

Arbeitsbericht NAB 20-09

**TBO Trüllikon-1-1:
Data Report
Dossier X
Petrophysical Log Analysis**

June 2021

S. Marnat & J.K. Becker

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

Hardstrasse 73
P.O. Box 280
5430 Wettingen
Switzerland
Tel. +41 56 437 11 11

www.nagra.ch

Arbeitsbericht NAB 20-09

**TBO Trüllikon-1-1:
Data Report**

**Dossier X
Petrophysical Log Analysis**

June 2021

S. Marnat¹ & J.K. Becker²

¹GPCI

²Nagra

Keywords:

TRU1-1, Zürich Nordost, TBO, deep drilling campaign,
stochastic log interpretation, MultiMin analyses,
petrophysical logs, lab data, Multi-Sensor Core Logger,
MSCL, mineralogy, clay content, clay typing, porosity

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

Hardstrasse 73
P.O. Box 280
5430 Wettingen
Switzerland
Tel. +41 56 437 11 11

www.nagra.ch

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

This NAB aims at reporting drilling results at an early stage. Additional borehole-specific data will be published elsewhere.

In the event of inconsistencies between dossiers of this NAB, the dossier addressing the specific topic takes priority. In the event of discrepancies between Nagra reports, the chronologically later report is generally considered to be correct. Data sets and interpretations laid out in this NAB may be revised in subsequent reports. The reasoning leading to these revisions will be detailed there.

This Dossier was prepared by a project team consisting of:

S. Marnat (data analyses, interpretation and writing)

J.K. Becker (project administration and writing)

Editorial work: P. Blaser and M. Unger

The Dossier has greatly benefitted from technical discussions with, and reviews by, internal experts. Their input and work are very much appreciated.

"Copyright © 2021 by Nagra, Wettingen (Switzerland) / All rights reserved.

All parts of this work are protected by copyright. Any utilisation outwith the remit of the copyright law is unlawful and liable to prosecution. This applies in particular to translations, storage and processing in electronic systems and programs, microfilms, reproductions, etc."

Table of Contents

Table of Contents.....	I
List of Tables.....	II
List of Figures.....	II
List of Appendices.....	III
List of Plates.....	IV
Abbreviations	V
1 Introduction.....	1
1.1 Context	1
1.2 Location and specifications of the borehole	2
1.3 Documentation structure for the TRU1-1 borehole	6
1.4 Scope and objectives of this dossier.....	7
2 Data preparation	9
2.1 Used log data	9
2.2 Used core data.....	11
2.3 Multi-sensor Core Logger (MSCL) data	11
2.4 MultiMin input dataset preparation.....	14
2.5 Preliminary calculations (Precalc)	14
3 Petrophysical log interpretation	15
3.1 MultiMin interpretation.....	15
3.2 Bad-hole treatment and quality of results.....	17
3.2.1 Indicator for input data quality (LQC_INDEX).....	17
3.2.2 Indicator for the mathematical model (CONDNUM and NFUN).....	18
3.2.3 Indicator for the MultiMin interpretation results (MULT_QC and QUALITY)	18
4 Results of the calibrated stochastic log interpretation	21
4.1 Comparison of interpretation results with core data.....	21
4.2 Main results of the core-calibrated log analyses in the TRU1-1 borehole	28
4.3 Main results of the core-calibrated log analysis in the Opalinus Clay (816.4 – 927.9 m).....	33
5 Summary	41
6 References.....	43

List of Tables

Tab. 1-1:	General information about the TRU1-1 borehole	2
Tab. 1-2:	Core and log depth for the main lithostratigraphic boundaries in the TRU1-1 borehole.....	5
Tab. 1-3:	List of dossiers included in NAB 20-09	6
Tab. 3-1:	List of MultiMin models used in TRU1-1	16

List of Figures

Fig. 1-1:	Tectonic overview map with the three siting regions under investigation	1
Fig. 1-2:	Overview map of the investigation area in the Zürich Nordost siting region with the location of the TRU1-1 borehole in relation to the boreholes Benken and Schlattingen	3
Fig. 1-3:	Lithostratigraphic profile and casing scheme for the TRU1-1 borehole	4
Fig. 2-1:	Petrophysical log availability and gaps in the borehole TRU1-1.....	10
Fig. 2-2:	XRF (black dots) and ECS (red curves) elements comparison.....	12
Fig. 2-3:	Core (black dots: spectral gamma ray, blue dots XRF Thorium) and wireline HNGS (red curves) spectral gamma ray elements comparison.....	13
Fig. 4-1:	Weight % of dry clay (y-axis) compared to core XRD data (x-axis) («Felsenkalke» + «Massenkalk» to the Schinznach Formation).....	22
Fig. 4-2:	Weight % of not potassic dry clay (y-axis) compared to core XRD data (x-axis) («Felsenkalke» + «Massenkalk» to the Klettgau Formation)	23
Fig. 4-3:	Weight of illite (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Klettgau Formation).....	24
Fig. 4-4:	Weight % of QF-silicates (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Bänkerjoch Formation).....	25
Fig. 4-5:	Weight % of carbonates (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Bänkerjoch Formation).....	26
Fig. 4-6:	Weight % of dolomite (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Bänkerjoch Formation).....	27
Fig. 4-7:	Total porosity (v/v, y axis) compared to core data (x axis) («Felsenkalke» + «Massenkalk» to the Bänkerjoch Formation).....	28
Fig. 4-8:	Dry clay weight percentage frequency histogram in the Opalinus Clay	33
Fig. 4-9:	Dry clay weight percentage frequency histogram in the upper section of Opalinus Clay (above 867 m).....	34
Fig. 4-10:	Dry clay weight percentage frequency histogram in the lower section of Opalinus Clay (below 867 m).....	35
Fig. 4-11:	Calcite weight percentage frequency histogram in the Opalinus Clay.....	36
Fig. 4-12:	Siderite weight percentage frequency histogram in the Opalinus Clay.....	37

Fig. 4-13: QF-silicates (quartz and feldspars) weight percentage frequency histogram
in the Opalinus Clay.....38

Fig. 4-14: Total porosity frequency histogram in the Opalinus Clay39

Fig. 4-15: Main log and core results in the Opalinus Clay40

List of Appendices

- App. A: Precalc parameters table
- App. B: Parameters used in the different MultiMin models
- App. C: List of MultiMin models

List of Plates

- Plate 1: Comparison of calculated log curves and measured petrophysical log curves
- Plate 2: Results of the core-calibrated petrophysical log interpretation

Note: In the digital version of this report the appendices and plates can be found under the paper clip symbol.

Abbreviations

ANHYDR	Anhydrite weight percentage from MultiMin
APLC	Corrected neutron hydrogen index from APS (limestone matrix)
APLC_PRED	APLC prediction by MultiMin
APS	Accelerator Porosity Sonde
B/E	Barns/Electron
BS	Drilling / Coring Bit Size
CALCITE	Calcite weight percentage from MultiMin
CALI	Caliper
CARBONATES	Carbonates weight percentage from MultiMin
CHLORITE	Chlorite weight percentage from MultiMin
COAL	Coal weight percentage from MultiMin
COMPOSITE	Composite log, validated logs dataset
CONDNUM	MultiMin model condition number
CT	Conductivity in the formation
CT_PRED	CT prediction by MultiMin
CU	Capture Unit, unit for sigma
CXO	Conductivity in the invaded zone
CXO_PRED	CXO prediction by MultiMin
DENS	Bulk density
DOLOMITE	Dolomite weight percentage from MultiMin
DRHO	Bulk density correction
DRY_CLAY	Dry clay weight percentage from MultiMin
dRRC	Rush corrected data
DWAL_WALK2	Dry weight fraction aluminium
DWCA_WALK2	Dry weight fraction calcium
DWFE_WALK2	Dry weight fraction iron
DWSI_WALK2	Dry weight fraction silicon
DWSU_WALK2	Dry weight fraction sulphur
DWSU_WALK2	Dry weight fraction sulphur from ECS
DTCO / DTC	Compressional wave slowness from far monopole mid frequency source compressional wave slowness
DTC_PRED	DTC prediction by MultiMin
DTSM	Shear wave slowness from inline X-Dipole (90°) source
DTS	Shear wave slowness

DTS_PRED	DTS prediction by MultiMin
ECGR_EDTC	Environmentally corrected Gamma Ray from EDTC
ECS	Elemental Capture Spectroscopy
EDTC	Enhanced Digital Telemetry Cartridge
EMS	Environment Measurement Sonde
FE_MIN	Iron-rich minerals (Siderite, pyrite, iron oxides)
FMI	Fullbore Formation Microimager
g/cm ³	Gram per cubic centimetre
GAPI	Unit of radioactivity used for natural Gamma Ray logs
GEOLOG	Emerson software used for logs interpretation
GPCI	Geneva Petroleum Consultants International
GPIT	General Purpose Inclinometry Tool
GR	Total Gamma Ray
GR_KCOR	Total Gamma Ray corrected for mud potassium
HALITE	Halite weight percentage from MultiMin
HDAR	Hole diameter from area
HDRA	Bulk density correction
HFK	Potassium concentration from HNGS
HI	Hydrogen Index
HNGS	Hostile Natural Gamma Ray Sonde
HRLT	High Resolution Laterolog array Tool
HSGR	HNGS Standard Gamma Ray
HTHO	Thorium concentration from HNGS
HURA	Thorium concentration from HNGS
HURA_PRED	HURA prediction by MultiMin
ILLITE	Illite weight percentage from MultiMin
KAOLIN	Kaolinite weight percentage from MultiMin
KEROGEN	Kerogen weight percentage from MultiMin
LEH.QT	Logging Equipment Head with Tension
LQC_INDEX	Log Quality Control Index
MCFL	Micro-Cylindrical Focused Log
MHF	Micro Hydraulic Fracturing
MSCL	Multi-sensor Core Logger
MULT_QC	MultiMin analysis quality flag

MULTIMIN	Multi mineral and multi fluid analysis module in geolog software
m MD	Metre measured depth
MSIP	Modular Sonic Imaging Platform
NFUN	Number of MultiMin iterations
NHI	Neutron Hydrogen Index
NHI_PRED	NHI prediction by MultiMin
NO_K_CLAYS	Not potassic clays weight percentage from MultiMin
NPHI	Corrected neutron hydrogen index (limestone matrix)
ORTHOCL	K-Feldspars weight percentage from MultiMin
p.u.	Porosity unit
PEF	Photoelectric factor
PEFZ	Photoelectric factor
PEFZ_PRED	PEFZ prediction by MultiMin
PHI_PICNO	Core pycnometer porosity
PHI_WL1	Core water-loss porosity (105 °C) using bulk wet density
PHI_WL2	Core water-loss porosity (105 °C) using grain density
PHIE	Effective porosity
PHIT	Total porosity
PLAGIO	Plagioclases weight percentage from MultiMin
PPC	Power positioning device and caliper tool
PRECALC	Precalculation module in the Geolog software
PYRITE	Pyrite weight percentage from MultiMin
QC	Quality Control
QUALITY	MultiMin analysis quality
QUARTZ	Quartz weight percentage from MultiMin
RCL	Reduced Composite Log
RHGE_WALK2	Matrix density from elemental concentrations (WALK2 model)
RHOG	Grain density from MultiMin
RHOS	Solids density
RHOZ	Bulk density
RHOZ_PRED	RHOZ prediction by MultiMin
RT_HRLT	HRLT true formation resistivity
RUGO	Borehole wall rugosity
RXOZ	Invaded formation resistivity filtered at 18 inches

SIDER	Siderite weight percentage from multimin
SIGF	Macroscopic cross section for the absorption of thermal neutrons, or capture cross section, of a volume of matter, measured in capture units [c.u.]
SIGF_PRED	SIGF prediction by MultiMin
QF_SILICATES	Matrix quartz and feldspars weight percentage from MultiMin
SLB	Abbreviation for Schlumberger Logging Company
SP	Spontaneous Potential
STOF	APS Stand-Off
Swe	Effective water saturation
Swt	Total water saturation
TLD	Three-detector Lithology Density
TNPH	Corrected neutron hydrogen index (limestone matrix, thermal)
TOC	Total organic carbon [w/w or wt.-%]
U	Volumetric photoelectric factor computed by Precalc [b/cc]
UBI	Ultrasonic Borehole Imager
v/v	Volume per volume
VCL	Volume of wet clay
VOL_ANHYDR	MultiMin volume of anhydrite
VOL_ANORTH	MultiMin volume of plagioclase
VOL_CALCITE	MultiMin volume of calcite
VOL_CHLOR	MultiMin volume of chlorites
VOL_DOLOM	MultiMin volume of dolomite
VOL_ILLITE	MultiMin volume of illite
VOL_ORTHOCL	MultiMin volume of potassic feldspars
VOL_SIDER	MultiMin volume of siderite
VP	Compressional waves velocity [m/s]
VS	Shear waves velocity [m/s]
VPVS	Compressional and shear waves velocity ratio
VPVS_INPUT	Array Monte-Carlo input for VP/VS
ECS WT.-%	Weight concentration
W/W	Weight per weight, concentration
WANH_WALK2	Dry weight fraction anhydrite/gypsum from ECS
WCAR_WALK2	Dry weight fraction carbonate from ECS
WCLA_WALK2	Dry weight fraction clay from ECS
WEVA_WALK2	Dry weight fraction salt from ECS

WPYR_WALK2	Dry weight fraction pyrite from ECS
WQFM_WALK2	Dry weight fraction quartz+feldspar+mica from ECS
WSID_WALK2	Dry weight fraction siderite from ECS
XRD	X-Ray Diffraction
$\mu\text{s}/\text{ft}$	Microsecond per foot (unit for sonic slowness)

1 Introduction

1.1 Context

To provide input for site selection and the safety case for deep geological repositories for radioactive waste, Nagra has drilled a series of deep boreholes in Northern Switzerland. The aim of the drilling campaign is to characterise the deep underground of the three remaining siting regions located at the edge of the Northern Alpine Molasse Basin (Fig. 1-1).

In this report, we present the results from the Trüllikon-1-1 borehole.

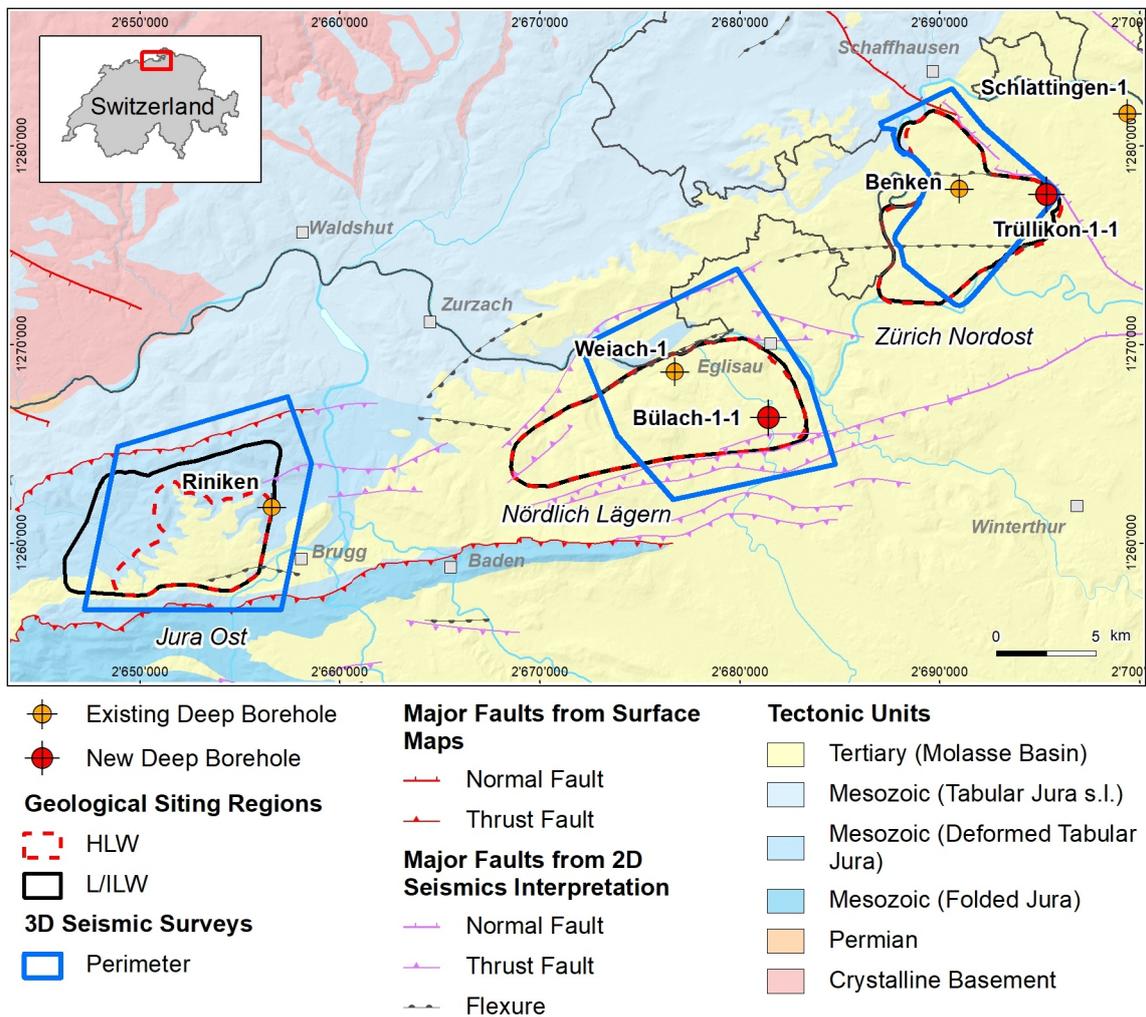


Fig. 1-1: Tectonic overview map with the three siting regions under investigation

1.2 Location and specifications of the borehole

The Trüllikon-1-1 (TRU1-1) exploratory borehole is the second borehole drilled within the framework of the TBO project. The drill site is located in the eastern part of the Zürich Nordost siting region (Fig. 1-2). The vertical borehole reached a final depth of 1'310 m (MD)¹. The borehole specifications are provided in Tab. 1-1.

Tab. 1-1: General information about the TRU1-1 borehole

Siting region	Zürich Nordost
Municipality	Trüllikon (Canton Zurich / ZH), Switzerland
Drill site	Trüllikon-1 (TRU1)
Borehole	Trüllikon-1-1 (TRU1-1)
Coordinates	LV95: 2'695'372.648 / 1'277'548.076
Elevation	Ground level = top of rig cellar: 475.07 m above sea level (asl)
Borehole depth	1'310.0 m measured depth (MD) below ground level (bgl)
Drilling period	15. August 2019 – 5. April 2020 (spud date to end of rig release)
Drilling company	PR Marriott Drilling Ltd.
Drilling rig	Rig-16 Drillmec HH102
Drilling fluid	Water-based mud with various amounts of different components such as ² : 46 – 712 m: Pure-Bore® 712 – 1'161 m: Potassium silicate 1'161 – 1'310 m: Sodium chloride & polymers

The lithostratigraphic profile and the casing scheme are shown in Fig. 1-3. The comparison of the core versus log depth³ of the main lithostratigraphic boundaries in the TRU1-1 borehole is shown in Tab. 1-2.

¹ Measured depth (MD) refers to the position along the borehole trajectory, starting at ground level, which for this borehole is the top of the rig cellar. For a perfectly vertical borehole, MD below ground level (bgl) and true vertical depth (TVD) are the same. In all Dossiers depth refers to MD unless stated otherwise.

² For detailed information see Dossier I.

³ Core depth refers to the depth marked on the drill cores. Log depth results from the depth observed during geophysical wireline logging. Note that the petrophysical logs have not been shifted to core depth, hence log depth differs from core depth.

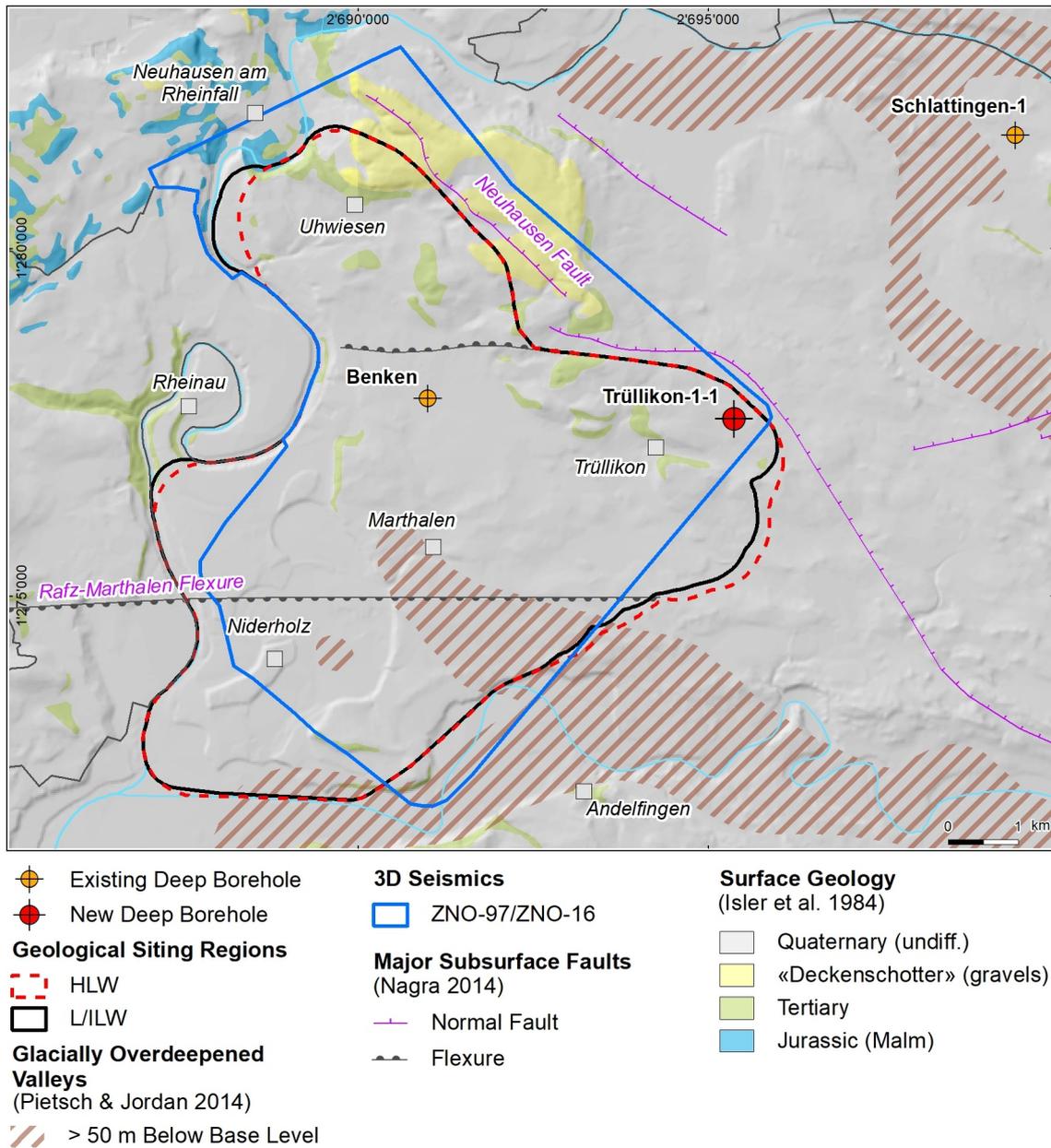


Fig. 1-2: Overview map of the investigation area in the Zürich Nordost siting region with the location of the TRU1-1 borehole in relation to the boreholes Benken and Schlattigen

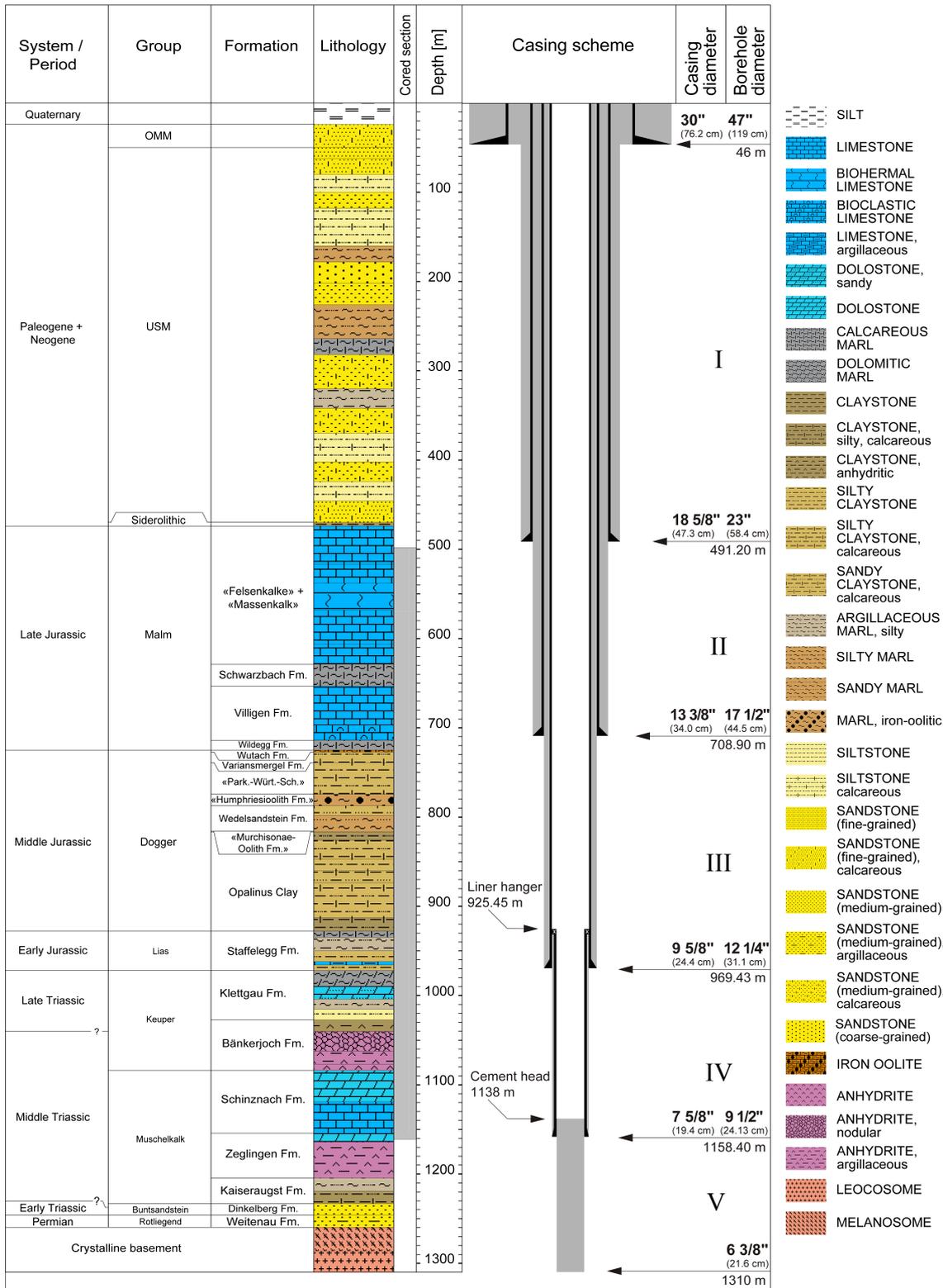


Fig. 1-3: Lithostratigraphic profile and casing scheme for the TRU1-1 borehole⁴

⁴ For detailed information see Dossier I and III.

Tab. 1-2: Core and log depth for the main lithostratigraphic boundaries in the TRU1-1 borehole⁵

System / Period	Group	Formation	Core depth in m (MD)	Log
Quaternary				
Paleogene + Neogene	OMM		24.0	—
	USM		50.0	—
	Siderolithic		470.0	—
			474.0	—
		«Felsenkalke» + «Massenkalk»		
	Malm	Schwarzbach Formation	628.87	628.75 —
		Villigen Formation	653.29	653.15 —
		Wildeggen Formation	714.00	714.00 —
		Wutach Formation	724.85	725.03 —
		Variansmergel Formation	727.13	727.27 —
Jurassic		«Parkinsoni-Württembergica-Schichten»	738.97	739.06 —
	Dogger	«Humphriesiolith Formation»	774.55	774.66 —
		Wedelsandstein Formation	787.50	787.55 —
		«Murchisonae-Oolith Formation»	815.51	815.50 —
		Opalinus Clay	816.42	816.43 —
	Lias	Staffellegg Formation	927.91	927.87 —
			971.68	971.55 —
	Keuper	Klettgau Formation	1027.22	1027.44 —
		Bänkerjoch Formation	1084.01	1084.22 —
Triassic		Schinznach Formation	1154.25	1154.43 —
	Muschelkalk	Zeglingen Formation		
		Kaiseraugst Formation	1204.5	—
			1233.2	—
	Buntsandstein	Dinkelberg Formation		
Permian	Rotliegend	Weitenau Formation	1246.1	—
			1259.7	—
		Crystalline Basement	1310.0	final depth

⁵ For details regarding lithostratigraphic boundaries see Dossier III; for details about depth shifts (core goniometry) see Dossier V.

1.3 Documentation structure for the TRU1-1 borehole

NAB 20-09 documents the majority of the investigations carried out in the TRU1-1 borehole, including laboratory investigations on core material. The NAB comprises a series of stand-alone dossiers addressing individual topics and a final dossier with a summary composite plot (Tab. 1-3).

This documentation aims at early publication of the data collected in the TRU1-1 borehole. It includes most of the data available approximately one year after completion of the borehole. Some analyses are still ongoing (e.g. diffusion experiments, analysis of veins, hydrochemical interpretation of water samples) and results will be published in separate reports.

The current borehole report will provide an important basis for the integration of datasets from different boreholes. The integration and interpretation of the results in the wider geological context will be documented later in separate geoscientific reports.

Tab. 1-3: List of dossiers included in NAB 20-09

Black indicates the dossier at hand.

Dossier	Title	Authors
I	TBO Trüllikon-1-1: Drilling	M. Ammen & P.-J. Palten
II	TBO Trüllikon-1-1: Core Photography	D. Kaehr & M. Gysi
III	TBO Trüllikon-1-1: Lithostratigraphy	M. Schwarz, P. Jordan, P. Schürch, H. Naef, T. Ibele, R. Felber & M. Gysi
IV	TBO Trüllikon-1-1: Microfacies, Bio- and Chemostratigraphic Analyses	S. Wohlwend, H.R. Bläsi, S. Feist-Burkhardt, B. Hostettler, U. Menkveld-Gfeller, V. Dietze & G. Deplazes
V	TBO Trüllikon-1-1: Structural Geology	A. Ebert, S. Cioldi, L. Gregorczyk, S. Rust, D. Böhni & M. Gysi
VI	TBO Trüllikon-1-1: Wireline Logging and Microhydraulic Fracturing	J. Gonus, E. Bailey, J. Desroches & R. Garrard
VII	TBO Trüllikon-1-1: Hydraulic Packer Testing	R. Schwarz, L. Schlickenrieder, H.R. Müller, S. Köhler, A. Pechstein & T. Vogt
VIII	TBO Trüllikon-1-1: Rock Properties, Porewater Characterisation and Natural Tracer Profiles	L. Aschwanden, L. Camesi, T. Gimmi, A. Jenni, M. Kiczka, U. Mäder, M. Mazurek, D. Rufer, H.N. Waber, P. Wersin, C. Zwahlen & D. Traber
IX	TBO Trüllikon-1-1: Rock-mechanical and Geomechanical Laboratory Testing	E. Crisci, L. Laloui & S. Giger
X	TBO Trüllikon-1-1: Petrophysical Log Analysis	S. Marnat & J.K. Becker
	TBO Trüllikon-1-1: Summary Plot	Nagra

1.4 Scope and objectives of this dossier

The present report describes the results of the stochastic petrophysical log analysis performed in the TRU1-1 borehole. The detailed workflow for this analysis is described in a methodology report (Marnat & Becker 2020, NAB 20-30), here, only a very short summary is given. The petrophysical logs record a measurement every $\frac{1}{2}$ foot (~ 15 cm) at standard resolution; using high resolution logs as input was not considered, as some of the wireline logs are not at high resolution (e.g. gamma-ray, sonic, ECS). For the Multimineral Log Analysis (abbreviation MultiMin throughout this report), a mineral content is assumed at each of these measurement locations, either from prior knowledge or from mineralogical lab analyses. A theoretical log response from this assumed mineral content for each available petrophysical log is calculated and compared to the actually measured log. Using optimisation techniques, the difference (i.e. the error) between calculated log responses and actual measured petrophysical logs is minimised by adjusting the assumed mineral content. Any deviation from this workflow is explained in this report.

The result of this analysis therefore are continuous profiles of the mineralogical content and other rock parameters (e.g. porosity) where the main aim of these calculations here were continuous profiles of the clay content and porosity.

The organisation of this dossier follows the necessary steps of the workflow. First, data is collected and quality checks (QC) are performed. In addition, necessary pre-calculations concerning important environmental parameters are performed (Chapter 2). This is followed by the actual analysis of the data (Chapter 3) and a short description of results in Chapter 4. Chapter 4 also includes an estimation of the fit of the results to available data from lab measurements.

All depths in this report are reported as measured depths from top rig cellar (MD) if not stated otherwise.

2 Data preparation

2.1 Used log data

The acquisition, QC (quality control) and generation of log composite of the petrophysical logs from the borehole TRU1-1 is described in more detail in Dossier VI, the raw corrected log data is also shown in Plate 1. Note that abbreviations in brackets in the list below are according to Schlumberger (SLB) mnemonics (as SLB was the log contractor responsible for the log acquisition). A detailed description of how the different tools measure the respective parameters and the underlying physics behind these measurements is not the focus of this report and can be found in Dossier VI. The petrophysical logs used for this study are listed below:

- Caliper log (EMS/PPC – Environment Measurement Sonde / Power Positioning device and Caliper tool)
The caliper log uses several arms (6 in this case) to continuously measure the borehole shape.
- Gamma Ray (GR, from the EDTC – Enhanced Digital Telemetry Cartridge)
This log measures the naturally occurring radioactivity which can be used to determine the mineral content (mainly clay)
- Spectral Gamma Ray (SGR, from the HNGS – Hostile Natural Gamma Ray Sonde)
This tool also measures the naturally occurring radioactivity. In addition to the total radioactivity, the tool is able to determine the amount (in ppm or wt.-%) of Uranium (U), Thorium (Th) and Potassium (K) in the rocks which can be used e.g. for clay typing.
- Neutron Hydrogen Index (NHI, from APS – Accelerator Porosity Sonde)
The APS is a tool that can measure the porosity (or more precise the NHI) in water saturated formations. Usually, the corrected NHI is used (in this case corrected for limestone porosity). SLB refers to this corrected NHI as APLC (Near/Array Corrected Limestone Porosity). In addition, the APS can be used to determine Sigma (SIGF), a measure to determine the water content and mineralogical characterisations.
- Density (TLD – Three-detector Lithology Density)
TLD is a gamma-gamma density type logging tool using a radioactive source to determine the density of the rock. In addition, the TLD records the photoelectric factor (PEF or PEFZ) which can also be used to determine the mineralogy.
- Element Spectroscopy (ECS – Elemental Capture Spectroscopy)
The ECS uses a radioactive neutron source to measure elemental concentrations in rocks and estimate the major matrix properties from them. The following element concentrations from the WALK2 closure model are used for this study: Silicon (DWSI_WALK2), Calcium (DWCA_WALK2), Iron (DWFE_WALK2), Sulphur (DWSU_WALK2) and Titanium (DWTI_WALK2).
- Resistivity (HRLT – High Resolution Laterolog array Tool)
The HRLT measures the true formation resistivity even in thinly bedded and deeply invaded formations.
- Sonic (MSIP – Modular Sonic Imaging Platform)
The MSIP measures the formation interval transit time, a measure of how fast seismic waves (compressional, shear and Stoneley waves) propagate through the formation.

An overview of the used petrophysical logs and their measurements in the borehole TRU1-1 is given in the Appendix in Plate 1.

Usable log data were available for analysis from 473.5 to 1'301.0 m (see Plate 1). Due to gaps between drilling sections and cased hole sections (see borehole report, Dossier VI), minor gaps or insufficient redundancy in log data were observed in the following intervals, as shown in Fig. 2-1:

- 481.6 – 504.6 m (Run 2.1.X, 7 7/8" casing at 504.2 m)
- 709.2 – 719.0 m (Between Run 2.1.X and cased hole Run 3.4.X at 720.0 m)
- 969.8 – 977.0 m (Between Run 3.4.X and cased hole Run 4.2.X at 976.9 m)

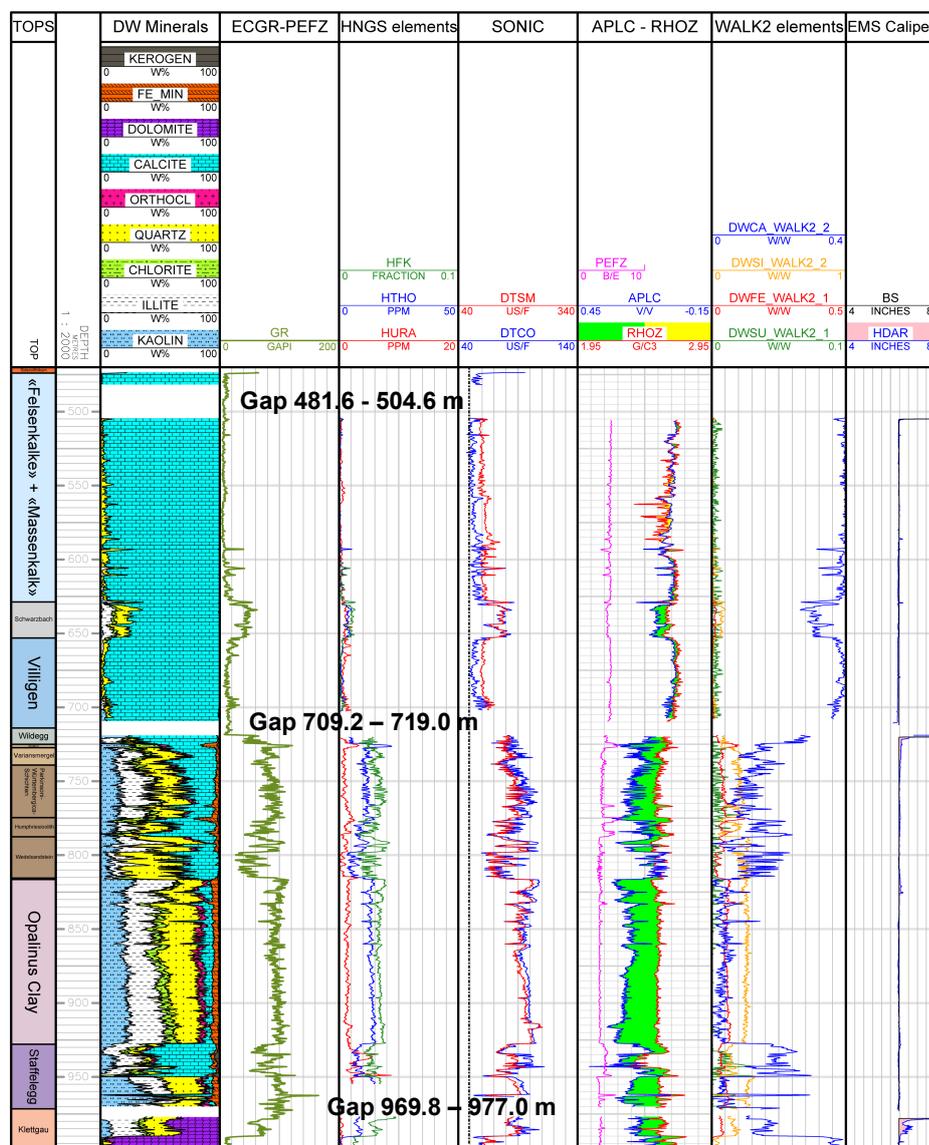


Fig. 2-1: Petrophysical log availability and gaps in the borehole TRU1-1

Please note that ECS elements are displayed as measured (in weight/weight, w/w) and are hence not converted to wt.-% (weight percentage) here.

In the upper interval (0 – 481.6 m), only technical logging was performed which is not suitable for the log interpretation routines used here. However, this interval is only of minor interest in terms of formation characterisation for the geological disposal of radioactive waste and, hence, was disregarded completely.

2.2 Used core data

As previously mentioned, the MultiMin algorithm requires an initial assumption of the mineralogical content. For the calibration of the log interpretation, core data (mainly lab measurements of mineralogy, porosity and density) were used (see Dossier VIII for more details on core data, some core data is shown in the Appendix in Plates 1 and 2). Over 184 core samples collected at depth ranging from 502.5 to 1'076.3 m were available of which 160 were analysed for porosity, 125 for XRD mineralogy and 50 for clay types. The analysed minerals were quartz, K-feldspars, plagioclase, calcite, dolomite/ankerite, siderite, anhydrite, celestite, pyrite, clay minerals and organic carbon. The 50 samples analysed for clay typing (in the interval 638.20 – 1'026.55 m) quantified the illite, smectite, kaolinite and chlorite endmembers. The mineral content was used to calibrate the MultiMin interpretation.

As mentioned earlier, porosities and grain densities are also included in the core data and hence used for this study. The three measured porosities (water-loss porosity (105 °C) using bulk wet density, water-loss porosity (105 °C) using grain density and pycnometer porosity) were accounted for. Some of the provided core data were measured on partially dried samples, these core data were dismissed, only data from fully saturated samples were selected and compared to the MultiMin total porosity (Φ_t). The relative errors of these measurements are provided as well. For more details on the exact measurement procedures of these parameters see Waber (2020).

The difference between core and log depth has been reported in Dossier V. As the reported depth differences are much smaller than the wireline logs vertical resolution, it was decided not to apply the shift to the core data in this study.

Part of the core data is also shown in the Appendix in Plate 2.

2.3 Multi-sensor Core Logger (MSCL) data

MSCL measurements from cores were available for parts of the borehole TRU1-1 (from 721.51 to 1'006.62 m). Measurements were performed in the interval of the host rock (Opalinus Clay) and its confining units. The following parameters were measured:

- Bulk density in g/cc
- Compressional (P) wave velocity in m/s
- Spectral gamma ray curves: potassium (K, %), thorium (Th, ppm) and uranium (U, ppm)
- XRF (X-ray fluorescence) elemental analysis: Iron (Fe), silicon (Si), calcium (Ca), aluminium (Al), titanium (Ti) and sulphur (S) are used for this study.

Some ECS data could not be acquired between drilling sections, leaving data gaps. In these same intervals, no MSCL-measurements could be performed, hence it was not possible to use to fill the gaps using XRF-data from MSCL-measurements.

For the remaining sections, the XRF elemental analysis results were compared with the same elements concentration from the ECS logging (WALK2 closure model). The MSCL data (also referred to as core logs in this report) covers the measured interval at variable sampling rates (0.05 to 0.10 m).

This comparison is shown in Fig. 2-2, the core logs were not depth shifted.

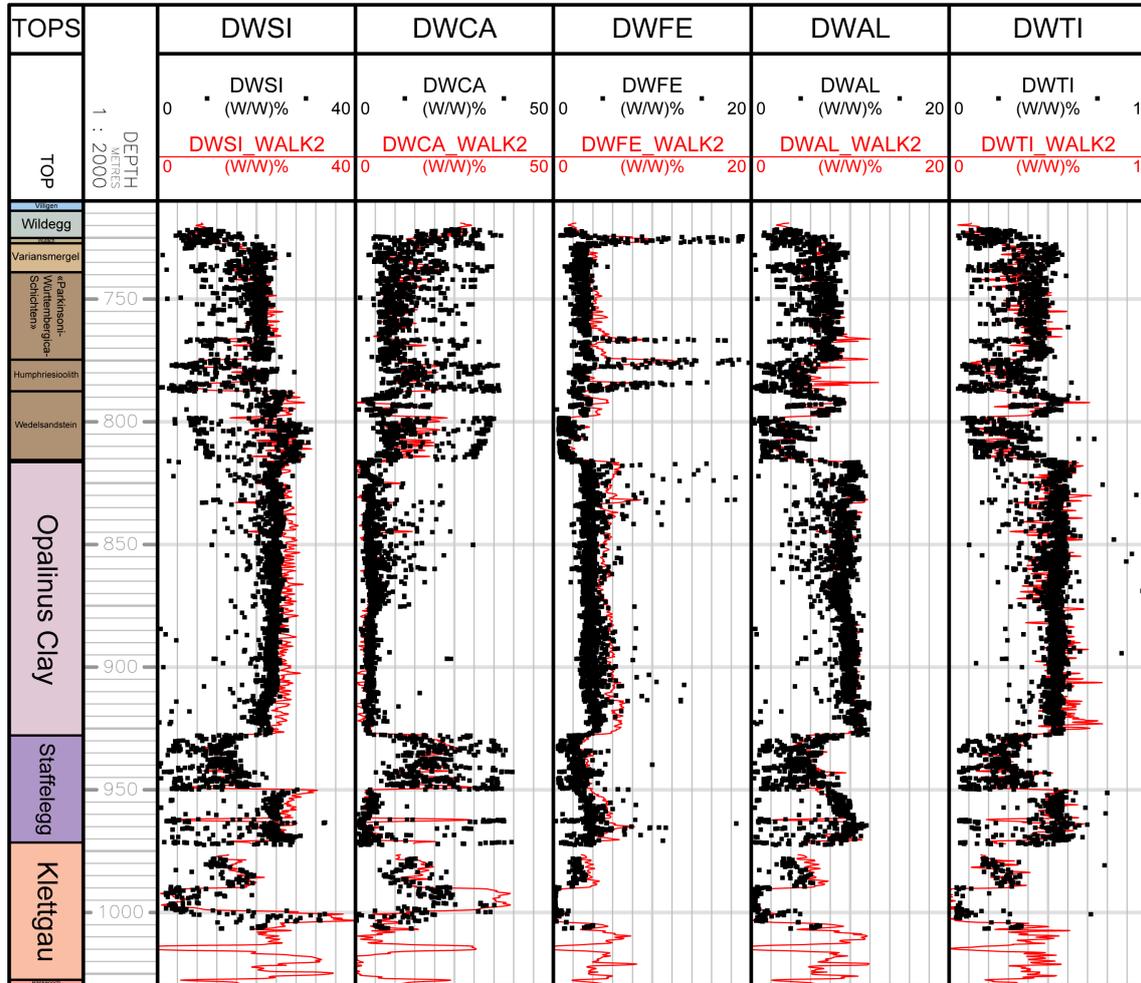


Fig. 2-2: XRF (black dots) and ECS (red curves) elements comparison

While the calcium, aluminium and titanium concentrations are almost similar, the XRF iron and silicon are lower than ECS WALK2 closure model.

The same check was done for the core and HNGS spectral gamma ray (see Fig. 2-3).

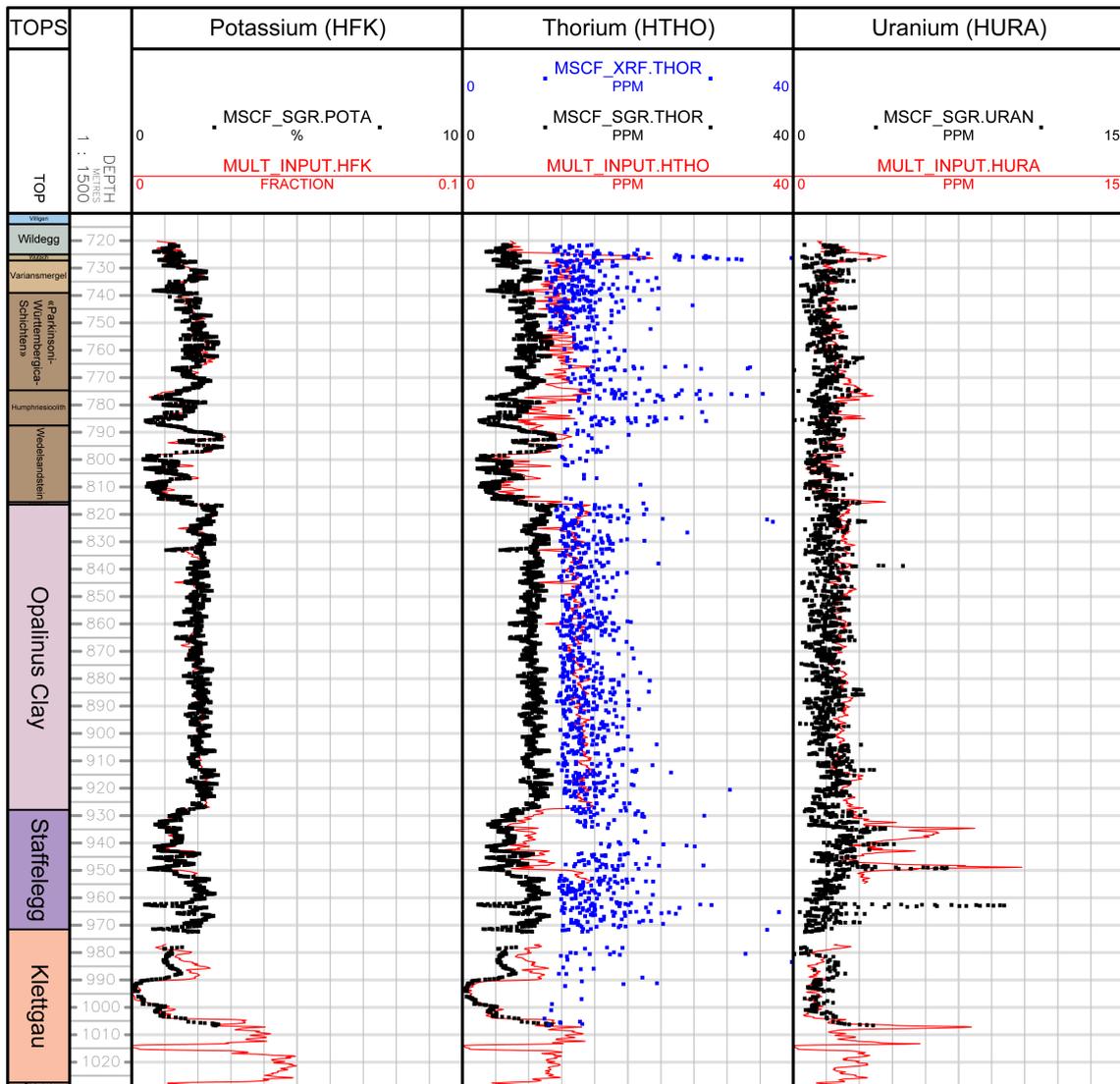


Fig. 2-3: Core (black dots: spectral gamma ray, blue dots XRF Thorium) and wireline HNGS (red curves) spectral gamma ray elements comparison

Uranium from the XRF scanner was not measured because it was below the detection limit of the scanner.

Concerning the SGR measurements, the potassium content is similar with both acquisitions, the uranium is close, but the HNGS thorium is significantly higher. When compared with the XRF thorium (blue dots), the range is similar to HNGS HTHO, but the dispersion of the core XRF Th is wide. U from XRF was not reported because it was below the detection limit of the used XRF scanner.

2.4 MultiMin input dataset preparation

The petrophysical composite log used as input for this study (see Dossier VI) represents a quality controlled, edited, corrected and merged dataset for a selection of the most important petrophysical logging data recorded in each section of the borehole. As mentioned earlier, some gaps in the coverage of the borehole with petrophysical logs occur. The original measurements and corrections of the petrophysical logs are reported in Dossier VI.

In a short interval (1'158.9 to 1'160.0 m), the ECS elements are missing in the Composite Log, but are available in Run 5.1.5. The following missing curves were inserted in the input dataset from 1'158.9 to 1'160 m: DWSI_WALK2 and DWCA_WALK2.

2.5 Preliminary calculations (Precalc)

As the wireline logs measure parameters under in situ conditions (e.g. temperatures depending on depth and temperature of the borehole fluid, infiltration of mud into the formation depending on the borehole fluid and its density etc.), these prevailing conditions in the borehole have to be taken into account to correctly predict/calculate the theoretical log response from the assumed mineral and fluid content (i.e. total porosity) at a certain depth. Continuous profiles of these environmental parameters were calculated using the Precalc module from the interpretation software Geolog. The main parameters used for the calculation of these environmental parameters are, for reasons of transparency and to be able to replicate exactly the analyses reported here, displayed in Appendix A.

The mud properties (mud density and resistivities) reported here were extracted from the validated SLB wireline log headers (see Dossier VI).

3 Petrophysical log interpretation

3.1 MultiMin interpretation

In the following, the petrophysical log interpretation and its results are shortly described. All necessary data treatment and environmental pre-calculations have been described in the previous chapters or are described in the Methodology report (Marnat & Becker 2020). Many qualitatively good wireline logs were available in most of the borehole, allowing the computation of many unknowns (fluids and minerals).

Significant hydrocarbon shows were neither described by the mudlogging nor inferred from cores or petrophysical logs. Consequently, the formations were treated as water wet (i.e. with saline water as the pore fluid).

The main minerals were inferred from the XRD measurements on core samples and regional knowledge (XRD-data from previously drilled boreholes Bülach1-1 (Dossier VIII) and Weiach-1 and Benken-1 from Mazurek 2017). Using the MultiMin approach, the mineral content for the following minerals were modelled:

- Clay mineral endmembers (kaolinite, illite, smectite and chlorites) and total clay mineral content. From the available wireline logs, the smectite cannot be differentiated from the kaolinite
- Silicates: quartz, potassic feldspars, plagioclases, muscovite (in the crystalline basement)
- Carbonates: calcite, siderite, dolomite/ankerite
- Iron oxide, to honour the ECS iron content in the formations just above the Opalinus Clay, as the measured siderite, pyrite and chlorite only cannot explain the DWFE_WALK2 values
- Evaporites: anhydrite
- Organic carbon (kerogen)

These compounds were modelled depending on the available data. In case not enough data were available for a given interval (e.g. where data was missing or of insufficient quality), some minerals were merged to a pseudo-mineral to reduce the number of unknowns (see Marnat & Becker (NAB 20-30) for more details).

Tab. 3-1 shows an example of the interpretation intervals, the available data and the MultiMin models names used in each interval. The intervals are defined based on their general (expected) mineralogy, available logs and consistent environmental parameters (e.g. mud system changes). Interpretation intervals may be subdivided further, e.g. to respect a reduced data quality. The full table with all intervals is available in Appendices B and C.

Tab. 3-1: List of MultiMin models used in TRU1-1

The intervals (column Interval Name) may include several MultiMin models if some of the input data were of bad quality or the particular section of the interval required special assumptions due to its assumed mineralogy. The full table is also available in Appendix C.

The column Cond Num stands for model condition number. Low values are typical for good mathematical models (below 4.00). Condition numbers above 4.00 highlighted in yellow correspond to fair models. See Section 3.2 for more information.

From [m]	To [m]	Interval [name]	MultiMin models	Cond. num.	Description
473.5	482.5	Int 1	tru11_int1	2.00	GR-Sonic only
504.7	506.7	Int 2	tru11_int2_top	2.71	No TLD-APS
506.7	701.8	Int 2	tru11_int2	3.07	All logs
701.8	706.9	Int 2	tru11_int2_bot1	2.81	No HNGS
706.9	709.4	Int 2	tru11_int2_bot2	1.99	GR-TLD only
718.5	720.5	Int 3_top	tru11_int3_ir	3.89	All logs
720.5	816.0	Int 3_top	tru11_int3_top	2.07	GR-Sonic-ECS
816.0	950.0	Int_3	tru11_int3	4.06	Opalinus Clay – Staffelegg
950.0	954.6	Int3_STA	tru11_int3_sta	3.34	Base Staffelegg
954.6	963.0	Int3_STA	tru11_int3_bot1	4.16	Base Staffelegg
963.0	970.0	Int3_STA	tru11_int3_bot2	4.51	Base Staffelegg
977.0	1'118.8	Int4	tru11_trias_dol	2.84	No modelled calcite
1'118.8	1'147.0	Int4A	tru11_trias_clc	3.41	Calcite and dolomite
1'147.0	1'156.9	INT4B	tru11_trias_4b	3.27	No HNGS
1'156.9	1'158.1	INT4B	tru11_trias_4b_bot1	2.57	No APS-HNGS
1'158.1	1'158.5	Int5	tru11_int5_top2	2.71	No APS-HNGS-Sonic
1'158.5	1'159.5	Int5	tru11_int5_top1	2.72	No APS-HNGS
1'159.5	1'204.8	Int5	tru11_trias_dol	2.84	No modelled calcite
1'204.8	1'233.0	Int6	tru11_int6	3.48	All logs, Kaiseraugst
1'233.0	1'245.6	Int7	tru11_int7	3.60	All logs, Dinkelberg
1'245.6	1'260.0	Int7a	tru11_int7a	3.89	All logs, Weitenau
1'260.0	1'286.2	Basement	tru11_bsmt	2.79	All logs, basement
1'286.2	1'291.6	Basement	tru11_bsmt_bot1	3.46	No TLD-HNGS, basement
1'291.6	1'301.0	Basement	tru11_bsmt_bot2	3.60	Sonic-GR-ECS only

Given the complexity of the MultiMin models applied to the TRU1-1 wireline logging data, an inverse linear modelling of the MultiMin endpoints could not be attempted in TRU1-1. Therefore, mineral and fluid endpoints were manually optimised to both reduce the difference between measured and predicted logs and match the core mineralogy and porosity. Greatly simplified, an endpoint can be regarded as a factor that is used to calculate the theoretical log response for each

mineral (e.g. if it is assumed that the endpoint for the density of calcite is 2.71 g/cc, a mineral content of 100% calcite should result in a density of 2.71 g/cc of the predicted density log. For a detailed explanation see Marnat & Becker, NAB 20-30).

Based on expert judgement, an uncertainty value for the petrophysical logs was estimated and used to adjust the weight given to the respective log in the MultiMin computation. Again, greatly simplified, if the uncertainty values are large, the corresponding log response will be predicted in the MultiMin interpretation, but it will not be used in the process of error minimisation and hence has no impact on the result of the MultiMin interpretation (for more details see Marnat & Becker 2020). High uncertainty values often apply to the Sonic curves, the PEFZ and the electrical conductivities.

The detailed parameters for all the MultiMin models are available in tables in Appendix B.

3.2 Bad-hole treatment and quality of results

The quality of the MultiMin interpretation relies in part on the quality of the input data. However, it also relies on the number of available curves and the number of unknowns (i.e. minerals) that need to be calculated. Hence, several quality indicators exist that either are informative about the quality of the input data (LQC-Index), the definition of the mathematical model (CONDNUM, NFUN) or the quality of the interpretation results (MULT_QC and QUALITY).

3.2.1 Indicator for input data quality (LQC_INDEX)

Bad-hole indicators are frequently calculated from some of the available wireline logs. They can be used as a quality measure of the data. In this report, a bad-hole indicator was calculated using the caliper log, the bulk density correction, Density-Neutron cross plots and borehole wall rugosity. A similar indicator is reported in Dossier VI (Appendix A7).

During each wireline logging, the borehole shape is determined using a caliper log. If the borehole shape deteriorates far from the bit size (BS) and bit shape (usually circular), some (or all) of the wireline logs may measure biased data, because the distance between the log and the borehole wall is too large. In that case, the response of a considerable amount of borehole fluid is measured by the tool and the measurements represent more the petrophysical parameters of the borehole fluid than of the formation. A log quality control flag (LQC_INDEX) was generated using the bad-hole indicators listed below. Each triggered indicator adds a value of 0.25 to the LQC-Index. Hence, the value of the LQC-Index must be between 0 and 1 (and can only have values of 0, 0.25, 0.5, 0.75 or 1).

1. Neutron-Density crossplot
2. $HDAR > 1.15 * \text{Bit Size}$
3. Borehole wall rugosity, $HDRA > 0.025 \text{ g/cc}$: HDRA (bulk density correction) is a correction of the bulk density measured with a gamma-gamma type logging device (here TLD). If this correction factor is larger than 0.025 g/cc, the indicator is triggered.
4. APS Neutron stand-off $> 0.35 \text{ in}$

If the values of the respective measurements are outliers (e.g. because they were measured in intervals with an enlarged borehole), this indicator is triggered (see also Dossier VI, Appendix A.7, Bad-hole Flags).

3.2.2 Indicator for the mathematical model (CONDNUM and NFUN)

CONDNUM

The CONDNUM stands for model condition number. Low values are typical for good mathematical models (below 4.00). Condition numbers above 4.00 correspond to fair models. A list of CONDNUMs for the different MultiMin interpretation intervals is given in Tab. 3-1. Please note that CONDNUM is not a proxy for the quality of the calculated output but only for the definition of the mathematical model to calculate the said output.

NFUN

NFUN indicates how many iterations were required to fulfil the constraints imposed by the available data where fewer numbers of iterations are indicative for a more robust model. NFUN is also shown in Plate 1. Please note that NFUN, as CONDNUM, is not a proxy for the quality of the calculated output but only for the definition of the mathematical model to calculate the said output.

3.2.3 Indicator for the MultiMin interpretation results (MULT_QC and QUALITY)

MULT_QC

The MultiMin results were not edited in TRU1-1 (e.g. less reliable data were not removed from the interpretation results), but an integrative MultiMin QC flag was generated (MULT_QC) combining several of the aforementioned quality indicators to inform the data user of potentially invalid results. As this flag relies on the availability of lab measurements, it is only available where a respective lab measurement is available. The MULT_QC flag relies on expert judgement and can have values of 2, 1 or 0 based on the three different scenarios detailed below:

- Suspicious porosity spikes occur and are correlated to an LQC-Index above or equal to 0.5, the quality curve (displayed in Plates 1 and 2, see below) shows values above 2 and the MultiMin results do not match the core measurements: MULT_QC = 2. A value of 2 in MULT_QC corresponds to most likely unreliable data.
- Suspicious porosity spikes occur but with an acceptable LQC_Index (0 or 0.25) and MultiMin quality curve values below 2: MULT_QC = 1. This value indicates that results can/should be used for the characterisation of the formation but should be treated with caution as the interpreted results are not a perfect fit with the available data.
- Otherwise, MULT_QC = 0. Interpreted results are reliable and can be used to characterise the formation.

QUALITY

In addition, a quality curve is shown in Plates 1 and 2. This curve is an indication of how well the observed measurements from wireline logs and the predicted results are part of the same population. At a value of QUALITY less than one, the calculated accuracy is within 95% compared to the original wireline logs and therefore the analysis is of good quality. If the value is consistently above one, log measurements are not well honoured by the predicted curves, hence the analysis must be regarded as less robust.

Please note that the quality curve only compares the results of the MultiMin interpretation with the petrophysical logs and does not take data quality of the petrophysical logs (e.g. in bad-hole sections) or lab measurements into account. The only indicator combining information on input data quality and interpretation result is the MULT_QC indicator detailed above.

4 Results of the calibrated stochastic log interpretation

In the following, the main results of the stochastic log interpretation are summarised. Plate 1 shows the measured wireline logs together with the calculated output from the MultiMin approach. The main results in terms of mineral content and porosity are displayed in Plate 2 as continuous curves. Plate 2 also shows the available lab measurements (from core data).

The aim of this chapter is not a detailed description and characterisation of the sedimentary sequence based on log interpretation results, but rather gives a more general description of the data and a general characterisation of the stratigraphic system or groups shown in Plate 2. Section 4.1 compares the interpretation results with core data giving an overview on the robustness of the interpreted mineralogical content in the borehole. Section 4.2 gives a general characterisation while Section 4.3 gives a more detailed description of calculated parameters in the Opalinus Clay.

4.1 Comparison of interpretation results with core data

Below, the MultiMin interpretations are compared to the mineralogical (bulk) and petrophysical measurements (porosity).

Due to the log database constraints and the need for robust mathematical MultiMin models (i.e. condition numbers ideally below 5 for fair to good models), the number of modelled minerals had to be adjusted. For the sake of easy comparison, the minerals had to be grouped:

- Quartz and feldspars (plagioclase and orthoclase) are grouped into a single pseudo mineral (called QF-silicates in Plate 2).
- Different clay minerals were computed when possible (kaolinite – smectite together, chlorites: not potassic clays, called NO_K_CLAYS, and illite). All clay minerals were added to a (total) clay content (DRY_CLAYS).
- Comparable to the clay minerals, different carbonate minerals were also calculated (calcite, dolomite and siderite). In Plate 2, next to the total amount of carbonates (called carbonates), also calcite and dolomite are displayed as the latter two can be used to distinguish between some formations, especially below the Opalinus Clay.

Figs. 4-1 to 4-6 show crossplots between mineral weight percentages from cores (X axis, from XRD lab analyses) and interpretation results from MultiMin (Y axis).

Fig. 4-7 shows the crossplot between total porosity from core (X axis, Water-loss porosity (105 °C) using grain density lab measurement) and interpretation results from MultiMin (Y axis).

All available data are displayed together, covering the interval from the «Felsenkalk» + «Massenkalk» to the Bänkerjoch Formation. The colour coding represents the formations, as per the attached legend.

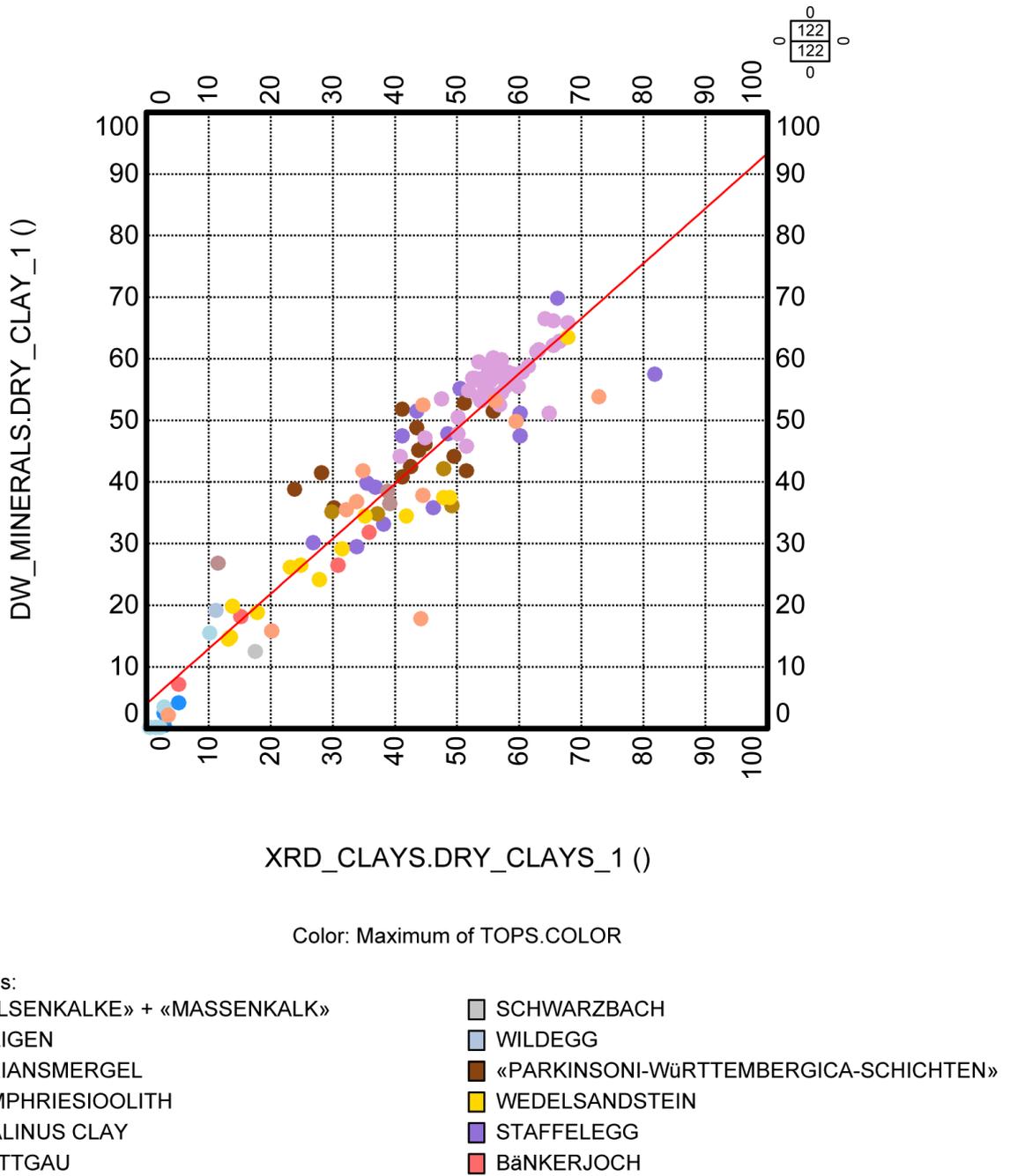
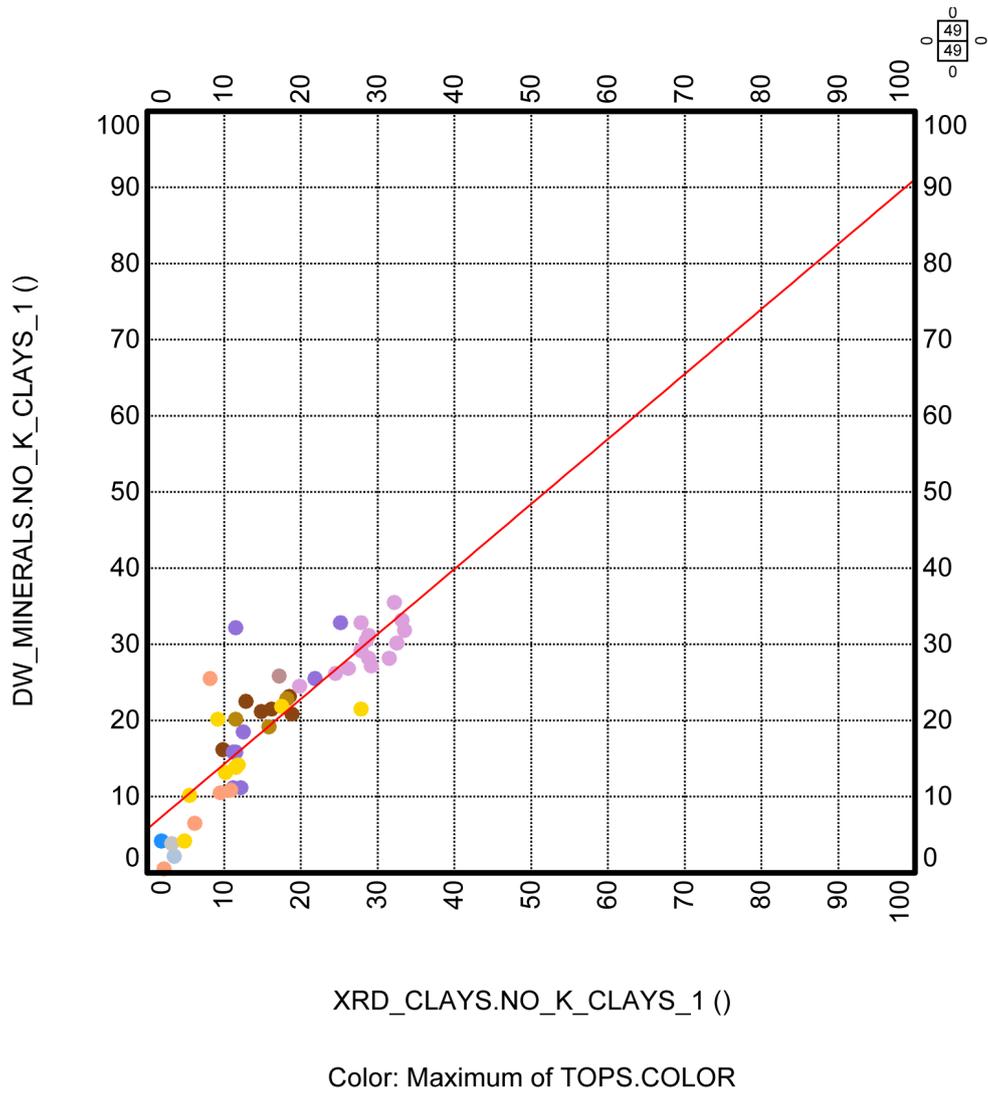


Fig. 4-1: Weight % of dry clay (y-axis) compared to core XRD data (x-axis) («Felsenkalke» + «Massenkalk» to the Schinznach Formation)

The MultiMin dry clay content is well correlated to the core XRD data, although slightly underestimated (cc = 0.94).



- Intervals:
- | | |
|---------------------------------------|--------------------|
| ■ SCHWARZBACH | ■ VILLIGEN |
| ■ WILDEGG | ■ VARIANSMERGEL |
| ■ «PARKINONI-WÜRTEMBERGICA-SCHICHTEN» | ■ HUMPHRIESIOOLITH |
| ■ WEDELSANDSTEIN | ■ OPALINUS CLAY |
| ■ STAFFELEGG | ■ KLETTGAU |

Fig. 4-2: Weight % of not potassic dry clay (y-axis) compared to core XRD data (x-axis) («Felsenkalk» + «Massenkalk» to the Klettgau Formation)

The XRD clay endmembers were not measured in all formations. The MultiMin not potassic clay content is well correlated to the core XRD data (cc = 0.87).

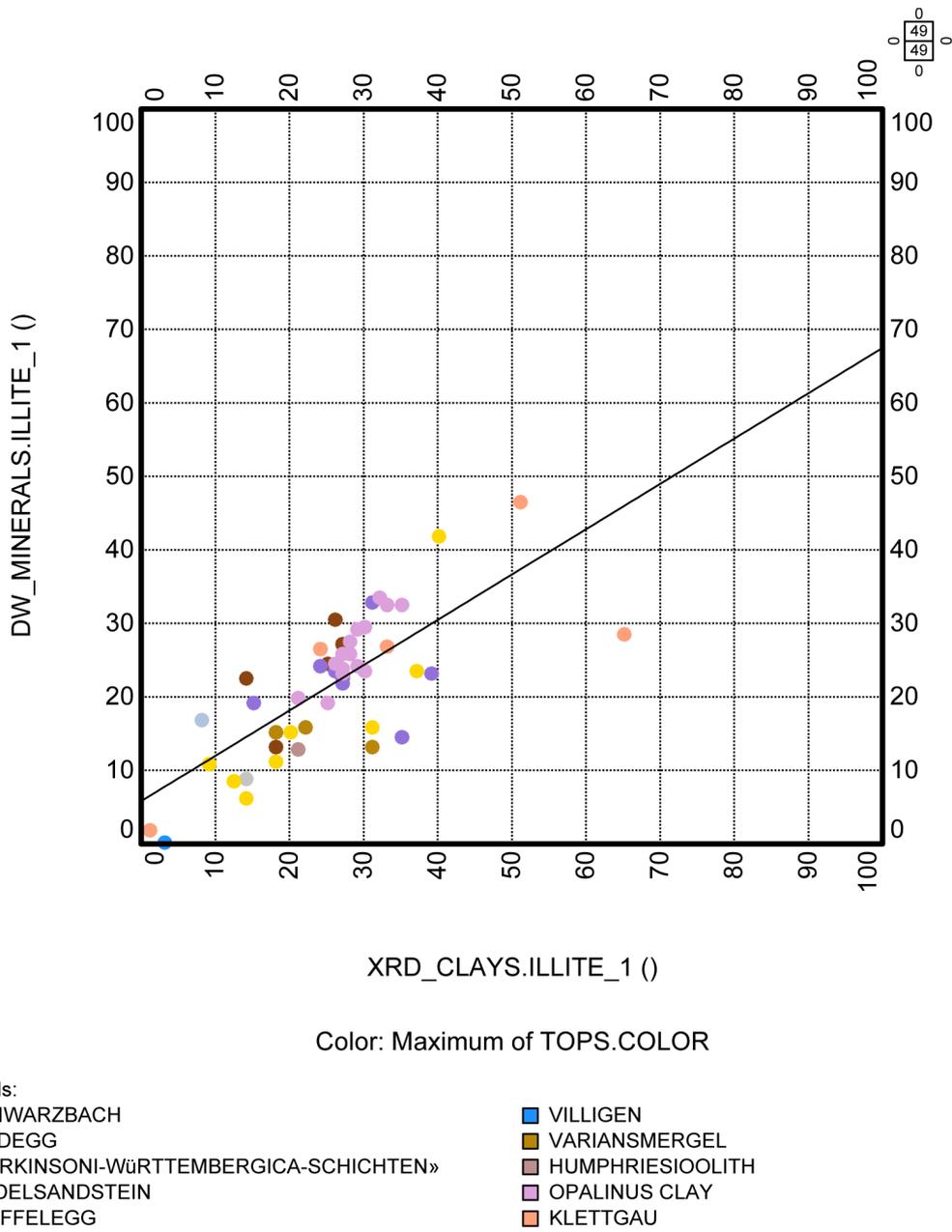


Fig. 4-3: Weight of illite (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Klettgau Formation)

The XRD clay endmembers were not measured in all formations. The MultiMin illite content is fairly correlated to the core XRD data (cc = 0.74) but often underestimated outside the Opalinus Clay (pale purple dots).

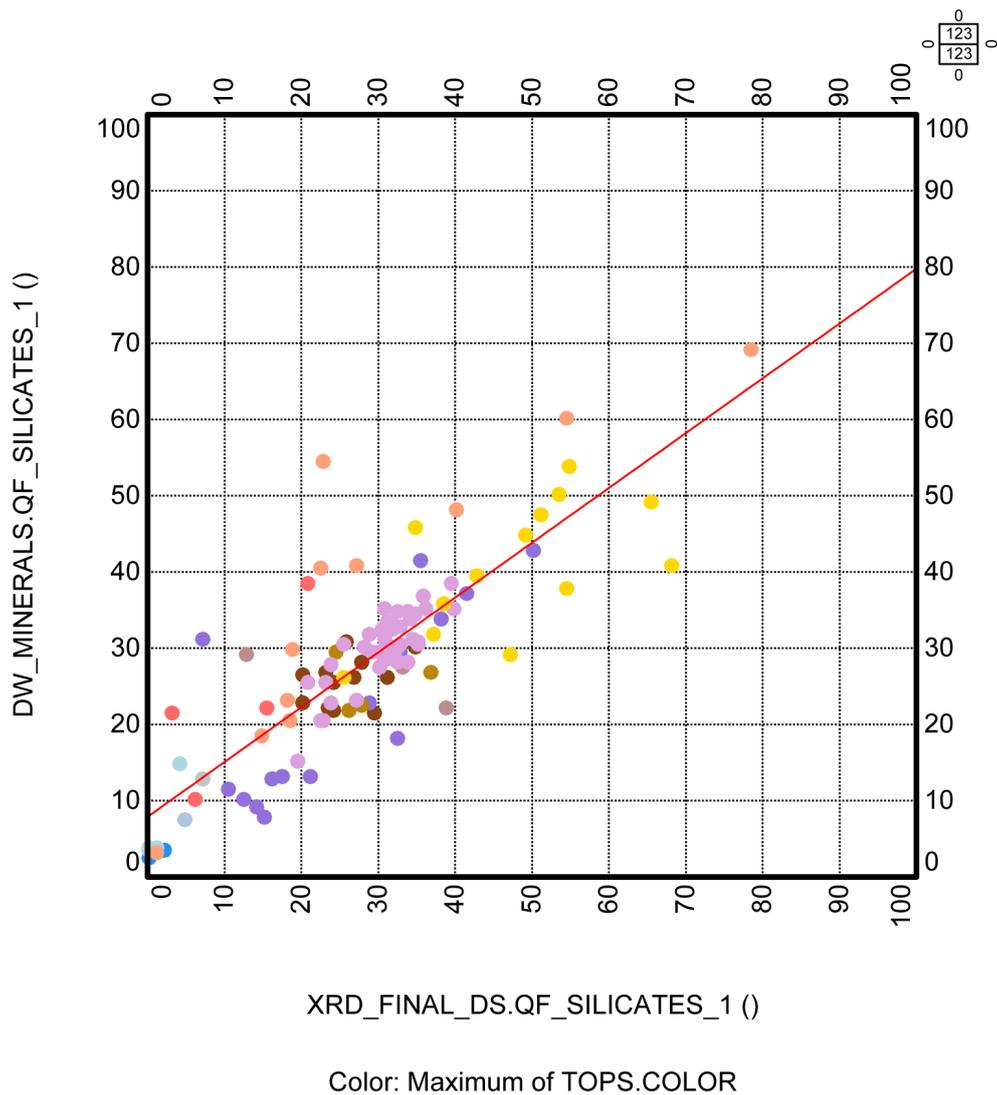
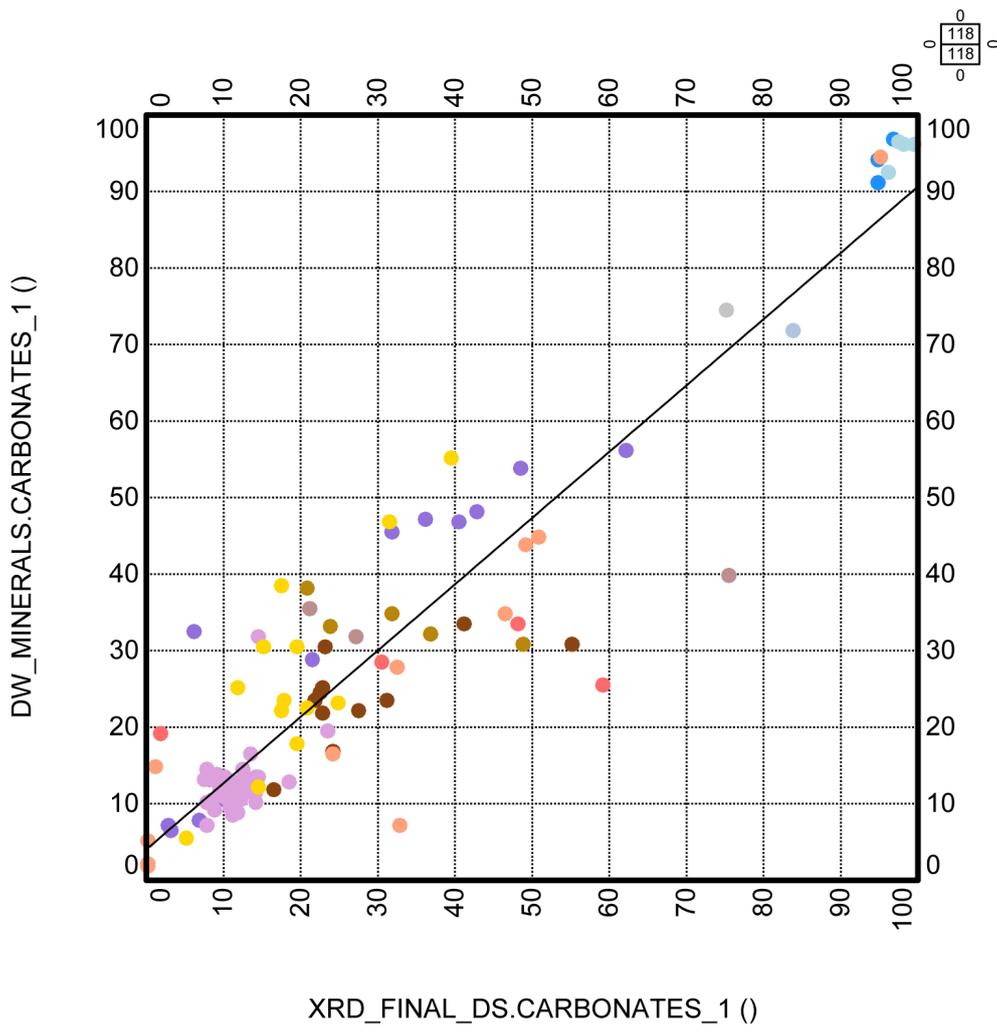


Fig. 4-4: Weight % of QF-silicates (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Bänkerjoch Formation)

The QF-silicates are the sum of quartz and feldspars. The calibration to core XRD data is good (cc = 0.84) despite some dispersion in the Triassic.



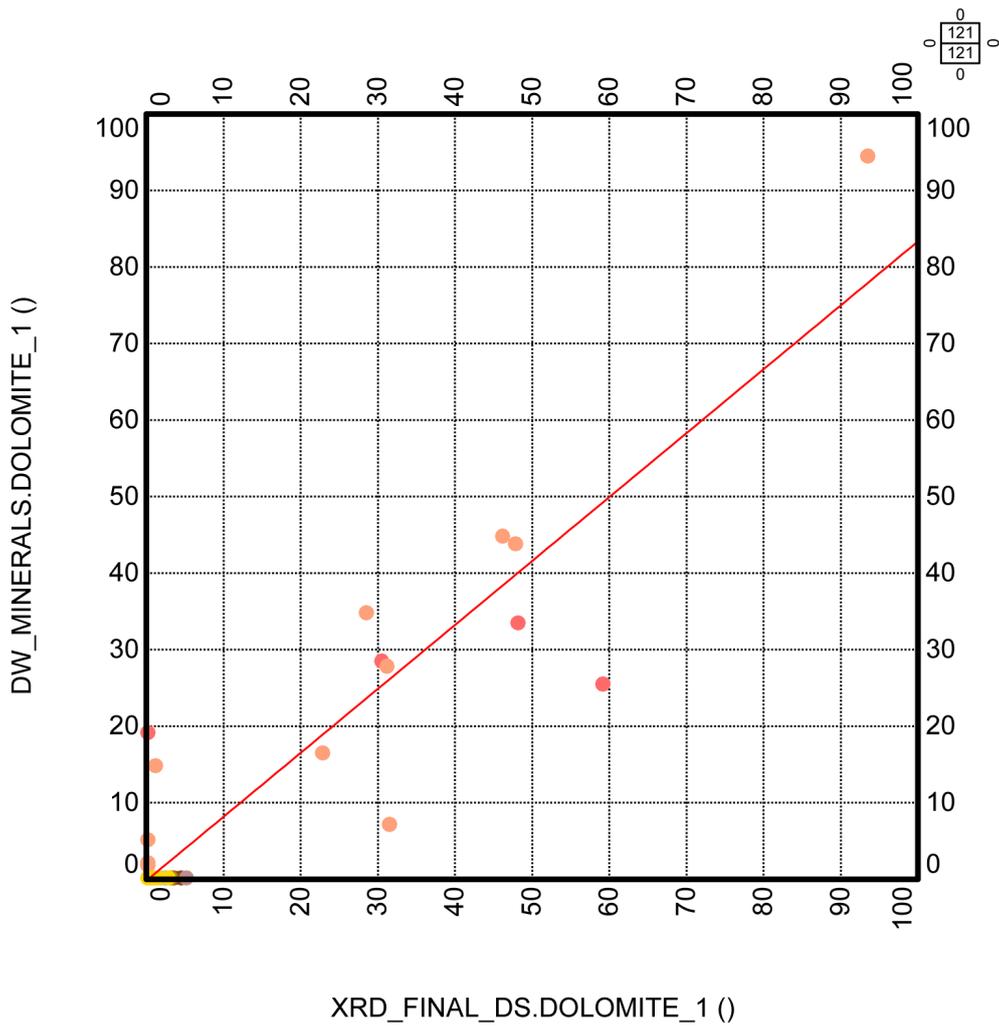
Color: Maximum of TOPS.COLOR

Intervals:

- | | |
|------------------------------|--------------------------------------|
| «FELSENKALKE» + «MASSENKALK» | SCHWARZBACH |
| VILLIGEN | WILDEGG |
| VARIANSMERGEL | «PARKINSONI-WÜRTEMBERGICA-SCHICHTEN» |
| HUMPHRIESIOOLITH | WEDELSANDSTEIN |
| OPALINUS CLAY | STAFFELEGG |
| KLETTGAU | BÄNKERJOCH |

Fig. 4-5: Weight % of carbonates (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Bänkerjoch Formation)

The carbonates include the calcite, dolomite and siderite content. The calibration to core XRD data is good (cc = 0.93), despite a few outliers and local heterogeneities.



Color: Maximum of TOPS.COLOR

- Intervals:
- | | |
|------------------------------|---------------------------------------|
| «FELSENKALKE» + «MASSENKALK» | SCHWARZBACH |
| VILLIGEN | WILDEGG |
| VARIANSMERGEL | «PARKINSONI-Württembergica-Schichten» |
| HUMPHRIESIOOLITH | WEDELSANDSTEIN |
| OPALINUS CLAY | STAFFELEGG |
| KLETTGAU | BÄNKERJOCH |

Fig. 4-6: Weight % of dolomite (x axis) compared to core XRD data (y axis) («Felsenkalke» + «Massenkalk» to the Bänkerjoch Formation)

The dolomites are mostly located in the Triassic, within complex mineralogical settings including anhydrite. The calibration to core XRD data is fair (cc = 0.93 but some dispersion in the dolomitic formations).

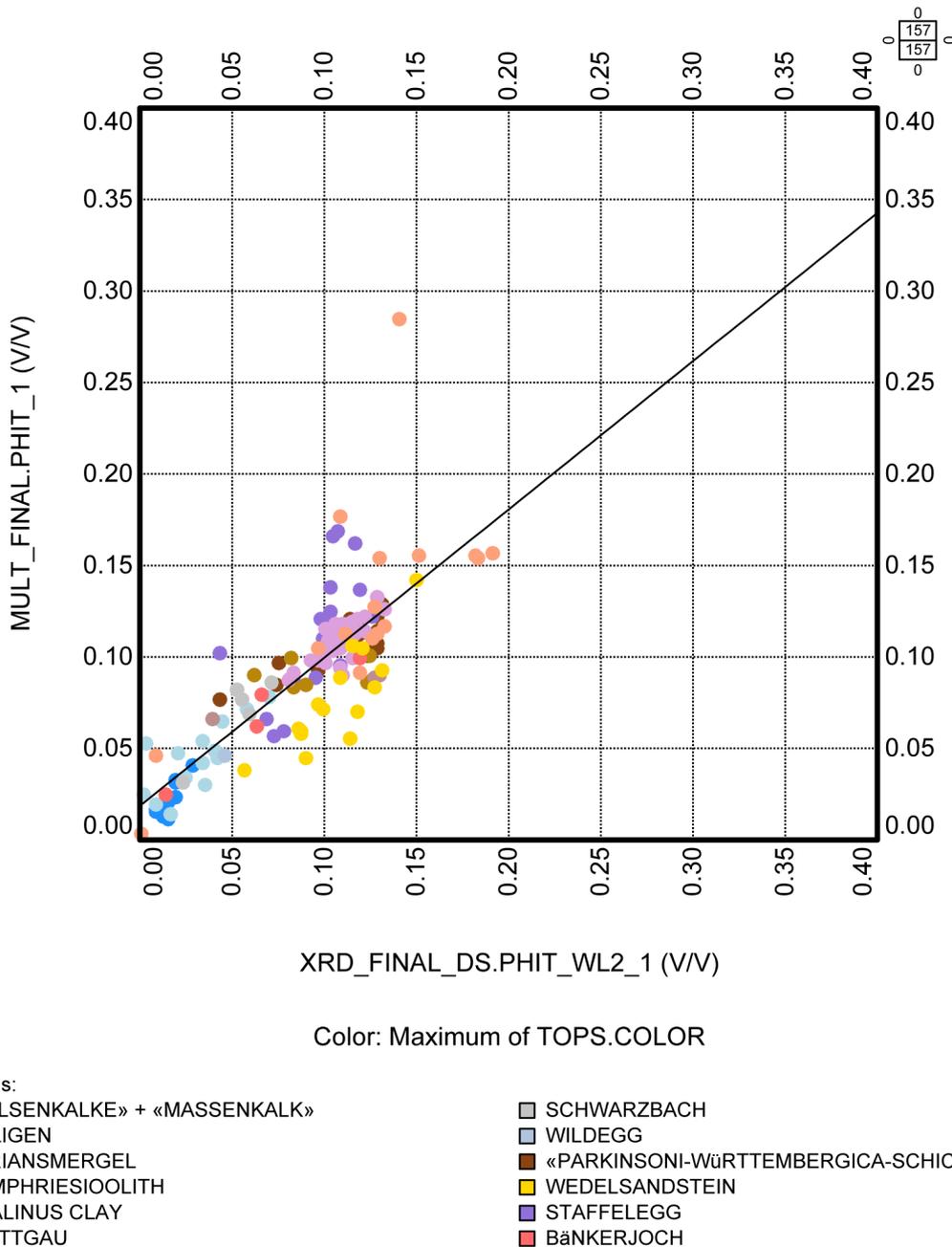


Fig. 4-7: Total porosity (v/v, y axis) compared to core data (x axis) («Felsenkalk» + «Massenkalk» to the Bänkerjoch Formation)

The lab porosity used for the comparison was water-loss porosity (105 °C) using grain density, at ambient conditions, i.e. no confining stress was applied during measurements. Therefore, cores and logs measurements are not fully equivalent as the logs evaluate in situ, wet formations. Nevertheless, the correlation between MultiMin and lab porosity is fair (cc = 0.82).

MultiMin porosity locally underestimates core porosity, for example in the «Humphriesiolith Formation» and Wedelsanstein Formation. In this interval, the MultiMin results could not be reconciliated with core porosities, as the core bulk density is lower than the TLD RHOZ, leading to lower MultiMin Phit. Additionally, some dispersion can be noticed in the Triassic, where the mineralogy is less accurately calibrated to core.

4.2 Main results of the core-calibrated log analyses in the TRU1-1 borehole

The main aim of the MultiMin interpretation were continuous curves of porosity and clay content of the borehole TRU1-1. Several other minerals have been determined (mainly QF-silicates and carbonates). Below is a summary of the main parameters of clay, carbonate, QF-silicate content and porosity for each system/group.

If not stated otherwise, clay content is used *sensu lato* meaning that clay content is used as a general term for the total clay mineral content of the formation (i.e. the sum of all clay minerals). Carbonates and QF-silicates are also used *sensu lato* where carbonates are regarded as the sum of all carbonate minerals (calcite, dolomite and siderite) while QF-silicates is used synonymous for the sum of quartz (*sensu stricto*) and feldspars.

Malm (474.0 – 725.0 m, «Felsenkalke» + «Massenkalk» Schwarzbach Formation, Villigen Formation and Wildegg Formation):

As the 7½" auxiliary casing shoe was installed at 504.2 m, the top part of the Malm could not be logged.

As expected, carbonates are the main constituents in the formations of the Malm, the mean calcite content is 92.4 wt.-% (median of 95.6 wt.-%). Lithological changes (e.g. at group boundaries) are sometimes reflected in a sharp negative peak (i.e. decreasing carbonate content at top Schwarzbach Formation), but in general variance of the carbonates in the Malm is low.

Only the Schwarzbach and Wildegg Formations are more argillaceous and correlatively less calcareous: respectively 11.7 wt.-% DRY_CLAY and 77.3 wt.-% CALCITE in the Schwarzbach Formation and 22.9% DRY_CLAY and 65.5 wt.-% CALCITE in the Wildegg Formation.

The carbonate content in the Malm is dominated by calcite, as no dolomite was calculated for this group (up to 3 wt.-% on core XRD data). Almost no siderite was measured on core XRD.

The QF-silicate content in the Malm is low (mean of 4.5 wt.-%, median of 3.3 wt.-%). The more clay-rich lithologies (Schwarzbach Formation and Wildegg Formation) show a slightly increased QF-silicate content (Mean / median of the Schwarzbach Formation: 10.6 / 11.0 wt.-%, Wildegg Formation: 8.4 / 8.0 wt.-%).

Generally, the dry clay content is low (mean of 2.9 wt.-%, median of 0.5 wt.-%) with locally higher values in the more argillaceous intervals (e.g. parts of the Schwarzbach or Wildegg Formations). In the Wildegg Formation, the maximum clay content is close to 33.9 wt.-% with a mean and median of 22.8 and 23.1 wt.-%.

Total porosity in the Malm ranges between 0 and 18.3% (mean of 4.1%, median of 3.7%). Some porosity peaks occur, especially at top «Felsenkalke» + «Massenkalk» and top Wildegg Formation. These must be treated with caution as they might represent artefacts due to a reduced data quality in these intervals.

Dogger (725.0 – 927.9 m, Wutach Formation, Variansmergel Formation «Parkinsoni-Württembergica-Schichten», «Humphriesoolith Formation», Wedelsandstein Formation, «Murchisonae-Oolith Formation», Opalinus Clay):

The boundary between the Malm and the Dogger is clearly marked by a sharp increase of the iron content (up to 10 wt.-%), the clay content (characterised by a gamma ray peak) and a sharp decrease of the carbonate content to the Wutach Formation.

The carbonate content in the Dogger is generally moderate, with a mean of 20.5 wt.-% and a median of 15.7 wt.-%. The carbonate content is dominated by the calcite above the Opalinus Clay (mean / median 29.7 wt.-% / 28.4 wt.-%), and the calcite plus siderite in the Opalinus Clay (mean / median calcite 8.2 wt.-% / 7.5 wt.-%; mean/median siderite 4.8 wt.-%).

Four calcite-rich thin streaks can be noticed in the upmost half of the Opalinus Clay, visible on the bulk density RHOZ and the calcium content DWCA_WALK2. These streaks are likely not well characterised due to the limited vertical resolution of the ECS tool.

When comparing the ECS iron content with the XRD iron-rich minerals, an excess of iron can be noticed. If the iron content measurement is valid, the presence of an additional iron-rich mineral species is possible. This was modelled as iron oxide with MultiMin.

The QF-silicate content in the Dogger ranges between 6.8 and 59.7 wt.-%. The mean and median values (29.8 and 29.2 wt.-%) are lifted up by the Wedelsandstein Formation (mean / median 41.1 / 41.8 wt.-%) and thin «Murchisonae-Oolith Formation», while the other formations are in the range between 6.8 and 41 wt.-%.

The Opalinus Clay in the Dogger certainly is the formation with the highest clay content, ranging between 34.8 and 70.2 wt.-% (mean / median of 55.6 / 56.1 wt.-%). The clay content is high but variable in the formations above (minimum 10.8 wt.-%, maximum 63.4 wt.-%, mean / median of 31.7 and of 30.6 wt.-%).

Total porosity of the Dogger also is very different between the different units. PHIT is not very variable in the Opalinus Clay (minimum / maximum 6.9 / 13.6%, mean / median 10.7 / 10.9% but a low standard deviation 1.1%). It is more variable in the overlying Dogger formations (minimum / maximum 2.7 / 19.9%, mean / median 9.1 / 9.0% and a standard deviation 2%). It must be reminded that the MultiMin Phit could not be reconciliated with the core porosity in the «Humphriesioolith Formation» and Wedelsandstein Formation.

Some porosity spikes occur mostly in the «Humphriesioolith Formation» iron-rich streaks, reaching values of 20% but these must be regarded as artefacts from the MultiMin interpretation (the quality indicator is above 2, suggesting a less reliable model).

Lias (927.9 – 971.5 m, Staffelegg Formation):

The formation boundary from the Opalinus Clay (Dogger) to the Staffelegg Formation (Lias) is characterised by a sharp drop of the clay content and a sharp rise of the carbonate (mostly calcite) content.

The carbonate content of the Lias reflects the lithology where the upper parts (Gross Wolf down to Grünscholzh Members) have a relatively high carbonate content (up to 70.4 wt.-%), while the lower part (Frick to Schambelen Members) have a relatively low carbonate content (mean / median 13.2 / 9.8 wt.-%). As in the previous groups, the carbonate content is dominated by calcite, no dolomite content has been calculated or measured from cores.

The QF-silicate content shows the reverse of the carbonate content. While the upper (Gross Wolf down to Grünscholzh Members) show a relatively low QF-silicate content (mean / median 12.6 /

11.5 wt.-%), the lower part (Frick Member) shows higher QF-silicate contents (mean / median 32.2 / 32.7 wt.-%).

The clay content follows the same trend, moderate in the upper part (mean / median 32.5 / 32.3 wt.-%) and high in the lower half (mean / median 53.7 / 55.1 wt.-%).

The Staffelegg formation is also characterised by high total organic carbon (TOC), not fully reconstructed by the MultiMin interpretation. The maximum TOC measured on cores was 7.84 wt.-% at 943.2 m.

The total porosity in the Staffelegg Formation ranges between 2.0 and 23%, the highest values in the Rietheim member likely being artefacts due to the poor calibration of the high TOC. Except in this member, the total porosity increases with the clay content, up to 12% at the base Frick Member.

The mean / median Phit in the Staffelegg Formation are 9.5 / 9.8%.

Keuper (971.5 – 1'084.2 m, Klettgau Formation, Bänkerjoch Formation):

In the Keuper, the top part of the Klettgau Formation (Gruhalde and Seebi Members) is characterised by a complex mineralogical mixture of carbonates (mostly dolomite) between 4 and 97 wt.-% (the latter represents a dolomite bed at the top half of the Seebi Member), silicates (quartz and feldspars) between 0 and 82.2 wt.-% and clays (dominant illite) between 0.7 and 63 wt.-%. The base of the Seebi Member is a sandstone, up to 82.2 wt.-% QF-silicates.

The Gansingen Member is an anhydrite bed, while the base Klettgau (Ergolz Member) Formation is an argillaceous formation (20 to 64 wt.-% clays, mean 45.7 wt.-%) with QF-silicates (15.5 to 62.5 wt.-%, mean 44.6 wt.-%).

The underlying Bänkerjoch Formation is dominated by anhydritic deposits: 0 to 86 wt.-% (mean 38 wt.-%). In addition, carbonates (dolomite), QF-silicates and clays are well represented in this formation.

The wireline log quality is often degraded above the Keuper, with a slightly enlarged Caliper (up to 9 in in a 6% in borehole) and HDRA above 0 g/cc suggesting wall rugosity. The combination of a complex mineralogy and low log quality made the porosity computation less accurate, the doubtful results were flagged by the MULT_QC curve (0 means good confidence, 1 suspicious porosity and 2 invalid porosity).

After filtering, keeping only MULT_QC = 1, the total porosity Phit ranges from 0 to 19.2% (mean 9.2% and median 9.6%). The low porosities correspond to the anhydrites.

Muschelkalk (1'084.2 – 1'233.2 m, Schinznach Formation, Zeglingen Formation, Kaiseraugst Formation):

The boundary from the Keuper to the Muschelkalk is marked by a sharp increase of the carbonate content which here is dolomite. The Asp and Stamberg Members are mostly dolomitic (except for a thin peak of QF-silicate and clay content in the uppermost part of the Muschelkalk, Asp Member), the top of the Liedertswil Member is the progressive transition to dolomitic limestones.

The carbonate content of the Schinznach Formation ranges from 0 to 100 wt.-% (mean 90.0 wt.-%, median 95.4 wt.-%): mean 83.8 wt.-% dolomite in the Asp and Stamberg Members

at the top, 31.4 wt.-% dolomite and 65.2 wt.-% calcite in the Liedertswil and Leutschenberg/Kienberg Members at base.

The top Zeglingen Formation is characterised by a sharp decrease of the calcite content, replaced by dolomite. The anhydrite content, well picked up by the ECS DWSU_WALK2 curve, increases downwards in the Dolomitzone Member, while the Sulfatzone Member is mostly anhydritic.

A sharp anhydrite to carbonates transition indicates the top Kaiseraugst Formation, with a complex mineralogical mixture of carbonates, QF-silicates and clays: mean 37.5 wt.-% carbonates, 29.7 wt.-% QF-silicates and 26.7 wt.-% clays. A thin anhydritic bed is seen at base Orbicularis-mergel Member.

Total porosity in the Muschelkalk is very variable and ranges between 0.2 and 20.6%. The lowest porosity rocks are the anhydrites and the dolomitic limestones in the Liedertswil and Leutschenberg/Kienberg Members at the base Schinznach Formation. The highest porosity interval is the dolomites of the Dolomitzone Member at the top Zeglingen Formation.

Buntsandstein (1'233.2 – 1'246.1 m, Dinkelberg Formation) and **Rotliegend** (1'246.1 – 1'259.7 m, Weitenau Formation):

The boundary from the Muschelkalk to the sandstones of the Buntsandstein and Rotliegend is characterised by a sharp increase of the QF-silicate content and a sharp decrease of the carbonate and clay contents. On the logs this corresponds to a sharp gamma ray decrease.

The QF-silicate content is uniformly high though higher in the Buntsandstein (mean / median of 88.4 / 90.6 wt.-%) than in the Rotliegend (mean / median: 71.8 / 72.1 wt.-%).

The clay content in the Buntsandstein (mean / median: 7.2 / 7.5 wt.-%, maximum 18.4 wt.-%) is lower than in the Rotliegend (mean / median: 22.1 / 22.7 wt.-%).

The carbonate content of these two groups is very low and ranges between 0 and 26.2 wt.-% (mean / median for the Buntsandstein: 4.4 / 2.5 wt.-%, for the Rotliegend: 4.8 / 4.4 wt.-%).

Total porosity in the Buntsandstein ranges from 3.6 to 21.6% (mean 12.5%, median 13.5%), while it is lower in the Rotliegend: 5.5 to 8.4% (mean and median 7.0%).

Crystalline Basement (1'259.7 – 1'310.0 m):

This interval was described from cuttings as gneiss featuring quartz, feldspars and sometime abundant micas.

Nevertheless, some intervals (e.g. 1'265.5 – 1'276 m) have high gamma ray, slow sonic, large density-neutron separation, suggesting possible significant clay content. Therefore, clay minerals were added in the MultiMin models for the Crystalline Basement.

The following minerals were modelled in the top of the interval, where all logs could be acquired, including ECS: Quartz, potassic feldspars, plagioclases, muscovite and clay minerals. As the logs coverages decrease downwards, the mineralogical assemblage was simplified to keep mathematical consistency.

4.3 Main results of the core-calibrated log analysis in the Opalinus Clay (816.4 – 927.9 m)

The main results in terms of total clay content, mineralogy and total porosity for the main focus interval (Opalinus Clay) are shortly described in this section. Figs. 4-8 to 4-14 show some general statistical values of the MultiMin analysis results within the Opalinus Clay.

Histogram of DW_MINERALS.DRY_CLAY

Well: TRU1-1

Interval: OPALINUS CLAY

Filter:

731
731

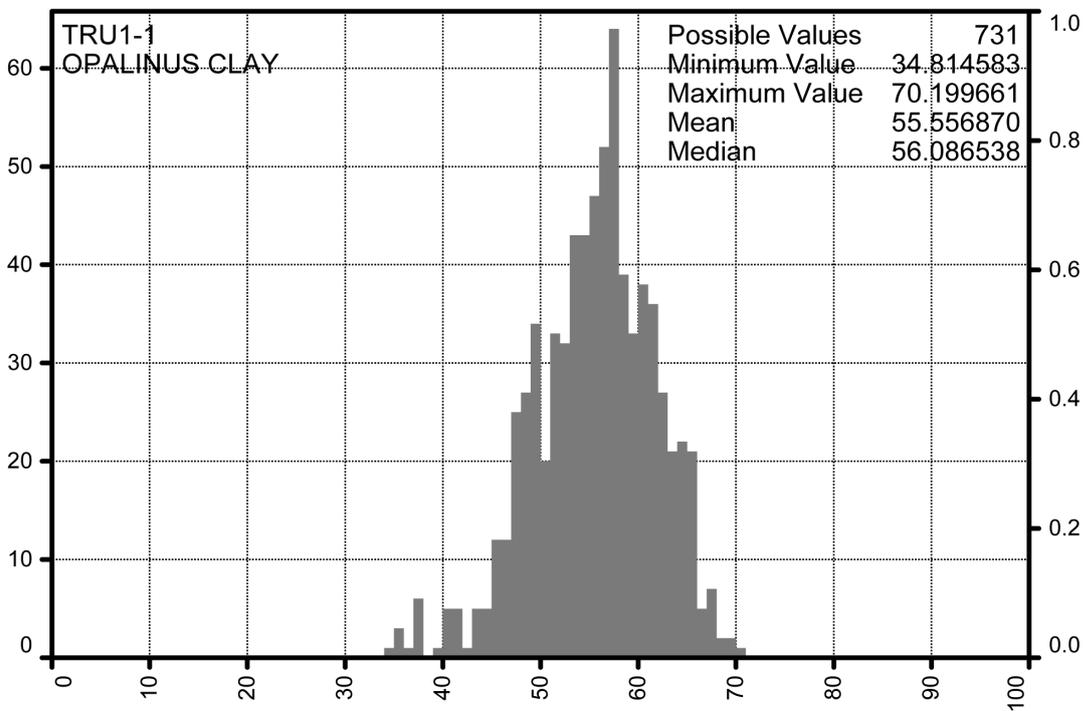


Fig. 4-8: Dry clay weight percentage frequency histogram in the Opalinus Clay
X axis is the dry clay wt.-% from MultiMin, y axis the number of points per bin (100 bins).

In the clay-rich Opalinus Clay, the mean and median dry clay contents are close to 55.6 and 56.1 wt.-%. The distribution is clearly monomodal and has a high variability, especially in the upper part.

The two next frequency histograms show a split of the Opalinus Clay in an upper and a lower part, showing that this last is slightly more argillaceous (Figs. 4-9 and 4-10).

Histogram of DW_MINERALS.DRY_CLAY

Well: TRU1-1

Interval: OPALINUS CLAY

Filter: DW_MINERALS.DEPTH<867

331
331

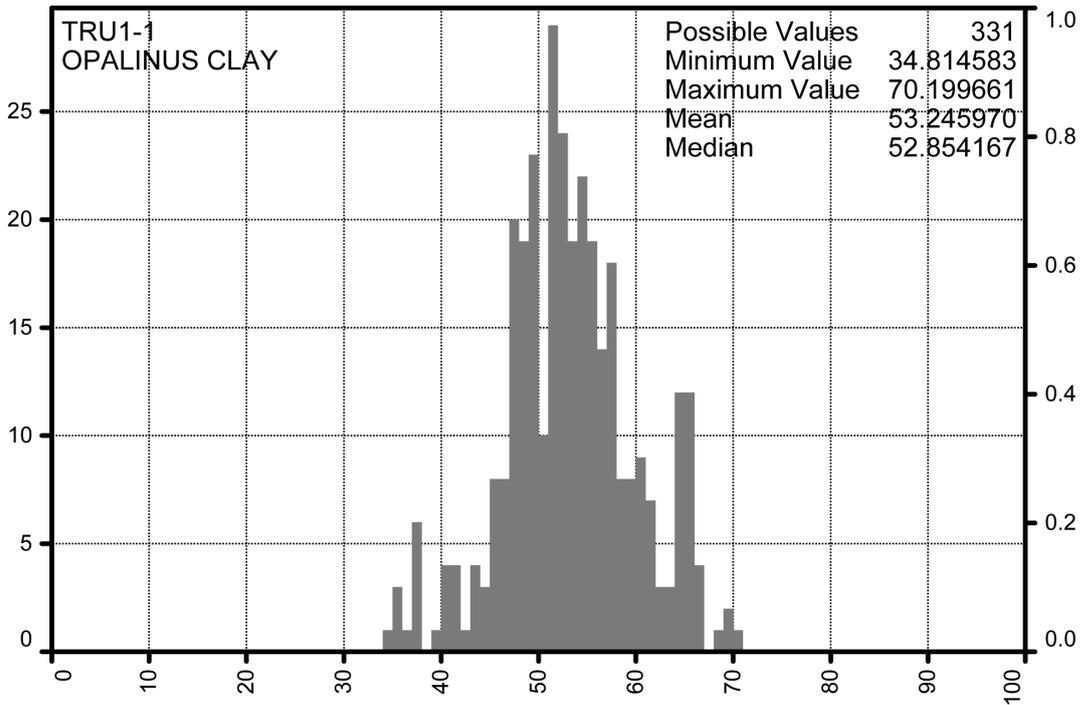


Fig. 4-9: Dry clay weight percentage frequency histogram in the upper section of Opalinus Clay (above 867 m)

X axis is the dry clay wt.-% from MultiMin, y axis the number of points per bin (100 bins).

In the upper part of the Opalinus Clay (above 867 m), the mean and median dry clay contents are close to 53.2 and 52.9 wt.-%. The top part of the formation is slightly less argillaceous than the bottom (see Fig. 4-10).

Histogram of DW_MINERALS.DRY_CLAY

Well: TRU1-1

Interval: OPALINUS CLAY

Filter: DW_MINERALS.DEPTH>=867

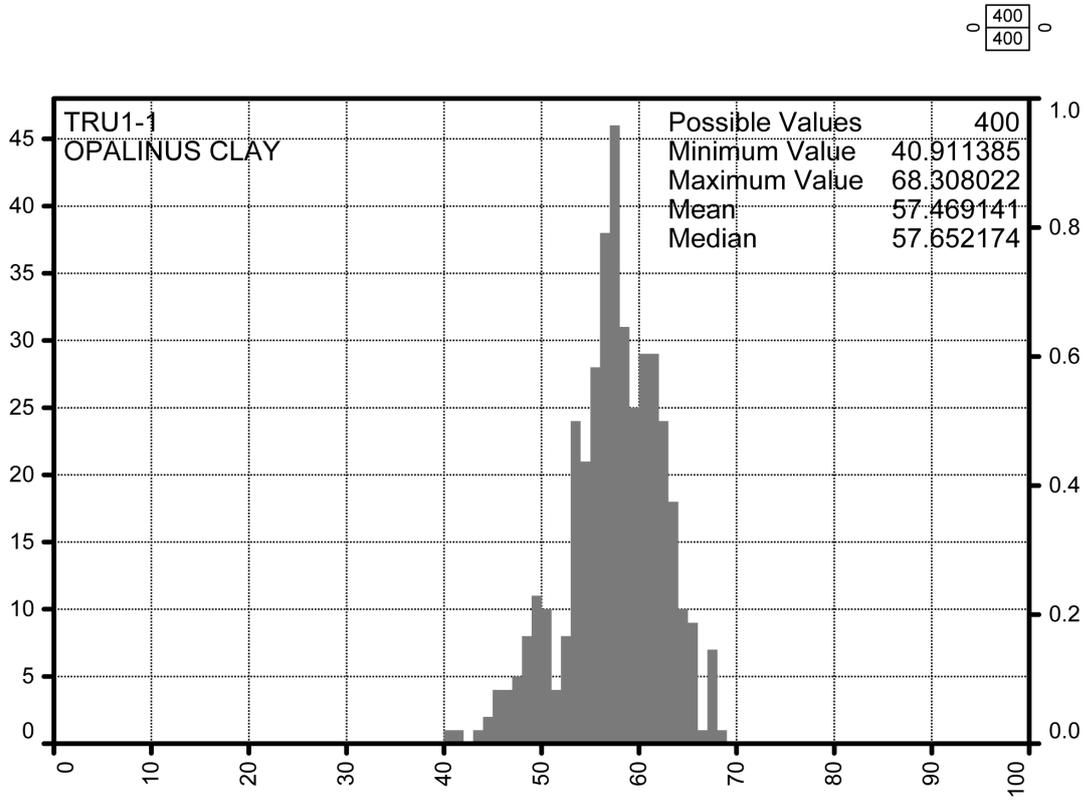


Fig. 4-10: Dry clay weight percentage frequency histogram in the lower section of Opalinus Clay (below 867 m)

X axis is the dry clay wt.-% from MultiMin, y axis the number of points per bin (100 bins).

The bottom part of the Opalinus Clay (below 867 m), is more argillaceous: the mean and median dry clay contents are close to 57.5 and 57.7 wt.-%.

Histogram of DW_MINERALS.CALCITE

Well: TRU1-1

Interval: OPALINUS CLAY

Filter:

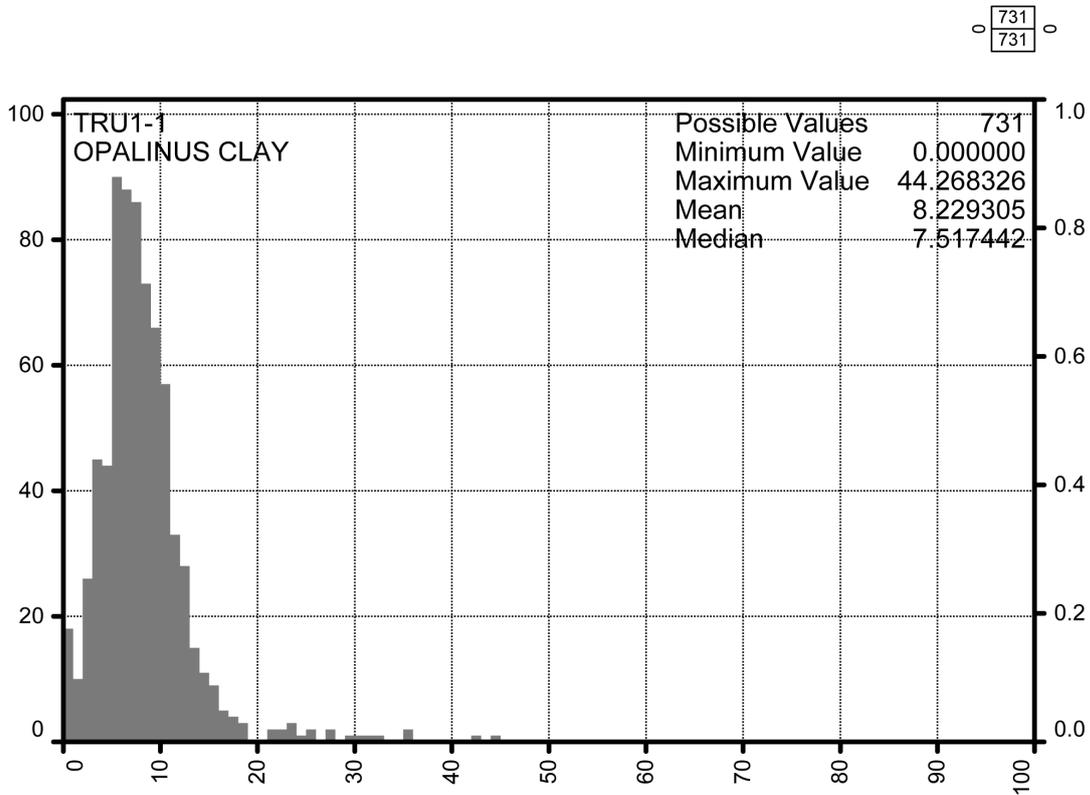


Fig. 4-11: Calcite weight percentage frequency histogram in the Opalinus Clay
 X axis is the calcite wt.-% from MultiMin, y axis the number of points per bin (100 bins).

The mean and median calcite contents are close to 8.2 and 7.5 wt.-%. The maximum values are up to 44.3 wt.-%, i.e. corresponding to thin, calcite-rich layers. In case these layers are thinner than the log resolution, the maximum calcite content would be higher than computed by MultiMin.

Histogram of DW_MINERALS.SIDER

Well: TRU1-1
 Interval: OPALINUS CLAY
 Filter:

o $\frac{731}{731}$ o

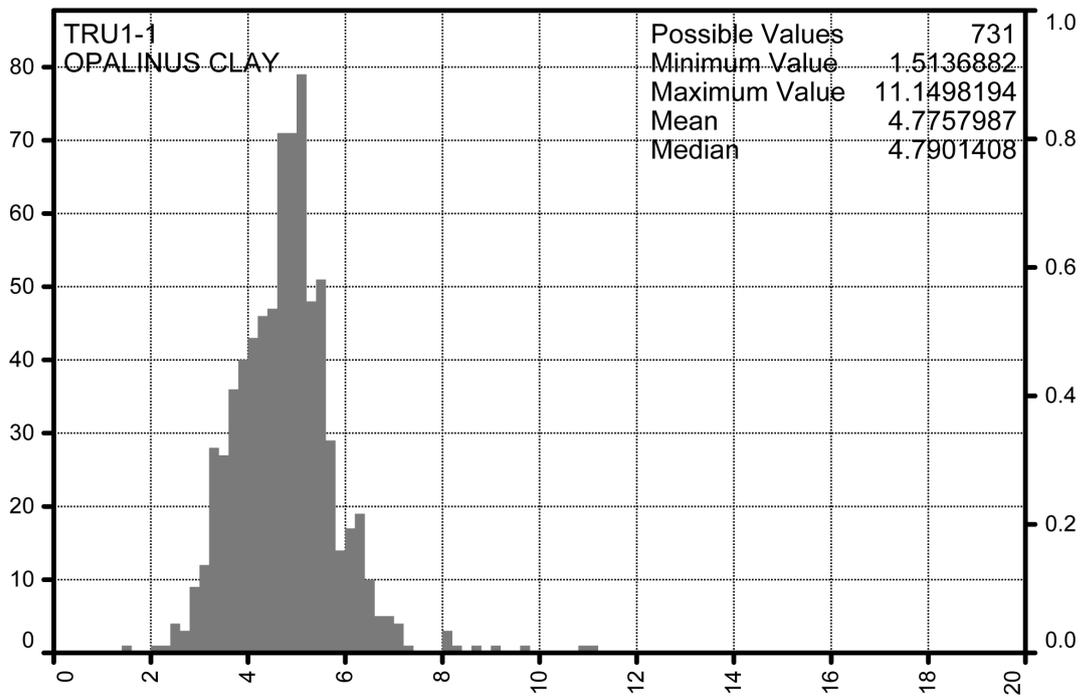


Fig. 4-12: Siderite weight percentage frequency histogram in the Opalinus Clay
 X axis is the siderite wt.-% from MultiMin, y axis the number of points per bin (100 bins).

The mean and median siderite contents are close to 4.8 wt.-%, with a maximum value of 11.2 wt.-% and minimum values close to 1.5 wt.-%. Please note that the siderite core calibration is less constrained than other minerals.

Histogram of DW_MINERALS.QF_SILICATES

Well: TRU1-1

Interval: OPALINUS CLAY

Filter:

731
731

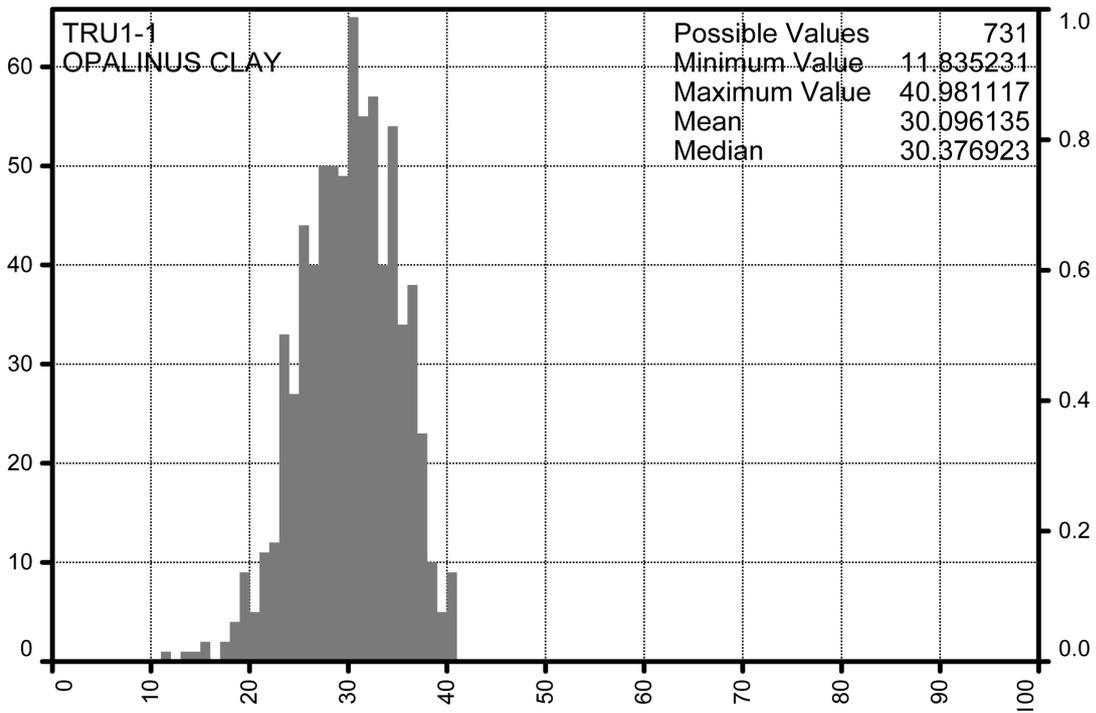


Fig. 4-13: QF-silicates (quartz and feldspars) weight percentage frequency histogram in the Opalinus Clay

X axis is the QF-silicates wt.-% from MultiMin, y axis the number of points per bin (100 bins).

The mean and median QF-silicates (quartz, plagioclases and potassic feldspars) contents are close to 30.1 and 30.4 wt.-%, much higher than the carbonates (close to 13.0 and 12.3 wt.-%).

From core XRD data, the quartz represents two thirds and feldspars the remaining third.

Histogram of MULT_FINAL.PHIT

Well: TRU1-1

Interval: OPALINUS CLAY

Filter:

○ $\frac{731}{731}$ ○

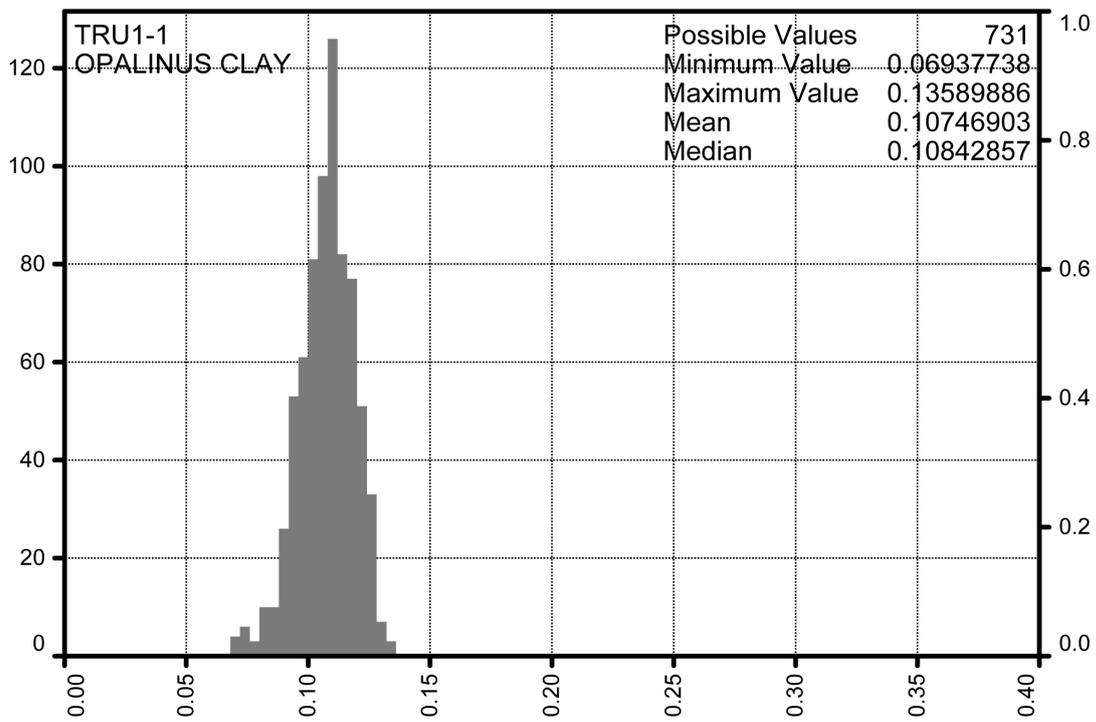


Fig. 4-14: Total porosity frequency histogram in the Opalinus Clay

X axis is the total porosity v/v from MultiMin, y axis the number of points per bin (100 bins).

The mean and median total porosities are 10.7 and 10.8%., with a range from 6.9 to 13.6%.

Fig. 4-15 summarises the main results in the Opalinus Clay.

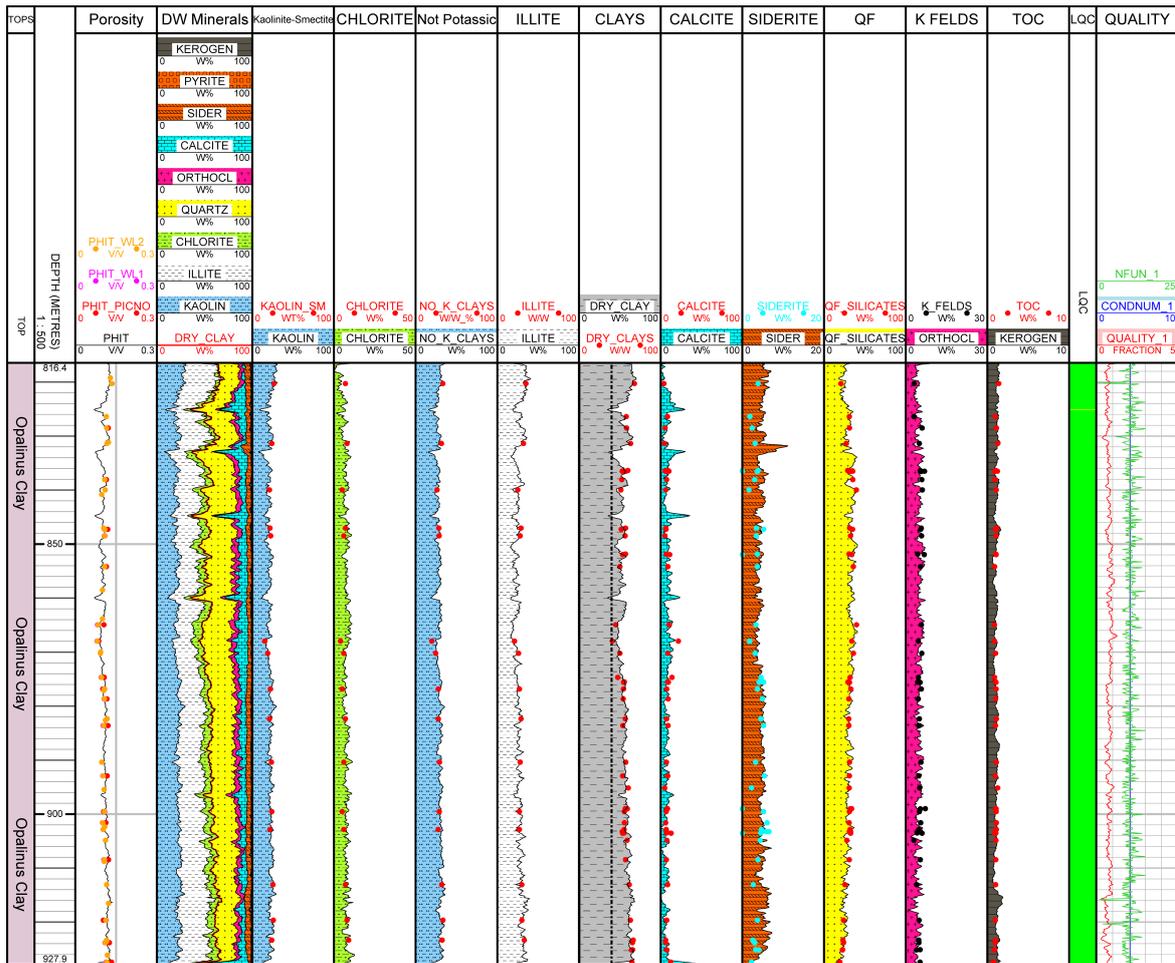


Fig. 4-15: Main log and core results in the Opalinus Clay

The wireline log quality was good in the Opalinus Clay, as shown by the green LQC flag.

The MultiMin quality curve always remains low, generally below 1.00, indicating an overall good curve prediction.

The total porosity and the main minerals dry weight are well calibrated to the core XRD measurements. The siderite and TOC calibration are less accurate.

The whole Opalinus Clay is very argillaceous, almost always above the 40 wt.-% (black line in the “All Clay minerals” track in Fig. 4-15). A few carbonates streaks in the top part have a lower clay content.

5 Summary

The MultiMin interpretation was successfully applied in the TRU1-1 borehole using the Paradigm Geolog MultiMin software (see Appendix Plate 1 and 2). On the basis of available petrophysical logs and formation mineralogical contents, several specific MultiMin interpretation intervals were designed. Some of these intervals needed to be further subdivided due to e.g. borehole conditions to ensure the best possible MultiMin interpretation result.

Core data from lab measurements were also available so that the mineralogical content and other parameters (e.g. density and/or porosity) were known at several points along the borehole. These core data included bulk rock XRD mineralogy, clay mineralogy, pycnometer and water loss porosity and grain density. The core data was used as a starting parameter set for the MultiMin interpretation where available.

The mineralogical MultiMin interpretation results were converted to weight percentages for a straightforward comparison with core XRD measurements. In general, the comparisons showed a good agreement between the mineralogy (and porosity) from the MultiMin interpretation and the core data. QF-silicates and carbonates show a good agreement with core data throughout the borehole even in the lowermost units. The differentiation between illite (potassic clay) and not potassic clays was fairly achieved, while the chlorite endmember remains less accurate. The total porosity is well calibrated to core measurements in the Opalinus Clay; the calibration was fair in the whole borehole, with occasional miscalibrations where the borehole quality was degraded (e.g. in the Keuper) or in organic-rich layers of the Staffelegg Formation.

The continuous curves from the MultiMin interpretation can be used to characterise the different formations (and hence members) occurring in TRU1-1. The Opalinus Clay shows a quite variable total clay content though in most locations it is well above 40 wt.-%.

In addition, boundaries between formations (and also between members) are often clearly marked by a decrease or increase of clay, QF-silicates and/or carbonate contents. The carbonate-rich formations can further be characterised according to the occurrence of dolomite (replacing calcite), especially in the lower part of the borehole (in the lithostratigraphic units of the Keuper and Muschelkalk).

6 References

- Isler, A., Pasquier, F. & Huber, M. (1984): Geologische Karte der zentralen Nordschweiz 1:100'000. Herausgegeben von der Nagra und der Schweiz. Geol. Komm.
- Marnat, S. & Becker, J.K. (2020): Petrophysical log analyses of deep and shallow boreholes: Methodology report. Nagra Arbeitsbericht NAB 20-30.
- Mazurek, M. (2017): Gesteinsparameter-Datenbank Nordschweiz – Version 2. Nagra Arbeitsbericht NAB 17-56.
- Nagra (2014): SGT Etappe 2: Vorschlag weiter zu untersuchender geologischer Standortgebiete mit zugehörigen Standortarealen für die Oberflächenanlage. Geologische Grundlagen. Dossier II: Sedimentologische und tektonische Verhältnisse. Nagra Technischer Bericht NTB 14-02.
- Pietsch, J. & Jordan, P. (2014): Digitales Höhenmodell Basis Quartär der Nordschweiz – Version 2013 (SGT E2) und ausgewählte Auswertungen. Nagra Arbeitsbericht NAB 14-02.
- Waber, H.N. (ed.) (2020): SGT-E3 deep drilling campaign (TBO): Experiment procedures and analytical methods at RWI, University of Bern (Version 1.0, April 2020). Nagra Arbeitsbericht NAB 20-13.