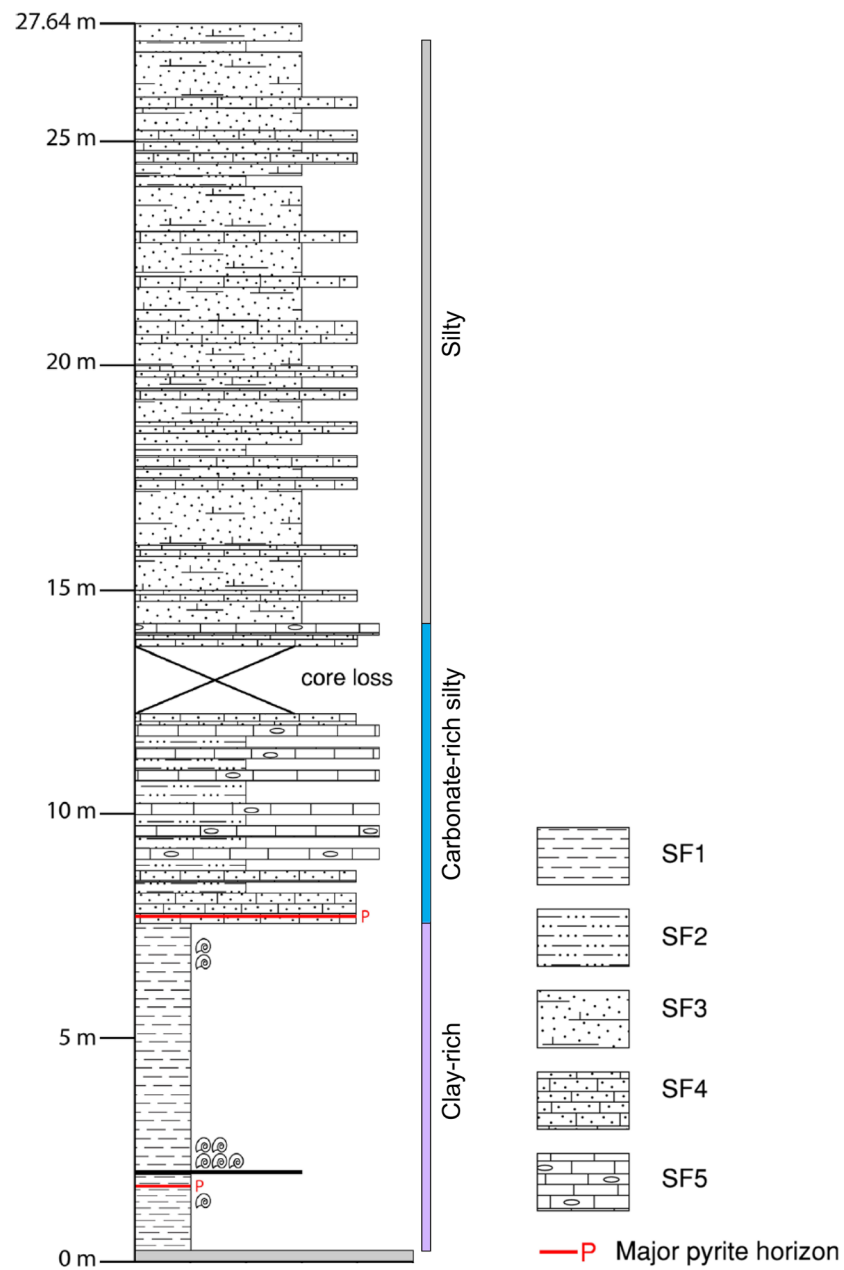


Fig. 2-17: Distribution of subfacies of the Opalinus Clay in borehole BDM-B2 at Mont Terri
Adapted from Lauper et al. (2018)

2.4 Parameterisation of sub-units in the Opalinus Clay

Given the existence of a consistent subdivision of the Opalinus Clay over the area of investigation, the sub-units can further be characterised by means of various laboratory measurements. For this purpose, the rock data base for the sedimentary rocks of Northern Switzerland (Mazurek 2017) was used, augmented by new mineralogical data for borehole BDB-1 from Mont Terri (Huber 2018). Mineralogical data from Beznau-1984 were excluded because they pertain only to the lowermost part of the Opalinus Clay.

2.4.1 Bulk mineralogy of sub-units

The mineralogical data for all sub-units are listed in Tab. 2-6. Fig. 2-18 and 2-19 show the data in the Füchtbauer triangle. In Fig. 2-20, the sub-unit-specific averages are shown relative to the bulk average of the Opalinus Clay. Fig. 2-21 shows the distribution of clay-mineral, quartz and calcite contents in boxplots. The following observations can be made:

- The carbonate-rich silty and the lower silty sub-units from Mont Terri deviate most strongly from the bulk of the data towards clay-poorer compositions (Fig. 2-18). The lower silty sub-unit at Lausen is distinctly richer in clay minerals.
- The upper silty sub-unit and the sub-unit with silty calcareous beds occupy relatively large fields in Fig. 2-18 and have intermediate positions between the lower silty and the clay-rich sub-units.
- The clay-rich sub-unit and the mixed clay-silt-carbonate sub-unit overlap widely in the clay-rich corner of Fig. 2-18.
- Some outliers towards more calcareous lithologies are found in all sub-units and are due to heterogeneities on the scale of centimetres to a few decimetres, such as calcareous nodules.
- As can be seen in Tab. 2-6 and Fig. 2-20, the ratio of quartz to feldspars is largely constant in all sub-units, with the exception of the carbonate-rich silty sub-unit at Mont Terri where it is substantially lower. This may indicate a less mature situation, possibly due to a shorter transport distance from the source area.
- Dolomite/ankerite is enriched in the carbonate-rich silty and the lower silty sub-unit at Mont Terri relative to the bulk average, while the opposite is observed for the sub-unit with silty calcareous beds (Fig. 2-20).
- Siderite is markedly enriched in the mixed clay-silt-carbonate sub-unit, whereas this is the case for pyrite in the sub-unit with calcareous beds (Fig. 2-20).

Tab. 2-6: Mineralogical composition of lithologic sub-units of the Opalinus Clay

Sub-unit		Quartz [wt.-%]	K-feldspar [wt.-%]	Plagioclase [wt.-%]	Calcite [wt.-%]	Dolomite/ Ankerite [wt.-%]	Siderite [wt.-%]	Pyrite [wt.-%]	C(org) [wt.-%]	Clay minerals [wt.-%]
All	Mean	23.2	2.6	1.0	13.7	0.9	3.5	1.1	0.7	53.1
	Median	22.6	2.3	1.0	11.0	0.8	2.4	0.9	0.7	56.3
	1 σ	7.4	1.4	0.7	9.4	1.4	4.8	0.8	0.3	14.2
	No.	159	159	159	233	233	233	155	233	159
With silty calcareous beds	Mean	23.5	2.4	0.9	16.8	0.3	3.0	1.7	0.8	51.9
	Median	23.0	2.3	1.0	13.0	0.0	0.0	1.4	0.7	54.0
	1 σ	5.0	1.2	0.4	11.3	0.5	7.9	1.2	0.5	12.3
	No.	28	28	28	43	43	43	24	43	28
Upper silty	Mean	26.7	2.9	1.1	13.6	0.6	3.1	1.2	0.6	49.8
	Median	26.2	3.0	1.0	11.4	0.8	2.5	0.9	0.7	50.0
	1 σ	6.8	1.3	0.7	6.8	0.6	2.8	0.6	0.2	11.2
	No.	17	17	17	25	25	25	15	25	17
Mixed clay-silt- carbonate	Mean	21.5	2.3	0.8	11.1	0.7	4.9	1.0	0.7	57.7
	Median	21.8	2.0	1.0	10.0	0.8	3.8	0.7	0.7	58.0
	1 σ	4.2	1.4	0.7	6.3	0.9	4.7	0.6	0.3	8.2
	No.	55	55	55	88	88	88	58	88	55
Lower silty	Mean	34.5	3.7	1.4	11.3	2.2	2.2	0.5	0.7	43.6
	Median	33.8	4.0	1.5	9.7	1.5	2.0	0.6	0.7	45.3
	1 σ	6.8	1.2	0.7	5.2	2.2	1.5	0.4	0.2	12.0
	No.	18	18	18	18	18	18	18	18	18
Carbonate- rich silty	Mean	28.0	4.1	2.0	32.5	3.1	3.0	1.1	0.5	25.8
	Median	27.9	4.1	2.0	31.4	1.9	2.5	0.8	0.4	22.5
	1 σ	2.9	1.0	0.6	16.1	2.8	1.6	1.1	0.2	14.9
	No.	12	12	12	12	12	12	12	12	12
Clay-rich	Mean	15.1	1.8	0.7	11.6	0.9	2.3	1.3	0.7	64.7
	Median	14.1	1.5	0.5	10.0	0.8	2.0	1.1	0.6	63.1
	1 σ	4.2	1.2	0.8	6.3	1.3	1.9	0.7	0.3	7.0
	No.	29	29	29	47	47	47	28	47	29

"No." = number of data points. Data from Beznau-1984 are excluded.

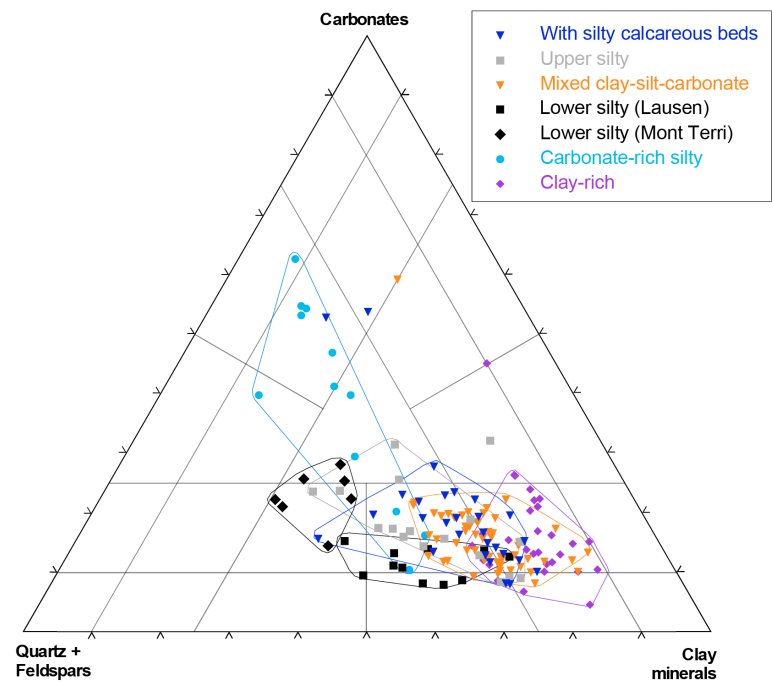


Fig. 2-18: Mineralogical composition of lithologic sub-units of the Opalinus Clay shown in the ternary plot

Füchtbauer (1988). Borders drawn around data of the sub-units may exclude some outliers.

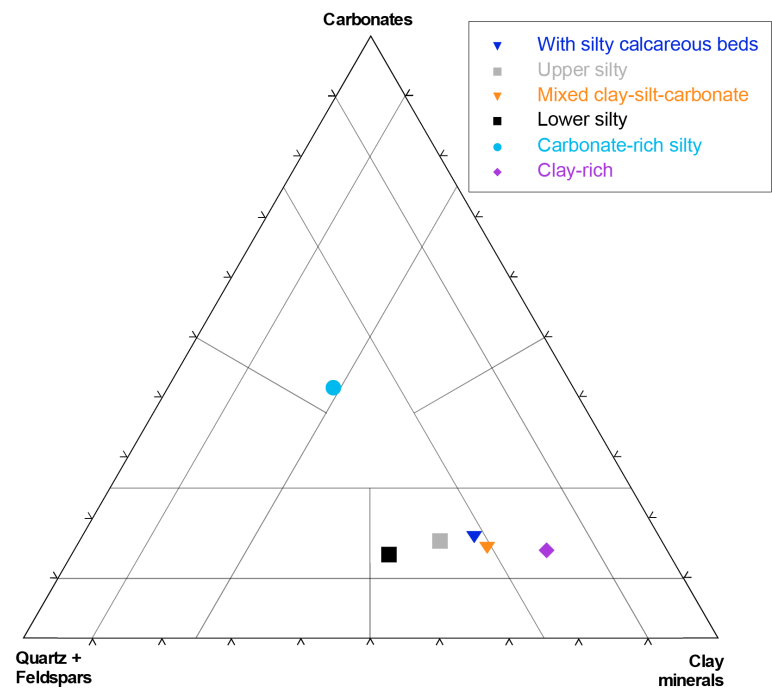


Fig. 2-19: Median values of mineral contents of lithologic sub-units of the Opalinus Clay shown in the ternary plot

Füchtbauer (1988)

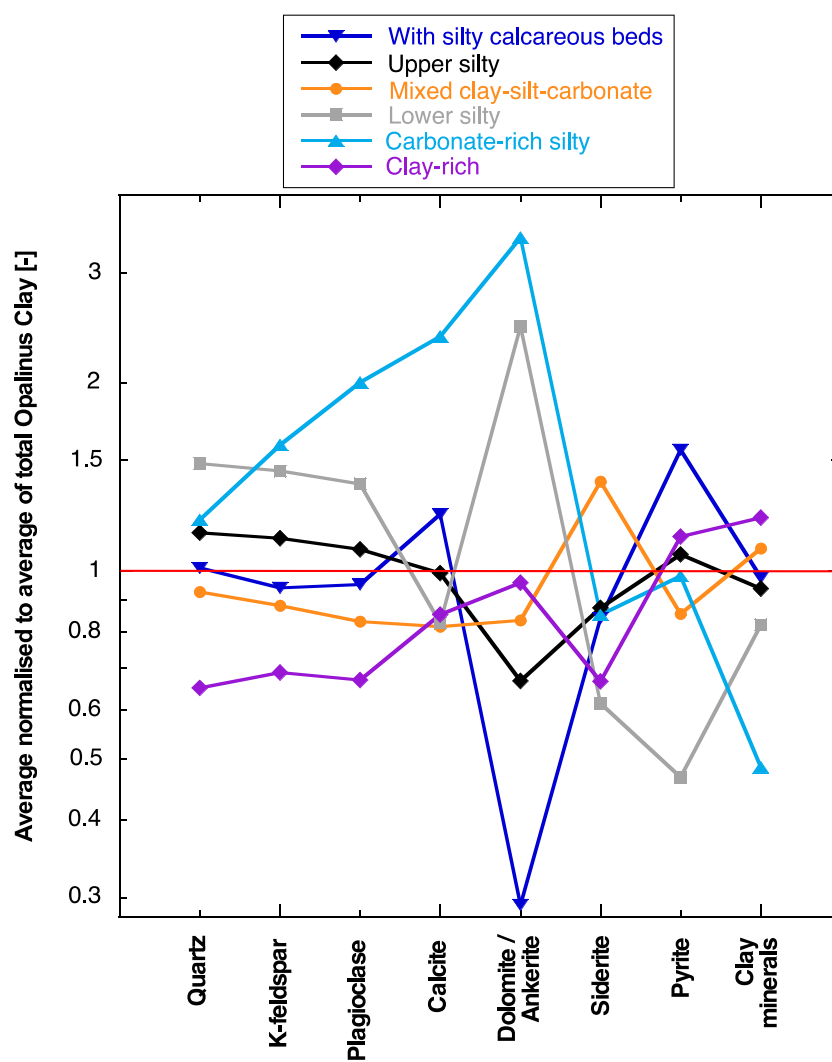


Fig. 2-20: Average mineralogical composition of sub-units normalised to the average of all data for the Opalinus Clay

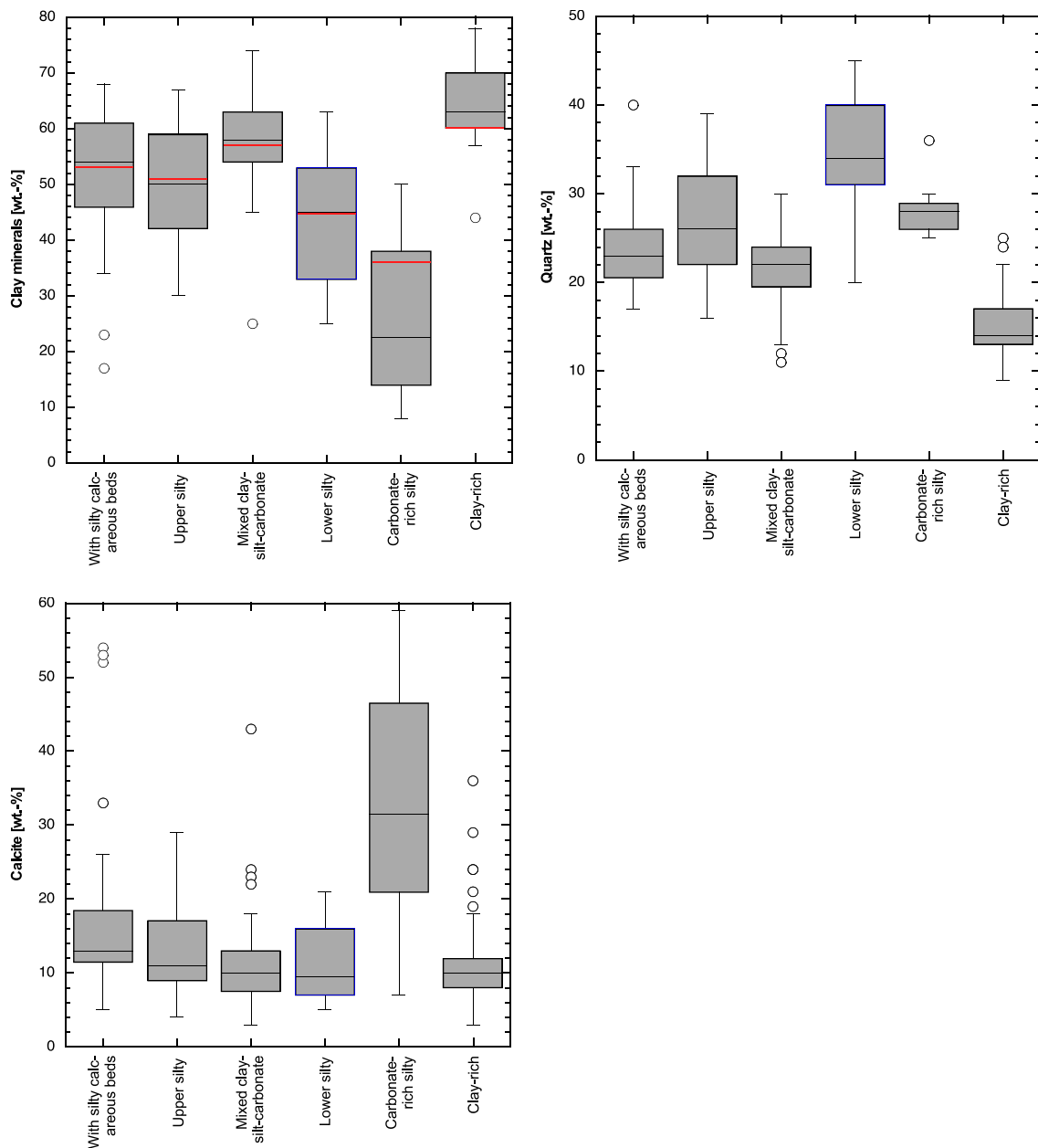


Fig. 2-21: Box plots showing the contents of clay minerals, quartz and calcite in the different sub-units of the Opalinus Clay

Each box shows the median and the lower and upper quartiles. Vertical lines indicate range $\pm 1.5 \times (\text{upper quartile} - \text{lower quartile})$. Data outside this range are shown by circles. Red lines indicate average clay-mineral contents obtained from geophysical logs.

2.4.2 Regional trends of bulk mineralogy

As the type and thickness of sub-units vary within the investigation area, the borehole-specific mineralogical composition of the Opalinus Clay is expected to show some degree of regional variation as well. The mineralogical data, organised by boreholes rather than by lithologic sub-units, are shown in Tab. 2-7, Fig. 2-22 and 2-23. Fig. 2-23 shows that the average clay-mineral content of the Opalinus Clay increases eastwards from Mont Terri towards Schafisheim/Riniken-1 and then decreases again in Benken and Schlattingen-1. Riniken-1 and Weiach-1 have the highest average clay-mineral contents in the region. Quartz contents indicate the inverse relationship. Calcite contents increase eastwards from Lausen to Schlattingen.

In addition to the data from drillcore investigations, clay-mineral contents derived from geophysical borehole logs were also analysed. The average clay-mineral contents for all sub-units and boreholes are listed in Tab. 2-8 and shown graphically in Fig. 2-24. It becomes evident that within each single sub-unit, Riniken-1 and Weiach-1 have the highest clay-mineral contents, which drop towards the west and to the east. Thus, it is not only the laterally evolving relative ratios of the different sub-units in any borehole profile, but also the composition of the same type of sub-unit evolves laterally.

The comparison of the mineralogical laboratory data (Tab. 2-6) and clay-mineral contents derived from geophysical logs (Tab. 2-8) in general yields a good consistency, which means that sampling bias of the laboratory data is small. Exceptions include the clay-rich sub-unit (laboratory data: 65 wt.-%; log data: 60 wt.-%) and in particular the carbonate-rich silty sub-unit (laboratory data: 26 wt.-%; log data: 36 wt.-%). In the latter case, laboratory sampling was deliberately focussed on clay-poor lithologies, which led to an underestimation of the average clay-mineral content.

Tab. 2-7: Mineralogical composition of the Opalinus Clay in different boreholes

Sub-unit		Quartz [wt.-%]	K-feldspar [wt.-%]	Plagioclase [wt.-%]	Calcite [wt.-%]	Dolomite/ Ankerite [wt.-%]	Siderite [wt.-%]	Pyrite [wt.-%]	C(org) [wt.-%]	Clay minerals [wt.-%]
Mont Terri BDB-1	Mean	26.5	3.5	1.5	19.2	1.9	2.7	1.1	0.6	43.1
	Median	26.3	3.4	1.2	16.0	1.1	2.4	1.0	0.6	46.5
	1 σ	8.4	1.4	0.8	12.4	2.2	1.6	0.7	0.2	16.9
	No.	44								
Lausen	Mean	29.5	3.0	0.9	7.8	1.2	2.0	0.8	0.8	54.2
	Median	30.5	2.7	1.0	7.9	1.4	1.0	0.6	0.8	53.9
	1 σ	7.9	1.2	0.5	2.4	0.7	1.9	0.7	0.1	9.6
	No.	14								
Schafisheim	Mean	22.3	2.5	0.9	10.5	1.1	3.8	1.3	0.5	59.4
	Median	23.1	2.4	1.0	10.0	1.0	2.0	1.3	0.5	59.8
	1 σ	3.5	1.8	1.0	3.8	0.9	5.6	0.7	0.2	4.2
	No.	14	14	14	36	36	36	10	36	14
Riniken-1	Mean	20.7	1.6	0.8	12.4	0.3	3.8	1.3	0.8	59.9
	Median	21.0	1.7	1.0	10.0	0.0	2.0	1.0	0.9	64.0
	1 σ	4.3	0.5	0.6	9.0	0.6	6.8	0.8	0.3	10.8
	No.	24	24	24	41	41	41	18	41	24
Weiach-1	Mean	18.8	1.7	0.4	12.5	0.3	4.0	1.0	0.8	61.1
	Median	18.0	2.0	0.0	10.0	0.0	2.0	0.6	0.8	63.9
	1 σ	5.8	1.3	0.5	9.9	0.6	5.8	0.8	0.4	14.3
	No.	20	20	20	55	55	55	26	55	20
Benken	Mean	20.3	2.2	0.9	15.3	0.7	4.6	1.1	0.6	54.4
	Median	20.8	2.3	0.9	12.6	0.8	4.6	1.0	0.6	55.9
	1 σ	4.7	1.0	0.3	9.4	0.4	2.4	0.9	0.3	10.3
	No.	22								
Schlat- tingen-1	Mean	22.7	2.6	0.8	15.1	1.4	2.9	1.4	0.4	52.5
	Median	23.0	2.0	1.0	14.0	1.2	2.4	0.9	0.3	54.0
	1 σ	8.0	1.3	0.7	5.9	1.9	2.3	1.1	0.2	10.2
	No.	21								

"No." = number of data points. Note that only the lower part of the Opalinus Clay was drilled at Lausen, and only data below the weathered zone (base at 23.65 m) were considered.

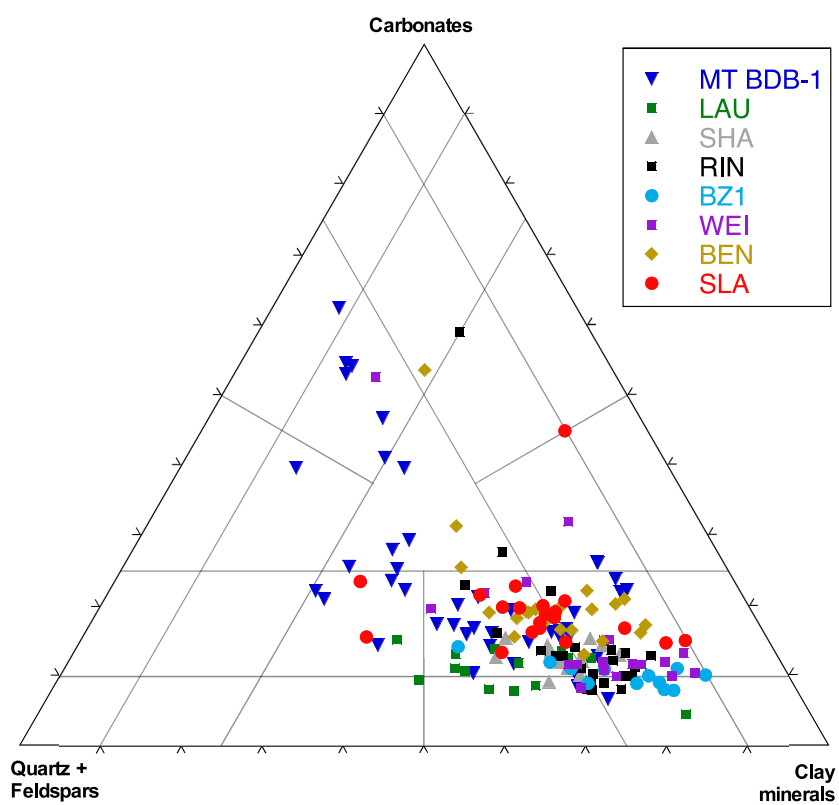


Fig. 2-22: Mineralogical composition of the Opalinus Clay in different boreholes shown in the ternary plot
Füchtbauer (1988)

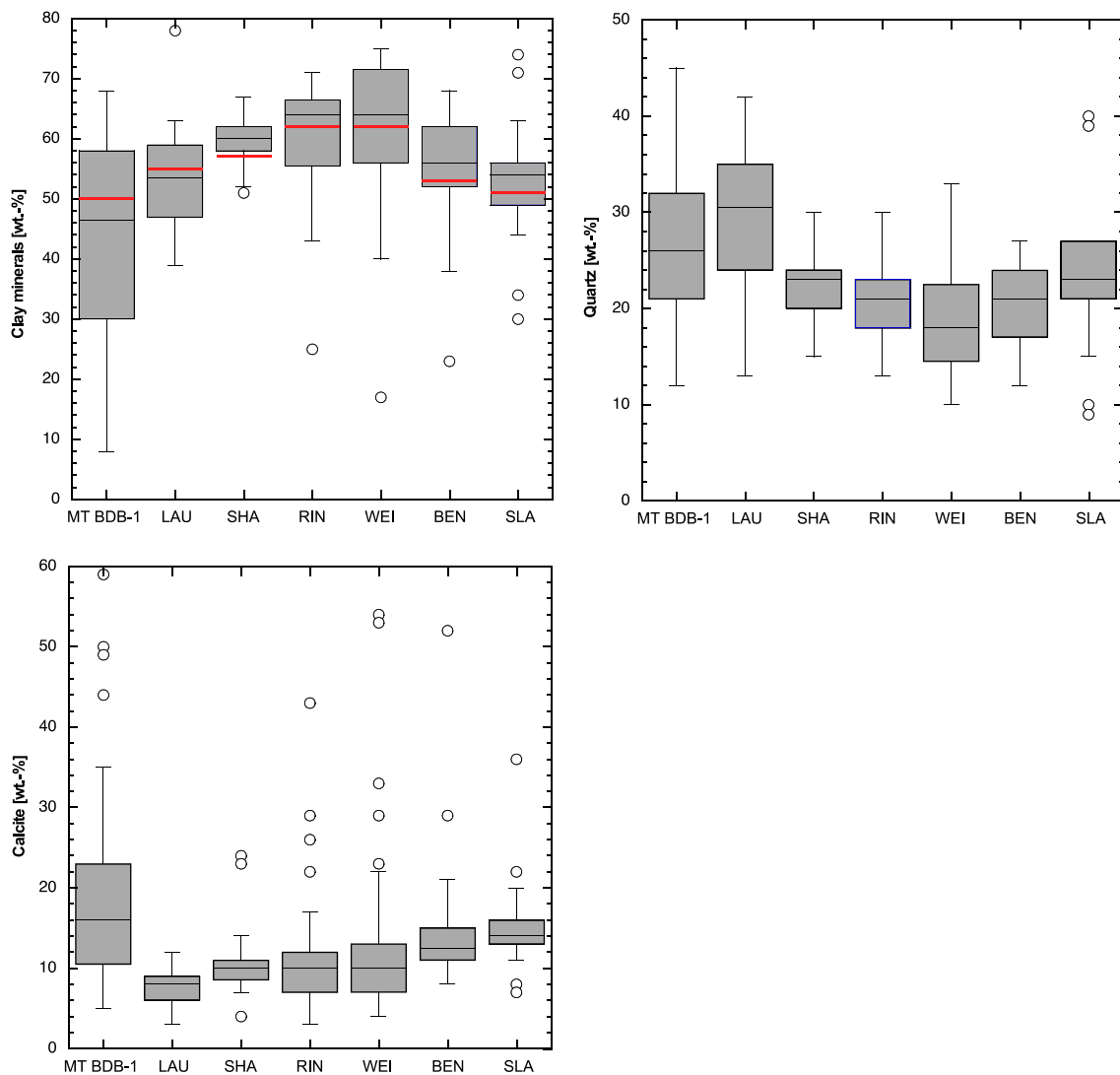


Fig. 2-23: Box plots showing the regional distribution of clay-mineral, quartz and calcite contents

Each box shows the median and the lower and upper quartiles. Vertical lines indicate range $\pm 1.5 \times (\text{upper quartile} - \text{lower quartile})$. Data outside this range are shown by circles. Red lines indicate average clay-mineral contents obtained from geophysical logs. Note that only the lower part of the Opalinus Clay was drilled at Lausen, and data below the weathered zone (base at 23.65 m) were considered.

Tab. 2-8: Average clay-mineral contents of boreholes and sub-units derived from geophysical logs

Data indicate averages in wt.-% $\pm 1 \sigma$. "ALL" is the average of the borehole-specific averages, i.e. each site has the same weight. Data for Schlattingen-1 are uncertain due to limited log quality

Sub-unit	MT BDB-1		LAU		SHA		RIN		WEI		BEN		SLA		ALL
With silty calcareous beds							55	± 8	55	± 9	52	± 7	50	± 5	53
Upper silty	45	± 5	No data		55	± 4	58	± 5	58	± 3	46	± 4	45	± 5	51
Mixed clay-silt-carbonate	52	± 3	No data		57	± 4	64	± 4	66	± 2	53	± 4	52	± 3	57
Lower silty	36	± 5	53	± 3											45
Carbonate-rich silty	36	± 7													36
Clay-rich	57	± 3	59	± 4	58	± 7	68	± 4	67	± 4	60	± 6	53	± 7	60
Total Opalinus Clay	50	± 8	55 ¹	± 4	57	± 5	62	± 7	62	± 7	53	± 6	51	± 5	56

¹ Refers to the section below the base of the weathered zone at 23.65 m

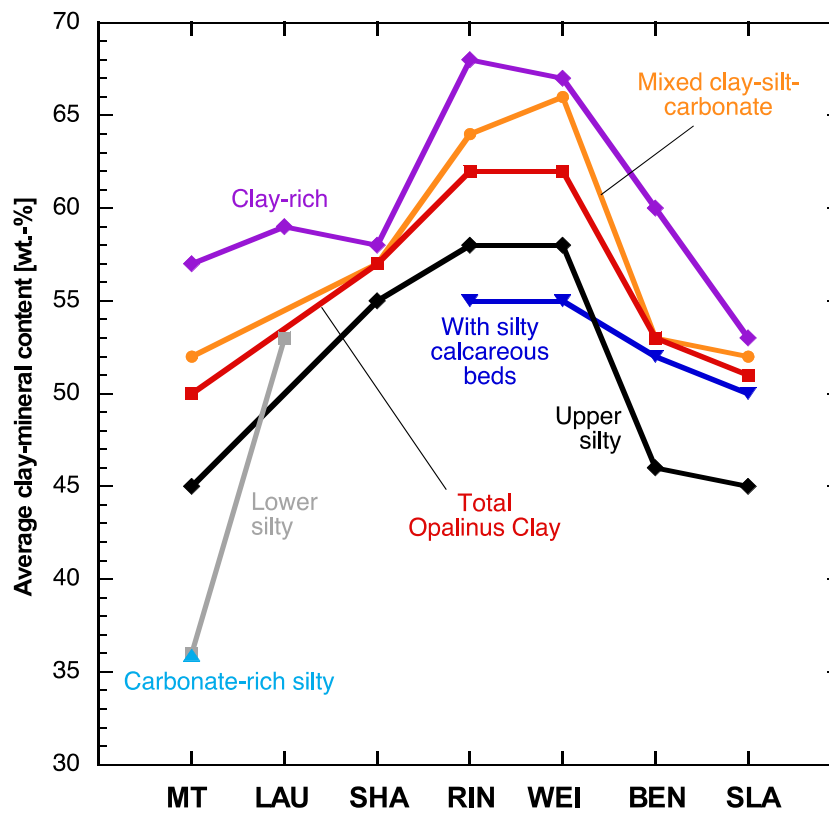


Fig. 2-24: Average clay-mineral contents of sub-units based on geophysical logs
Data for Schlattingen-1 are uncertain due to limited log quality.

2.4.3 Clay mineralogy of sub-units

Clay minerals include illite, illite-rich illite-smectite mixed layers (ill/sm ML), kaolinite and chlorite. While the total clay-mineral content varies, the relative proportions of the different clay minerals are essentially constant, as shown in Tab. 2-9, Fig. 2-25 and 2-26. There are no systematic differences between lithologic sub-units or between boreholes (but note that the number of analyses is small for some sub-units). It is concluded that the relative proportions of clay minerals have a quite limited variability in both the vertical and the horizontal dimensions.

Tab. 2-9: Clay-mineral composition of lithologic sub-units of the Opalinus Clay

Sub-unit		Illite	Ill/Sm ML	Kaolinite	Chlorite	Illite	Ill/Sm ML	Kaolinite	Chlorite
		[wt.-% of total rock]				[wt.-% of clay fraction]			
All	Mean	18.9	14.7	15.9	6.4	32.9	27.3	28.3	11.5
	Median	17.1	15.0	16.0	6.0	30.6	27.0	28.1	11.1
	1 σ	7.9	6.7	5.0	2.9	9.5	12.1	5.3	4.2
	No.	80							
With silty calcareous beds	Mean	18.6	13.1	16.1	5.5	34.2	25.4	30.1	10.3
	Median	18.2	14.0	15.5	4.0	30.7	26.0	30.0	8.2
	1 σ	7.7	6.8	5.5	3.0	9.8	13.1	7.0	4.7
	No.	17							
Upper silty	Mean	17.1	12.7	13.5	6.4	32.8	27.4	27.2	12.6
	Median	14.0	12.0	13.0	6.0	31.3	26.1	26.2	12.8
	1 σ	8.2	6.2	4.1	3.0	8.6	13.1	3.6	3.8
	No.	11							
Mixed clay-silt-carbonate	Mean	19.2	16.7	17.0	7.1	34.2	25.4	30.1	10.3
	Median	17.0	16.0	16.2	7.0	30.7	26.0	30.0	8.2
	1 σ	7.5	7.0	4.0	2.9	9.8	13.1	7.0	4.7
	No.	31							
Lower silty	Mean	9.3	9.3	6.0	3.7	32.0	32.3	21.9	13.7
	Median	7.0	8.0	6.0	4.0	28.0	30.8	23.1	16.0
	1 σ	4.0	3.2	1.0	1.5	7.9	5.3	6.7	7.0
	No.	3							
Carbonate-rich silty	Mean	2.0	2.0	3.0	1.0	25.0	25.0	37.5	12.5
	Median	2.0	2.0	3.0	1.0	25.0	25.0	37.5	12.5
	No.	1							
Clay-rich	Mean	22.4	15.7	18.0	7.1	35.2	25.4	28.3	11.1
	Median	20.0	17.0	18.0	6.2	31.7	26.3	29.5	10.0
	1 σ	7.1	5.5	3.8	2.5	9.6	9.4	4.5	3.3
	No.	17							

"No." = number of data points. Data from Beznau-1984 are excluded.

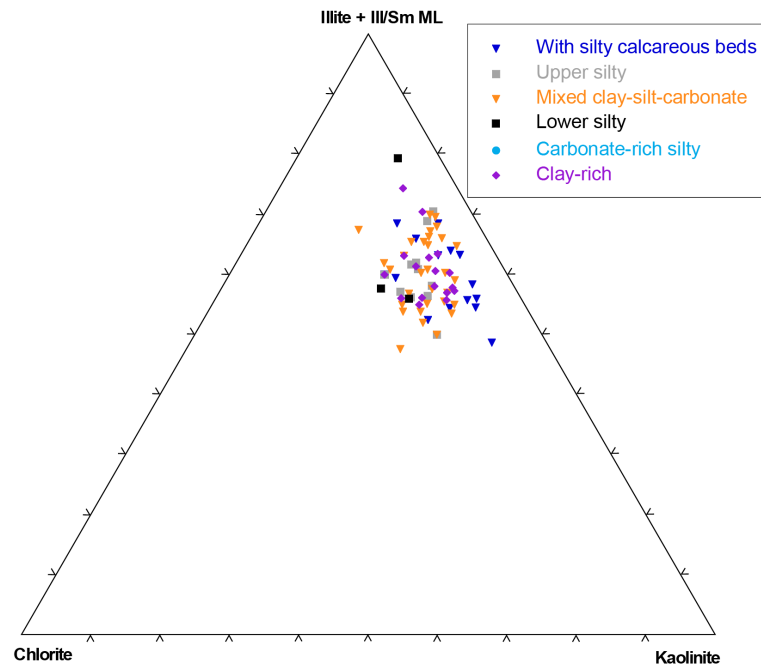


Fig. 2-25: Clay-mineral composition of lithologic sub-units of the Opalinus Clay shown in a ternary plot

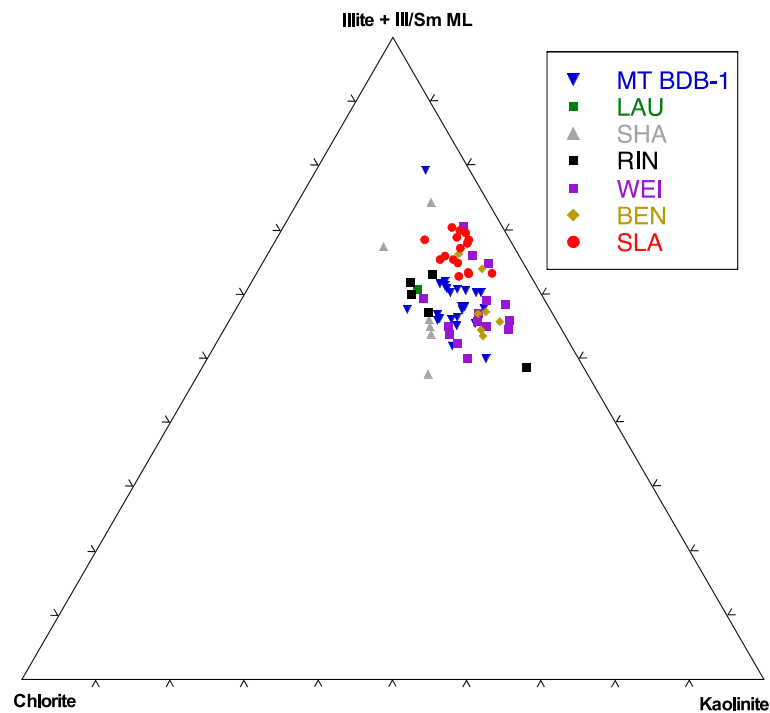


Fig. 2-26: Clay-mineral composition of the Opalinus Clay in different boreholes shown in a ternary plot

2.4.4 Petrophysical parameters

Available petrophysical data are listed in Tab. 2-10. All existing measurements of bulk dry density (including the pycnometer porosity calculated from it) have been excluded because drying of clay-rich samples leads to shrinkage and therefore potentially to an overestimation of density. In contrast, bulk density of saturated samples (bulk wet density) is unaffected by such artefacts and permits the calculation of realistic bulk-dry density data. Because bulk wet densities were only measured in the more recent campaigns (Schlattingen-1, Mont Terri BDB-1, Lausen), Tab. 2-10 shows bulk-density data originating from these boreholes only. Similarly, water content, water-loss porosity and data obtained from isotope diffusive exchange experiments are limited to Benken, Schlattingen-1, Mont Terri BDB-1 and Lausen. Grain-density data and BET surfaces obtained by N₂ adsorption are available for all boreholes. The main findings are as follows:

- There is a tendency towards lower porosity with increasing depth below surface (Fig. 2-27). This can be explained either by different burial depths in the past (Mazurek et al. 2006 considered the maximum burial to be about 1'000 m deeper than the current position throughout the investigation area) and/or an effect of decompaction that is expressed more intensely at shallow positions of the Opalinus Clay. Calculated decompaction curves (Nagra 2014) fit well with the trend of the measured data. In any case, the dependence of porosity on clay-mineral content (Fig. 2-28) is more substantial than the variability with depth.
- The most substantial data sets pertinent to porosity are available for Mont Terri BDB-1 and Schlattingen-1. As shown in Fig. 2-28, water-loss porosity correlates positively with clay-mineral content, but the correlation lines are different for the two sites. For a given clay-mineral content, porosity is higher at Mont Terri. As discussed above, this is due to different maximum burial depths or to effects related to decompaction. The clay-rich sub-unit and the mixed clay-silt-carbonate sub-unit have the highest, and the carbonate-rich silty sub-unit have the lowest porosity.
- Given the fact that sub-units within the Opalinus Clay occur at different depths in different boreholes, bulk-density and porosity data include the combined effects of mineralogy and the depth location. It is therefore not useful to merge the available data from sub-units at different locations. For Mont Terri BDB-1, the data set is sufficient to explore the porosities of individual sub-units, as illustrated in Fig. 2-29. The highest porosities (and clay-mineral contents) are found in the mixed clay-silt-carbonate and clay-rich sub-units, while the carbonate-rich silty sub-unit has by far the lowest porosity.
- The different methods to measure porosity show good agreement. Data obtained from density measurements (pycnometer porosity) yield porosities that are, on the average, 6 %_{rel} higher than water-loss porosities (Fig. 2-30, left). The discrepancy may be explained by the fact that pore water is not completely removed at 105 °C, which is the standard temperature used to measure water content. Porosities obtained from isotope diffusive exchange experiments are 13 %_{rel} higher than water-loss porosities (Fig. 2-30, right).
- The correlation between clay-mineral content with BET surface area (Fig. 2-31) is better than that with porosity. The slope of the correlation is similar for all sub-units.
- Cation-exchange capacity, expressed as the consumption of the index cation Ni, shows fair correlations with clay-mineral content and water-loss porosity.

Tab. 2-10: Petrophysical parameters of the Opalinus Clay

Sub-unit		Bulk wet density [g/cm ³]	Bulk dry density calc. from bulk wet density [g/cm ³]	Grain density [g/cm ³]	Pycnometer porosity [%]	Wet water content [wt.-%]	Water-loss porosity [%]	Wet water content from isotope diffusive exchange [wt.-%]	Porosity from isotope diffusive exchange [%]	BET surface [m ² /g rock]	Total surface [m ² /g rock]	CEC: Consumption of the index cation [meq/kg rock]
All	Mean	2.488	2.363	2.711	12.98	4.91	12.24	5.57	13.8	24.3	84	116
	Median	2.476	2.347	2.703	13.33	5.01	12.47	5.76	14.2	24.4	88	114
	1 σ	0.039	0.056	0.027	1.70	0.92	2.12	1.04	2.3	6.1	21	10
	No.	61	61	123	61	83	83	54	54	63	11	8
Mont Terri BDB-1	Mean	2.475	2.345	2.706	13.34	5.17	12.8	5.88	14.4	21.2		¹⁾
	Median	2.472	2.335	2.703	13.61	5.52	13.6	6.18	15.1	22.0		
	1 σ	0.030	0.045	0.014	1.37	0.94	2.2	1.06	2.4	5.8		
	No.	37	37	52	37	43	43	28	28	24		
Lausen	Mean	2.457	2.316	2.709	14.48	5.74	14.2	6.17	15.1	24.6		126
	Median	2.453	2.314	2.710	14.56	5.54	13.7	6.06	14.8	24.3		126
	1 σ	0.034	0.045	0.011	1.63	0.60	1.3	0.61	1.4	1.9		16
	No.	8	8	8	8	8	8	8	8	6		2
Schafis- heim	Mean			2.717						27.8		
	Median			2.695						28.0		
	1 σ			0.041						0.8		
	No.			8						5		
Riniken-1	Mean			2.712						31.8		
	Median			2.711						32.0		
	1 σ			0.017						4.0		
	No.			12						4		
Weiach-1	Mean			2.684						32.8		
	Median			2.689						32.5		
	1 σ			0.032						2.0		
	No.			15						6		
Benken	Mean			2.723		4.44	11.2	5.55	13.7	24.2	77	114
	Median			2.724		4.64	11.7	5.84	14.3	26.7	90	114
	1 σ			0.014		0.77	1.9	0.73	1.7	10.4	33	6
	No.			12		16	16	4	4	4	4	3
Schlat- tingen-1	Mean	2.535	2.427	2.739	11.38	4.24	10.8	4.61	11.7	22.7	88	110 ²
	Median	2.534	2.421	2.744	11.51	4.23	10.9	4.70	11.8	23.3	88	111
	1 σ	0.018	0.022	0.035	1.25	0.35	0.8	0.55	1.3	3.5	12	9
	No.	16	16	16	16	16	16	14	14	14	7	3

"No." = number of data points

¹ Data are available from various other locations at Mont Terri but not from borehole BDB-1.² One sample from Mäder & Waber (2017) was added to the data reported by Mazurek (2017). Another 6 measurements given in Wersin et al. (2013) are not included because they were obtained by the Co-hex method, which is not directly comparable to the Ni-en method on which all listed data are based (see Hadi et al. 2019 for details).

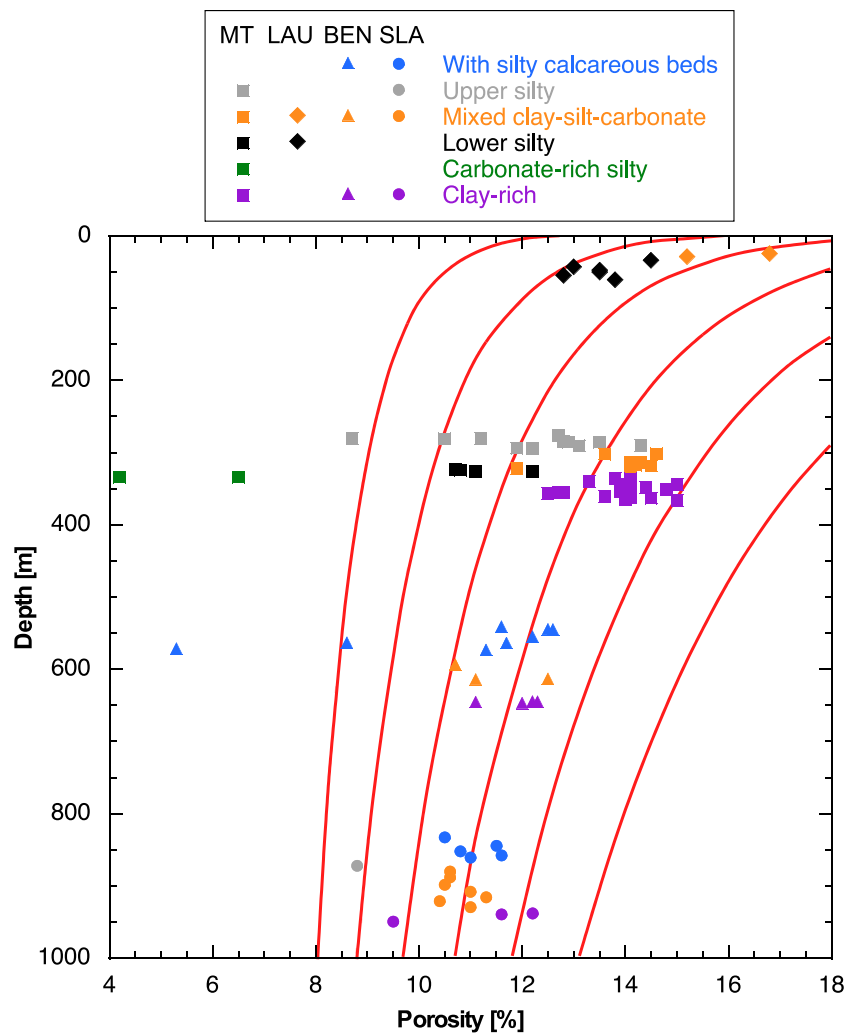


Fig. 2-27: Water-loss porosity of the Opalinus Clay in different boreholes as a function of current depth

Red lines represent the decompaction behaviour of the Opalinus Clay according to different rock-mass models. Left curve is for intact rock mass (matrix only), the other curves represent progressively weaker rock mass due to the presence of discrete discontinuities (from Nagra 2014).

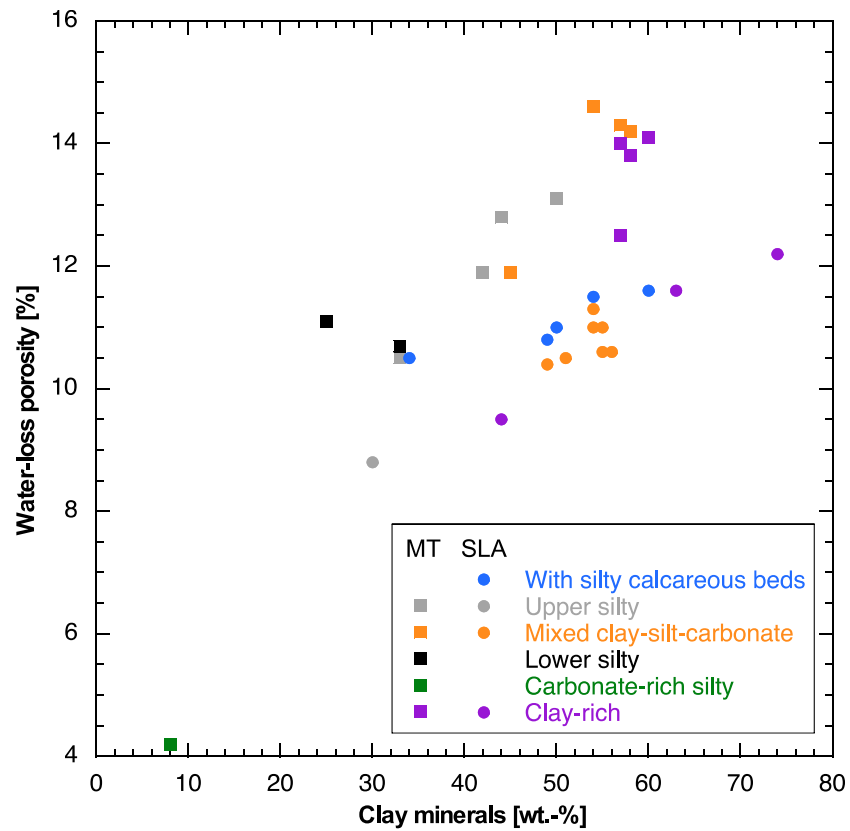


Fig. 2-28: Water-loss porosity of lithologic sub-units at Mont Terri and Schlattingen-1 as a function of clay-mineral content

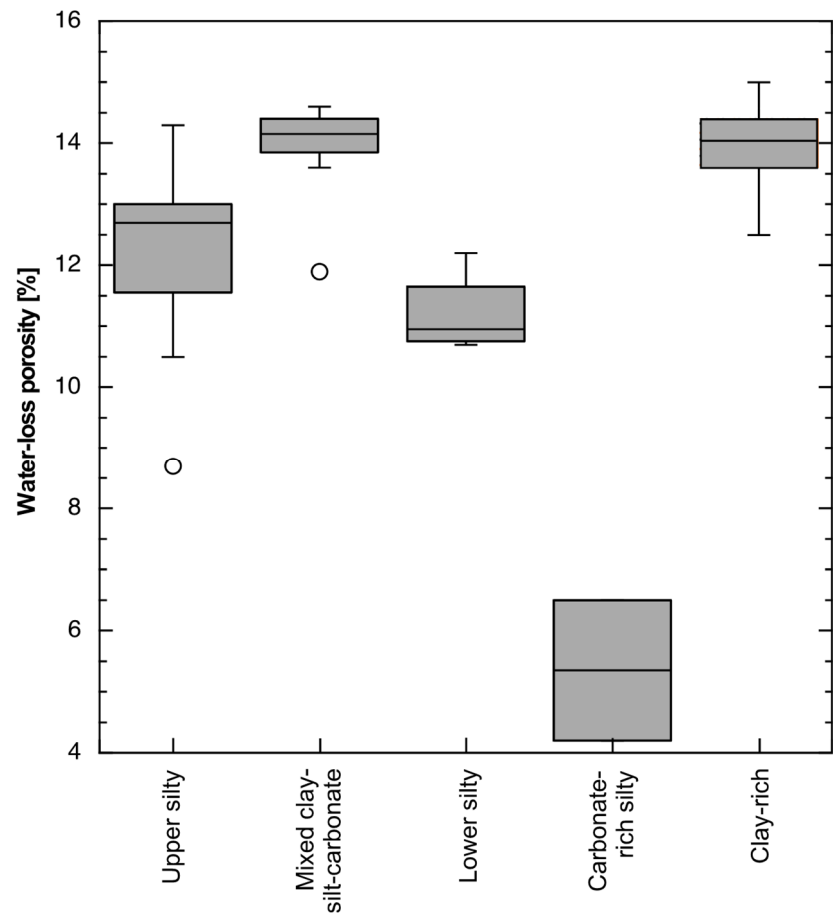


Fig. 2-29: Water-loss porosity of sub-units at Mont Terri BDB-1

Each box shows the median and the lower and upper quartiles. Vertical lines indicate range $\pm 1.5 \times (\text{upper quartile} - \text{lower quartile})$. Data outside this range are shown by circles.

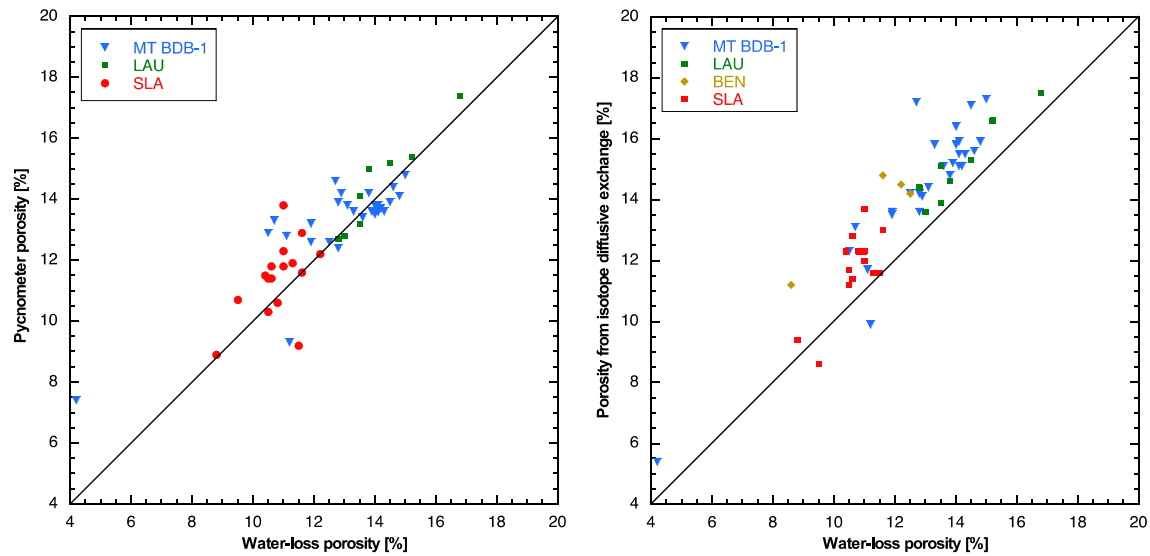


Fig. 2-30: Comparison of porosity data obtained by different methods

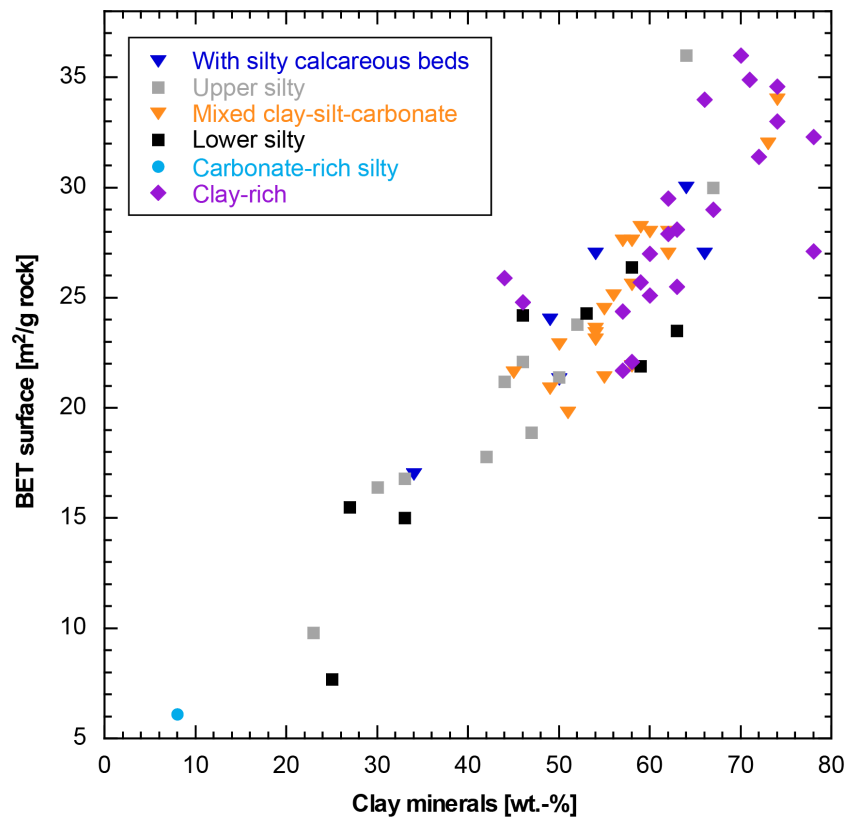


Fig. 2-31: External surface (BET method) as a function of clay-mineral content

3 Texture and diagenesis of the Opalinus Clay and its confining units

The objective of this chapter is to provide a general overview of the diagenetic history of the Opalinus Clay. This includes descriptions of the various diagenetic minerals, textures and their spatial distribution within the region of interest (Sections 3.2 – 3.6), the relative temporal sequence of mineral precipitation and the relationship of mineral precipitation to various stages of diagenesis (i.e. eo- and mesogenesis; Section 3.7), as well as the effects of diagenesis and compaction on porosity and permeability of the rock (Section 3.8).

Studies pertinent to diagenesis in clay-rich lithologies are rather challenging. This is mainly due to the nanometric pore-space architecture of clay-mineral aggregates, where cementation generally does not occur and/or is not resolvable by optical and SEM techniques. However, cementation may occur in more calcareous domains of the rock. During diagenesis, clay-rich lithologies lose their originally high porosity mainly by mechanical compaction, by reorientation of clay platelets, as well as by recrystallisation of clay minerals if temperature is high enough. In contrast, porosity loss by cementation does not play a major role (Bläsi 2002). This study does not strictly focus on the diagenesis of the Opalinus Clay alone but also includes the more calcareous and/or silty confining units, in which diagenetic features are more strongly expressed (see e.g., Burley & Worden 2003).

Diagenetic mineralisation in the rock matrix is described separately from that in veins. This is mainly because matrix mineralisation is considered to be of regional extent, whereas vein mineralisation potentially depends on the local tectonic history.

3.1 Data base

Information on petrography and diagenesis of the Opalinus Clay and its confining units is documented in a variety of reports and publications. Additionally, new thin-section investigations were conducted. The localities for which literature is available and thin sections were analysed are listed in Tab. 3-1. The locations of the sites are documented in Tab. 2-1 (coordinates) and in Fig. 2-1 (map). For the boreholes at Schafisheim and Weiach-1, the only information available is on vein mineralisation, and no data pertinent to diagenesis are available for the borehole at Lausen.

Boreholes Berlingen-1, Herdern-1, Kreuzlingen-1 and Lindau-1 were drilled by SEAG in the period 1962 – 1982 for hydrocarbon exploration. Given the thick Molasse overburden, the Mesozoic in these boreholes occurs at deeper levels and also experienced a higher maximum burial depth and temperature during diagenesis. The centre of the Opalinus Clay is located at 1'788 – 2'222 m below surface, i.e. more than 1000 m deeper in comparison to most of the other boreholes. Given the fact that the diagenetic evolution of the Mesozoic from these four boreholes is similar (Bläsi et al. 1996), these will be called "SEAG boreholes in Northeastern Switzerland" in the following.

Tab. 3-1: Investigated sites and literature references

Locality	Units	Literature references	New thin-section investigations
Mont Terri URL	Opalinus Clay	Bläsi et al. (1991), Pearson et al. (2003), Peters et al. (2011), Lerouge et al. (2015), Mazurek & de Haller (2017)	Yes (borehole BWS-1)
Schafisheim	Opalinus Clay	Nagra (1992)*	No
Bözberg SB 2/13	Opalinus Clay	-	Yes
Riniken-1	Opalinus Clay	Nagra (1990)*, Lerouge (2016)	No
Weiach-1	Opalinus Clay	Nagra (1989)*, Waber & Schürch (1999)*	No
Benken	Opalinus Clay	Langer et al. (2001), Bläsi (2002), Lerouge et al. (2014)	Yes
Schlattingen-1	Opalinus Clay, confining units	Wersin et al. (2013), Mazurek et al. (2018)	No
Lindau-1	Confining units	Bläsi et al. (1996), Bläsi et al. (1999)	No
Herdern-1	Confining units	Bläsi et al. (1996), Bläsi et al. (1999)	No
Berlingen-1	Confining units	Bläsi et al. (1996), Bläsi et al. (1999)	Yes
Kreuzlingen-1	Confining units	Bläsi et al. (1996), Bläsi et al. (1999)	No
Meersburg-1	Confining units	Bläsi et al. (1996), Bläsi et al. (1999)	No

* Exclusively information on vein mineralisation

3.2 Bioturbation

Bioturbation refers to churning and reworking of soils and sediments by animals or plants. In marine sediments, the activity of organisms is commonly restricted to the uppermost metre below the water/sediment interface, while laterally it may cover an area of tens to hundreds of square kilometres (Gingras & Smith 2015). Bioturbation manifests itself in a wide range of structures of various shapes, sizes and complexity depending on the type of organism, activity and substrate. In marine sediments, typical structures are burrows, tracks, trails, mounds and pellets. Such structures often disrupt bedding and layering, potentially affect the mobility of early diagenetic fluids and alter both porosity and permeability of the sediment.

In the case of the Opalinus Clay, information on bioturbation and its effect on rock properties is rather sparse. A study by Lauper et al. (2018) quantified bioturbation in the Opalinus Clay at Mont Terri (drillcore BDM-B2) by using the scheme of Lazar et al. (2015). Accordingly, based on visual inspection of the drill core, a bioturbation index of 0 to 5 was assigned to the various sub-units of the Opalinus Clay: 0 indicates "not bioturbated" – i.e. no visible burrows and all sedimentary structures preserved, whereas 5 indicates "churned" – i.e. bedding completely obliterated, rock fully homogenised and individual burrows difficult to recognise. Lauper et al. (2018) determined bioturbation indices of 3 – 5 for the silty, 2 – 5 for the carbonate-rich silty and 1 for the clay-rich sub-unit (Fig. 3-1). While no detailed studies are available for the Northeastern part of the study area, the textures are analogous at least in qualitative terms, so similar degrees of bioturbation appear likely.

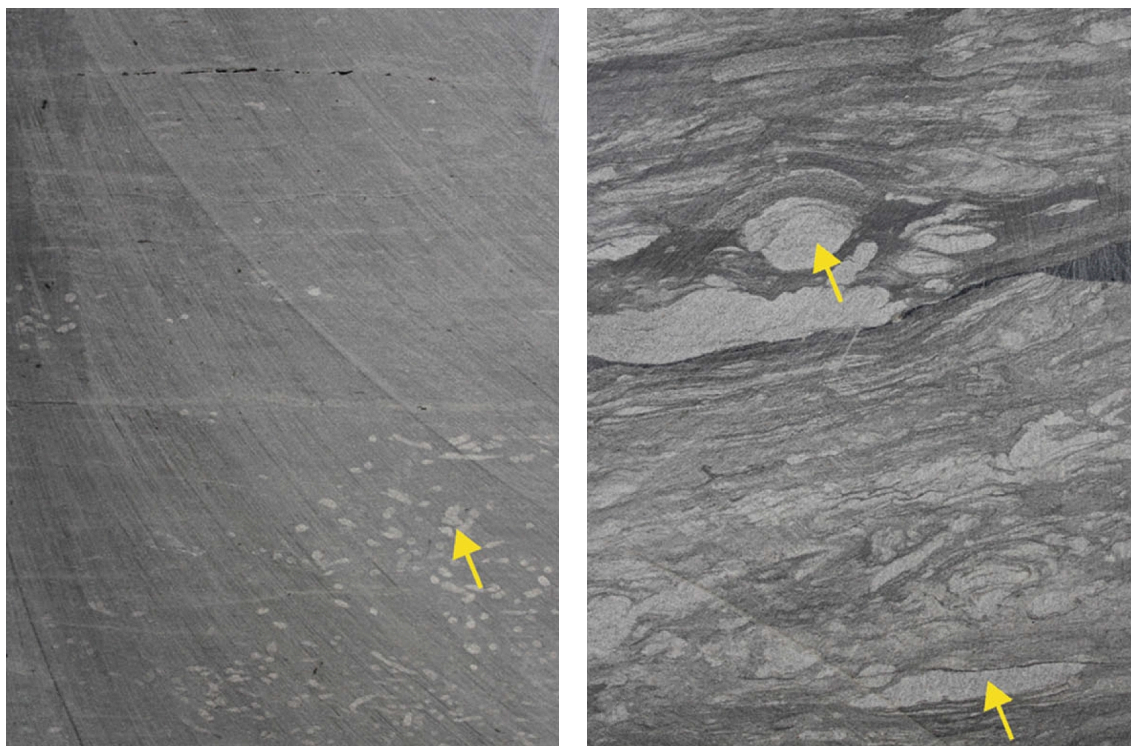


Fig. 3-1: Textures related to bioturbation in the Opalinus Clay at Mont Terri

Left: Lens-shaped bioturbational structures (shown by arrow) in the clay-rich sub-unit. Right: Intense bioturbation (shown by arrows) in the silty sub-unit. Width of pictures is 8 cm. Lauper et al. (2018)

3.3 Diagenetic minerals in the rock matrix

Tab. 3-2 below lists the regional occurrence of the identified diagenetic minerals. In this Section, these are described in chronological order, i.e. according to their relative timing of precipitation. However, textural relationships are not always available and sufficiently clear to allow the definition of an unequivocal time sequence. Thus, uncertainties exist in the chronology of mineralisations, so the sequence presented here is a rough guideline that is further discussed in Section 3.7.

3.3.1 Aragonite/Mg-calcite

Known occurrences in the Opalinus Clay: Mont Terri (Peters et al. 2011), Bözberg SB 2/13, Benken (Bläsi 2002). *Known occurrences in the confining units:* Benken (Staffelegg Fm., Klettgau Fm.; Langer et al. 2001), Schlattigen-1 ('Brown Dogger', Staffelegg Fm.; Wersin et al. 2013), SEAG boreholes in Northeastern Switzerland ('Brown Dogger', Staffelegg Fm., Klettgau Fm.; Bläsi et al. 1996; Tab. 3-2).

In the still soft sediment, fibrous aragonite and Mg-calcite grew around bioclasts, thus supporting one another. However, both minerals are metastable and have been completely replaced by more stable blocky calcite I cement during diagenesis (see Section 3.3.4). Accordingly, the only evidence of their existence are the characteristic fibrous and short prismatic crystal shapes of calcite I cement surrounding bioclasts (Fig. 3-2). Quantitatively, aragonite /Mg-calcite is of minor importance.

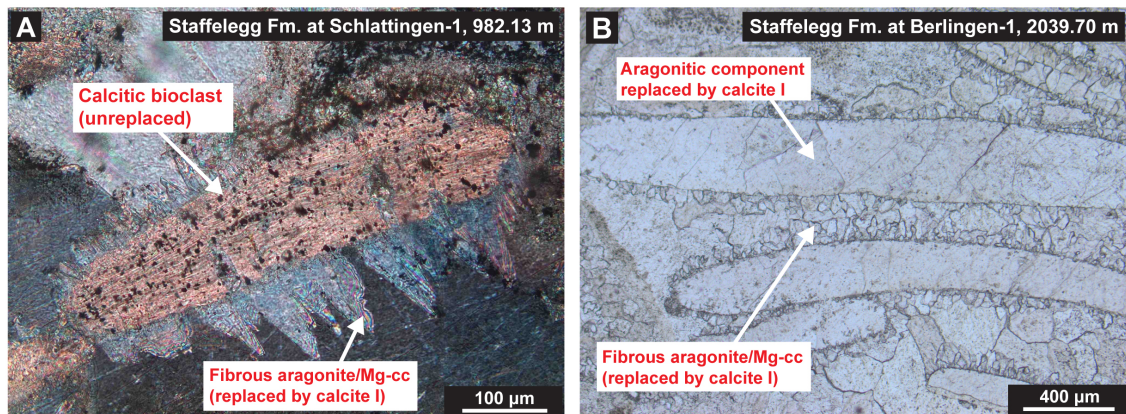


Fig. 3-2: Early diagenetic fibrous aragonite and Mg-calcite surrounding bioclasts

(A) Calcite I replaces early diagenetic, fibrous or short prismatic aragonite or Mg-calcite that grew around calcitic bioclasts (cross polarised, transmitted light microscopy; Wersin et al. 2013). (B) Same features as in (A) but fibrous aragonite/Mg-calcite grew around an aragonitic bioclast. Both bioclast and cement have been replaced by calcite I (plane polarised, transmitted light microscopy)

3.3.2 Pyrite I

Known occurrences: all investigated sites in the Opalinus Clay and its confining units (Tab. 3-2).

According to Tab. 2-6, the average pyrite content (including the contribution of accessory pyrite II, see below) in the Opalinus Clay is 1.1 wt.-%. Pyrite I is commonly associated with early carbonate cements and occurs as massive pyrite concretions, framboids (disseminated isolated framboids or several agglomerated framboids; Fig. 3-3A), as single euhedral grains disseminated within the rock matrix (or in bioturbations; Fig. 3-3B) and as replacement of fossil calcite/aragonite structures (Fig. 3-3C; Bläsi et al. 1996, Wersin et al. 2013). Framboidal pyrite forms due to bacterial sulphate reduction (BSR) within the uppermost 1 – 5 m of the soft sediment. The textural relationship of framboidal pyrite with respect to the disseminated single crystals of pyrite or with respect to the pyrite that replaces fossil calcite/aragonite structures is not clear.

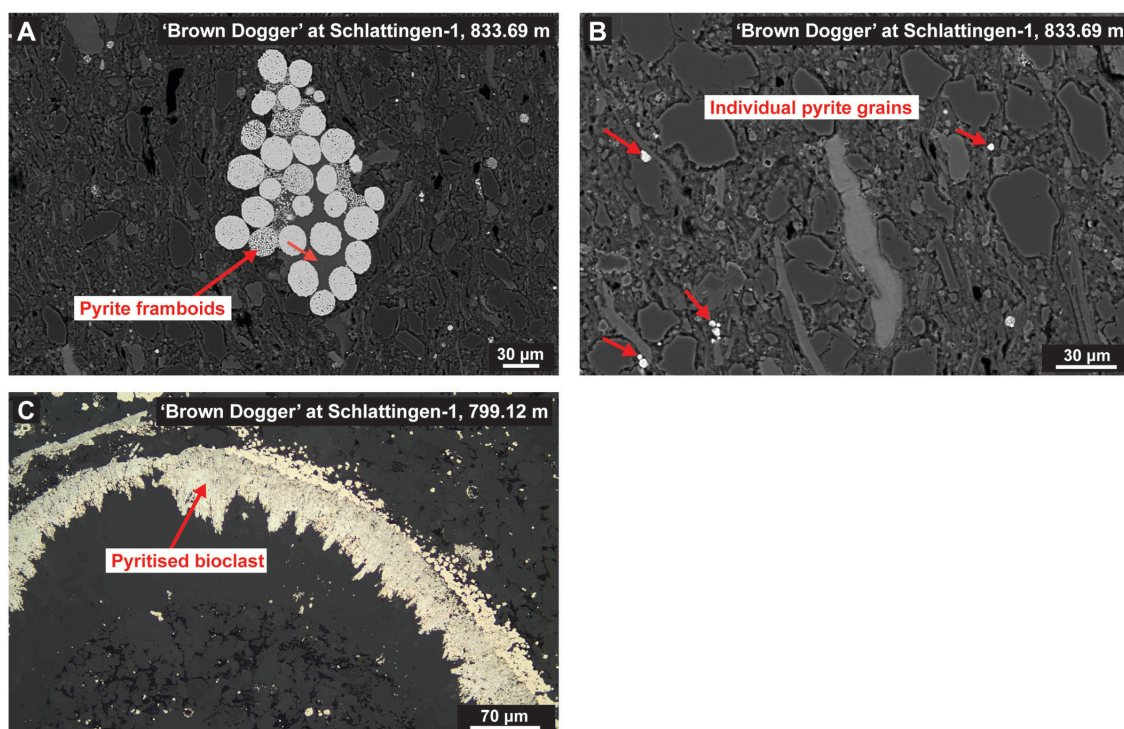


Fig. 3-3: Occurrence and textures of diagenetic pyrite I

Diagenetic pyrite I occurs as (A) agglomerated framboids, (B) individual grains or framboids disseminated in the rock matrix or (C) replacing bioclasts (A,B: SEM-BSE images; Wersin et al. 2013; C: reflected-light microscopy; Wersin et al. 2013).

3.3.3 Siderite

Known occurrences: all investigated sites in the Opalinus Clay and its confining units (Tab. 3-2).

Siderite constitutes a major diagenetic mineral in the Opalinus Clay and its confining units. According to Tab. 2-6, the average siderite content in the Opalinus Clay is 3.5 wt.-%, and it shows a variety of different textures:

- *Concretions* of variable size, ranging from <mm-sized clusters that are the predominant siderite texture at Riniken-1 and at Mont Terri (Lerouge 2016), to centimetric yellowish concretions elongated along the bedding, well documented for boreholes Benken (Fig. 3-4A; Lerouge et al. 2014, Lerouge 2016) and Schlattigen-1 (Wersin et al. 2013). Both types of concretions consist of agglomerated µm-sized subhedral–euhedral siderite crystals (Fig. 3-4B; Lerouge et al. 2015).

Siderite concretions constitute early diagenetic products that form during shallow burial of the still unconsolidated sediment, preferably within the first tens of metres (Blome & Albert 1985, Pye et al. 1990, Mozley 1996, Raiswell & Fisher 2004). The growth of the concretions either proceeds concentrically or pervasively (e.g. Coleman et al. 1985, Mozley 1996, Raiswell & Fisher 2004, Loyd et al. 2014). In the former case rigid, fully cemented layers are added to the outer surface of the concretion, whereas during pervasive growth, siderite crystals grow simultaneously throughout the entire volume of the concretion. The two models result in distinctly different mineralogical, isotopic and element geochemical

trends across the concretions. Siderite concretions in the Opalinus Clay have not been investigated in great detail and so no reliable statements about their style of growth can be made.

The trigger for the precipitation of authigenic siderite is considered to be microbial decomposition of organic matter under anoxic conditions. The most important biogeochemical processes are (1) dissimilatory ferric iron reduction, (2) bacterial sulphate reduction, and (3) methanogenesis (Baumann et al. 2016 and references therein). Siderite precipitation in the Opalinus Clay occurs only once dissolved sulphate in the pore water has been consumed by precipitation of pyrite I, which constitutes the thermodynamically favoured pool for reduced iron.

Regardless of the processes triggering siderite precipitation, concretions only form in discrete zones of the sediment. Accordingly, siderite supersaturation may occur uniformly throughout the entire sediment but concretions only form where nuclei (e.g. biogenic components) are present ("equilibrium model" by Raiswell & Fisher 2000). However, the majority of documented siderite concretions lack nuclei (Baumann et al. 2016 and references therein). Alternatively, siderite supersaturation may be spatially heterogeneous caused by localised biogeochemical activity resulting from a heterogeneous distribution of organic matter ("local-equilibrium model" of Raiswell & Fisher 2000). Siderite concretions in the Opalinus Clay are not known to contain any nuclei (at least macroscopically), which indicates that the variable amounts and sizes of siderite concretions observed at the different sites across the study area could result from local differences in the availability of organic matter.

- *Finely disseminated, crystals (< 10 µm)* in the rock matrix.
- *Hollow siderite* consists of idiomorphic crystals with a near-circular cavity in the centre. Often, this cavity is filled with Mg-rich carbonate (Fig. 3-4C; Wersin et al. 2013). It is not exactly known whether hollow siderite represents a separate siderite type or whether it may be part of e.g. concretions.
- *Polycrystalline siderite coronas* form agglomerations lining the walls of µm-sized cavities in the rock matrix. Often these cavities are filled with dolomite I (Fig. 3-4D; Wersin et al. 2013). Hollow siderite and siderite coronas are documented for the 'Brown Dogger' at Schlattingen-1 (Wersin et al. 2013) and for the Opalinus Clay at Mont Terri (Lerouge et al. 2015).

Lerouge et al. (2015) analysed the chemical composition of siderite in samples from Mont Terri (borehole BDB-1) and from Schlattingen-1 by electron microprobe (EPMA). Samples originated from both the Opalinus Clay and the confining units. The results, discussed in more detail in Section 3.5, show that siderite from concretions or siderite-rich layers is Ca-poor and Fe-rich, whereas disseminated siderite or siderite from coronas is Ca- and Mg-rich. Accordingly, these textural types constitute different generations that are not coeval.

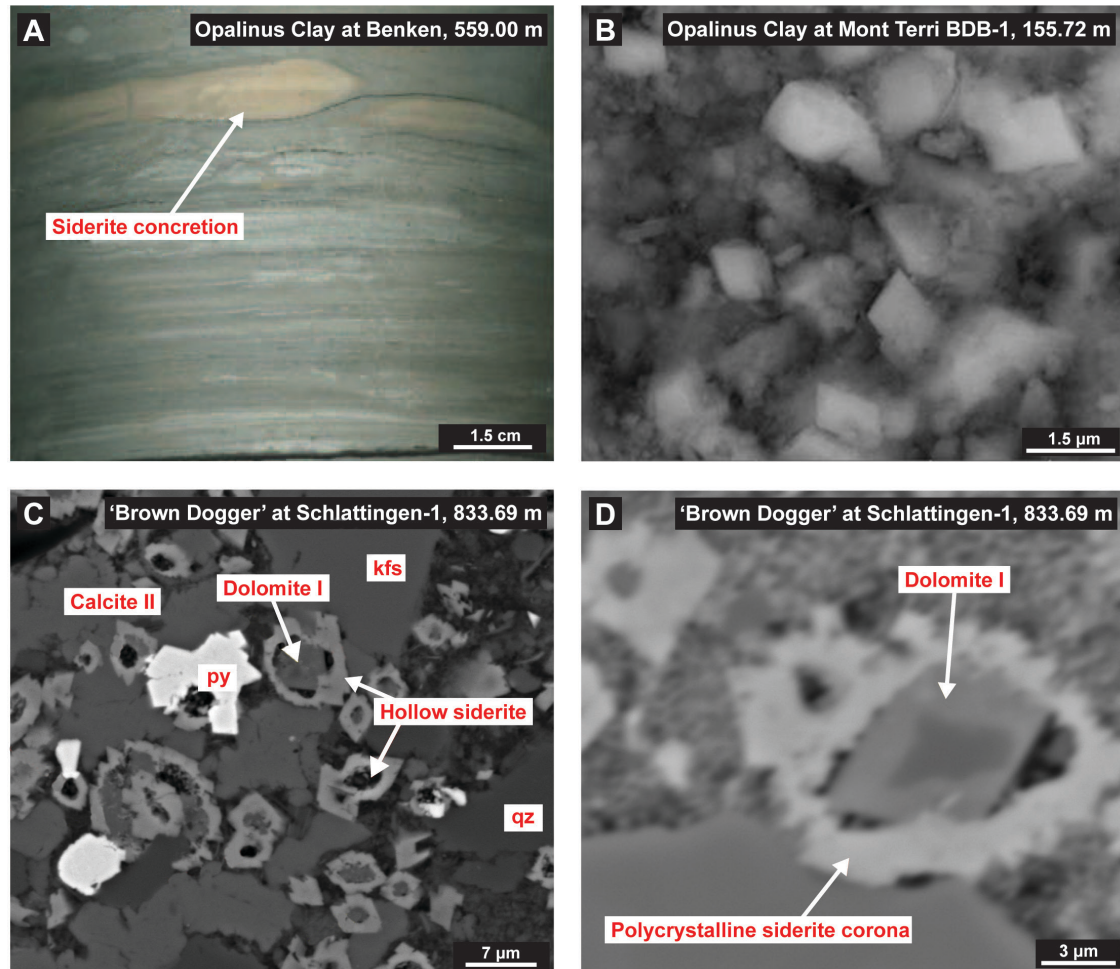


Fig. 3-4: Occurrence and textures of diagenetic siderite

(A) Macroscopic siderite concretion consisting of μm -sized, agglomerated, subhedral-euhedral siderite crystals shown in (B). (C) Idiomorphic hollow siderite with Mg-rich carbonate filling the central cavity. (D) Polycrystalline siderite coronas lining the walls of μm -sized cavities in the rock matrix. Often dolomite I fills such cavities (A: reflected light photograph of drill core; Lerouge et al. 2014; B: SEM-BSE image; Lerouge et al. 2015; C & D: SEM-BSE images; Wersin et al. 2013).

3.3.4 Calcite I

Known occurrences in the Opalinus Clay: Mont Terri (Peters et al. 2011), Bözberg SB 2/13, Riniken-1, Benken (Bläsi 2002). *Known occurrences in the confining units:* Benken (Staffelegg Fm., Klettgau Fm.; Langer et al. 2001), Schlattigen-1 ('Brown Dogger', Staffelegg Fm.; Wersin et al. 2013), SEAG boreholes in Northeastern Switzerland ('Brown Dogger', Staffelegg Fm., Klettgau Fm.; Bläsi et al. 1996; Tab. 3-2).

Iron-bearing calcite I represents a minor to major diagenetic phase, which occurs as blocky cement replacing the early fibrous cements and filling empty pore space. It is particularly frequent in beds enriched in bioclastic components (i.e. mainly aragonitic) and poor in clay matrix. The development and spatial distribution of such bioclastic beds is detailed in Section 2.3.2. Early diagenetic dissolution of the bioclasts (< 100 m overburden; Bläsi 2002; see Section 3.7) is considered to have provided the solutes for cement precipitation (Fig. 3-5).

Lerouge et al. (2014, 2015) and Lerouge (2016) documented calcite cement in the Opalinus Clay at Benken, Riniken-1 and at Mont Terri. This calcite occurs as rare euhedral crystals disseminated in the rock matrix. Considering the differences in texture and occurrence, it is unclear whether it genetically corresponds to the one described above. However, what the two calcite cements have in common is that they postdate aragonite/Mg-calcite but predate calcite II, which represents a main phase of carbonate cementation in the Opalinus Clay and its confining units and which occurs at all investigated sites (see Section 3.3.15).

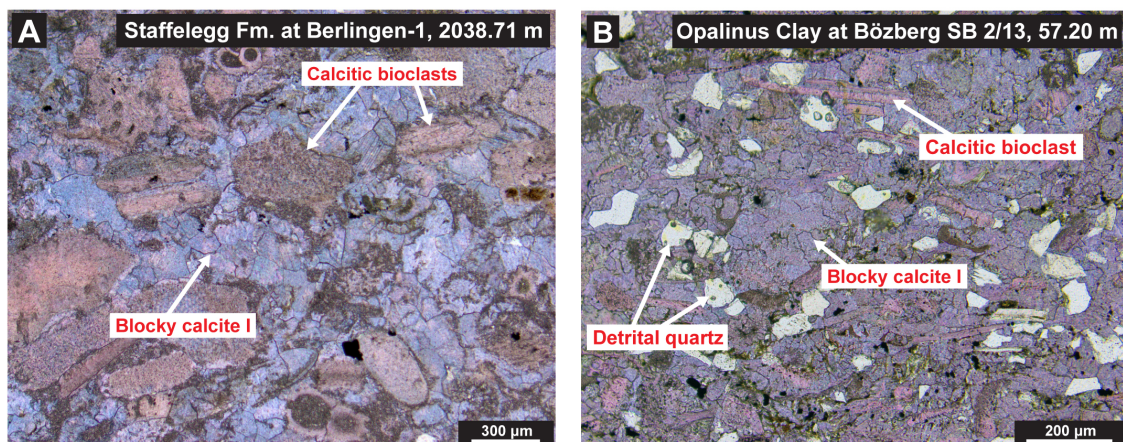


Fig. 3-5: Occurrence and textures of diagenetic calcite I

(A, B) Diagenetic calcite I (blue) mainly occurs as blocky cement in bioclast-rich rock domains where it replaces early fibrous aragonite/Mg-calcite cements and fills the interparticle pore space, as well as moulds left by the dissolution of aragonitic bioclasts (A,B: plane polarised, transmitted light microscopy).

3.3.5 Limonite

Known occurrences in the Opalinus Clay: Mont Terri (Bläsi et al. 1991). *Known occurrences in the confining units:* Benken (Staffelegg Fm.; Langer et al. 2001), Schlattingen-1 ('Brown Dogger'; Wersin et al. 2013).

Limonite is a collective term for hydrous Fe-oxides and includes various phases, such as goethite or jarosite. In the Opalinus Clay and its confining units, limonite is observed in distinct stratigraphic horizons, typically hardgrounds or Fe-oolites, where it gives a yellowish colour to the rock (Fig. 3-6; Bläsi pers. comm.). On the basis of X-ray diffraction, Wersin et al. (2013) found that the colour of the condensation horizon constituting the Anceps-Athleta- and Macrocephalus-Schichten (top Dogger) in Schlattingen-1 is due to the presence of 8 wt.-% goethite. Goethite is thought to have formed very shortly after deposition within only a few centimetres below the seafloor, just before the redox conditions turned reducing and pyrite I started to precipitate (see Section 3.3.2).

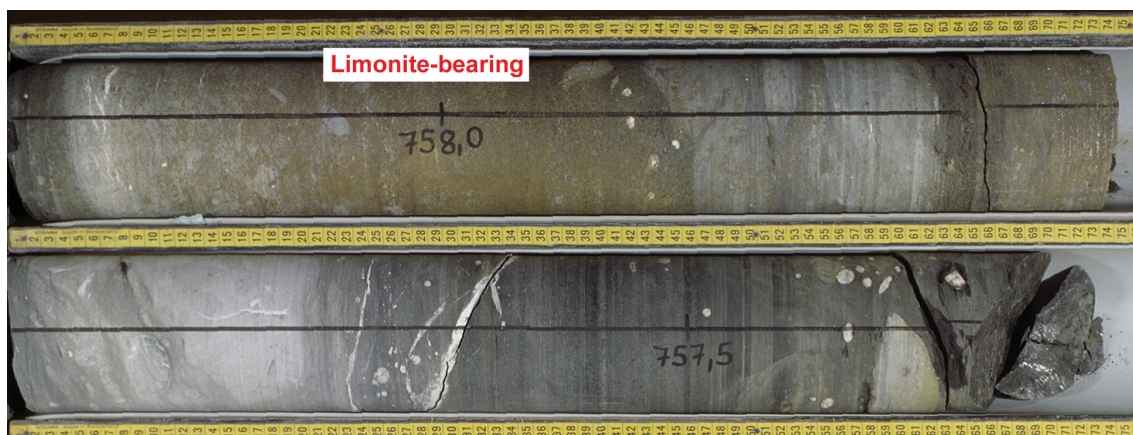


Fig. 3-6: Occurrence of limonite in the Schlattingen-1 core
Depth range 757.0 – 758.5 m, Anceps-Athleta- and Macrocephalus-Schichten

3.3.6 Glauconite

Known occurrences in the Opalinus Clay: Mont Terri (Bläsi et al. 1991), Riniken (Lerouge 2016), Benken (Lerouge et al. 2014; Tab. 3-2).

Glauconite constitutes an accessory mineral phase and occurs as greenish pellets in clay-rich layers (Fig. 3-7).

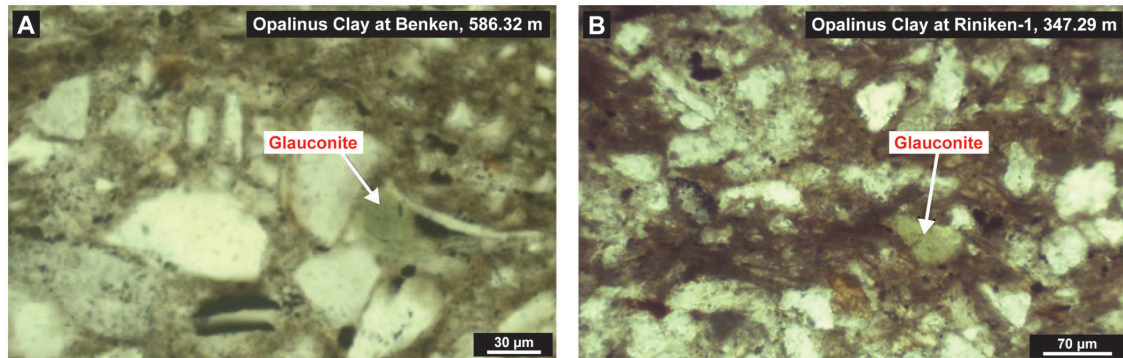


Fig. 3-7: Occurrence and texture of diagenetic glauconite

(A, B) Glauconite occurs as green pellets in clay-rich layers (A: plane polarised, transmitted light microscopy; Lerouge et al. 2014, Lerouge 2016)

3.3.7 Ti-oxides

Known occurrences in the Opalinus Clay: Mont Terri (Pearson et al. 2003, Lerouge et al. 2015). *Known occurrences in the confining units:* Schlattingen-1 ('Brown Dogger'; Wersin et al. 2013), SEAG boreholes in Northeastern Switzerland ('Brown Dogger' and Staffelegg Fm.; Bläsi et al. 1996; Tab. 3-2).

Ti-oxides (e.g. anatase or brookite) constitute an accessory phase in the Opalinus Clay and in its confining units (Fig. 3-8). However, it is not entirely clear whether all the observed Ti-oxides grew diagenetically or whether they have at least partially a detrital origin (Wersin et al. 2013).

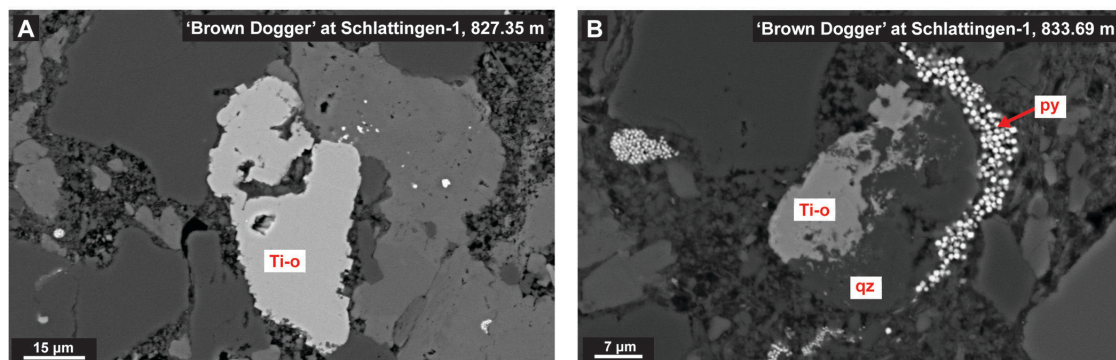


Fig. 3-8: Occurrence and texture of Ti-oxide

(A) Ti-oxide occurs as rare rounded or irregularly-shaped grains disseminated in the rock matrix or (B) inter-grown with quartz (A,B: SEM-BSE images; Wersin et al. 2013)

3.3.8 Dolomite I

Known occurrences: all investigated sites in the Opalinus Clay and its confining units (Tab. 3-2).

Abundance and texture of dolomite I vary over the area of investigation. At Riniken-1 it constitutes an accessory phase, whereas at the other sites it represents a minor to major cementation event (Tab. 3-2). Generally, it either occurs (1) as poikilitic cement filling the interparticle pore space in silty lenses (Fig. 3-9A), (2) replacing blocky calcite I in bioclastic areas (Fig. 3-9B; Bläsi pers. comm.) or (3) as disseminated or agglomerated euhedral crystals (predominantly occurring in clay lenses in bioclastic areas; Fig. 3-9C). At Schlattingen-1, Benken, Riniken-1 and Mont Terri, the dolomite crystals occasionally show an ankerite rim (Fig. 3-9D; Wersin et al. 2013, Lerouge et al. 2014, Lerouge et al. 2015, Lerouge 2016, Pekala et al. 2018). Individual dolomite crystals in physical contact with calcite I occasionally show solid inclusions of calcite I and indentations along their grain boundaries (Fig. 3-9E), thus again indicating replacement of calcite I.

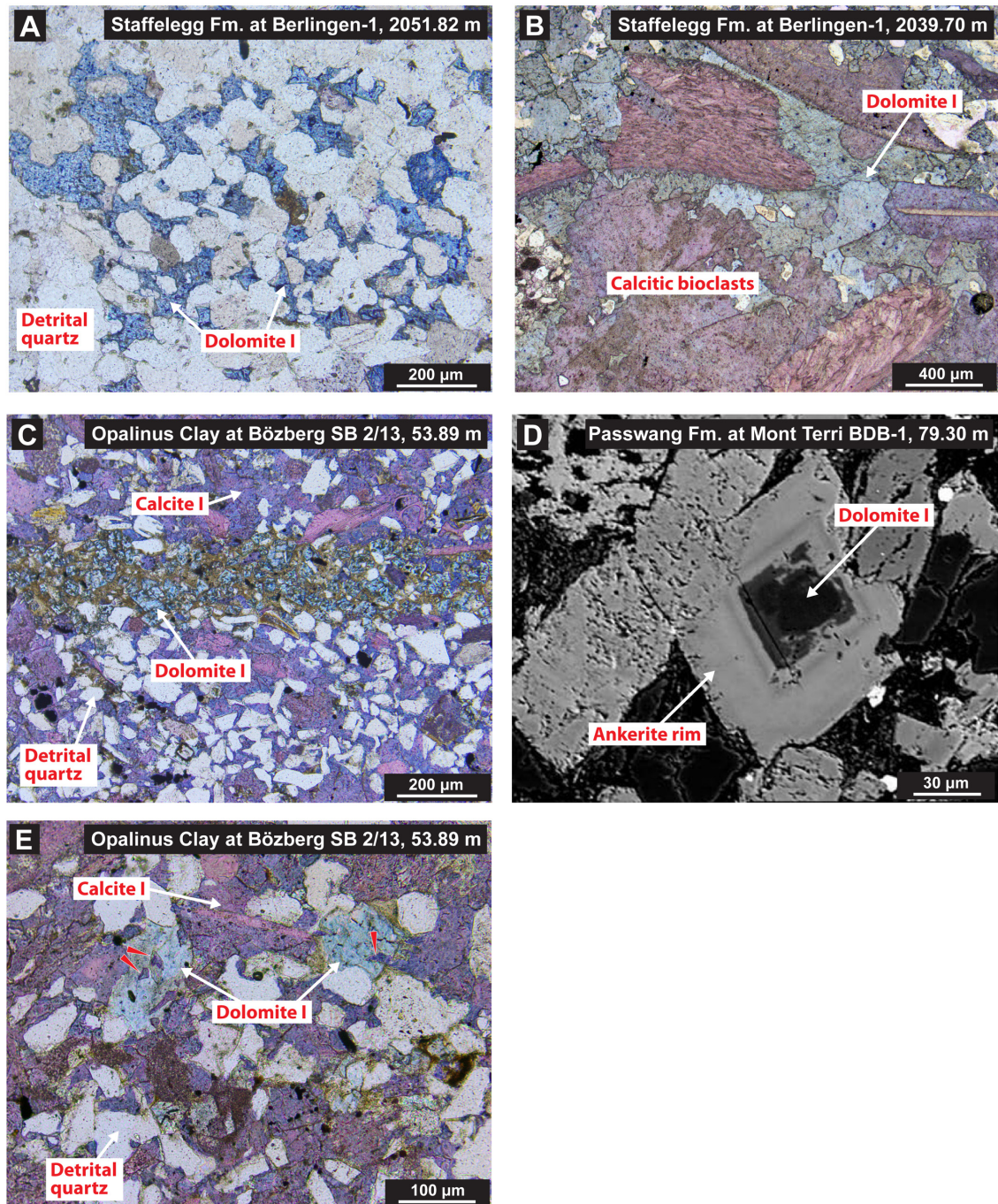


Fig. 3-9: Occurrence and textures of diagenetic dolomite I

Diagenetic dolomite I either occurs as (A) poikilitic cement in silty lenses, (B) replacing blocky calcite I in bioclastic areas or (C) disseminated or agglomerated euhedral crystals in clay lenses. (D) Ankerite growing over dolomite crystal cores. (E) Dolomite crystals in physical contact with calcite I occasionally show solid inclusions of calcite I and indentations (red arrows) along the grain boundaries (A–C & E: plane polarised, transmitted light microscopy; D: SEM-BSE image).

3.3.9 Quartz

Known occurrences in the Opalinus Clay: Mont Terri (Peters et al. 2011), Bözberg SB 2/13, Benken (Bläsi 2002). *Known occurrences in the confining units:* Benken (Klettgau Fm.; Langer et al. 2001), Schlattingen-1 ('Brown Dogger'; Wersin et al. 2013), SEAG boreholes in Northeastern Switzerland ('Brown Dogger', Staffelegg Fm. and Klettgau Fm.; Bläsi et al. 1996; Tab. 3-2).

In both the Opalinus Clay and its confining units, diagenetic quartz predominantly occurs in silty lenses where it constitutes syntaxial overgrowth on detrital quartz grains (Fig. 3-10A; Bläsi 2002, Peters et al. 2011). The onset of this authigenic overgrowth is commonly marked by a distinct line of impurities, i.e. solid grains (e.g. pyrite) or fluid inclusions surrounding the detrital quartz grains.

Whether authigenic quartz formed during diagenesis was mainly controlled by the presence of biogenic components in the silty lenses. Their dissolution during early diagenesis served as a source of solutes for aragonite/Mg-calcite and calcite I cementation that would occlude the pore space, thus leaving no space for later quartz cements. In contrast, in the absence of bioclasts the surfaces of detrital quartz grains remained free for authigenic quartz growth in optical continuity with the detrital grain.

Syntaxial quartz overgrowth is also present when the interparticle pore space was cemented by calcite II and anhydrite, occasionally also when kaolinite filled the pore space (Fig. 3-10A-C). It follows that authigenic quartz predates these diagenetic minerals. In the confining units of the SEAG boreholes in Northeastern Switzerland, the syntaxial quartz cement shows two different growth generations, i.e. a first non-luminescent generation and a second luminescent generation (Fig. 3-10D; Bläsi et al. 1996). Whether this also applies to the Opalinus Clay is not known.

From a quantitative point of view, syntaxial quartz represents an accessory diagenetic mineral phase in the Opalinus Clay (< 1 – 2 vol.-%; Bläsi pers. comm.), whereas in the confining units at the SEAG boreholes in Northeastern Switzerland the amount of quartz cement reaches distinctly higher levels of 5 – 11 vol.-% (Bläsi et al. 1996).

Apart from syntaxial overgrowths on detrital grains, diagenetic quartz sporadically also occurs as microcrystalline aggregates within intergrain pores in the confining units of the SEAG boreholes in Northeastern Switzerland. Finally, a last type of diagenetic SiO₂ is present in the 'Brown Dogger' at Schlattingen-1, where it occurs as replacement (probably chalcedony) of bioclasts.

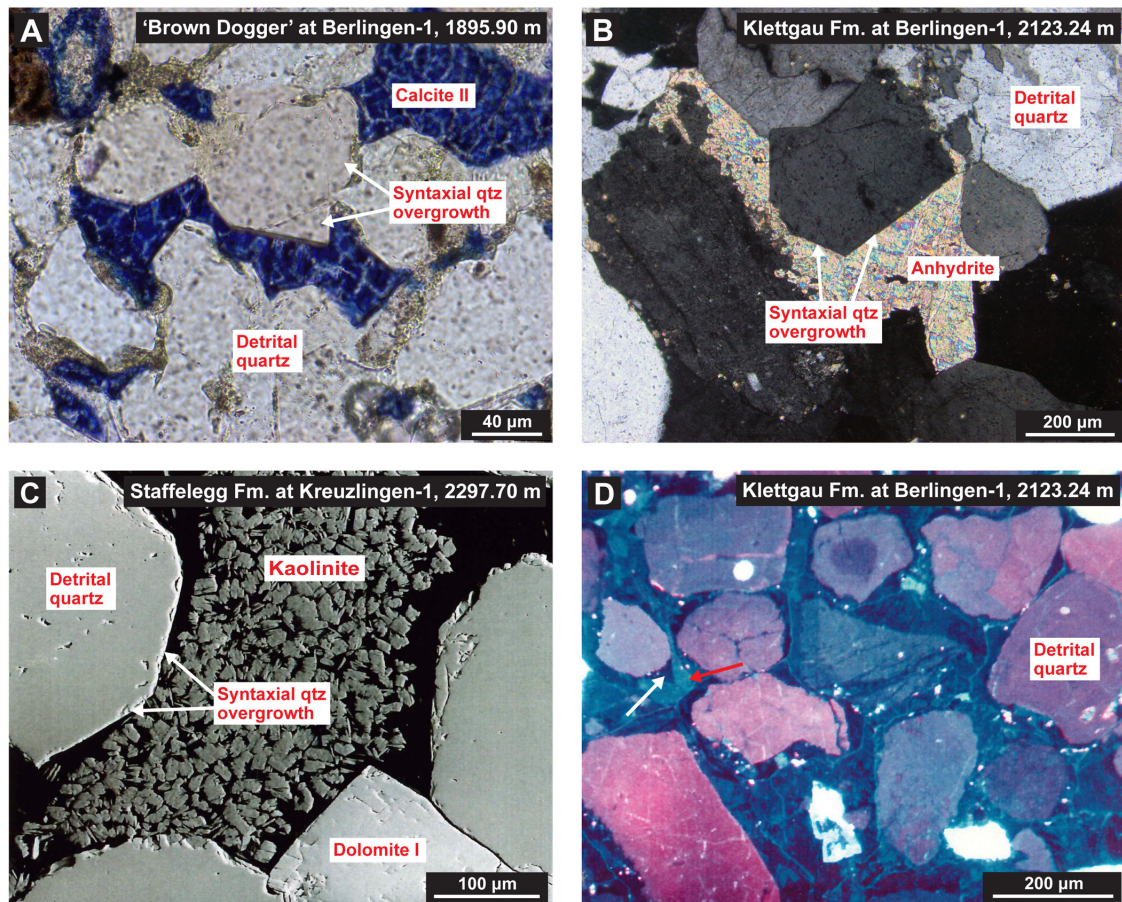


Fig. 3-10: Occurrence and texture of diagenetic quartz

(A) Syntaxial overgrowth of detrital quartz. The interparticle pore space is filled with poikilitic calcite II (plane polarised, transmitted light microscopy). (B) Authigenic quartz overgrowth on detrital quartz grains evidenced by the idiomorphic crystal faces. Diagenetic anhydrite fills the interparticle pore space (cross polarised, transmitted light microscopy). (C) Syntaxial quartz overgrowth in a pore later filled by kaolinite (SEM-BSE image; Bläsi et al. 1996). (D) Detrital quartz (blue and red) totally cemented by authigenic quartz. The first generation of quartz is non-luminescent (white arrow), in contrast to a second generation (red arrow; cathodoluminescence image; Bläsi et al. 1996).

3.3.10 Feldspar

Bläsi et al. (1996) and Bläsi (2002) reported small amounts of diagenetic feldspar as syntaxial cement lining detrital grains for the Opalinus Clay and the Klettgau Fm. at Benken. However, no detailed documentation is available, and more recent studies did not confirm these findings. The presence of considerable amounts of diagenetic kaolinite at Schlattingen-1 (Wersin et al. 2013) and clear petrographic evidence for the dissolution of detrital feldspar in the SEAG boreholes in Northeastern Switzerland (Bläsi et al. 1996) place further question marks on the presence of diagenetic feldspar.

3.3.11 Kaolinite

Known occurrences in the Opalinus Clay: Mont Terri (Peters et al. 2011). *Known occurrences in the confining units:* Schlattingen-1 ('Brown Dogger'; Wersin et al. 2013), SEAG boreholes in Northeastern Switzerland ('Brown Dogger', Staffelegg Fm. and Klettgau Fm.; Bläsi et al. 1996; Tab. 3-2).

Quantitatively, kaolinite is considered to be of minor to major importance. In both the Opalinus Clay and its confining units kaolinite cement is characterised by uncompacted, vermicular hexagonal platelets either filling empty pore space or forming a fine-grained diagenetic matrix between silty and biogenic components, predominantly in clay-poor areas and where carbonate cementation is incomplete (Fig. 3-11).

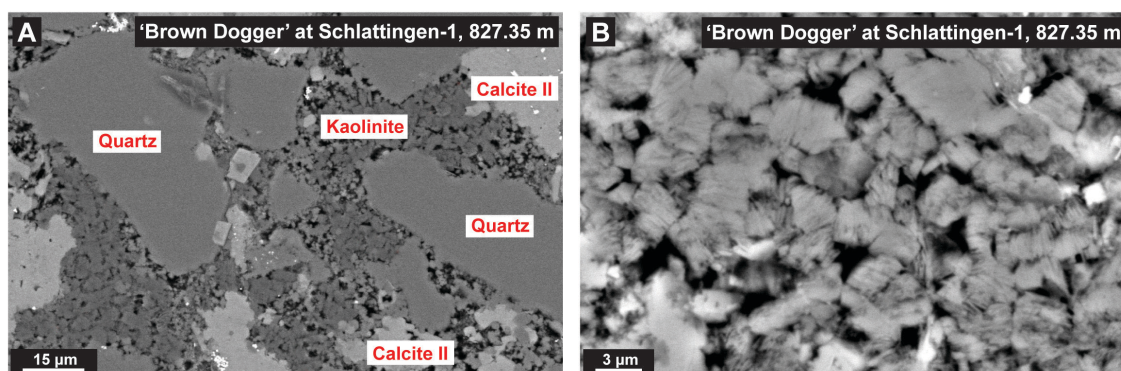


Fig. 3-11: Occurrence and texture of diagenetic kaolinite

(A) Diagenetic kaolinite filling the intergranular pore space between detrital quartz grains. Its texture is characterised by (B) vermicular hexagonal platelets (A,B: SEM-BSE images; Wersin et al. 2013).

3.3.12 Pyrite II

Known occurrences in the Opalinus Clay: Mont Terri (Lerouge et al. 2015). *Known occurrences in the confining units:* Benken (Staffelegg Fm., Klettgau Fm.; Langer et al. 2001), Schlattingen-1 ('Brown Dogger'; Wersin et al. 2013), SEAG boreholes in Northeastern Switzerland ('Brown Dogger', Staffelegg Fm.; Bläsi et al. 1996; Tab. 3-2).

Pyrite II constitutes an accessory mineral and refers to a younger generation of pyrite, which is not associated with early carbonate cements but occurs together with younger carbonate cements (Lerouge et al. 2015). Its content is substantially lower in comparison to pyrite I. It fills moulds left by the dissolution of biogenic calcite/aragonite structures (Fig. 3-12; Wersin et al. 2013). Moreover, in the SEAG boreholes in Northeastern Switzerland, pyrite II replaces detrital grains and fills the pore space that has been left after quartz cementation (see Section 3.3.9; Bläsi et al. 1996).

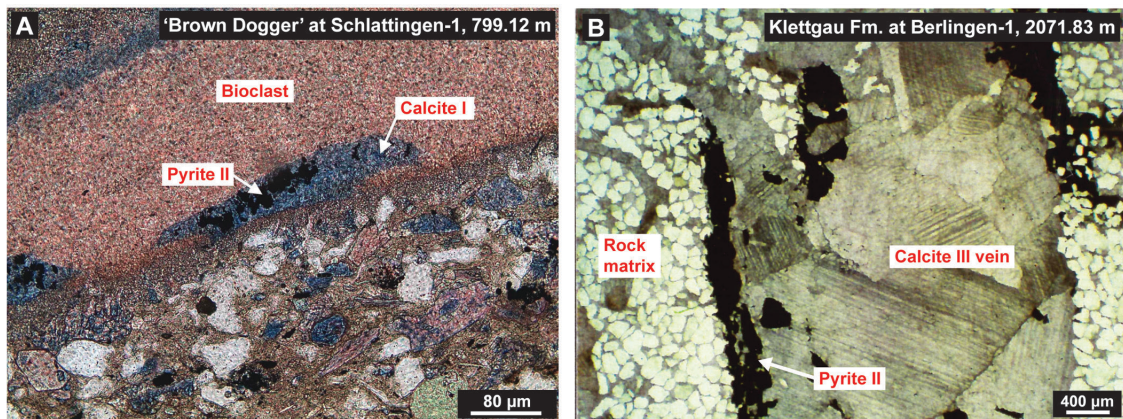


Fig. 3-12: Occurrence of diagenetic pyrite II

(A) Pyrite II filling a intraparticle pore in a calcitic bioclast (plane polarised, transmitted light microscopy; Wersin et al. 2013); (B) pyrite II associated with late diagenetic calcite III as infill of veins (plane polarised, transmitted light microscopy; Bläsi et al. 1999).

3.3.13 Sphalerite

Known occurrences in the Opalinus Clay: Mont Terri (de Haller et al. 2014, Lerouge et al. 2015), Benken (Lerouge et al. 2014). *Known occurrences in the confining units:* Schlattingen-1 ('Brown Dogger'; Wersin et al. 2013; Tab. 3-2).

Sphalerite constitutes an accessory mineral phase that generally occurs as < 50 µm-sized anhedral-euhedral crystals disseminated (or occasionally agglomerated) within the rock matrix (Fig. 3-13) or rarely as 300 – 400 µm-sized euhedral crystals growing into empty pore space (Lerouge et al. 2014).

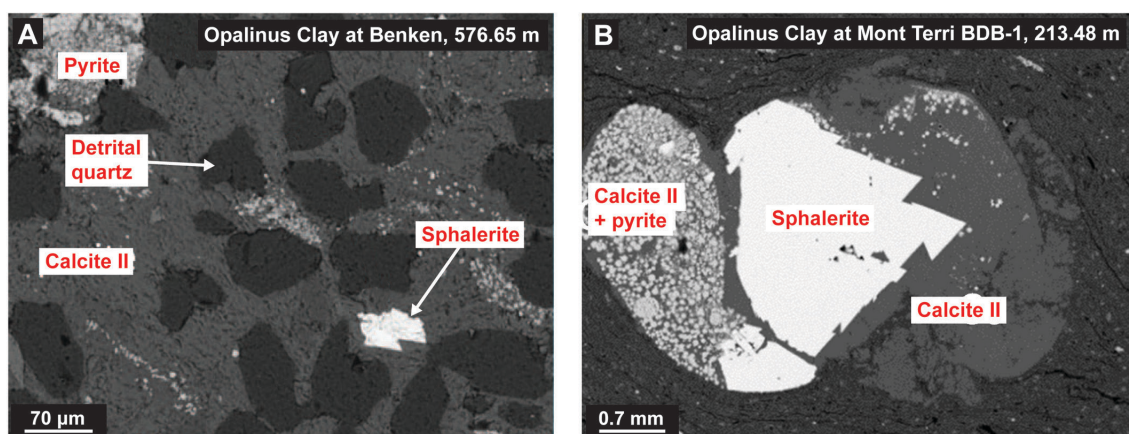


Fig. 3-13: Occurrence and texture of diagenetic sphalerite

(A) Euhedral sphalerite disseminated in the rock matrix (SEM-BSE image; Lerouge et al. 2014). (B) Euhedral sphalerite filling intrafossil pore space and overgrown by calcite II (SEM-BSE image; Lerouge et al. 2015)

3.3.14 Galena

Galena is reported in one sample from the Opalinus Clay at Benken. It occurs in association with calcite II as infill of empty pore space in a pyrite concretion, but also in a micro-crack that cuts across the pyrite concretion (Fig. 3-14; Lerouge et al. 2014; Tab. 3-2).

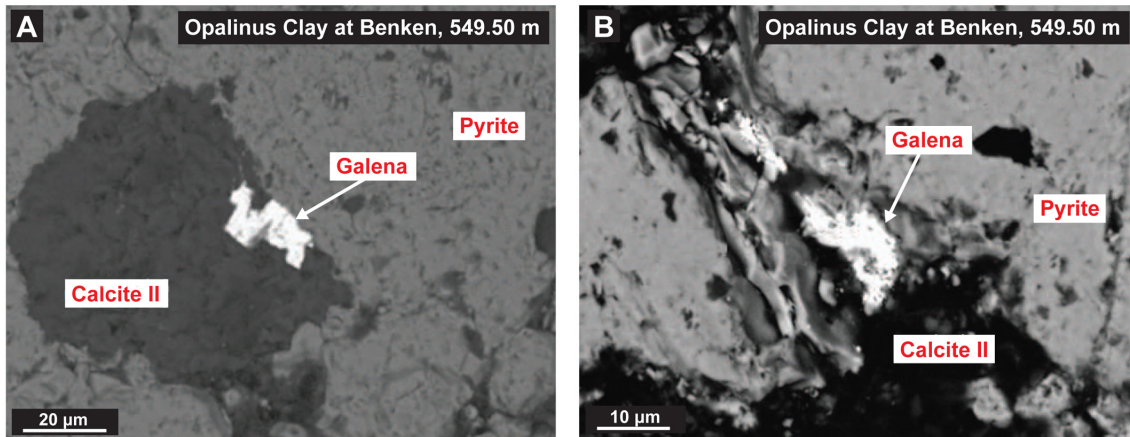


Fig. 3-14: Occurrence and texture of diagenetic galena

(A) Euhedral galena and younger calcite II filling the interparticle pore space in a pyrite concretion. (B) Micro-crack filled with late calcite and galena cutting across the pyrite concretion from (A) (A,B: SEM-BSE image; Lerouge et al. 2014).

3.3.15 Calcite II

Known occurrences: all investigated sites in the Opalinus Clay and its confining units (Tab. 3-2).

Throughout the region of interest, the precipitation of calcite II represents one of the major cementation events. It occurs as late diagenetic infill of interparticle pore space, predominantly in silty lenses (Fig. 3-15) which lack large amounts of biogenic components. Early diagenetic dissolution of biogenic components would promote precipitation of pore-occluding calcite I, thus leaving no space for later calcite II cement. Calcite II is insignificant or absent in the clay-rich bulk of the Opalinus Clay. Various authors use different terms to describe the texture of this cement (Wersin et al. 2013: "continuous"; Bläsi et al. 2002: "poikilitic"; Lerouge et al. 2015: "sparitic").

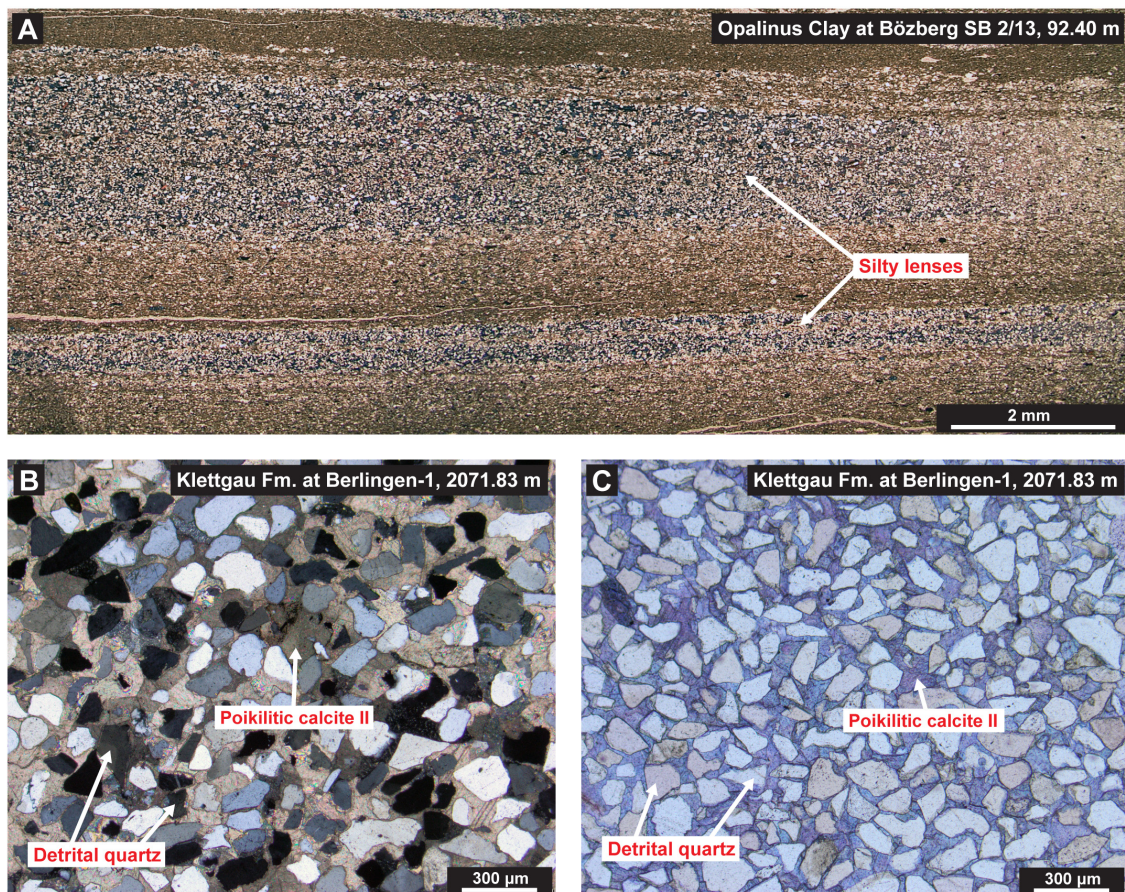


Fig. 3-15: Occurrence and texture of calcite II

(A) Silty lenses in the Opalinus Clay. (B,C) Poikilitic calcite II cement filling the interparticle pore space in silty lenses. (A,B: cross polarised, transmitted light microscopy; C: plane polarised, transmitted light microscopy).

3.3.16 Illite and chlorite

Known occurrences in the Opalinus Clay: Possibly in the Main Fault at Mont Terri (to be confirmed; Clauer et al. 2017). *Known occurrences in the confining units:* sandy lithologies of the SEAG boreholes in Northeastern Switzerland ('Brown Dogger', Staffelegg Fm. and Klettgau Fm.; Bläsi et al. 1996).

Quantitatively, illite is of minor importance, whereas chlorite occasionally constitutes a major diagenetic phase (Tab. 3-2). Illite either forms tangential linings on detrital quartz grains or bridges between individual quartz grains. Chlorite on the other hand forms thin seams of fan- or rosette-shaped aggregates lining detrital grains or older cements (Fig. 3-16; Bläsi et al. 1996).

In a detailed study dedicated to the Main Fault in the Opalinus Clay at Mont Terri, Clauer et al. (2017) interpreted nanoscale illite as a neoformation that precipitated during faulting, even though Laurich et al. (2018) also mention alternative genetic explanations (detrital or due to cataclasis).

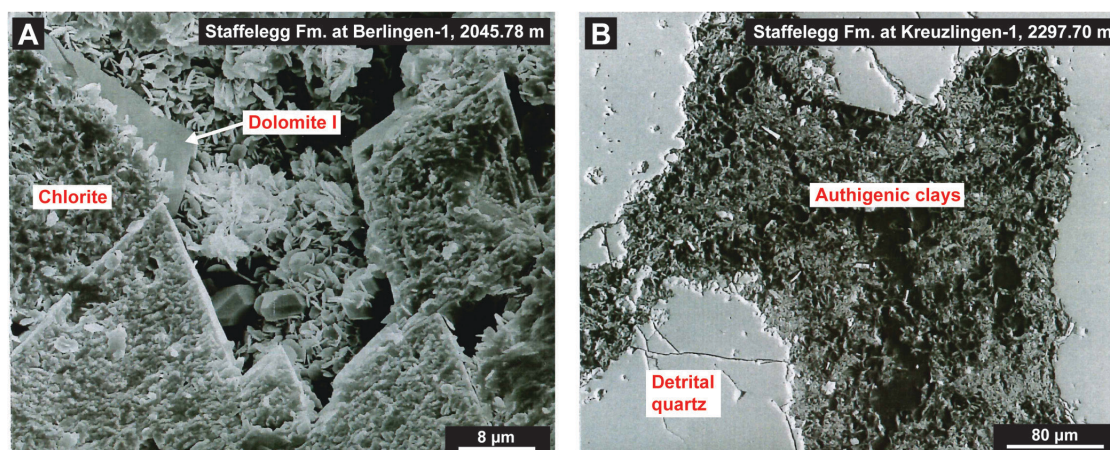


Fig. 3-16: Occurrence and texture of diagenetic illite and chlorite

(A) Dolomite I crystals overgrown by fan-shaped chlorite (SEM-SE image; Bläsi et al. 1996). (B) Authigenic clays filling the interparticle pore space between detrital quartz grains. Quartz does not show any syntaxial overgrowth (see Section 3.3.9; SEM-BSE image; Bläsi et al. 1996).

3.3.17 Celestite and Ba-Sr sulphate

Known occurrences in the Opalinus Clay: Mont Terri (Lerouge et al. 2015), Benken (Lerouge et al. 2014). *Known occurrences in the confining units:* Schlattingen-1 ('Brown Dogger', Staffelegg Fm.; Wersin et al. 2013), SEAG boreholes in Northeastern Switzerland (Staffelegg Fm., Klettgau Fm.; Bläsi et al. 1996; Tab. 3-2).

Celestite and Ba-Sr sulphate constitute accessory mineral phases that are rather difficult to identify if they are not specifically searched. In both the Opalinus Clay and the confining units, Ba-Sr sulphate and celestite mainly occur as fillings of interstices and as xenomorphic, fibrous cement in the rock matrix (Fig. 3-17; Bläsi et al. 1996, Wersin et al. 2013, Lerouge et al. 2014). These occurrences are rather rare and only few samples contain Ba-Sr sulphate and celestite grains that are large enough to be identified by conventional transmitted light microscopy.

Sulphate minerals are of particular importance for pore-water investigations: A striking observation is that at Schlattingen-1 the sulphate concentration obtained by aqueous extraction and back-calculated to in-situ pore water is consistently much higher than sulphate concentrations measured in seepage waters at Mont Terri or in squeezed waters (i.e. "excess sulphate"; Wersin et al. 2013). Accordingly, dissolution of celestite or barite, in addition to the pore-water sulphate, is considered to contribute to sulphate concentrations in the aqueous extracts. Based on the difference between sulphate obtained from extraction and that obtained from squeezing experiments, Wersin et al. (2013) postulated a sulphate mineral content of 0.02 – 0.06 wt.-% for the Opalinus Clay.

Energy-dispersive X-ray spectroscopy (EDX) of sulphate minerals indicates highly variable barium and strontium contents in sulphate minerals (Wersin et al. 2013). According to Lerouge et al. (2015), 1 – 24 % of the strontium is replaced by barium, indicative of a solid solution between celestite and barite. Note that to date barite has solely been documented for the Opalinus Clay at Benken (Langer et al. 2001).

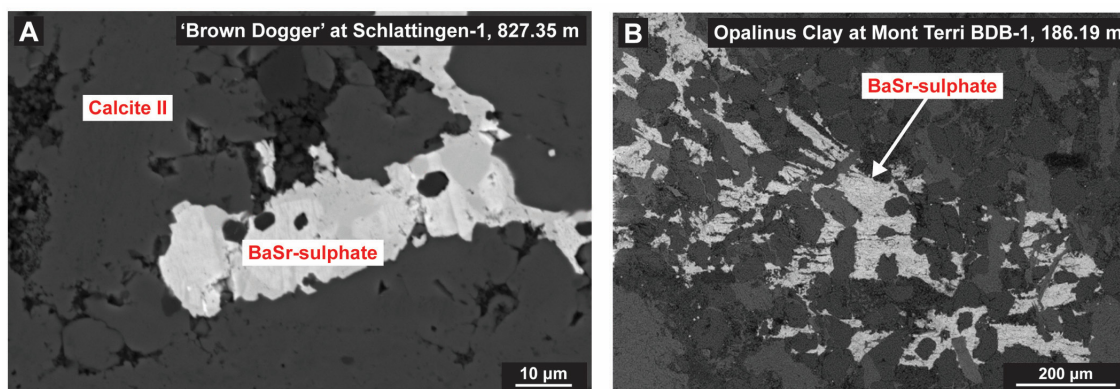


Fig. 3-17: Occurrence and texture of diagenetic Ba-Sr sulphate

(A) Diagenetic Ba-Sr sulphate filling residual intergrain pore space left after cementation by calcite II (SEM-BSE image; Wersin et al. 2013). (B) Fibrous Ba-Sr-sulphate cementing detrital quartz grains (SEM-BSE image; Lerouge et al. 2015).

Jenni et al. (2019) conducted a detailed study targeted at the identification of sulphur-bearing minerals in the Opalinus Clay on two samples from the clay-rich and silty sub-units at Mont Terri and two samples from Schlattingen-1. The methods included element mapping using EPMA-WDX analysis (wavelength-dispersive analysis on an electron microprobe) and SEM-EDX (energy-dispersive analysis on a scanning electron microscope) with the QEMSCAN setup. Both methods have in common that the sampled rock volume for each point analysis has a diameter in the order of 1 – 2 µm, which is larger than the grain sizes of many minerals in the studied samples. This means that analyses of minerals with similar and smaller grain sizes will represent mixtures of different phases.

In the sample from the clay-rich sub-unit at Mont Terri, celestite with typical grain sizes of 2 – 4 µm was identified by EPMA, in addition to few grains of up to 10 µm diameter. The maximum content was estimated at 0.01 – 0.03 vol.-%. Even smaller contents of Sr-free barite were observed. Areas with high Ca contents containing S but no Sr and Fe were interpreted as calcite and/or apatite. The S inventory in calcite and apatite is substantially larger than that in celestite. Rough estimates of the S contents in S-rich calcite and in apatite are around 1.2 and 1.5 wt.-%, respectively.

In the sample from the silty sub-unit at Mont Terri, celestite grains with sizes of 10 – 20 μm were observed. Rough estimates of their contents are 0.006 – 0.008 vol.-%. Although smaller grains dominate by number (Fig. 3-18), their contents are below 0.005 vol.-%. As for the clay-rich sample, the inventory of S is dominated by calcite and apatite, with similar S contents. In conclusion, celestite was identified with a satisfactory level of confidence in all four studied samples. While the number of samples and the studied surface area within each sample (in the range of 2 – 400 mm^2) are far away from being representative, the findings nevertheless support the existence of small amounts of celestite finely disseminated in the rock matrix. The S inventory is dominated by calcite and apatite, whereas the contribution of celestite is of lesser quantitative importance, probably insufficient to explain in full the "excess sulphate" in aqueous extracts.

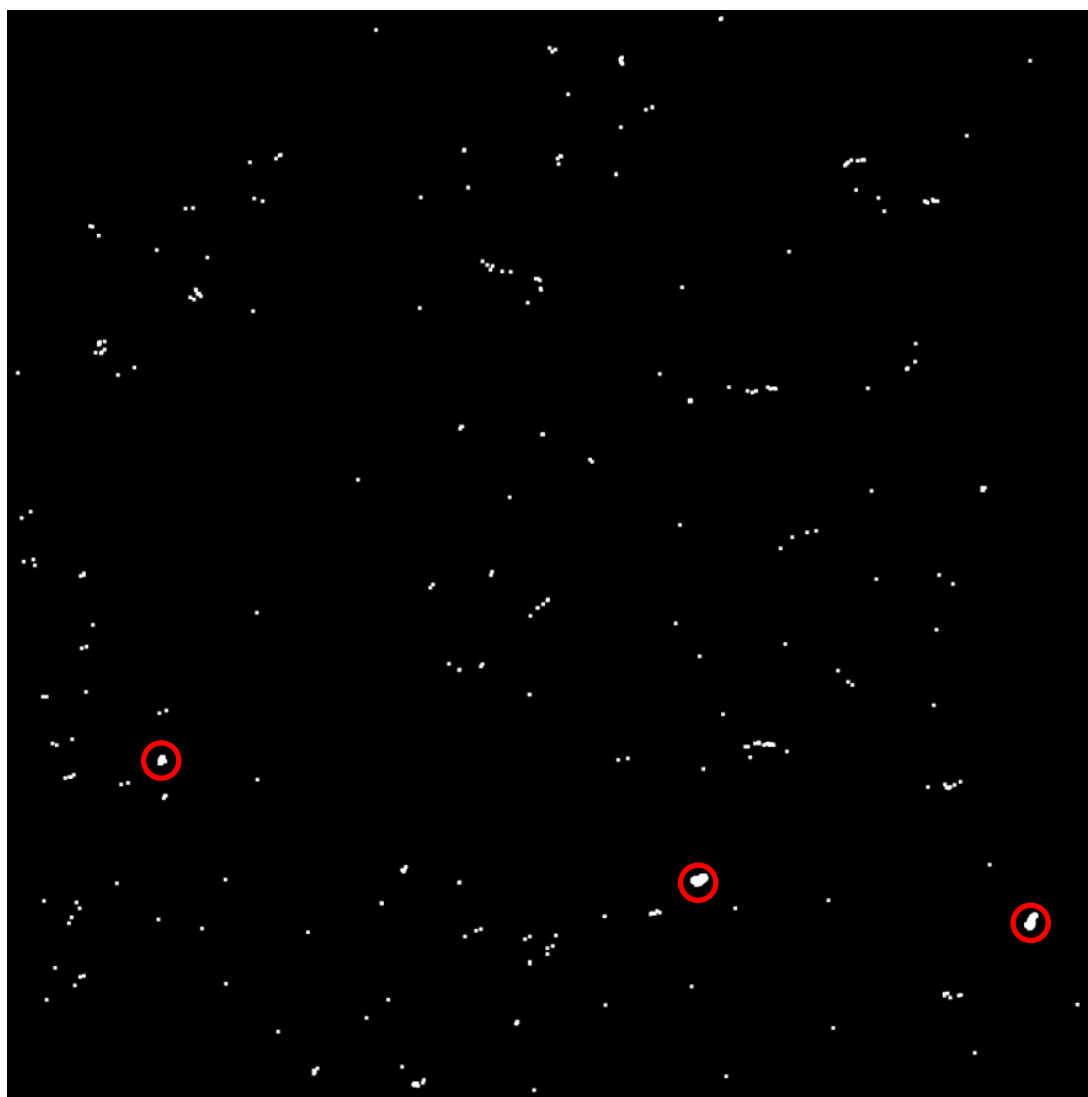


Fig. 3-18: Combination of high Sr and high S element maps with pyrite excluded suggesting the distribution of celestite (segmented binary map, $4 \times 4 \text{ mm}^2$)

Sample from the silty sub-unit of the Opalinus Clay at Mont Terri. Data acquired using SEM-EDX with the QEMSCAN setup, pixel size is $2 \times 2 \mu\text{m}^2$. Grains are enlarged for better visibility. The large grains detected by QEMSCAN as pure celestite are encircled. Jenni et al. (2019).

3.3.18 Anhydrite

One single occurrence of diagenetic anhydrite in the Opalinus Clay was identified by Bläsi et al. (1996) at Mont Terri. Other occurrences were reported by Bläsi et al. (1991, 1996) for the SEAG boreholes in Northeastern Switzerland, where anhydrite occurs as cement, replacing older cements and detrital components (Fig. 3-19, Tab. 3-2).

For Mont Terri, Bläsi et al. (1996) also described the occurrence of gypsum, often in association with pyrite. However, it is likely that gypsum is a product of oxidation since the time of tunnel excavation and does not occur in the undisturbed formation.

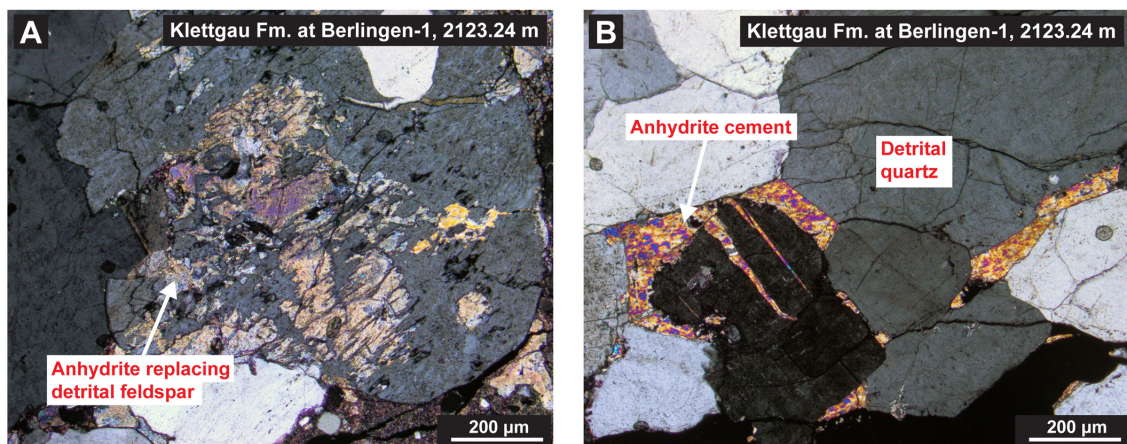


Fig. 3-19: Occurrence and texture of diagenetic anhydrite

(A) Diagenetic anhydrite (coloured mineral) replacing detrital feldspar. (B) Anhydrite cement filling the interparticle pore space between detrital quartz grains in silty lenses (A,B: cross polarised, transmitted light microscopy).

3.3.19 Native sulphur

At Mont Terri, one single occurrence of diagenetic native sulphur has been reported by Pearson et al. (2003). It occurs as μm -sized grains in the rock matrix.

3.3.20 Iron-bearing trace phases in the Opalinus Clay

In addition to the Fe-bearing phases discussed above, some further minerals occur in trace amounts and have been identified by dedicated techniques. In an investigation of the natural magnetisation of the Opalinus Clay from Mont Terri, Aubourg et al. (2008) suggested the presence of pyrrhotite, magnetite and hematite and estimated maximum concentrations of 50 ppmv, 170 ppmv and 0.1 vol.-%, respectively. Magnetite and pyrrhotite are considered to be products of burial diagenesis (see also Aubourg & Pozzi 2010, Aubourg et al. 2012, Kars et al. 2012). On the other hand, the presence and origin of hematite appears to be more controversial. Furthermore, while Aubourg & Pozzi (2010) identified goethite in the Callovo-Oxfordian at Bure, they do not mention its presence in the Opalinus Clay. Goethite occurs in specific horizons, such as Fe-oolites (see Section 3.3.5), but there is no clear evidence for its presence outside these beds.

Mazurek et al. (2017a) applied Mössbauer spectroscopy to identify Fe-bearing phases in the Lausen borehole where the Opalinus Clay is exposed on the surface. In samples below the surficial oxidation zone (about > 20 m), pyrite, siderite $\pm$ clay minerals are the main carriers of Fe^{2+} . Fe^{3+} occurs mainly in clay minerals (illite/smectite, kaolinite). No evidence was found for goethite, even though a small amount of nanogoethite could not be excluded.

3.4 Mineralisations in tectonic veins

3.4.1 Calcite III

Known occurrences: all investigated sites in the Opalinus Clay and its confining units (Tab. 3-3).

Calcite III fills tectonic veins and constitutes one of the major events of vein mineralisation (Fig. 3-20, 3-21). It may be associated with celestite (see Section 3.4.3) or anhydrite (see Section 3.4.2).



Fig. 3-20: Calcite III as infill of a slickensided fracture crosscutting bedding.

3.4.2 Anhydrite

Known occurrences in the confining units: Schafisheim (Klettgau Fm.; Nagra 1992), Benken (Klettgau Fm.; Langer et al. 2001), SEAG boreholes in Northeastern Switzerland (Staffelegg Fm., Klettgau Fm.; Bläsi et al. 1996, 2002; Tab. 3-3).

Anhydrite is an accessory mineral in veins (Nagra 1992, Bläsi et al. 1991, 1996), often associated with calcite III and/or (Fe-)dolomite II (Fig. 3-21, 3-23A).

Gypsum was also reported as a diagenetic mineral (e.g. Bläsi et al. 1991). However, it is likely that it is a product of oxidation since the time of sampling and so does not represent a diagenetic mineral phase.

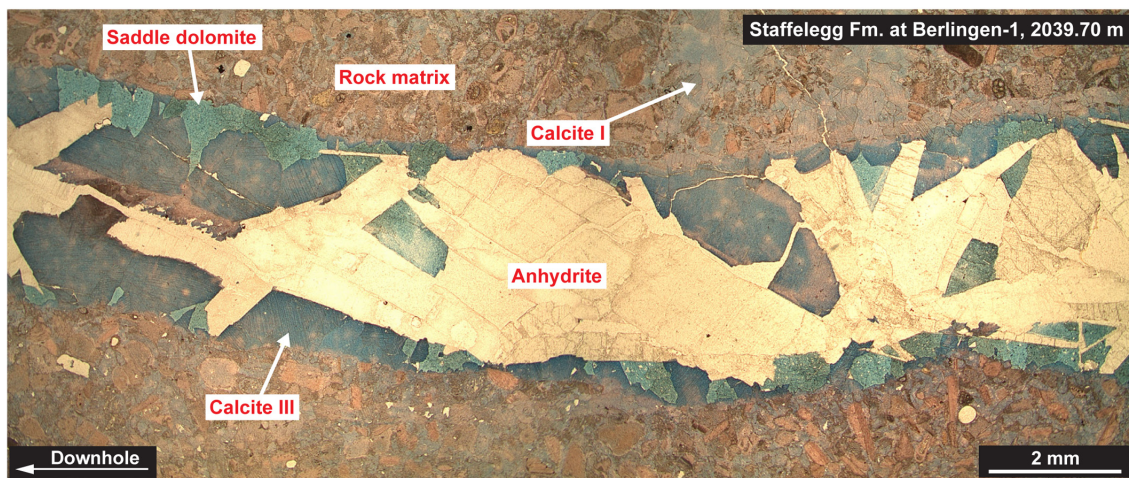


Fig. 3-21: Occurrence and texture of diagenetic anhydrite in tectonic veins

Vein consisting of anhydrite (white), saddle dolomite (bright blue) and calcite III (dark blue; plane polarised, transmitted light microscopy).

3.4.3 Celestite

Known occurrences in the Opalinus Clay: Mont Terri (Bläsi et al. 1991, de Haller et al. 2011, 2014, Laurich et al. 2014, Lerouge et al. 2015), Weiach-1 (Waber & Schürch 1999), Benken (Langer et al. 2001, Lerouge et al. 2014). *Known occurrences in the confining units:* Schlattingen-1 (Mazurek et al. 2018; Tab. 3-3).

Celestite occurs as infill of fractures, joints and faults, often associated with calcite III (Fig. 3-22). Apart from the occurrence at Mont Terri, celestite constitutes an accessory vein mineral, which is rather difficult to identify if not specifically searched. In contrast, at Mont Terri, there are veins with celestite as dominant infill. In particular, it occurs in the Main Fault (Laurich et al. 2014, Mazurek & de Haller 2017) where its origin is related to thrusting of the Jura fold-and-thrust-belt. No celestite has been reported for the SEAG boreholes in Northeastern Switzerland (Tab. 3-3).

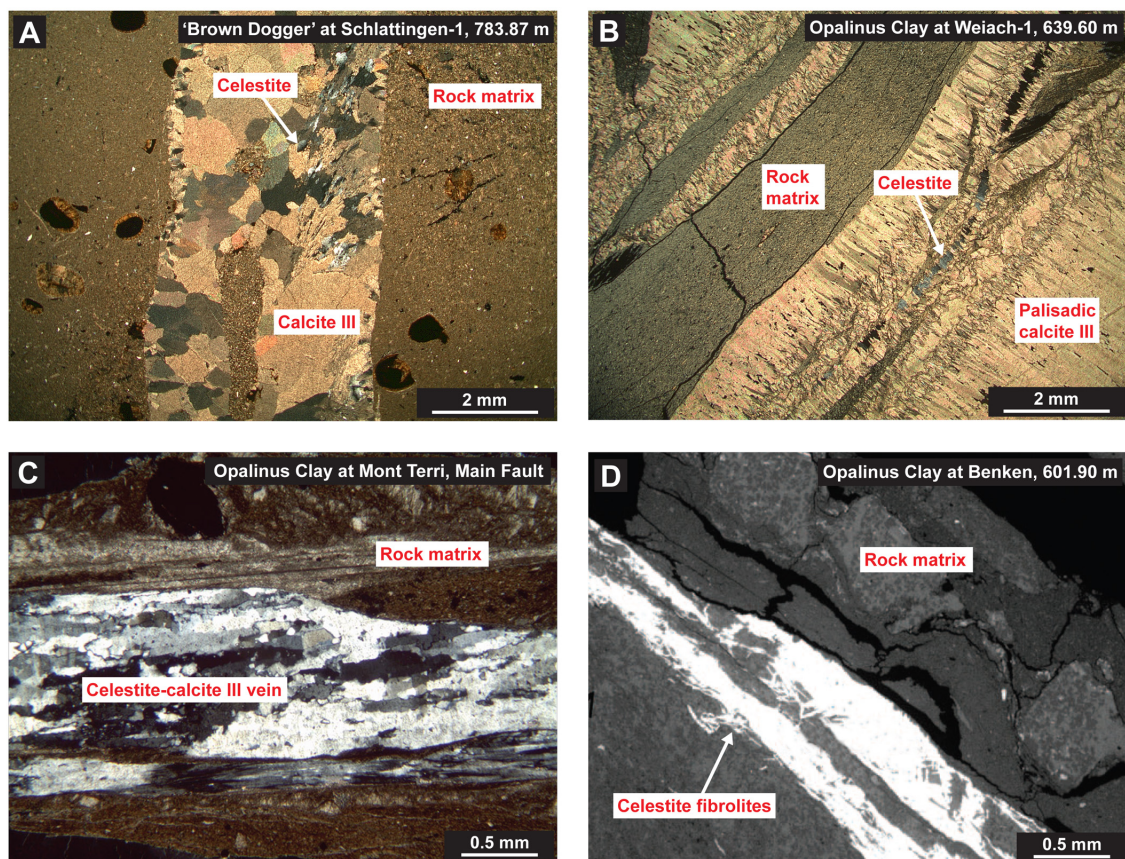


Fig. 3-22: Occurrence and texture of diagenetic calcite II and celestite in tectonic veins

(A) Calcite III vein with accessory amounts of celestite (plane polarised, transmitted light microscopy). (B) Celestite as late accessory infill of a calcite III vein. The calcite has a palisadic texture (plane polarised, transmitted light microscopy). (C) Celestite-calcite vein with fibrous texture (plane polarised, transmitted light microscopy; Mazurek & de Haller 2017). (D) Celestite fibrolites as vein infill (SEM-BSE image; Lerouge et al. 2015).

3.4.4 Pyrite II

Known occurrences in the Opalinus Clay: Mont Terri (de Haller et al. 2014). *Known occurrences in the confining units:* Schlattingen-1 (Staffelegg Fm., Wersin et al. 2013; Tab. 3-3).

Traces of pyrite II occur in calcite-celestite veins. At Mont Terri, these are likely associated with the formation of the Jura fold-and-thrust belt. Note that pyrite II in veins may not be genetically linked to pyrite II in the rock matrix (Section 3.3.12). The only commonality between these pyrite types is the fact that they postdate early diagenetic pyrite I.

3.4.5 (Fe-)dolomite II

(Fe-)dolomite II was solely reported for the deeply buried confining units in the SEAG boreholes in Northeastern Switzerland (Tab. 3-3) where it represents a major event of vein mineralisation. (Fe-)dolomite II refers to diagenetic Fe-bearing dolomite, which often shows characteristic undulose optical extinction (Fig. 3-23A) and curved crystal faces (Fig. 3-23B; Bläsi et al. 1996, Bläsi 2002). These textures are highly diagnostic for saddle dolomite (Davis & Smith 2006).

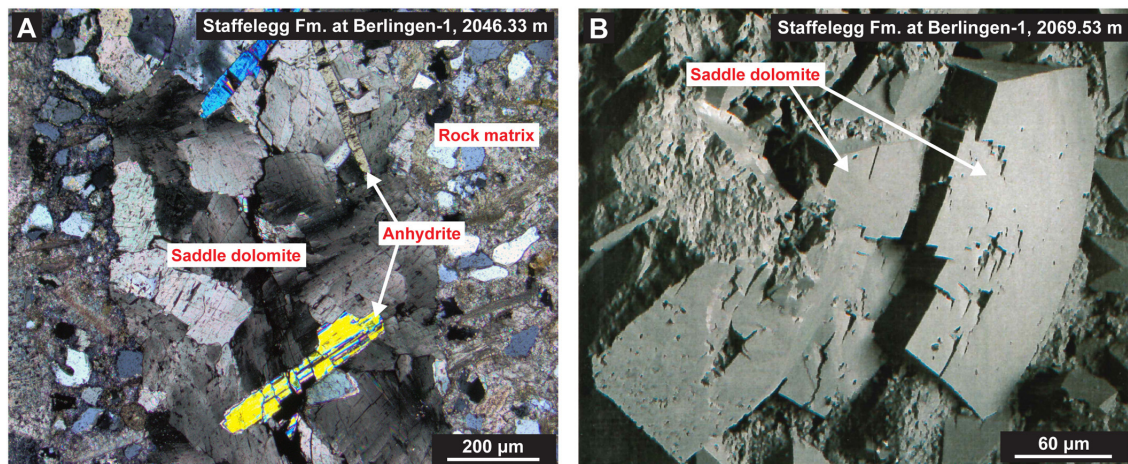


Fig. 3-23: Occurrence and textures of late diagenetic (Fe-)dolomite II in tectonic veins

(A) (Fe-)dolomite II in association with anhydrite as infill of veins. Often individual crystals show characteristic undulose optical extinction and (B) curved crystal faces. Such textures are diagnostic for saddle dolomite (A: cross polarised, transmitted light microscopy; B: SEM-SE image; Bläsi et al. 1999).

3.4.6 Bitumen

Traces of bitumen were reported for the Staffelegg Fm. and the Klettgau Fm. at the SEAG boreholes in Northeastern Switzerland (Bläsi et al. 1996), where they occur in brittle tectonic structures (Fig. 3-24A) and as infill of pores in the rock matrix (Fig. 3-24B). Generally, bitumen is associated with (Fe-)dolomite II. No bitumen is documented for any of the sites further to the west (Tab. 3-3).

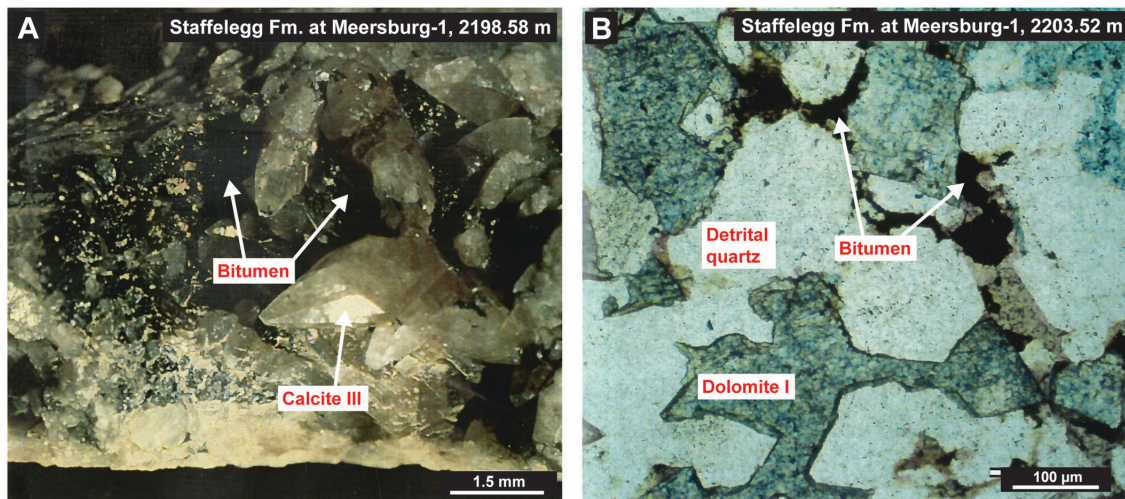


Fig. 3-24: Occurrence of bitumen in tectonic veins

(A) Bitumen (black) in a partly open vein filled by late calcite and anhydrite (reflected light photograph of drill core; Bläsi et al. 1999). (B) Bitumen (black) filling the interparticle pore space between detrital quartz grains and dolomite I (plane polarised, transmitted light microscopy; Bläsi et al. 1996).

3.5 Chemical composition of matrix carbonate and sulphate minerals

3.5.1 Carbonate minerals

Pekala et al. (2018) and Lerouge et al. (2015) analysed the chemical composition of carbonate minerals in the rock matrix of samples from Mont Terri (borehole BDB-1) and from Schlattingen-1 by scanning electron microscopy (SEM-EDS) and by electron microprobe (EPMA). Samples originated from both the Opalinus Clay and the confining units. Reliable data could only be obtained on crystals with sizes exceeding several μm , which made the analysis of some types of carbonate difficult, such as of micritic calcite or of siderite (only Lerouge et al. 2015 provide data on the latter). For these methodological reasons, calcite analyses may have been biased towards sparitic cement (calcite II) and to bioclasts. The results, shown in Fig. 3-25, are as follows:

- The measured data suggest that calcite contains only small amounts of Fe and Mg, typically with a molar fraction of Fe+Mg below 0.05. Note that at such low concentrations the measured values are close to or within the expected method uncertainty. Moreover, clay-sample preparation was challenging and based on the available results it cannot be ruled out that the measured Fe and Mg are affected by contamination by clay minerals. The

composition of cements overlaps completely with that of (recrystallised) bioclasts. Some rare occurrences of Fe-rich calcite were identified by Lerouge et al. (2015) in recrystallised bioclasts, often with a corona of siderite.

- Dolomite mostly constitutes the cores of individual grains, whereas ankerite forms the rims (Fig. 3-9D). More complex situations with a rhythmic zonation were also observed. Nevertheless, the chemical data in Fig. 3-25 indicate that dolomite and ankerite form two chemically distinct groups with a clear gap. Dolomite is invariably Fe-poor, with $\text{Fe}/(\text{Fe}+\text{Mg}) < 0.05$ in most cases. In contrast, this value is typically in the range 0.3 – 0.4 for ankerite. In addition to the occurrence in rims around dolomite cores, ankerite can also form individual euhedral grains or cements. All types of ankerite cover the same narrow field in Fig. 3-25.
- Siderite compositions obtained by Lerouge et al. (2015) occupy a relatively wide field in Fig. 3-25. Siderite from concretions or siderite-rich layers lie in the Ca-poor and Fe-rich corner, whereas disseminated siderite or siderite from coronas around calcite are Ca- and Mg-rich.

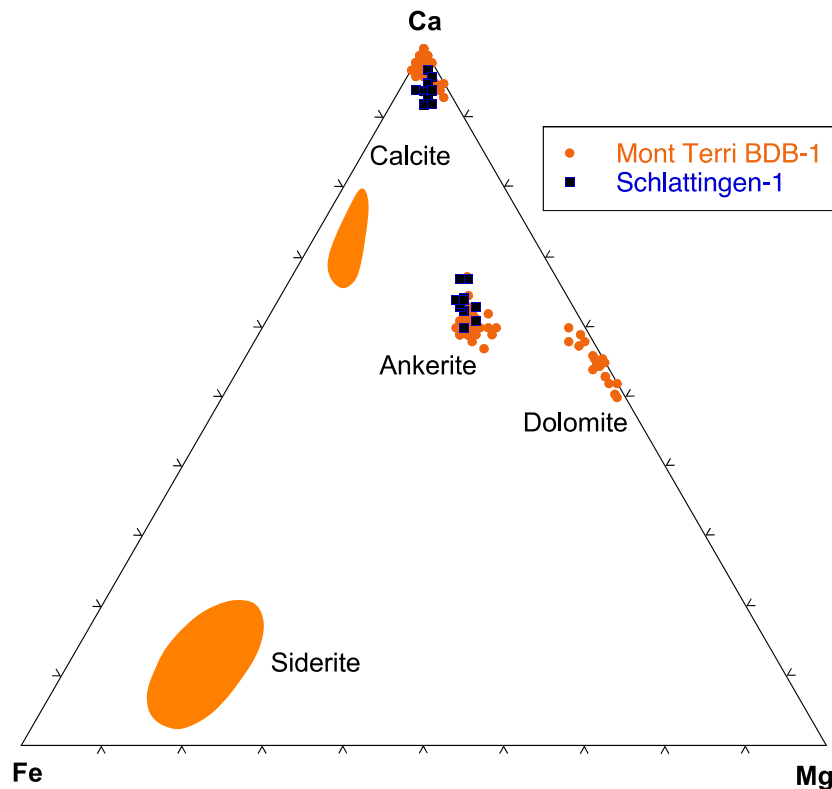


Fig. 3-25: Chemical composition of carbonate minerals

Data points from Pekala et al. (2018), fields for siderite and Fe-rich calcite from Lerouge et al. (2015). The fields obtained by Lerouge et al. (2015) for Fe-poor calcite, ankerite and dolomite overlap completely with those of Pekala et al. (2018) and are not shown.

3.5.2 Sulphate minerals

In Section 3.3.17, a detailed study by Jenni et al. (2019) was documented in which S-bearing minerals were searched by element mapping using EPMA and SEM techniques. In all 4 studied samples, celestite or a Sr-Ba sulphate were qualitatively identified. However, due to the small grain size, often smaller than the sampled rock volume, no quantitative data on the chemical composition could be obtained. In this Section, quantitative analyses are presented that were performed on some infrequent, relatively large crystals identified in thin sections.

In the 12 samples of the Opalinus Clay and its confining units from Mont Terri and Schlattingen-1 that were studied by Pekala et al. (2018), one single occurrence of a Sr-Ba sulphate mineral was identified by optical microscopy in the lower silty sub-unit at Mont Terri in the form of isolated clusters of elongated or fibrous crystals in the rock matrix (Fig. 3-26). Lerouge et al. (2015) studied 24 samples from Mont Terri and also found only one sulphate-bearing sample (the same as Pekala et al. 2018) by optical methods.

Individual crystals are up to ca. 100 μm long and ca. 10 μm thick. The shape of the crystals and their relation with surrounding cement indicate that the mineral was formed late, i.e. during burial diagenesis. The chemical variability, expressed as $\text{Ba}/(\text{Ba}+\text{Sr})$, covers a wide molar range of 0 – 0.27 (Fig. 3-27). As seen in Fig. 3-26, the chemical heterogeneity is identified on the μm scale, i.e. even within single crystals.

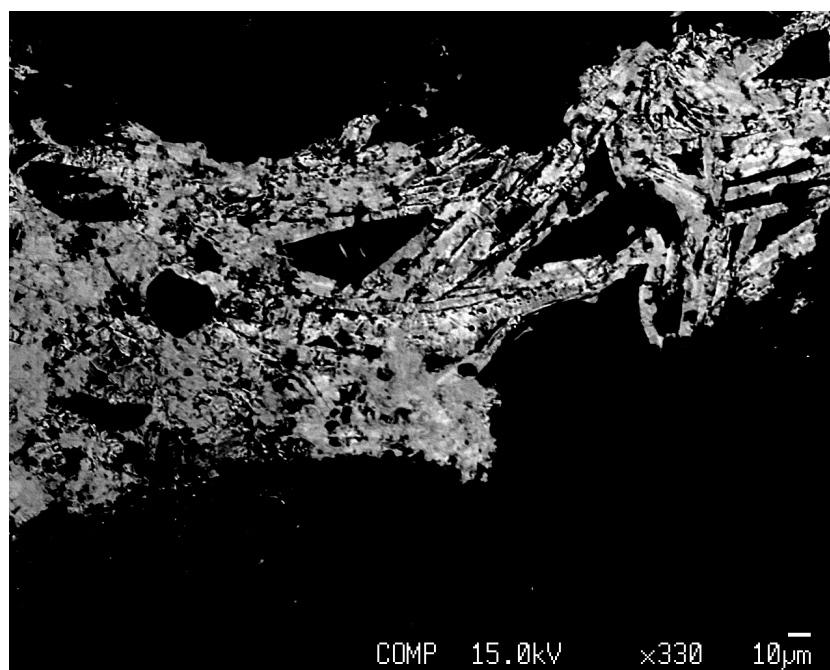


Fig. 3-26: Sr-Ba sulphate in sample 186.19 from Mont Terri, borehole BDB-1 (BSE image by EPMA)

Brighter areas indicate a higher Ba content. The chemical variability occurs on a length scale of around 1 μm . Pekala et al. (2018).

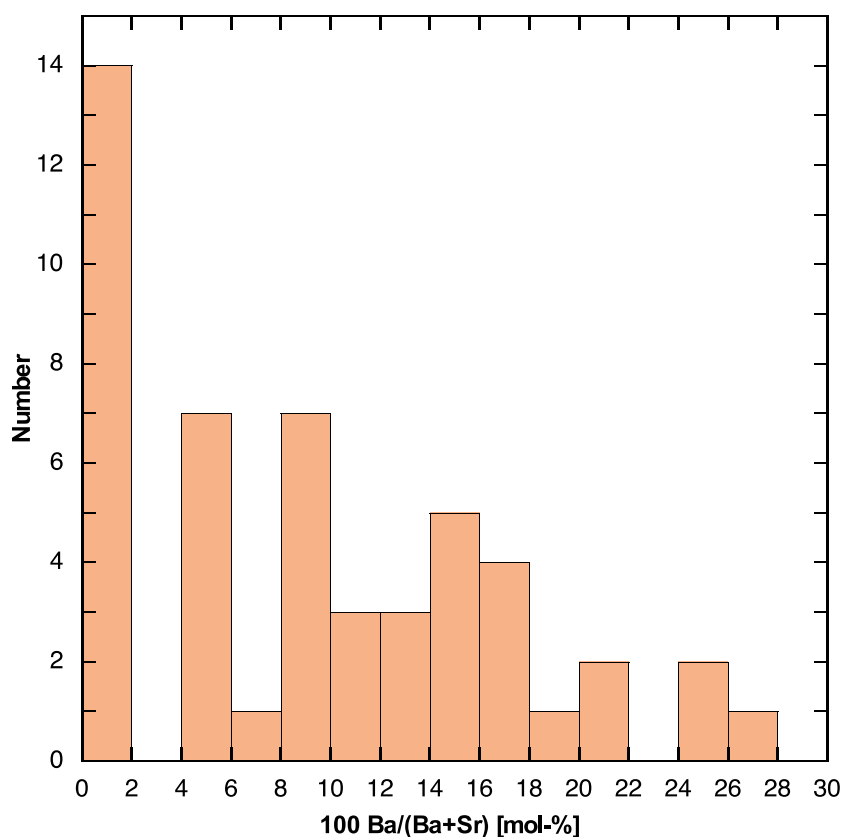


Fig. 3-27: Chemical composition of Sr-Ba-sulphate in sample 186.19 from Mont Terri, borehole BDB-1

Data obtained by SEM-EDX and EPMA by Pekala et al. (2018)

3.6 Overview of the occurrence and abundance of diagenetic minerals

Tab. 3-2 lists the occurrence and the relative abundance of diagenetic minerals in the rock matrix of the Opalinus Clay and its confining units at the investigated sites across Northern Switzerland. Tab. 3-3 shows vein mineralisations in the same format.

The differentiation between major, minor and accessory phases remains on a qualitative level except when quantitative mineralogical data are available, e.g. for dolomite I, siderite and pyrite I. The representativity of some of the studies for the whole formation is limited because of the limited number of samples that were analysed. For example, Wersin et al. (2013) only analysed one sample from the Opalinus Clay and accordingly these results cannot be considered representative for the entire rock unit. Distinctly more samples were analysed in the confining units. Further, it needs to be noted that samples for diagenetic studies were predominantly taken from silty and/or calcareous portions of the rocks, including e.g. hardgrounds and Fe-oolites. This is because diagenetic mineralisations in such lithologies are more strongly developed and therefore better suited for diagenetic studies. On the other hand, clay-rich lithologies, such as the bulk of the Opalinus Clay, are underrepresented.

Tab. 3-2: Occurrence of diagenetic minerals in the rock matrix of the Opalinus Clay and its confining units

	Mont Terri: Opalinus Clay (Bläsi et al. 1991, Peters et al. 2011, Lerouge et al. 2015, NTSI)	Bözberg SB 2/13: Opalinus Clay (NTSI)	Rimiken-1: Opalinus Clay (Lerouge 2016)	Benken: Opalinus Clay (Bläsi 2002, Lerouge et al. 2014, NTSI)	Benken: Staffelegg Fm. (Langer et al. 2001)	Benken: Klettgau Fm.n (Langer et al. 2001)	Schlattingen-1: 'Brown Dogger' (Wersin et al. 2013)	Schlattingen-1: Opalinus Clay (Wersin et al. 2013)	Schlattingen-1: Staffelegg Fm. (Wersin et al. 2013)	SEAG boreholes in NE Switzerland: 'Brown Dogger' (Bläsi et al. 1996, NTSI)	SEAG boreholes in NE Switzerland: Staffelegg Fm. (Bläsi et al. 1996, NTSI)	SEAG boreholes in NE Switzerland: Klettgau Fm. (Bläsi et al. 1996, NTSI)
Aragonite/Mg-calcite	x	x		xx	xx	xx	xx		xx	xx	xx	xx
Pyrite I	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx	xx
Siderite	xxx	xx	xxx	xxx	x		x	xxx	xx	xxx	xx	x
Calcite I	xx	xx	xx	xx	xx	xx	xx		xx	xxx	xxx	xxx
Limonite	x				x		x					
Illite and chlorite	1)									xx	xx	x
Glauconite	x		x	x								
Ti-oxides	x						x			x	x	
Dolomite I	xx	xx	x	xx	xx	xxx	xx	xx	xxx	xx	xx	
Quartz	x	x		x		x	x			xx	xx	xx
Kaolinite	xx						xx			xx	xxx	xx
Pyrite II	x				x	x	x			x	x	
Sphalerite	x			x			x					
Galena				x								
Calcite II	xxx	xxx	xxx	xxx	xxx	xxx	xxx	xxx	xxx	xxx	xxx	xxx
Celestite and Ba-Sr sulphate	x			x			x		x		x	x
Anhydrite	x									x		x
Native sulphur	x											

XXX: major phases; XX: minor phases; X: accessory phases; NTSI: new thin-section investigations. An empty field means "no information" or "not reported".

¹ Authigenic illite was suspected in the Main Fault by Clauer et al. (2017)

Tab. 3-3: Vein mineralisations in the Opalinus Clay and its confining units

	MT	Schafisheim				Riniken-1		Weiach-1			Benken			Schlattingen -1		SEAG		
	Opalinus Clay (Bläsi et al. 1991; Mazurek & de Haller 2017)	Passwang Fm. (Nagra 1992)	Opalinus Clay (Nagra 1992)	Staffelegg-Klettgau Fm. (Nagra 1992)	Opalinus Clay (Nagra 1990)	Staffelegg-Klettgau Fm. (Nagra 1990)	'Brown Dogger' (Nagra 1989)	Opalinus Clay (Nagra, 1989; Waber & Schürch 1999)	Staffelegg-Klettgau Fm. (Nagra 1989)	'Brown Dogger' (Langer et al. 2001)	Opalinus Clay (Bläsi 2002; Lerouge et al. 2014)	Staffelegg-Klettgau Fm. (Langer et al. 2001)	'Brown Dogger' (Mazurek et al. 2018)	Opalinus Clay (Mazurek et al. 2018)	Staffelegg-Klettgau Fm. (Mazurek et al. 2018)	'Brown Dogger' (Bläsi et al. 1996)	Staffelegg-Klettgau Fm. (Bläsi et al. 1996, 1999, 2002)	
Calcite III	xxx	xxx	xxx	xxx	xxx	See footnote 2	xx	xxx	xxx	xxx	xxx	xxx ¹	xxx	xxx	xxx	xxx	xxx	xxx
Anhydrite	x			xx ³									x ³					x
Celestite	xx							x			x			x		x		
Pyrite II	x ⁴															x ⁴		
(Fe-)dolo. II																	xxx	xxx
Bitumen																		x ⁶

XXX: major phases; XX: minor phases; X: accessory phases. An empty field means "no information" or "not reported". MT = Mont Terri; SEAG = SEAG boreholes in Northeastern Switzerland.

¹ Presence of calcite III in veins reported by Nagra (2001)

² Staffelegg Fm.: No vein infills reported; Klettgau Fm.: No data

³ Only in Klettgau Fm.

⁴ From de Haller et al. (2014)

⁵ Only in Staffelegg Fm.; from Wersin et al. (2013)

⁶ Bitumen also occurs as infill of intergrain pores in the rock matrix

Apart from the cementation by calcite II, which is considered to occur under several hundred metres of overburden (see Section 3.7), the effects of early diagenesis, i.e. processes that occur within the uppermost 100 m of the sediment, are quantitatively particularly important. They mainly include the precipitation of aragonite/Mg-calcite, pyrite I, siderite, calcite I and dolomite I. In general, the contents of pyrite I, siderite and dolomite I do not correlate with clay-mineral content, which means that these precipitation events affected all lithologies, including those that are clay-rich. Fig. 3-28 shows the absent or weak correlations between clay-mineral content and contents of early diagenetic minerals, based on XRD whole-rock analysis (data base of Mazurek 2017). The only systematic features that can be identified are the higher dolomite I contents in the carbonate-rich silty and the lower silty sub-units (see Section 2.3.1 for definitions) and the lower pyrite contents in the lower silty sub-unit, even though the fields are overlapping.

In contrast, later mineralisations related to burial diagenesis are more strongly expressed in silty/calcareous lithologies but only weakly in clay-rich rocks. When a clay-rich sample of the Opalinus Clay is immersed in distilled water, it will disaggregate completely over time, which illustrates the only limited, if not absent diagenetic cementation. The main cement precipitated during burial diagenesis in silty/calcareous zones is calcite II.

There are no major systematic differences in the diagenetic mineralisation over the region of interest, and no evident distinctions between the Opalinus Clay and the confining units can be made (except for the fact that diagenetic effects are quantitatively more strongly expressed in the latter). One exception are the SEAG boreholes in Northeastern Switzerland (Berlingen-1, Herdern-1, Kreuzlingen-1, Lindau-1) in which the Mesozoic was (and still is) more deeply buried than further to the west (the centre of the Opalinus Clay is at 1'788 – 2'222 m below surface, see Tab. 2-1). Authigenic illite and chlorite, as well as (Fe-)dolomite II, occur only in these boreholes, which is consistent with comparatively higher burial temperatures during diagenesis.

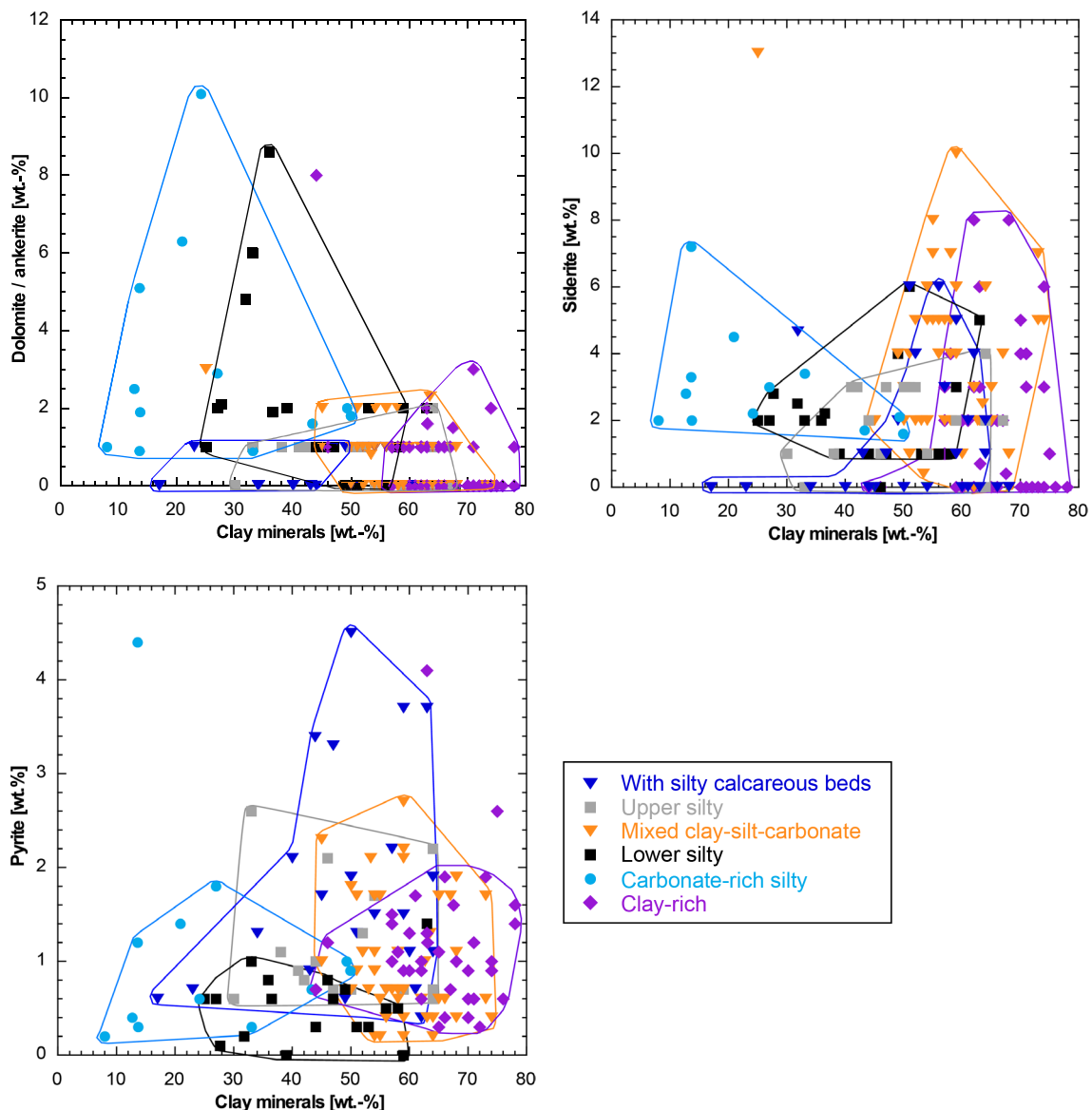


Fig. 3-28: Contents of diagenetic minerals in different sub-units of the Opalinus Clay as a function of clay-mineral content

Borders drawn around data of the sub-units exclude some outliers.

3.7 Relative temporal sequence of mineral precipitation

Fig. 3-29 illustrates the relative temporal sequence of diagenetic mineral precipitation in the Opalinus Clay and in its confining units at the investigated sites. It is based on information from the literature, which has been assessed and updated where required, and by new thin-section investigations. Due to the scarcity of clear textural relationships between the different minerals, the determination of mineral parageneses was challenging and not always feasible.

Accordingly, the individual groups of minerals illustrated in Fig. 3-29 should not be viewed as mineral parageneses *sensu stricto* (i.e. groups of co-genetic minerals) but as groups of minerals which formed during certain diagenetic stages. For the Opalinus Clay, 5 different stages of diagenetic mineral precipitation were identified. These stages can be correlated across the investigation area, indicating that the burial was a regional, spatially homogeneous process over the area between Mont Terri in the west and Schlattingen-1 in the east. Differences exist between lithologies (e.g. quantitatively stronger diagenetic effects in clay-poor units) but not among locations.

The oldest, eogenetic stage of mineral precipitation (i.e. burial depths of less than 100 m) includes precipitation of aragonite/Mg-calcite, framboidal pyrite I, calcite I and siderite. *Aragonite/Mg-calcite* precipitated as fibrous and short prismatic crystals encrusting bioclasts, thus supporting one another (see Section 3.3.1). This is a common phenomenon in marine diagenesis and occurs very early, in the still soft sediment (Tucker & Wright 1992). However, both minerals are metastable and were either dissolved or replaced by more stable low-magnesium *calcite I* (see Section 3.3.4). These processes of dissolution and replacement commonly occur spontaneously (i.e. without involvement of meteoric fluids) during marine eogenesis (Melim et al. 1995, 2001, Cherns & Wright 2000, 2009).

Framboidal *pyrite I*, as well as *siderite*, commonly form by anaerobic, sulfidic diagenesis related to microbial decomposition of organic matter (Blome & Albert 1985, Pye et al. 1990, Bläsi et al. 1996, Mozley 1996, Raiswell & Fisher 2004, Lerouge et al. 2014). In the organic-rich Opalinus Clay, corresponding conditions prevailed a few decimetres below the sediment-water interface onwards and so, same as aragonite/Mg-calcite, both pyrite and siderite are thought to have formed during shallow burial of the still unconsolidated sediment, preferably within the first tens of metres. In theory, siderite should only precipitate once dissolved sulphate in the pore water has been consumed by the precipitation of pyrite, which constitutes the thermodynamically favoured pool for reduced iron. Due to the absence of petrographic relationships, such a precipitation sequence was not observed in the Opalinus Clay, and so pyrite and siderite are placed into the same group of minerals in Fig. 3-29.

In the Opalinus Clay, *dolomite I* partially replaces and therefore postdates calcite I (see Section 3.3.8). Considering the epicontinental, shallow marine deposition environment of the Opalinus Clay (Nagra 2002), the favoured model for dolomitisation is a "penecontemporaneous" model as described by Machel (2004). According to this model, sea water is the dolomitising fluid and dolomite precipitates shortly after deposition of the sediment. Often, this model of dolomitisation is linked to the so-called "microbial" or "organogenic" model, which suggests that dolomitisation is promoted by bacterial sulphate reduction. According to Lerouge et al. (2014), this is the case for the Opalinus Clay. However, penecontemporaneous or microbial dolomitisation produces only a few wt.-% dolomite, which is characterised by microcrystalline textures and non-stoichiometric chemical composition with relatively high Ca contents (Machel 2004). All these characteristics match the characteristics of dolomite I in the Opalinus Clay (see Section 3.3.8, Fig. 3-25, 3-28 and Pekala et al. 2018). Accordingly, in the Opalinus Clay

dolomitisation is likely to be associated with eogenesis shortly after sediment deposition. This finding is in agreement with the studies by Bläsi et al. (1996) and Lerouge et al. (2014) who, based on petrographic observations, suggest an early diagenetic formation of dolomite.

In contrast to the eogenetic mineralisations, fluid-inclusion studies and oxygen isotope investigations in authigenic *quartz* and *calcite II* at Benken and Weiach-1 indicate that these minerals precipitated at temperatures of $\leq 50 - 65$ °C (Bläsi et al. 2002, Lerouge et al. 2014), thus clearly indicating burial conditions and formation during mesogenesis. Further evidence for a mesogenetic association of authigenic quartz and calcite II is provided by the occurrence of authigenic quartz whose formation is mainly controlled by the presence of biogenic components in the silty lenses. Their dissolution during early diagenesis serves as a source of solutes for eogenetic aragonite/Mg-calcite and calcite I cementation that would occlude the pore space, thus leaving no space for later quartz cements. In contrast, in the absence eogenetic aragonite/Mg calcite and calcite I cements the surfaces of detrital quartz grains remain free for authigenic quartz growth (see Section 3.3.9). These observations indicate that authigenic quartz postdates the eogenetic calcite I cement. Later during diagenesis calcite II filled the pore space in silty lenses and grew over authigenic quartz (see Section 3.3.9).

Ba-Sr sulphate, *kaolinite*, *sphalerite* and *galena* are considered to also have precipitated during mesogenesis, however, due to the lack of petrographic evidence, a more detailed determination of their relative ages is not feasible. Quantitatively, eogenetic effects dominate those of mesogenetic mineralisations.

The SEAG boreholes in Northeastern Switzerland, where only the confining units ('Brown Dogger', Staffelegg Fm., Klettgau Fm., see Bläsi et al. 1996) but not the Opalinus Clay were cored, all show a somewhat different evolution when compared to the sites further west. The differences include the occurrence of authigenic *illite*, *chlorite* and *(Fe-)dolomite II* (saddle dolomite, restricted to veins). On the basis of microtextural relationships, illite and chlorite clearly postdate dolomite I (Fig. 3-16). However, textural criteria documenting the relative ages with respect to quartz and calcite II are not available. Given the fact that the precipitation of authigenic clay minerals is expected to occur at elevated temperatures, it is likely that illite and chlorite are linked to relatively late stages of diagenesis. The Mesozoic of the SEAG boreholes experienced a deeper burial than at all sites further to the west. Even today, the Opalinus Clay is buried more than 1000 m deeper in comparison to the other sites. Fluid-inclusion studies in authigenic quartz and calcite II yield precipitation temperatures of > 72 °C (Bläsi et al. 1996, 2002). Furthermore, clay authigenesis, as well as the occurrence of (Fe-)dolomite II with saddle textures indicate burial temperatures of $> 60 - 80$ °C (Worden & Morad 2003, Davis & Smith 2006 and references therein). Nevertheless, apart from these minerals related to burial diagenesis, there are no major differences of diagenetic effects between the confining units at the SEAG boreholes and the Opalinus Clay and its confining units at the sites further west.

Vein mineralisations postdate burial diagenesis but are currently not well constrained in terms of timing. In contrast to diagenesis in the matrix that appears to be homogeneous over the entire study area (except for the deeper burial in the extreme east), veins formed in response to a number of tectonic events that affected the investigation area to different degrees. More detail is provided in Chapter 5.

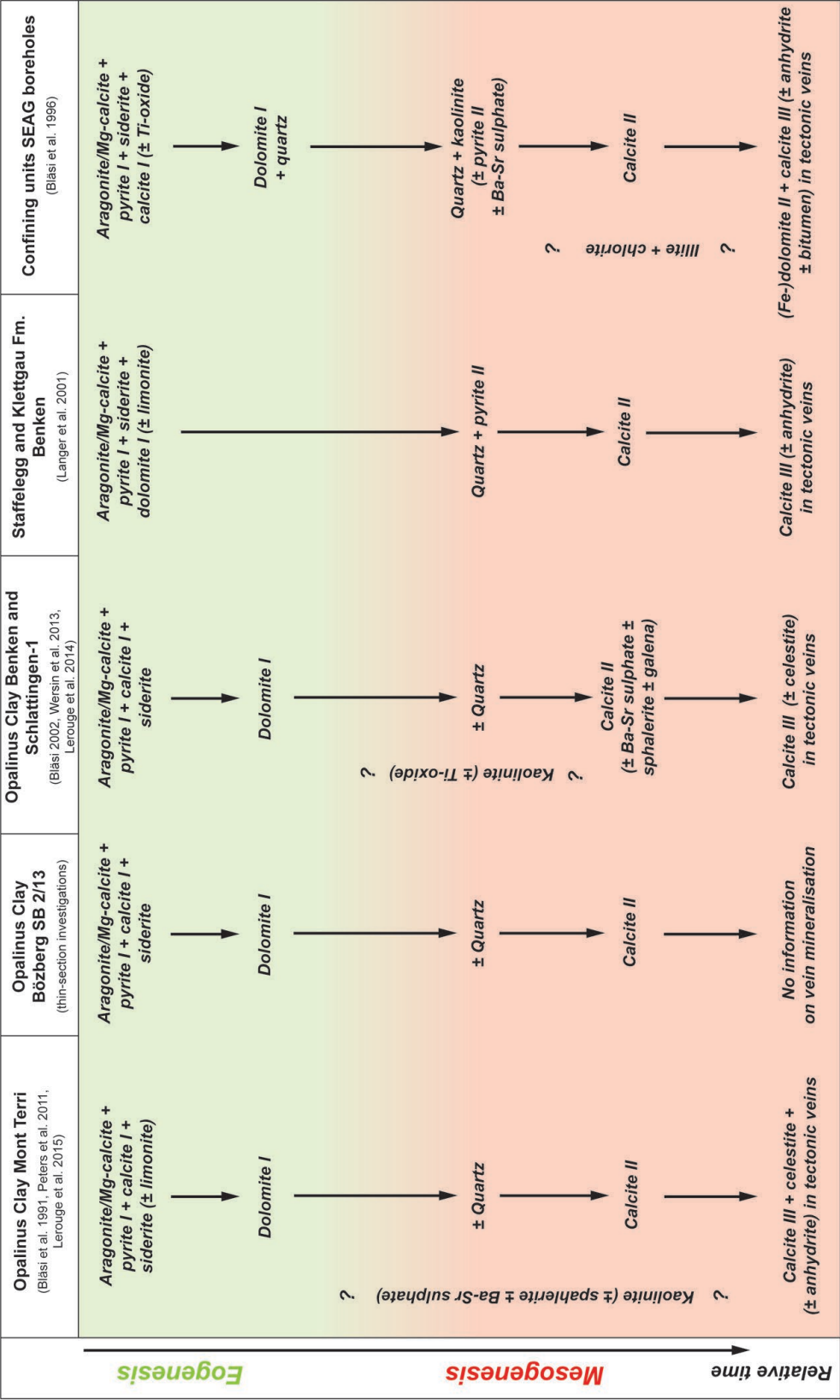


Fig. 3-29: Relative temporal sequence of diagenetic mineral precipitation and mineralisation of tectonic veins in the Opalinus Clay and in its confining units at the investigated sites

3.8 Effect of cementation on compaction and on hydromechanical rock properties

In argillaceous sediments, mechanical compaction (consolidation) during burial mainly involves an increase of the packing density of particles, the mechanical rearrangement of particles (i.e. development of a preferred orientation perpendicular to the direction of maximum stress), as well as the expulsion of interstitial water. These processes reduce the porosity of argillaceous muds from 75–90 vol.-% close to the seafloor to 30–35 vol.-% within the first 250–300 m of burial (Fig. 3-30; Müller 1967, Rieke & Chilingarian 1974, Wygrala 1989). At this depth, the clay is already lithified and cohesive (e.g. the Boom Clay in Belgium). Upon further burial, reduction of porosity occurs more slowly and mainly involves mechanical deformation of particles and further expulsion of pore water.

In addition to mechanical compaction, diagenetic processes such as cementation may contribute to lithification and enhance cohesion, stiffness and the mechanical strength of a mudstone (Müller 1967). Bjørlykke & Høeg (1997) and Nygård et al. (2004) also showed that cementation has a large impact on the hydro-mechanical properties of mudstones. However, cementation is not a prerequisite for the lithification of argillaceous sediments – numerous lithified mudstones devoid of cementation are found at considerable depths, the clay particles being kept together by cohesive bonds (Müller 1967, Rieke & Chilingarian 1974, Jones 1978, Rutter 1983).

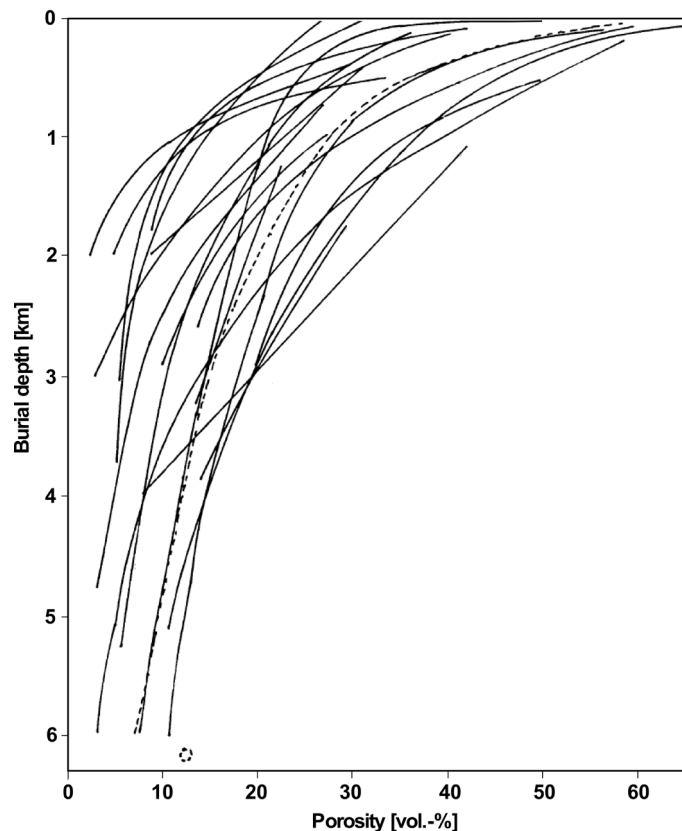


Fig. 3-30: Porosity-depth trends for argillaceous sediments
Compilation of literature data, adapted from Wygrala (1989).

In the Opalinus Clay, rock sections most strongly affected by cementation relate to bioclastic beds (aragonite/Mg-calcite and calcite I cements) and silty/calcareous lithologies (calcite II cements in silty-calcareous lenses). The clay-rich bulk of the rock is less strongly affected (or even unaffected) by cementation (siderite, minor dolomite I).

Favero et al. (2016) and Crisci et al. (2019) investigated the effect of compaction and cementation on the hydro-mechanical behaviour of the Opalinus Clay by oedometric compression experiments on intact and remoulded samples. The samples used for the studies originated from Lausen, Schlattingen-1 and Mont Terri. The results of the oedometric tests revealed a considerably greater stiffness for the intact samples compared to the remoulded specimens at a given effective stress. Moreover, at stresses similar to the effective vertical stress during maximum burial (15 MPa were estimated for Lausen) the void ratios of the intact samples were 40 – 60 % lower than those of the remoulded samples (example in Fig. 3-31). These differences were attributed to diagenetic cementation.

Similar to porosity, permeability of the tested samples decreased during oedometric compression. However, no distinct differences in permeability between intact and remoulded samples were observed during the experiments. Accordingly, Favero et al. (2016) concluded that diagenetic cementation has no severe impact on permeability. They suggested that cementation occurs mainly in larger pores, such as in silty or calcareous lenses, which are completely embedded in the clay matrix with nanometric pore apertures. Thus, in agreement with microstructural evidence (see Chapter 4), permeability is thought to be determined by the clay matrix. Because the larger pores ("storage pores" of Favero et al. 2016) are connected only via the clay matrix, the degree of cementation of these pores has limited effects on bulk permeability.

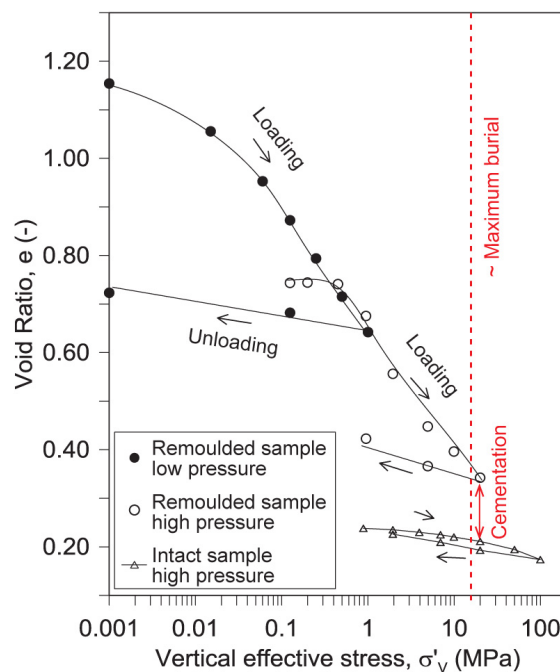


Fig. 3-31: Results of oedometric compression experiments on Opalinus Clay samples

Sample from the Lausen borehole. The majority of the calcite constitutes diagenetic cement. The difference in void ratio between intact and remoulded samples at the estimated effective stress during maximum burial is considered to reflect the contribution of cementation. Modified after Crisci et al. (2019).

3.9 Summary and conclusions

There are no major systematic differences in the diagenetic mineralisation over the region of interest, and no evident distinctions between the Opalinus Clay and the confining units can be made except for the fact that diagenetic effects are quantitatively more strongly expressed in the latter. Accordingly, it is concluded that in the Opalinus Clay burial and diagenesis proceeded relatively homogeneously across the entire study area. The only exception are the SEAG boreholes in the Northeastern part of the study area where burial was deeper and temperatures higher, documented by authigenic illite, chlorite and (Fe-)dolomite II (saddle dolomite). Diagenesis in the rock matrix is mainly determined by eogenetic and mesogenetic processes, thus occurring at a time when uniform burial conditions prevailed throughout the basin, i.e. before spatially heterogeneous Cenozoic tectonic events affected the basin.

Porosity and pore-size distribution depend on the sedimentary facies, on the burial and uplift history and on the nature and intensity of diagenetic effects, such as cementation. Because diagenesis and sedimentary facies (or lithology) of individual sub-units within the Opalinus Clay do not show regional variability, porosity and pore-size distribution of a specific sub-unit can be considered to depend mainly on the maximum burial depth and on the current depth location (i.e. the degree of uplift). This also means that porosity and pore-size distribution data are transferrable among sites with comparable burial and uplift histories.

As the inventory of detrital and diagenetic minerals present in the Opalinus Clay does not vary over the study area, it can further be concluded that the mechanisms by which the rock controls the chemical composition of the pore water are regionally constant and can be treated in one single pore-water model.

It has been shown that the effects of early diagenesis, i.e. processes that occur within the first 100 m of burial, are quantitatively particularly important and mainly include the precipitation of aragonite/Mg-calcite, pyrite I, siderite, calcite I and dolomite I. The precipitation of siderite, pyrite I and (Fe-)dolomite affected all lithologies, including those that are clay-rich. In contrast, precipitation of aragonite/Mg-calcite and calcite I only occurred in areas rich in bioclastic material whose early diagenetic dissolution provided the solutes for pore-occluding cement precipitation. On the other hand, later mineralisations related to burial diagenesis, such as authigenic quartz and calcite II, are more strongly expressed in silty/calcareous lithologies but only weakly in the clay-rich bulk of the rock. Furthermore, they only occur in the absence of bioclastic material and associated pore-occluding cements. As a consequence, the presence or absence of bioclastic material has a considerable effect on the style by which diagenesis overprints the Opalinus Clay and its confining units.

Oedometric compression experiments showed that cementation has a distinct impact on the porosity of the Opalinus Clay, whereas permeability is not significantly affected. According to Favero et al. (2016), this is due to selective cementation by which mineral precipitation predominantly occurs in larger storage pores (typically in silty or calcareous domains), whereas smaller connecting pores (clay matrix) that control the transport properties remain unaffected.

In contrast to the regional extent of matrix mineralisation, vein mineralisation shows local differences regarding the mineral inventory and abundance of individual minerals: (1) (Fe-)dolomite II (saddle dolomite) and bitumen are solely reported for the SEAG boreholes in Northeastern Switzerland, (2) celestite has been reported for the southwestern parts of the study area, however, no celestite is observed at the SEAG boreholes in Northeastern Switzerland, (3) at Benken and Schlattigen-1 celestite constitutes an accessory vein mineral, whereas, at Mont Terri there are veins with celestite as dominant infill. Apart from these differences calcite III is consistently present at all investigated sites. Vein mineralisations reflect the tectonic

history of a specific site. The style and degree of deformation of the Opalinus Clay, as well as the timing of vein mineralisation vary over the region and depend on the tectonic position of a borehole within the basin (see Chapter 5 and Mazurek et al. 2018). Accordingly, it is not surprising that the inventory and abundance of vein minerals are heterogeneous across the investigation area.

4 Microstructural characterisation

4.1 Introduction

The water-filled pore space of the Opalinus Clay includes intergranular (or external) porosity between mineral grains and interlayer (or internal) porosity in swelling clay minerals, essentially smectite. The relative proportions of these reservoirs and the pore apertures can be estimated on the basis of a simple geometric calculation. The average internal surface of the Opalinus Clay, i.e. that associated with interlayers in smectite, can be approximated by subtracting the external surface (obtained from BET N₂ adsorption, 25 m²/g according to Tab. 2-10) from the total surface (about 90 m²/g according to Gimmi 2003), yielding 65 m²/g. Assuming that the interlayers contain 2 water molecules with an interlayer thickness of 0.56 nm (corresponding to the size of 2 water molecules) leads to a porosity of 4.4 % that is associated with interlayers. The average total porosity of the Opalinus Clay is 13 % (Tab. 2-7), so about one third of the pore space is associated with smectite interlayers (4.4 %) and two thirds with interparticle porosity (8.6 %).

The mean aperture of the interparticle porosity can be obtained by dividing the interparticle pore volume of a specific rock mass by half the external surface area of that mass (assuming slab geometry with 2 surfaces bounding each pore). This calculation yields an average aperture of about 3 nm. This rough estimation illustrates the fact that the pore space of the Opalinus Clay is nanometric and therefore difficult to visualise. For example, scanning electron microscopy generally only resolves a porosity of 1 – 3 % because it detects only the larger pores. The nanoporous nature of the Opalinus Clay and other shales is further confirmed by pore-size distributions obtained by water and N₂ adsorption (Nagra 2002).

However, the average pore size alone is just a statistical value, as the pore space in clay-rich rocks has a pore-size spectrum ranging over several orders of magnitude, from the μm range to below 1 nm. In order to capture the main features of the pore space at different scales, a combination of different analytical instruments is needed. The resolution of scanning electron microscopy (SEM) lies at 10 – 20 nm, so this technique captures only a fraction of all pores. Other techniques, such as transmission electron microscopy (TEM), offer a substantially better resolution. Further information can be obtained from adsorption isotherms (e.g. N₂, H₂O, CO₂).

In recent years, technological innovations have provided new approaches to the characterisation of microtexture and porosity down to the nanometre scale. These include micro-computed X-ray tomography (μCT) and broad- and focussed ion-beam (BIB, FIB) milling of surfaces for study by scanning electron microscopy (SEM), and other methods with even higher resolution (Fig. 4-1). FIB milling is also used for the preparation of lamellae for transmitted electron microscopy (TEM) and of cylinders for scanning transmitted electron microscopy (STEM), the latter yielding 3D information (tomography). In addition, new freezing and freeze-drying techniques were developed to minimise artefacts related to sample drying and related shrinkage. Reviews are provided in Uchic et al. (2007), Marschall et al. (2016), Desbois et al. (2016), NEA (2013) and Schäfer et al. (2016).

Surface milling using a focussed ion beam (FIB) is applicable to surface areas of a few μm^2 at most, as compared to several mm^2 or more for broad-ion beam (BIB) milling. Typically, the small areas for FIB studies are selected on the basis of BIB-SEM studies on a larger scale. One major advantage of FIB-SEM is the possibility to sequentially ablate the surface and so obtain 3D information (nano-tomography, FIB-SEM-nt). On this basis, the 3D connectivity of the pore space and transport parameters can be constrained, including information on anisotropy.

The better the spatial resolution, the smaller the area or volume of the studied sample. For SEM and TEM studies, the sample dimensions lie in the range of μm or less, and the question arises how representative the information is for the larger scale. The definition of representative elementary areas and volumes (REA, REV) are important issues, as are techniques of upscaling (see Keller et al. 2013a, 2015a).

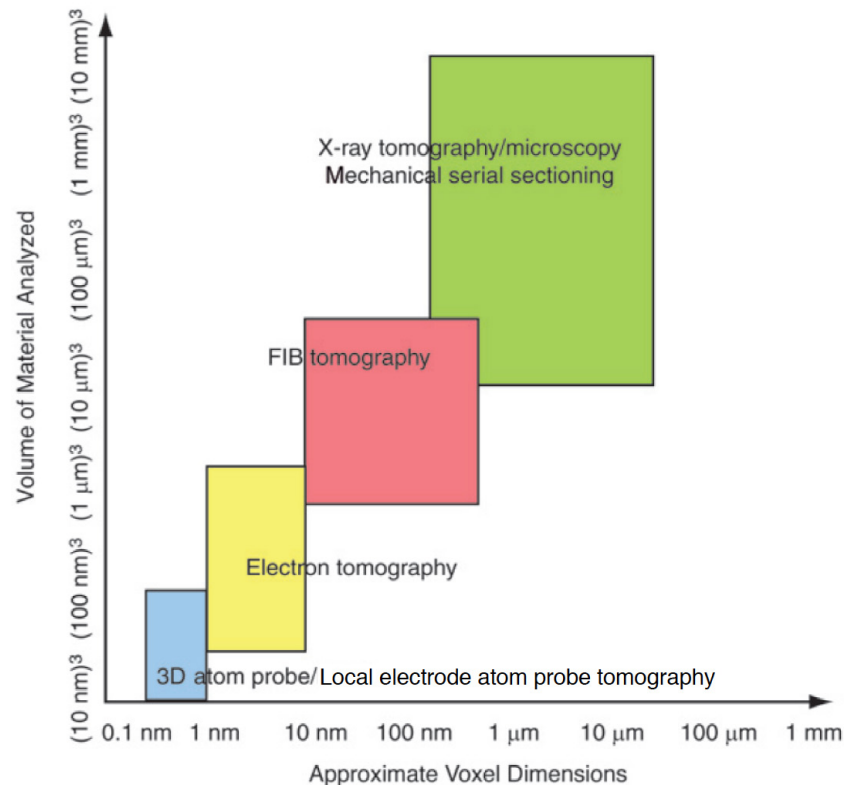


Fig. 4-1: Methods to characterise the 3-dimensional pore architecture of nanoporous materials at different scales

Adapted from Uchic et al. (2007)

4.2 Petrography and pore geometry by BIB-SEM

In a BIB-SEM study on samples from the clay-rich sub-unit of the Opalinus Clay from Mont Terri, Houben et al. (2013) distinguished the following pore types:

- **Porous clay matrix:** A scheme of pore morphologies developed by Desbois et al. (2009); illustrated in Fig. 4-2 for the Boom Clay is also applicable to Mont Terri and includes (I) elongated pores between similarly oriented clay sheets, (II) crescent shaped pores in saddle reefs of folded sheets of clay, and (III) large jagged pores surrounding mineral grains. Pores in the clay matrix of the Opalinus Clay are also shown in Fig. 4-3.
- **Porous fossil fragments:** Calcitic fossil shells, such as bivalves, may preserve their primary structure and porosity, or pores are generated by mineral dissolution (Fig. 4-4). They constitute the most conspicuous pore type with comparatively large mean pore size around 100 nm, even though some pores may be even larger (up to several μm). Note that the

Opalinus Clay contains various types of calcite, and not all calcites are porous. Clastic grains without resolvable porosity are frequently observed.

- Diagenetic siderite frequently forms idiomorphic, rhombic crystals that have hollow cores with jagged surfaces (Fig. 4-5).
- Diagenetic pyrite framboids show substantial porosity with pore sizes up to 1 μm (Fig. 4-6).
- Large bedding-parallel cracks with high aspect ratios and lengths in the range of μm to mm are seen in the clay matrix (Fig. 4-7). They are clear artefacts of sample preparation and drying. They are most strongly expressed in air-dried samples but also occur in freeze-dried samples.

In summary, the natural pore space consists of primary pores (clay matrix, fossils) and diagenetic pores (siderite, pyrite). Pore sizes in fossils, siderite and pyrite may reach sizes of 100 – 1'000 nm, but they are connected only via the nanoporous clay matrix. Quartz, mica and organic matter are not associated with any pore spaces at the resolution of the instrument. Note that Keller et al. (2013b) found substantial porosity in organic matter by FIB-SEM.

After pore segmentation, Houben et al. (2013) quantified the visible porosity of the different pore types, and the results for two samples are shown in Tab. 4-1. The applied magnification of 20'000 – 25'000x is large enough to distinguish different pore types but still allows the study of areas sufficiently large for a statistically significant evaluation (the minimum representative elementary area [REA] was determined by box counting and lies around $100 \times 100 \mu\text{m}^2$). When ignoring cracks that are probably artefacts, the visible porosity amounts to 1.5 – 2.3 %. About 60 – 64 % of the total originate from the clay matrix, 33 – 36 % from fossils and 3 – 4 % from siderite. The contribution of pyrite is much lower. By absolute number and therefore by pore surface, pores in the clay matrix dominate by far.

The average porosity of the clay-rich sub-unit of the Opalinus Clay at Mont Terri obtained from water-content measurements is about 14 % (Mazurek et al. 2017b). This means that only about a tenth of the entire pore space can be imaged by SEM, while the remainder of the pore space has apertures below the resolution at around 10 nm. This pore space is associated with the clay matrix, including the external porosity as well as the interlayers in smectite.

The mineral fabric of the clay-rich sub-unit of the Opalinus Clay is clearly matrix-supported, i.e. larger grains of quartz, calcite and other minerals are completely embedded in the clay matrix (Houben et al. 2013, 2014). Therefore, the hydraulic, transport and mechanical properties are essentially determined by the properties of the matrix. This may not be the case at least on the cm scale in the silty sub-units of the Opalinus Clay throughout the area of investigation, where silty lenses and ripples with typical dimensions of 1 cm $\times$ 10 cm occur (Keller et al. 2013a; Fig. 2-5c, 6-1h,i). These lenses can have a grain-supported fabric with clay in the interstitial space. Philipp et al. (2017) identified a more limited degree of compaction of the clay matrix and therefore a higher porosity in such situations (Fig. 4-8) and attributed this to a pressure-shadow effect. It is worth noting that on a decimetric or larger scale, the silty lenses as a whole can nevertheless be considered to be matrix-supported, given the fact that their extent is limited in all dimensions and so they are embedded in clay-rich material. This is probably not the case for the carbonate-rich silty sub-unit, where the fabric is grain-supported even on larger scales.

In addition to studying the microfabric, Philipp et al. (2017) also conducted laboratory experiments on centimetric samples to measure permeability of the Opalinus Clay from Mont Terri. They obtained higher porosity but lower permeability values for the clay-rich sub-unit when compared to the silty sub-unit, contrary to the general trend of permeability increasing with increasing porosity (and therefore clay-mineral content). This is explained by the pore-size distribution, which is dominated by nanometric pores in the clay matrix, whereas larger pore apertures are found in silty lithologies.

Tab. 4-1: Selected results of the BIB-SEM study conducted by Houben et al. (2013) on samples from the clay-rich sub-unit of the Opalinus Clay from Mont Terri

Note that only a relatively small fraction of the total porosity can be imaged by SEM. Thus, the reported median pore radius refers to the visible part of the pore space, while it would be much smaller when considering the total pore space.

Sample	Drying	Magnification	Pixel size [nm]	Visible porosity [%]	Visible porosity, excluding cracks [%]	Porous phase	Number of pores	Contribution to visible porosity [%]	Contribution to visible porosity, excluding cracks [%]	Median pore radius [nm]
BCS-2/5	Air-dried	25'000×	11.7	2.69	2.3	Clay matrix	36'632	51	60	34
						Fossils	4'748	31	36	51
						Siderite	770	3	4	38
						Cracks	1'709	15		71
BCS-2/3	Freeze- dried	20'000×	14.7	2.1	1.5	Clay matrix	25'226	47	64	26
						Fossils	3'434	24	33	42
						Siderite	185	2	3	57
						Cracks	1'099	27		75

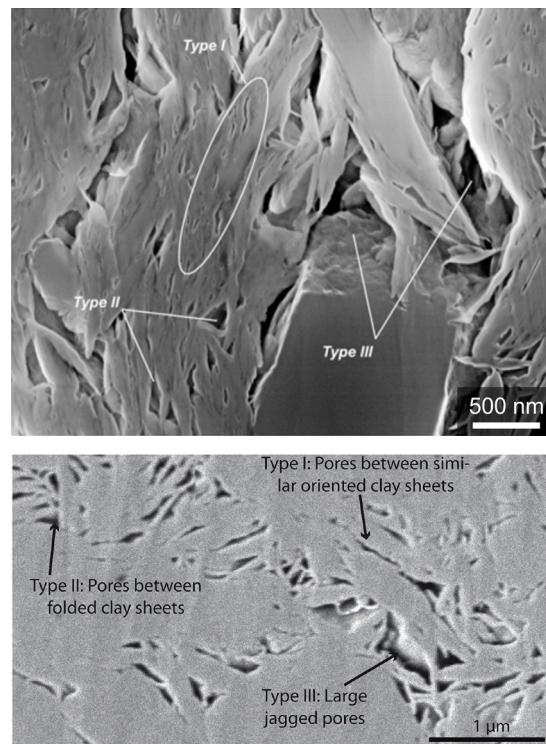


Fig. 4-2: Different pore morphologies identified by BIB-SEM in the matrix of clays and shales

Top: Boom Clay, from Desbois et al. (2009). Bottom: Clay-rich sub-unit of the Opalinus Clay at Mont Terri, from Houben et al. (2014). Type I – elongated pores between similarly oriented clay sheets; type II – crescent shaped pores in saddle reefs of folded sheets of clay; type III – large jagged pores surrounding mineral grains.

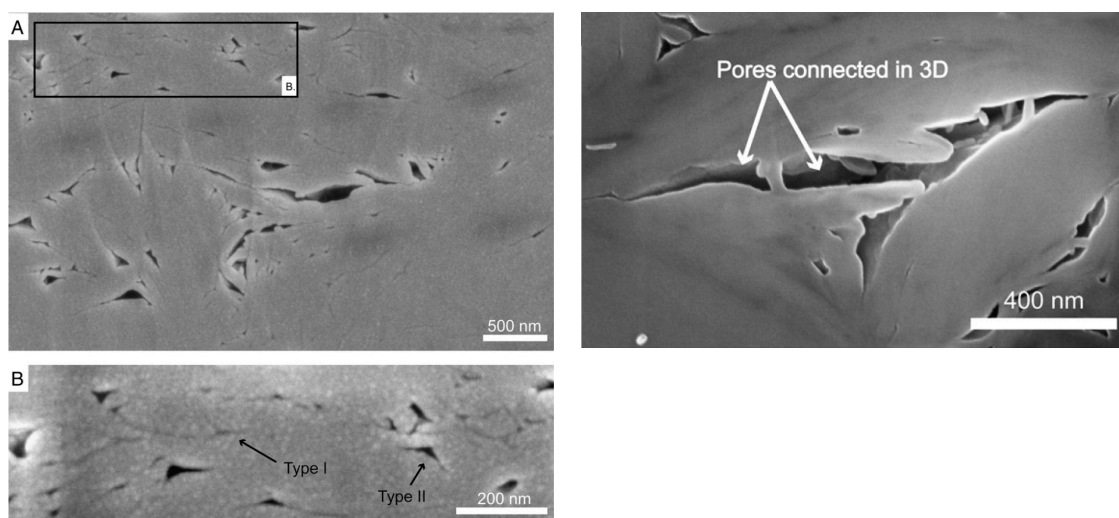


Fig. 4-3: Pores in the clay matrix of the Opalinus Clay

BIB-SEM images from Houben et al. (2013), clay-rich sub-unit of the Opalinus Clay at Mont Terri.

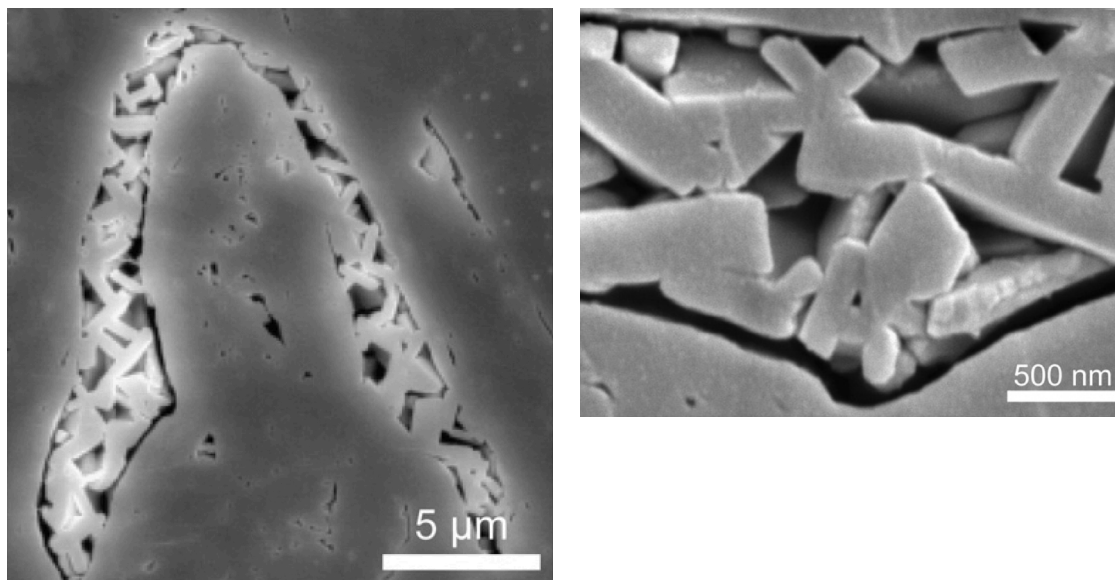


Fig. 4-4: Pores in fossil fragments in the Opalinus Clay

BIB-SEM images from Houben et al. (2013), clay-rich sub-unit of the Opalinus Clay at Mont Terri.

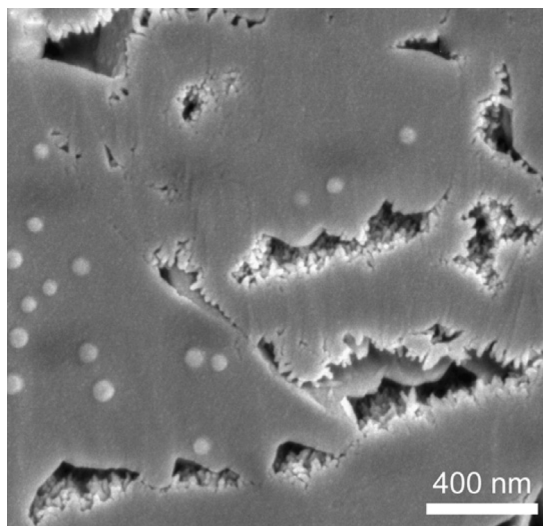


Fig. 4-5: Pores in diagenetic siderite in the Opalinus Clay

BIB-SEM image from Houben et al. (2013), clay-rich sub-unit of the Opalinus Clay at Mont Terri.

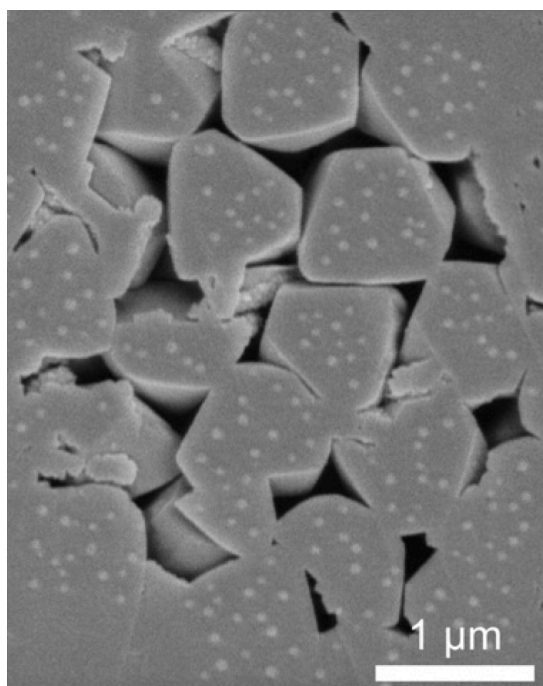


Fig. 4-6: Pores in a diagenetic pyrite framboid in the Opalinus Clay
BIB-SEM image from Houben et al. (2013), clay-rich sub-unit of the Opalinus Clay at Mont Terri.

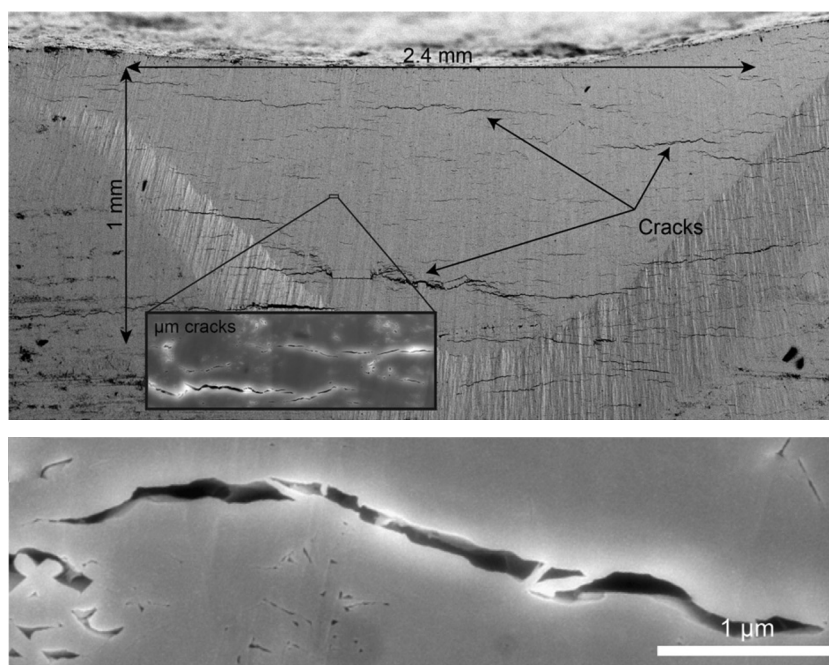


Fig. 4-7: Artificial drying cracks in the clay matrix of an air-dried Opalinus Clay sample at different scales
BIB-SEM images from Houben et al. (2013), clay-rich sub-unit of the Opalinus Clay at Mont Terri.

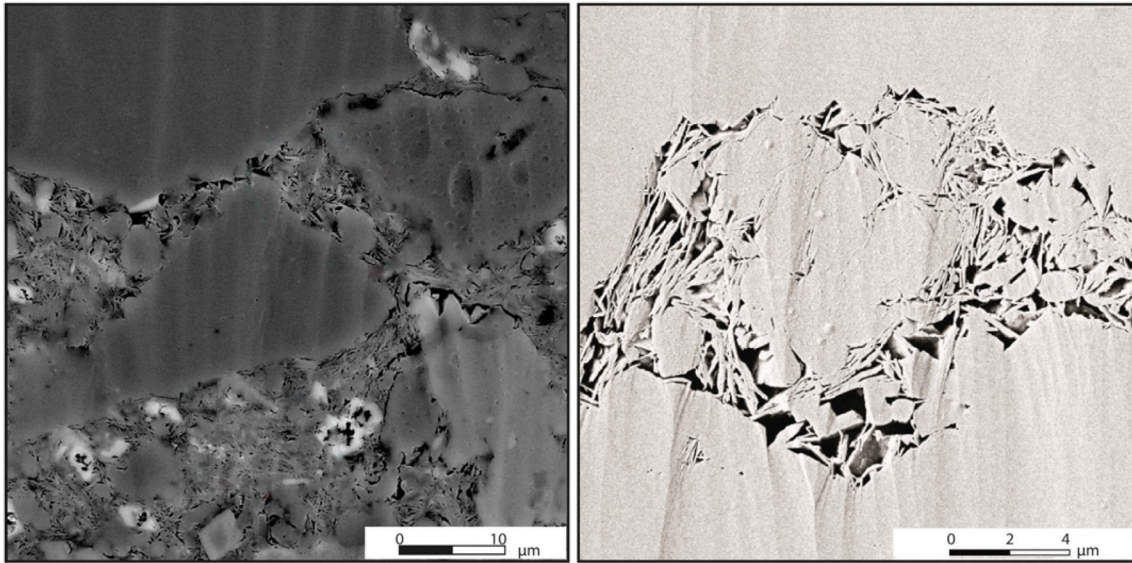


Fig. 4-8: Weakly compacted and porous clay matrix in a grain-supported zone of the silty sub-unit of the Opalinus Clay at Mont Terri
BIB-SEM image from Philipp et al. (2017).

4.3 μ CT, FIB-SEM and STEM studies

Keller et al. (2013b) studied the clay-rich sub-unit of the Opalinus Clay at Mont Terri by μ CT, FIB-SEM and STEM nanotomography and so covered a wide range of scales. By μ CT, the resolved porosity was 0.6 %, compared to 2 – 3 % that were resolved by FIB-SEM-nt. By STEM and N_2 adsorption, 10 – 13 % were obtained, which is close to the total porosity obtained by water loss or densitometry. The different porosities obtained reflect the resolution of the respective analytical tool. Fig. 4-9 shows the pore-size distributions obtained. Note that at least for STEM tomography, the studied volume is far below the REV size and so not directly comparable to the results obtained by the other techniques on the same sample.

The study of Keller et al. (2013b) focussed on the characterisation of porosity in the Opalinus Clay on different scales. The majority of the pore spaces were found to be due to geometric incompatibilities at contacts between individual clay particles. Enhanced porosity was frequently identified at the contacts between larger clastic grains (mainly quartz and calcite) and the embedding matrix (Fig. 4-10). These pores add to the connectivity of pores in the clay matrix. Similar conclusions were obtained by Sammartino et al. (2003) and Yven et al. (2007) for the Callovo-Oxfordian shale in France. These authors described larger pores associated to quartz and calcite grain boundaries. In the matrix-supported shale, higher porosity and larger apertures associated with larger clastic grains were found to be connected via the lower-aperture pores in the embedding clay matrix.

The 3D information obtained from μ CT or FIB-SEM tomography can further be used for a quantitative analysis of the pore space. For example, Keller et al. (2015b) and Robinet et al. (2012) applied synchrotron X-ray tomography to reconstruct the mesostructure (spatial arrangement of minerals on the μ m to mm scale) of the Opalinus Clay and the Callovo-Oxfordian shale in eastern France, respectively. Conceptually, both considered the rock fabric to consist of a porous clay matrix containing isolated grains of non-porous larger grains (mainly calcite and quartz). They simulated solute diffusion through the reconstructed shale and

characterised geometric parameters, such as tortuosity and constrictivity. The simulations yielded only weak anisotropy, which means that the pronounced anisotropy of transport (diffusion coefficient, permeability) and mechanical parameters that is observed in laboratory experiments is not due to the mesostructure but to anisotropy on a smaller scale, in particular within the clay matrix.

As a further example, Grochimund et al. (2016) applied a synchrotron X-ray technique to reconstruct the 3-dimensional distribution of calcite, clay and pyrite in the Opalinus Clay on a sub-millimetric scale and imaged the transport of Cs through the pore space (Fig. 4-11).

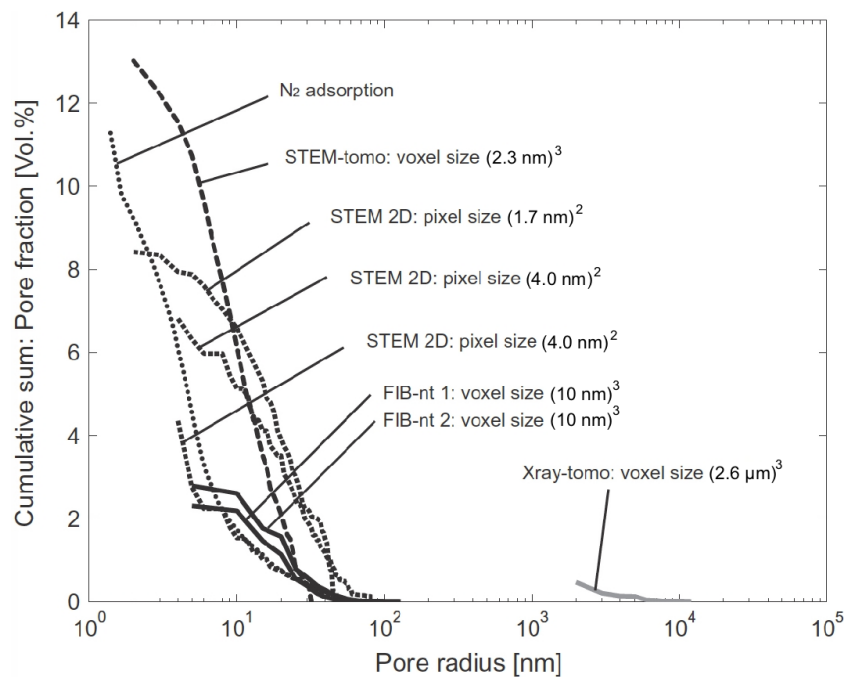


Fig. 4-9: Pore-size spectra of a sample from the clay-rich sub-unit of the Opalinus Clay obtained by various investigation tools
Keller et al. (2013b).

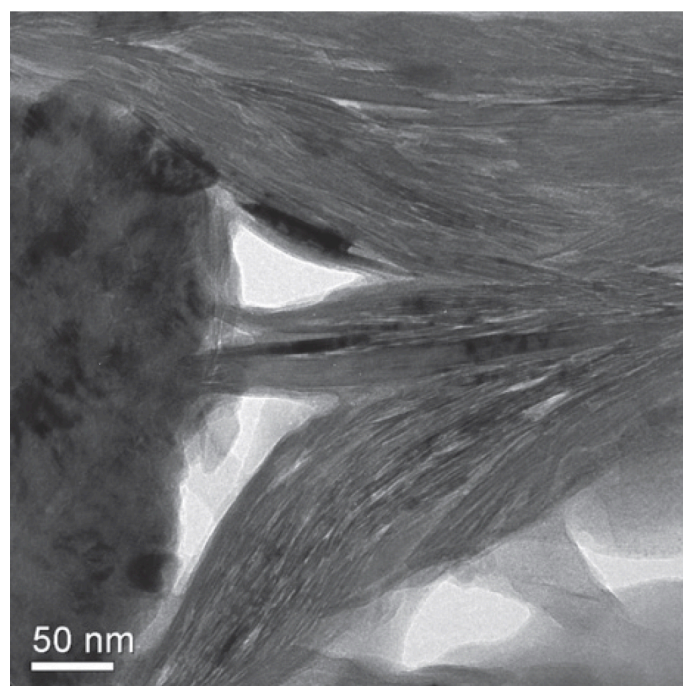


Fig. 4-10: TEM picture showing porosity at the contact between a clastic grain (left) and the clay matrix

Keller et al. (2013b).

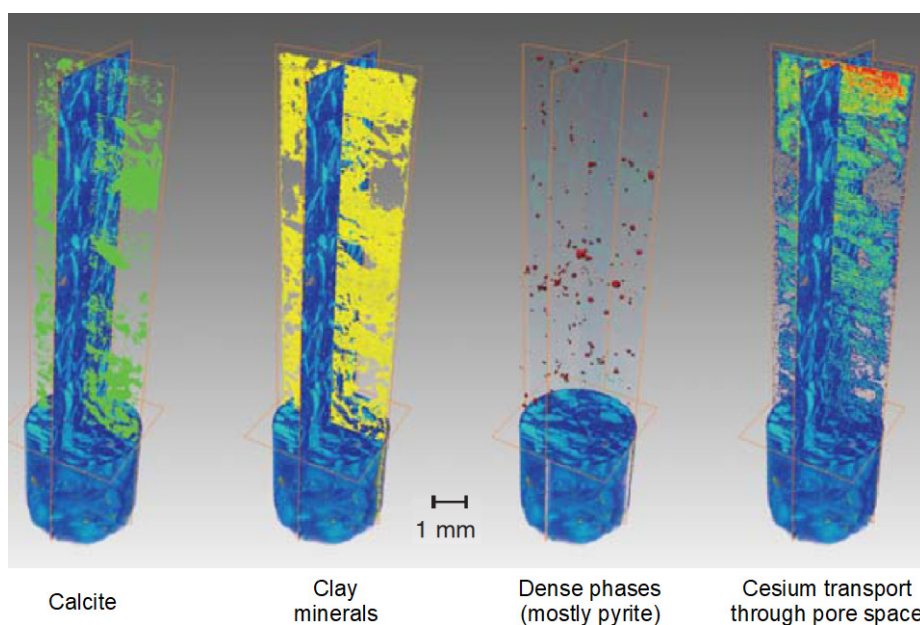


Fig. 4-11: Distribution of minerals and diffusive transport of cesium in a sample from the Opalinus Clay

Data were obtained by synchrotron X-ray absorption-edge difference tomography, augmented by micro-XRF and micro-XRD for phase identification. Blue volumes and slices image the absorption contrast. The source of Cs is on the top, and migration direction is downward (image to the right). Adapted from Grolimund et al. (2016).

5 Structural features

In this report, the characterisation of brittle structures in the Opalinus Clay is limited to cored boreholes and tunnel observations in the case of Mont Terri. While borehole-wall imaging was performed in several percussion boreholes, the interpretation remains uncertain in the absence of core. Surface mappings of brittle structures in the Opalinus Clay were performed in quarries and are documented in Nagra (2002). These findings are not repeated here.

The degree of detail to which structural features have been studied varies. The most detailed information is available for Mont Terri, while it is limited for the older boreholes in Northern Switzerland (in particular Schafisheim, Riniken-1 and Weiach-1). The new boreholes in the frame of the Stage 3 investigations (from 2019 onwards) will be drilled with a triple-core barrel technique and are expected to provide substantial structural information.

5.1 Mont Terri

Given the fact that the Mont Terri underground laboratory is located within an anticline of the Jura fold-and-thrust belt, the Opalinus Clay is strongly deformed. According to Nussbaum et al. (2011), the most frequent fault set is a SSE-dipping, essentially bedding-parallel system that is interpreted as due to flexural slip during folding of the anticline. On the average, larger faults of this system occur every 10 m. Including smaller structures, the frequency ranges from 0.2 to 20 faults per metre. A magnetic fabric also developed during deformation along this fault set, meaning that a penetrative fabric is related to this stage of deformation (Nussbaum et al. 2011).

The most prominent structure at Mont Terri is the Main Fault, a thrust fault that extends laterally over at least 100 m (Fig. 5-1, 5-2). A detailed characterisation and structural interpretation is found in Nussbaum et al. (2011) and Jäggi et al. (2017). Outcrops in two parallel tunnels (Ga98 and Ga08) 55 m apart indicate a major lateral change of deformation style. In Ga98, the Main Fault is narrower (about 1 m) and intensely deformed, whereas in Ga08 deformation is more distributed across a 3 – 5 m thick structure. On a large scale, the fault orientation is about 20° steeper than bedding. The fraction of scaly clay (see below) in the outcrop cross-section decreases with decreasing fault thickness, suggesting a more localised deformation in the narrower part of the fault. In the conceptual model of Jäggi et al. (2017) shown in Fig. 5-2, zones of scaly clay are located along the external parts of the fault, with sharp boundaries. A continuous band of fault gouge constitutes the upper boundary, but thinner gouge horizons occur throughout the fault. Slickensides are ubiquitous and constitute the elementary building blocks of the fault.

On the meso- and microscopic scales, Laurich et al. (2014) distinguished the following structural elements (Fig. 5-3):

- *Slickensides* record highly localised shear deformation and are characterised by striated, shiny surfaces, which consist of an about 1 µm thick layer of clay minerals that are strictly oriented along the structure (Fig. 5-3a–c). This layer has no porosity that would be resolved by scanning electron microscopy.
- *Calcite and celestite veins* are linked to small-scale extensile relay zones along the slickensides (fibres) and are due to syntectonic precipitation in pressure shadows (Fig. 5-3a,d). They are typically thin (max. 1 mm) but can extend over several centimetres along the slickensides. Crack-seal textures indicate repeated crack opening and mineral precipitation.

- *Scaly clay* consists of fish-like flakes bounded by slickensides (Fig. 5-3f). Structures of this type occur on the mesoscopic scale but similar features are also found at smaller scales, with flake thicknesses down to 300 μm or less. Zones of scaly clay vary in size from 1 cm to 1 m. On a macroscopic scale, shear bands and drag folds are identified (Jäggi et al. 2017).
- *Fault gouges* occur but are volumetrically insignificant, with thicknesses often below 1 mm but sometimes up to 2 cm (Fig. 5-3e). Grain size is smaller than in the surrounding rock. Calcite content of the gouges is also distinctly lower, suggesting effects of pressure solution. Porosity resolvable by BIB-SEM is below 1 %, i.e. less than in the undeformed rock. A detailed characterisation of the fault gouge is provided by Laurich et al. (2018).



Fig. 5-1: The Main Fault in the Gallery 98 of the Mont Terri underground laboratory
Upper picture shows the whole fault in the right half of the window. Detail in the lower picture illustrates a zone with a high degree of shear deformation, including drag folding.

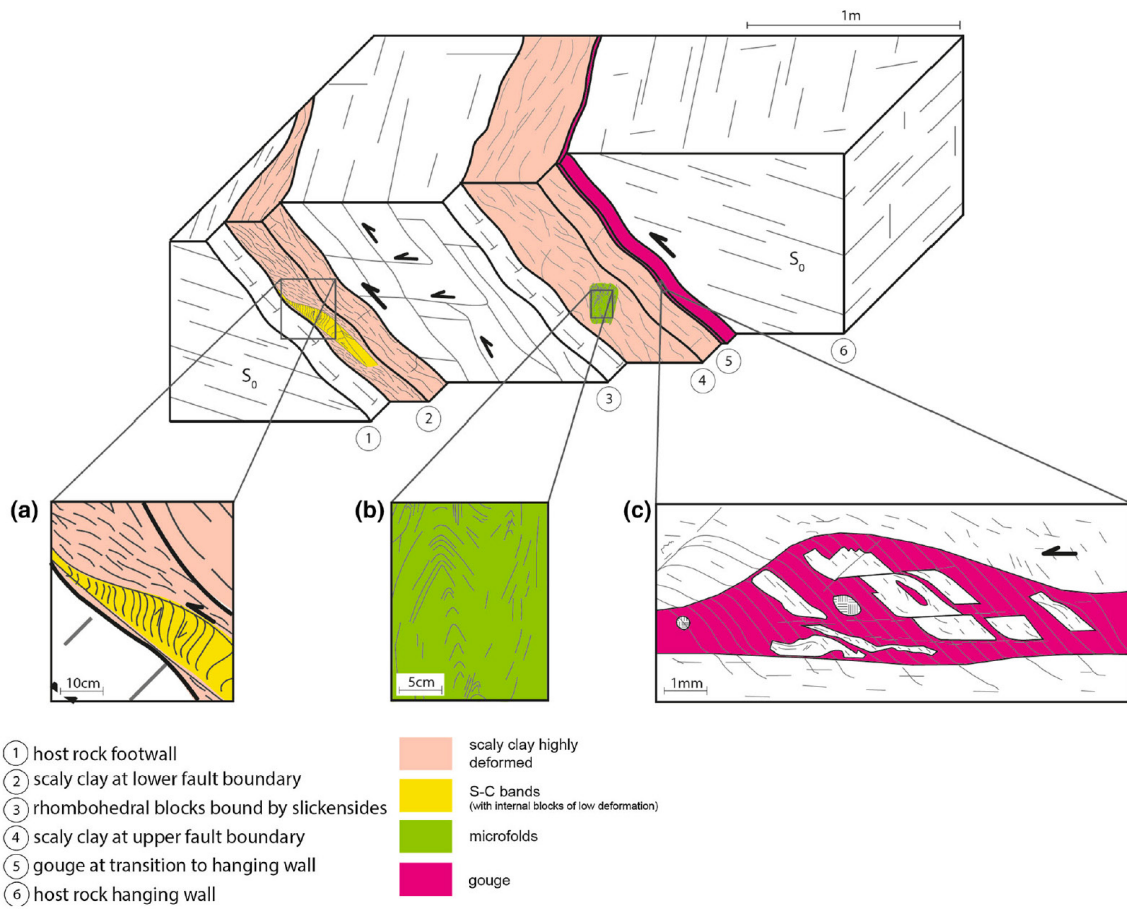


Fig. 5-2: Conceptual block model of the Main Fault at Mont Terri
 Jäggi et al. (2017).

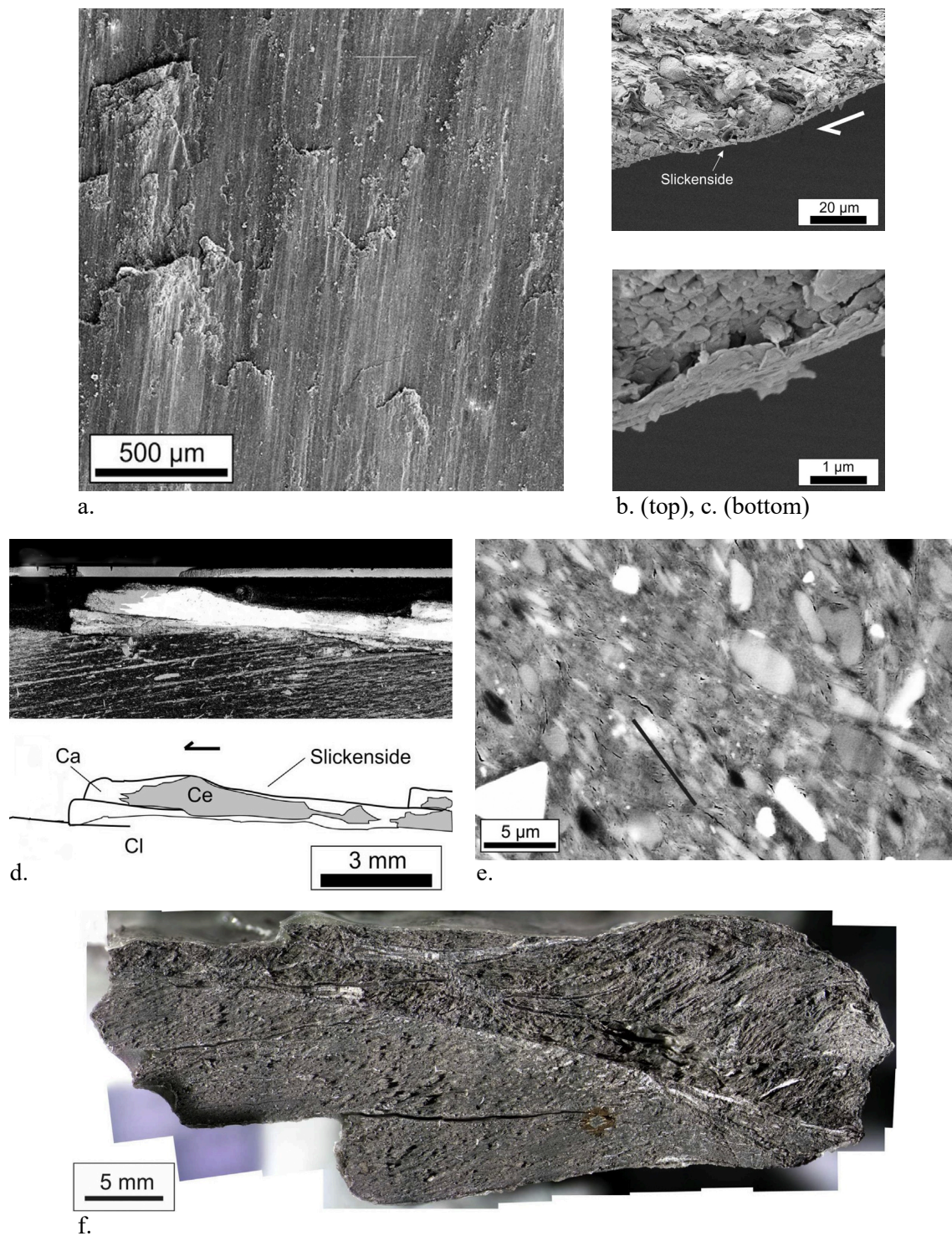


Fig. 5-3: Small-scale structural elements of the Main Fault at Mont Terri

Adapted from Laurich et al. (2014).

- a. Surface view of a slickenside with calcite-celestite fibres (SEM image)
- b. Cross-section view of a slickenside, showing the thin layer of oriented clay minerals (SEM image)
- c. Detail of b.
- d. Cross section of a slickenside surface with a calcite-celestite fibre (photograph)
- e. Fault gouge with planar fabric (SEM image)
- f. Scaly clay (photograph)

5.2 Lausen

Brittle structures were logged by Vogt et al. (2016) on the basis of core and borehole-image data. The frequency of joints is high within the weathered zone and down to about 40 m. Joints are subordinate at deeper levels, suggesting that they are related to the decompaction of the Opalinus Clay. Three fault surfaces occur in the deeper part of the Opalinus Clay, in addition to some slickensided fractures. They are bedding-parallel, i.e. horizontal. Faults in the underlying units have the same orientation, indicating that these structures are of tectonic origin, unrelated to decompaction.

5.3 Schafisheim

The upper part of the Opalinus Clay, down to about 1'050 m, is only weakly affected by deformation and contains few slickensided fractures with dip angles around 45°. Fracture frequency increases below this depth and reaches a maximum in the lowermost 10 m of the Opalinus Clay, with frequencies up to 4 m⁻¹ (Matter et al. 1988b; Fig. 5-4, 5-6). Some but not all fractures in this lowermost zone show slickensides. They have dip angles of up to 50° and so are discordant to the flat-lying bedding. A conspicuous calcite vein infill at 1'056.66 m is associated with a 45° dipping slickensided fracture (Fig. 5-5).

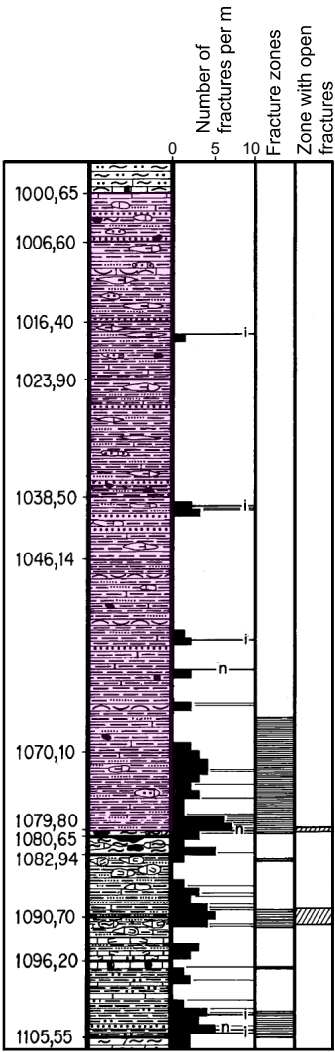


Fig. 5-4: Structural core log of the Opalinus Clay from the Schafisheim borehole

Opalinus Clay shown in pink. n = normal, i = inverse. Adapted from Matter et al. (1988b)



Fig. 5-5: Slickensided fracture sealed with vein calcite at 1'056.66 m in the Schafisheim core

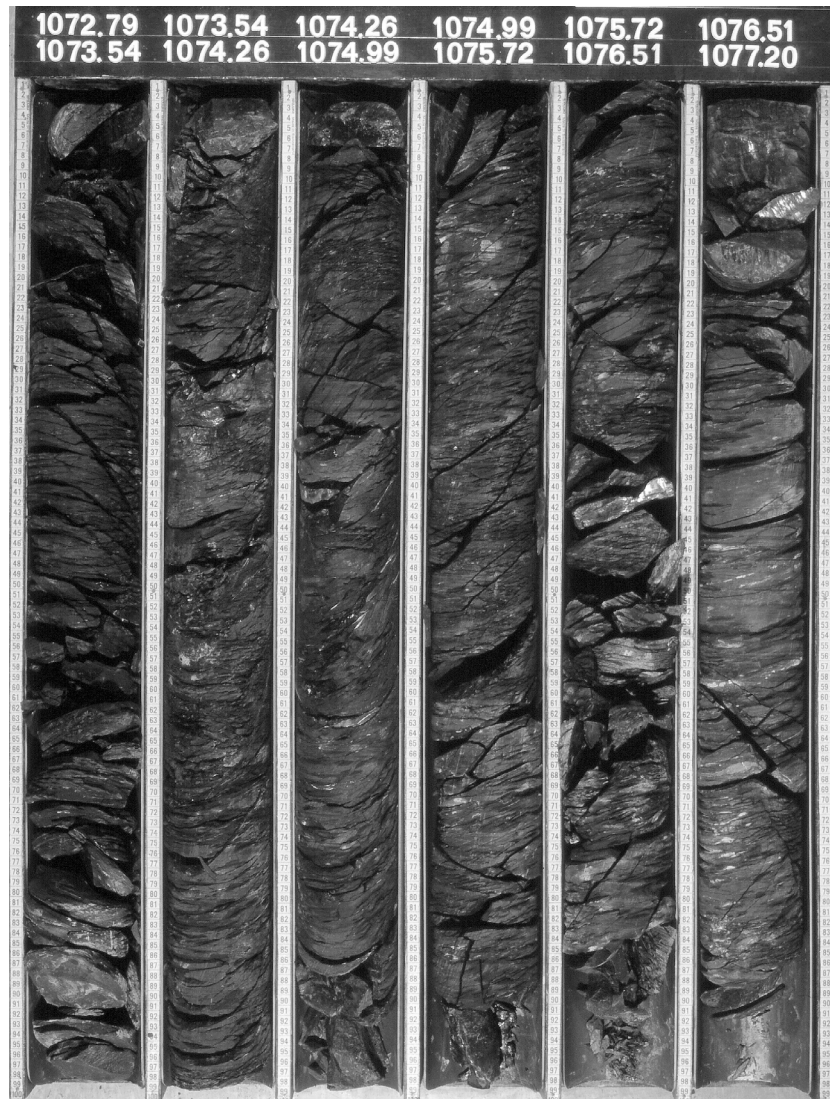


Fig. 5-6: Core photographs of the highly deformed base of the Opalinus Clay in the Schafisheim borehole

5.4 Riniken-1

The upper and central parts of the Opalinus Clay are essentially undeformed, while the lowermost 30 m show high fracture density (Matter et al. 1987; Fig. 5-7). Two fault zones, each about 2 m thick, were identified at 429 and 436 m, with fractures dipping with $25 - 45^\circ$ and $40 - 60^\circ$ to the NNW, respectively. Thus, these fault zones are parallel to the strike of the Jura fold-and-thrust belt and the underlying Permo-Carboniferous trough. They consist of individual fault surfaces, slickensides and joints. Fracture infills consist of clay minerals (probably fault gouges) and minor calcite.

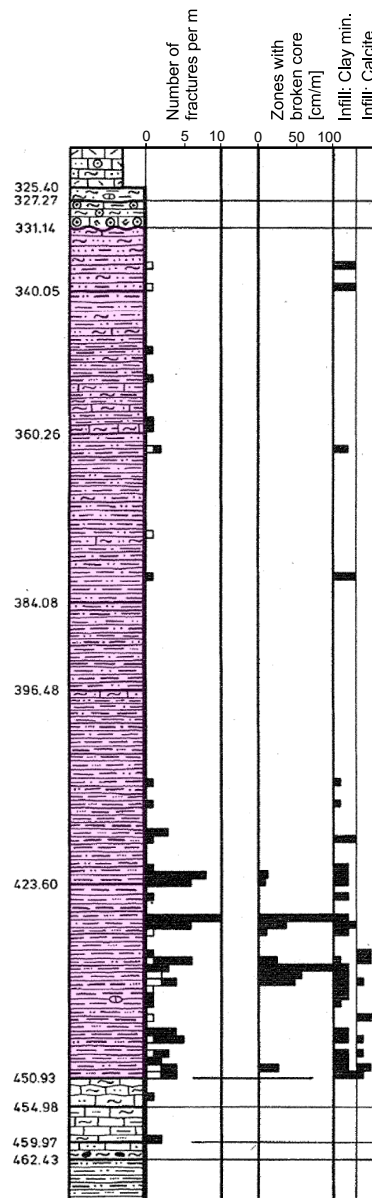


Fig. 5-7: Structural core log of the Opalinus Clay from the Riniken-1 borehole

Opalinus Clay shown in pink. Black bars in column "Number of fractures per m": fracture in continuous core; white bars: core broken along fracture. Adapted from Matter et al. (1987).

5.5 Weiach-1

In the lowermost 25 m, a limited degree of fracturing can be identified, even though much less strongly expressed than in Riniken-1 and Schafisheim (Matter et al. 1988a). The rest of the Opalinus Clay is essentially undeformed.

5.6 Benken

The Opalinus Clay is essentially undeformed, except for some single fault surfaces and a 10 cm thick fault (Nagra 2002).

5.7 Schlattingen-1

The Opalinus Clay itself is only mildly affected by shear deformation (one fault surface, 18 slickensides) and almost devoid of vein infills (Albert et al. 2012a, Mazurek et al. 2018). The embedding units, i.e. the overlying 'Brauner Dogger' and the underlying Staffelegg Formation, are more strongly deformed, mostly by dip-slip normal faulting. The structural style as well as age dating of calcite veins that infill part of the faults indicate a genetic relationship to the formation of the Bodensee-Hegau graben in the Miocene (Mazurek et al. 2018). The present-day stress field, in particular in the deeper parts of the borehole, is also compatible with a normal-faulting regime, with a possible strike-slip component ($\sigma_h < \sigma_H \leq \sigma_V$, Klee 2012).

5.8 Conclusions

The degree of deformation of the Opalinus Clay varies over the investigation area and depends on the tectonic position of the borehole in which it was drilled. The main findings are summarised in Tab. 5-1. In boreholes Weiach-1 and Benken, the Opalinus Clay is almost undeformed, consistent with their position considerably northeast of the Jura fold-and-thrust belt (even though some degree of deformation may have been expected at Weiach, given the position within the Deformed Tabular Jura). Even farther to the northeast, some degree of normal faulting is identified at Schlattingen, which is likely due to the proximity of the Miocene Bodensee-Hegau graben.

In Riniken-1 and Schafisheim, the lowermost part of the Opalinus Clay is strongly affected by faulting. This is likely due to effects of the distant push that affected the Mesozoic during the formation of the Jura fold-and-thrust belt. Schafisheim is located south of this belt, while Riniken-1 is located to the north in the Deformed Tabular Jura ("Vorfallenzzone"). As stated by Madritsch (2015), this tectonic unit, which terminates at the Mandach fault, is a part of the Jura fold-and-thrust belt and its compressive regime.

The degree of deformation in the lower part of the Opalinus Clay at Lausen is low, corresponding to its position in the Tabular Jura.

Finally, the high and penetrative degree of deformation of the Opalinus Clay at the Mont Terri underground laboratory is in line with its location in an anticline of the Jura fold-and-thrust belt.

Tab. 5-1: Summary of brittle-deformation features in cored boreholes

Borehole	Tectonic unit	Deformation of the Opalinus Clay	Deformation style
Mont Terri	Jura fold-and-thrust belt	Penetrative deformation	Mainly thrusting
Lausen	Tabular Jura	Essentially undeformed (except for surficial decompaction)	-
Schafisheim	Molasse Basin within the range of the Jura décollement	Strong faulting in the lowermost 10 m, essentially undeformed in the hanging wall	Thrusting and/or strike-slip
Riniken-1	Deformed Tabular Jura	Strong faulting in the lowermost 30 m, essentially undeformed in the hanging wall	Thrusting and/or strike-slip
Weiach-1	Deformed Tabular Jura	Essentially undeformed	-
Benken	Molasse Basin outside the range of the Jura décollement	Essentially undeformed	-
Schlattingen-1	Molasse Basin outside the range of the Jura décollement, within range of the Hegau-Bodensee graben	Weakly deformed	Normal faulting

6 Conceptual characterisation of the Opalinus Clay on different scales

The structure of the Opalinus Clay on scales between tens of km to 1 nm, i.e. over a length-scale range of 13 orders of magnitude, is illustrated in Fig. 6-1. The main methods and sources of information include, in the order of decreasing scale, geophysical borehole logs, macroscopic core inspection, thin-section analysis, SEM imaging and TEM imaging.

On a regional scale (Fig. 6-1a), a number of sub-units can be distinguished and correlated laterally. The correlation, including marker horizons in geophysical borehole logs, is straightforward in the Northeastern part of the investigation area. Towards the southwest, the correlatability ends along a WNW-ESE-trending zone bounded by Lausen and Wölflinswil-2 in the northwest and Schafisheim and Triemli in the southeast (Fig. 2-10). This zone correlates with a region of low thickness of the Opalinus Clay, i.e. it separates depocentres to the northeast and to the southwest, as well as realms with different directions of palaeo-currents (Allia 1996, Wetzel & Allia 2003). To the southwest of the zone, correlatable marker horizons in geophysical logs are virtually absent, and two silty sub-units represent the main heterogeneities.

On the borehole scale (Fig. 6-1b), sub-units with thicknesses in the range of metres to a few dekametres can be defined by core inspection and geophysical borehole logs, which in most cases yield highly consistent information. Discrete heterogeneities, such as calcareous beds/nodules with a thickness in the range of 0.1 – 0.6 m (Tab. 2-4), are frequent within the upper part of the formation in the Northeastern part of the investigation area. These heterogeneities are the defining feature of the *sub-unit with silty calcareous beds*. Let us note that even in this sub-unit, clay-mineral contents remain at levels > 40 wt.-%, with local excursions to lower levels (Fig. 2-8, 2-18). While the sub-unit with silty calcareous beds can be correlated among boreholes, individual heterogeneities often cannot, indicating limited lateral extents. In the underlying *upper silty sub-unit*, particularly silt-rich, 1.7 – 5 m thick zones can be distinguished (Tab. 2-4, Fig. 2-8). The average clay-mineral contents in these zones remain > 40 wt.-%. The underlying *mixed clay-silt-carbonate sub-unit* is present over the whole investigation area, whereas the occurrence of the *lower silty sub-unit* and the *carbonate-rich silty sub-unit* is limited to the extreme west. The smaller-scale characteristics of the *mixed clay-silt-carbonate sub-unit* are not illustrated in Fig. 6-1 because this sub-unit contains elements of all other sub-units to some degree. Along the base of the Opalinus Clay, the *clay-rich sub-unit* extends across the whole investigation area, with clay-mineral contents well above 50 wt.-%.

On this basis, the building blocks of the Opalinus Clay, illustrated in Fig. 6-1c–e, can be conceptually simplified to

- clay matrix with variable contents of disseminated quartz and calcitic fossil fragments, occurring (and mostly dominating) in all sub-units
- calcareous beds/nodules, mostly within the sub-unit with silty calcareous beds
- silty lenses, most frequently occurring in the silty sub-units

The small-scale calcareous and silty heterogeneities in all sub-units are embedded in a clay-rich matrix, which is the dominant building block. This fact is illustrated by arrows pointing from Fig. 6-1c–e towards Fig. 6-1j.

Calcareous beds/nodules are illustrated in Fig. 6-1f–g on the thin-section scale. They consist of fossil fragments, silty particles and a calcite cement, with only small amounts of clay minerals.

Fig. 6-1h–i illustrate silty lenses on a microscopic scale. These can contain clay minerals (see e.g., Fig. 4-8) or, as shown in Fig. 6-1h–i, consist of almost pure quartz $\pm$ feldspars. Given the originally large pore apertures, the lenses are mostly cemented by sparitic and/or poikilitic calcite cement.

The clay-rich matrix is the quantitatively dominating building block of the Opalinus Clay and is illustrated in Fig. 6-1j–n. It embeds variable amounts of disseminated quartz and calcitic fossil fragments (Fig. 6-1j–k). Note that under the SEM, only a fraction of the pore space can be visualised, given the limited resolution (at best around 10 nm). Fig. 6-1l–m visualise the clay matrix by TEM. Visible pores are due to geometric incompatibilities between clay aggregates or between clay and non-clay minerals. While pores with even smaller, nanometric apertures constitute a substantial part of the pore space, they are difficult or impossible to image and so illustrated by a conceptual sketch in Fig. 6-1n. A part of the porosity is located in the interlayer space of swelling minerals, in particular smectite (within illite/smectite mixed-layer minerals). Pore water in the interlayers (and along the external surfaces of smectite) has distinct properties in terms of chemical composition and mobility, given the fact that it is affected by the surface charge and electrostatic potential of clay surfaces. The so-called free or mobile pore water resides in the central parts of larger pores. The 3-dimensional architecture and connectivity of the different pore types determine macroscopic properties, such as transport parameters (e.g. permeability, diffusion coefficient) and their anisotropy, ion exclusion and various coupled processes.

Apart from the cementation by a number of calcite generations, siderite and pyrite are quantitatively relevant diagenetic neoformations and occur in all sub-units of the Opalinus Clay (Fig. 6-1o–p). Siderite can be found in concretions with sizes in the range of centimetres or as disseminated crystals in the clay matrix. Pyrite occurs in the form of 1 – 10 μm -sized framboids or as larger crystals. Concretions are also found, even though much less frequently than in the case of siderite.

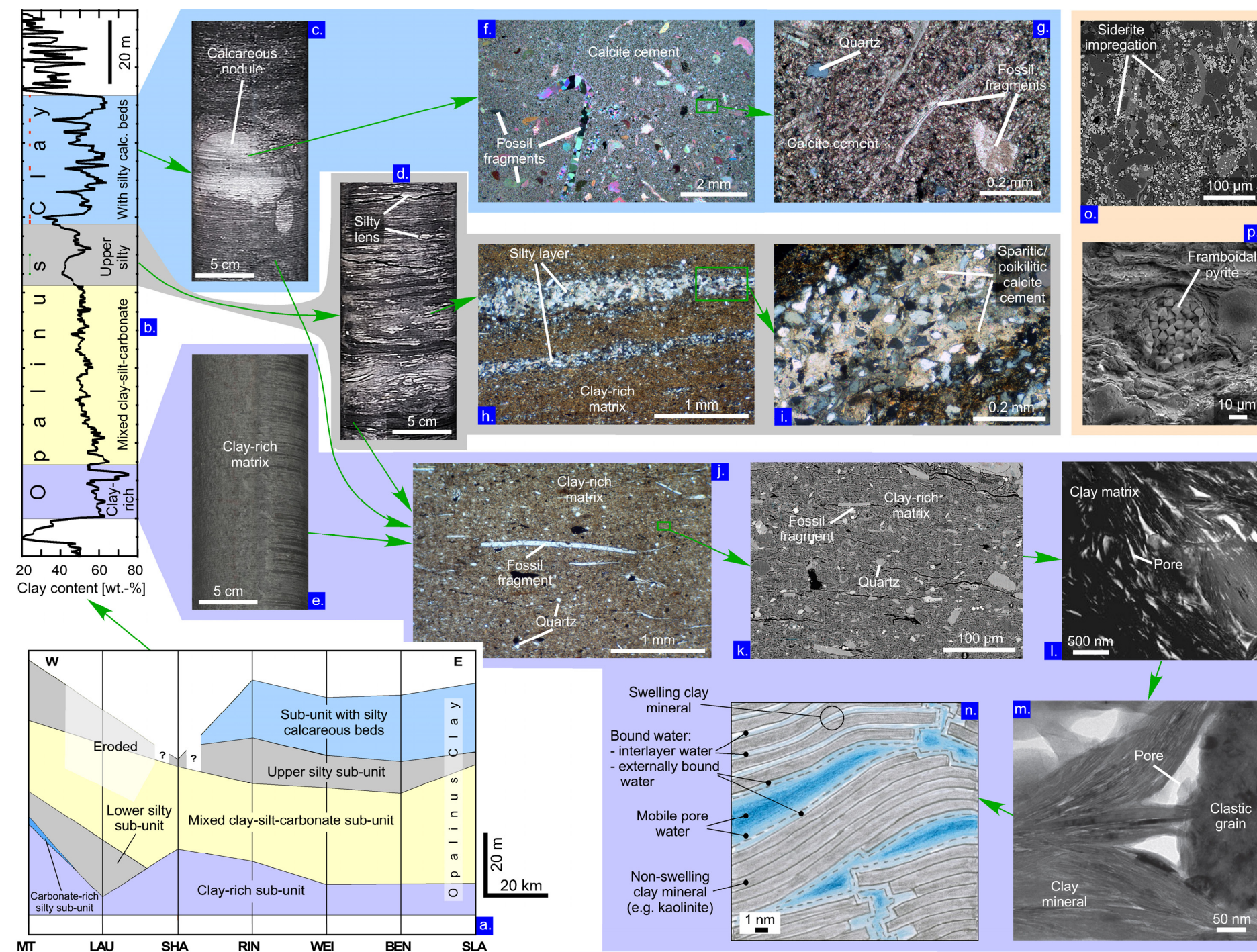


Fig. 6-1: Conceptual representation of the structure of the Opalinus Clay over a length-scale range of 13 orders of magnitude

- a. Regional distribution of sub-units
- b. Typical borehole profile with sub-units, discrete heterogeneities and clay-mineral log (Benken borehole)
- c. Calcareous nodule in the sub-unit with silty calcareous beds (BEN 549.22)
- d. Silty sub-unit (BEN 582.83)
- e. Clay-rich basal sub-unit (MT BDB-1 220.74)
- f. Thin-section photograph of a calcareous nodule from the sub-unit with silty calcareous beds (SLA 852.80, transmitted light, crossed polars)
- g. Detail from f.
- h. Thin-section photograph from the silty sub-unit showing two silty lenses (BEN 575.35, transmitted light, parallel polars)
- i. Thin-section photograph from the silty sub-unit showing a close-up of a silty lens cemented by sparitic/poikiloblastic calcite (MT 808.40, transmitted light, crossed polars)
- j. Thin-section photograph from the clay-rich sub-unit (MT 968.50, transmitted light, parallel polars)
- k. SEM image from the clay-rich sub-unit (Mont Terri FE tunnel, from Seiphoori et al. 2017)
- l. TEM image of the clay matrix (from Keller & Holzer 2013)
- m. TEM image of the clay matrix (Mont Terri sample, from Keller et al. 2013b)
- n. Artist's view of the clay structure on the nanometre scale (from Nagra 2002)
- o. Siderite impregnation in a concretion (SLA 833.69, from Wersin et al. 2013)
- p. Pyrite framboid (Mont Terri FE tunnel, from Seiphoori et al. 2017)

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