Arbeitsbericht NAB 21-22

TBO Bözberg-2-1: Data Report

Dossier X
Petrophysical Log Analysis

April 2022

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for the Disposal of
Radioactive Waste

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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.

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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 raw corrected data
DTCO	Compressional wave slowness from far monopole mid frequency source compressional wave slowness
DTCO_PRED	DTCO prediction by MultiMin
DTSM	Shear wave slowness from inline X-Dipole (90°) source
DTSM_PRED	DTSM prediction by MultiMin
DWAL_WALK2	Dry weight fraction aluminium, ECS WALK2 closure model
DWCA_WALK2	Dry weight fraction calcium, ECS WALK2 closure model
DWFE_WALK2	Dry weight fraction iron, ECS WALK2 closure model
DWFE_CORR	Dry weight fraction iron, calibrated to XRF iron content
DWSI_WALK2	Dry weight fraction silicon, ECS WALK2 closure model

DWSU_WALK2	Dry weight fraction sulphur, ECS WALK2 closure model
DWTI_WALK2	Dry weight fraction titanium from ECS, ECS WALK2 closure model
DWAL_MGWALK	Dry weight fraction aluminium, ECS MGWALK closure model
DWCA_MGWALK	Dry weight fraction calcium, ECS MGWALK closure model
DWFE_MGWALK	Dry weight fraction iron, ECS MGWALK closure model
DWMG_MGWALK	Dry weight fraction magnesium, ECS MGWALK closure model
DWSI_MGWALK	Dry weight fraction silicon, ECS MGWALK closure model
DWSU_MGWALK	Dry weight fraction sulphur, ECS MGWALK closure model
DWTI_MGWALK	Dry weight fraction titanium, ECS MGWALK closure model
ECS	Elemental Capture Spectroscopy
EDTC	Enhanced Digital Telemetry Cartridge
EMS	Environment Measurement Sonde
FE_MIN	Iron-rich minerals (Siderite, pyrite, iron oxides)
FLAG_BADHOLE_DN	Badhole flag from the Density-Neutron crossplot
FLAG_BADHOLE_ OVERGAUGE	Badhole flag from the Caliper
FLAG_BADHOLE_RUGO	Badhole flag from the Density correction
FLAG_BADHOLE_STOF	Badhole flag from the Neutron stand-off
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
GR_KCOR_PRED	GR_KCOR prediction by MultiMin
HAEMATITE	Haematite weight percentage from MultiMin
HALITE	Halite weight percentage from MultiMin
HDAR	Hole diameter from area
HDRA	Bulk density correction
HFK	Potassium concentration from HNGS
HFK_DWK	Potassium concentration from ECS

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	Uranium 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
NO_K_CLAYS	Not potassic clays weight percentage from MultiMin
ORTHOCL	K-Feldspars weight percentage from MultiMin
p.u.	Porosity unit
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
QF_SILICATES	Matrix quartz and feldspars weight percentage from MultiMin
QUALITY	MultiMin analysis quality
QUARTZ	Quartz weight percentage from MultiMin
RCL	Reduced Composite Log
RHGE_WALK2	Matrix density from elemental concentrations (WALK2 model)
RHOB_CALC	Bulk density computed from core data
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
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
TOC	Total organic carbon [w/w or wt.-%]
U	Photoelectric cross-section 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
WT.-%	Weight concentration
W/W	Weight per weight, concentration
WANH_WALK2	Dry weight fraction anhydrite/gypsum from ECS (WALK2 model)
WCAR_WALK2	Dry weight fraction carbonate from ECS (WALK2 model)
WCLA_WALK2	Dry weight fraction clay from ECS (WALK2 model)
WEVA_WALK2	Dry weight fraction salt from ECS (WALK2 model)
WPYR_WALK2	Dry weight fraction pyrite from ECS (WALK2 model)
WQFM_WALK2	Dry weight fraction quartz+feldspar+mica from ECS (WALK2 model)
WSID_WALK2	Dry weight fraction siderite from ECS (WALK2 model)
XRD	X-Ray Diffraction
µs/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 ("Tiefbohrungen", TBO) 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 Bözberg-2-1 borehole.

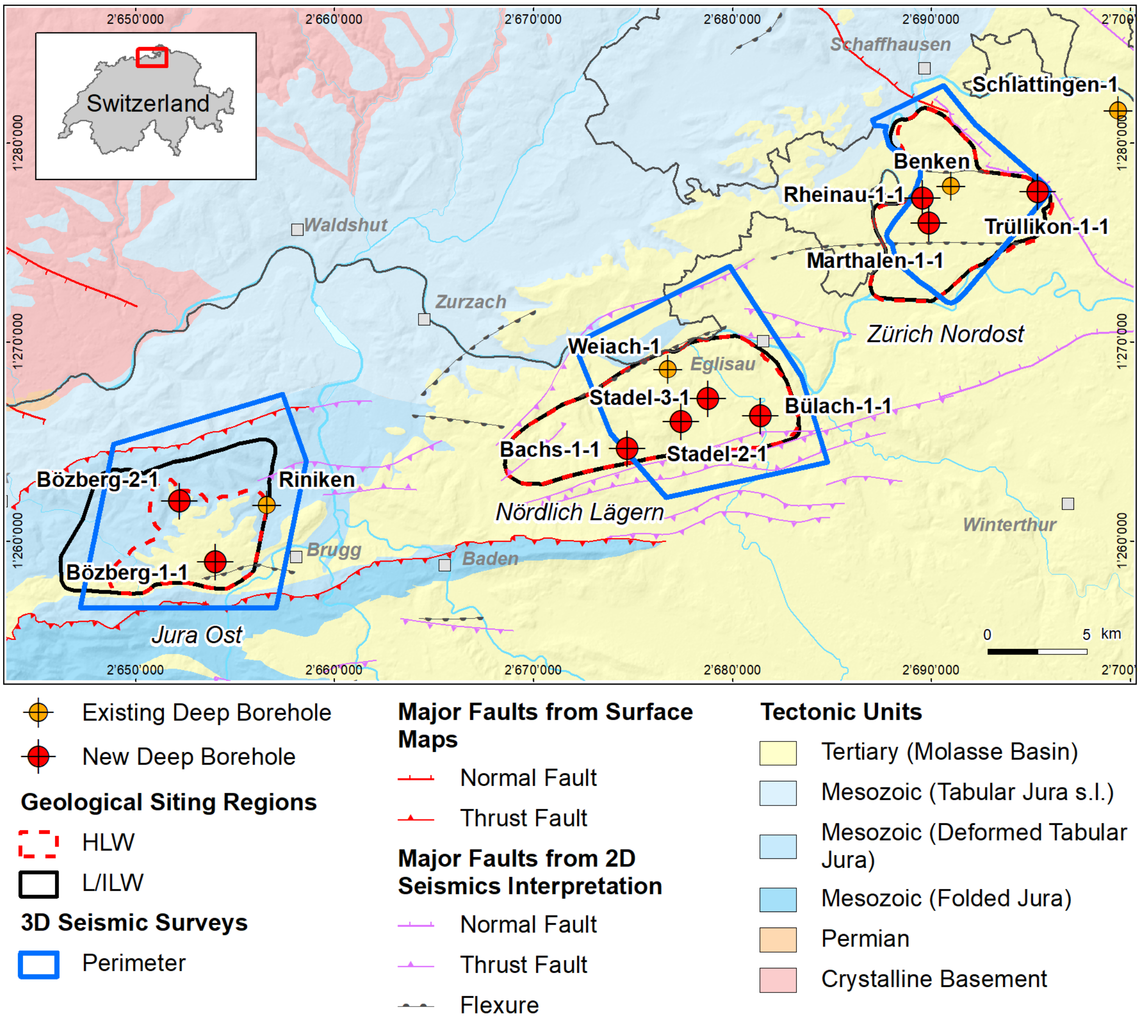

Fig. 1-1: Tectonic overview map with the three siting regions under investigation

1.2 Location and specifications of the borehole

The Bözberg-2-1 (BOZ2-1) exploratory borehole is the fifth borehole drilled within the framework of the TBO project. The drill site is located in the northern part of the Jura Ost siting region (Fig. 1-2). The vertical borehole reached a final depth of 829.11 m (MD)[1]. The borehole specifications are provided in Tab. 1-1.

Tab. 1-1: General information about the BOZ2-1 borehole

Siting region	Jura Ost
Municipality	Bözberg (Canton Aargau / AG), Switzerland
Drill site	Bözberg-2 (BOZ2)
Borehole	Bözberg-2-1 (BOZ2-1)
Coordinates	LV95: 2'652'218.764 / 1'261'985.437
Elevation	Ground level = top of rig cellar: 624.33 m above sea level (asl)
Borehole depth	829.11 m measured depth (MD) below ground level (bgl)
Drilling period	11th August – 14th December 2020 (spud date to end of rig release)
Drilling company	Daldrup & Söhne AG
Drilling rig	Wirth B 152t
Drilling fluid	Water-based mud with various amounts of different components such as[2]: 0 – 370 m: Bentonite & polymers 370 – 615 m: Potassium silicate & polymers 615 – 829.11 m: Pure-Bore®

The lithostratigraphic profile and the casing scheme are shown in Fig. 1-3. The comparison of the core versus log depth[3] of the main lithostratigraphic boundaries in the BOZ2-1 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.

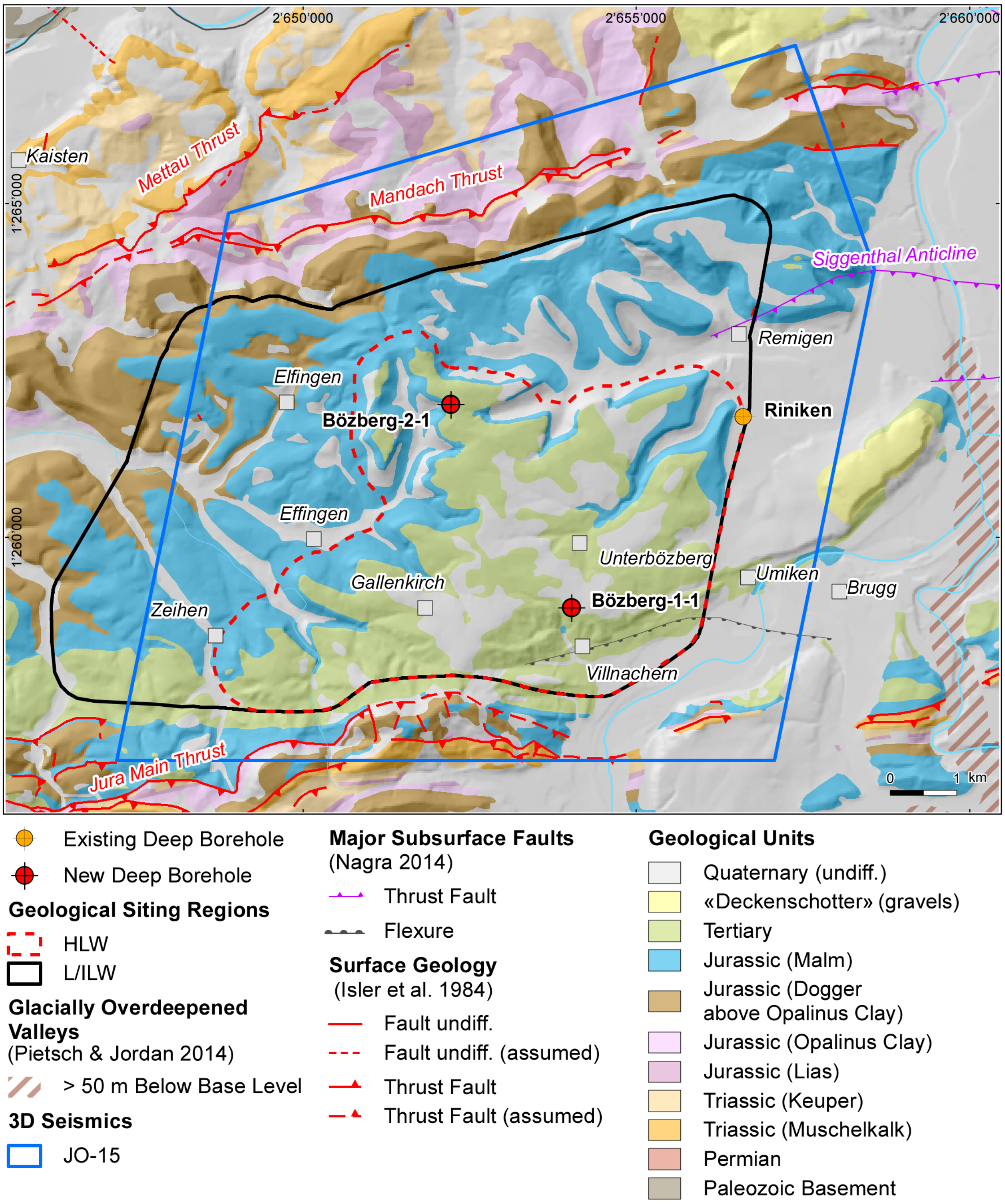

Fig. 1-2: Overview map of the investigation area in the Jura Ost siting region with the location of the BOZ2-1 borehole in relation to the boreholes Riniken and BOZ1-1

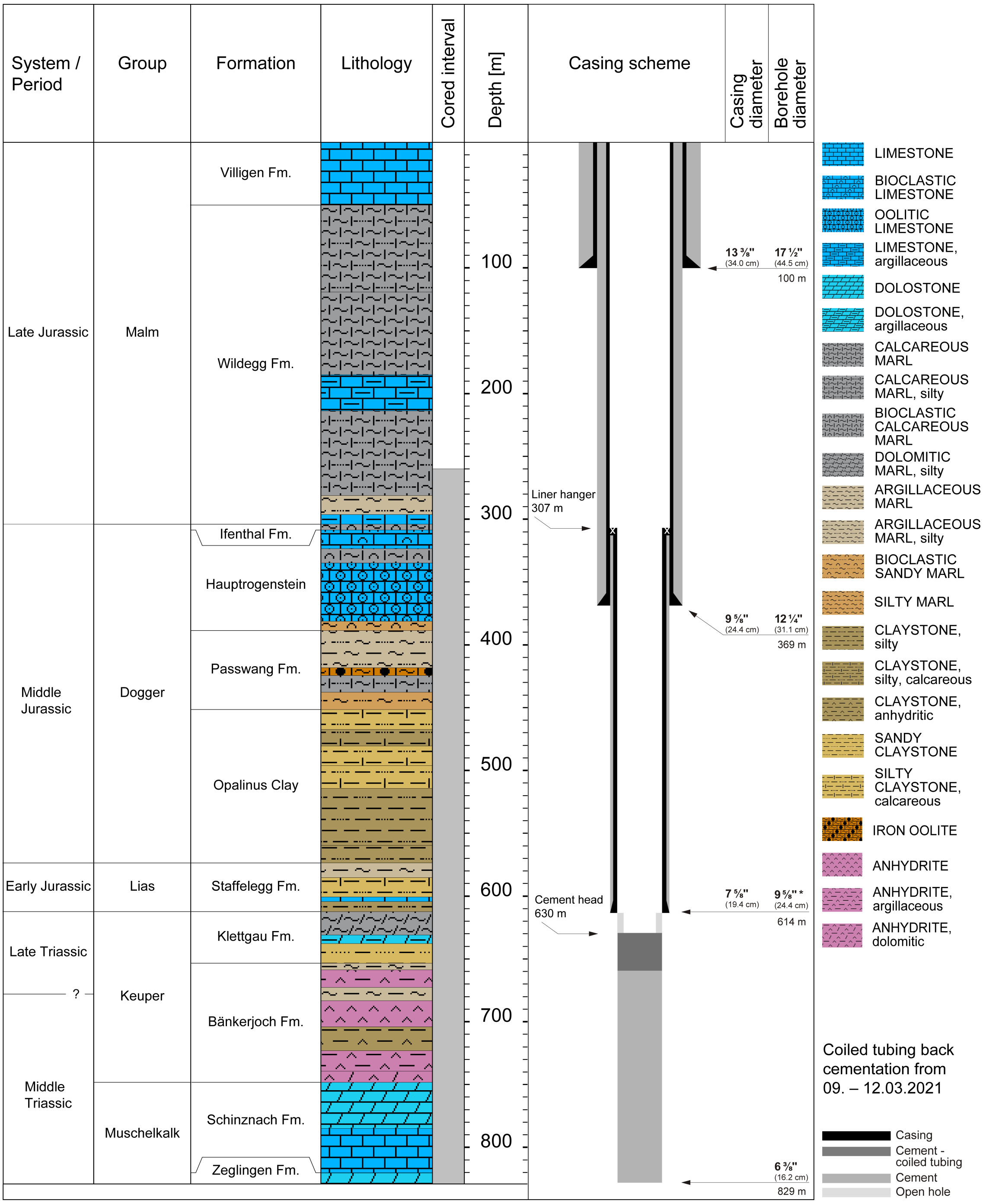

Fig. 1-3: Lithostratigraphic profile and casing scheme for the BOZ2-1 borehole[4]

[4] For detailed information see Dossier I and III.

Tab. 1-2: Core and log depth for the main lithostratigraphic boundaries in the BOZ2-1 borehole[5]

System / Period	Group	Formation	Core depth in m (MD)	Log depth in m (MD)
Jurassic	Malm	Villigen Formation		
			50.0	
		Wildegg Formation		
			303.95	304.38
	Dogger	Ifenthal Formation		
			308.70	309.07
		Hauptrogenstein		
			388.54	388.97
		Passwang Formation		
			451.54	451.90
		Opalinus Clay		
			573.68	573.89
	Lias	Staffelegg Formation		
			612.46	**612.76**
Triassic	Keuper	Klettgau Formation		
			653.45	654.70
		Bänkerjoch Formation		
			748.27	749.52
	Muschelkalk	Schinznach Formation		
			820.32	821.09
		Zeglingen Formation	829.11	829.88
			final depth	

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

1.3 Documentation structure for the BOZ2-1 borehole

NAB 21-22 documents the majority of the investigations carried out in the BOZ2-1 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 BOZ2-1 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 21-22

Black indicates the dossier at hand.

Dossier	Title	Authors
I	TBO Bözberg-2-1: Drilling	P. Hinterholzer-Reisegger
II	TBO Bözberg-2-1: Core Photography	D. Kaehr & M. Gysi
III	TBO Bözberg-2-1: Lithostratigraphy	P. Jordan, P. Schürch, H. Naef, M. Schwarz, R. Felber, T. Ibele & M. Gysi
IV	TBO Bözberg-2-1: Microfacies, Bio- and Chemostratigraphic Analyses	S. Wohlwend, H.R. Bläsi, S. Feist-Burkhardt, B. Hostettler, U. Menkveld-Gfeller, V. Dietze & G. Deplazes
V	TBO Bözberg-2-1: Structural Geology	A. Ebert, L. Gregorczyk, S. Cioldi, E. Hägerstedt & M. Gysi
VI	TBO Bözberg-2-1: Wireline Logging, Micro-hydraulic Fracturing and Pressure-meter Testing	J. Gonus, E. Bailey, J. Desroches & R. Garrard
VII	TBO Bözberg-2-1: Hydraulic Packer Testing	R. Schwarz, M. Willmann, S. Reinhardt, S.M.L. Hardie, M. Voß & A. Pechstein
VIII	TBO Bözberg-2-1: Rock Properties, Porewater Characterisation and Natural Tracer Profiles	T. Gimmi, L. Aschwanden, L. Camesi, E. Gaucher, A. Jenni, M. Kiczka, U. Mäder, M. Mazurek, D. Rufer, H. N. Waber, P. Wersin, C. Zwahlen & D. Traber
IX	TBO Bözberg-2-1: Rock-mechanical and Geomechanical Laboratory Testing	E. Crisci, L. Laloui & S. Giger
X	TBO Bözberg-2-1: Petrophysical Log Analysis	S. Marnat & J.K. Becker
	TBO Bözberg-2-1: Summary Plot	Nagra

1.4 Scope and objectives of this dossier

The dossier at hand describes the results of the stochastic petrophysical log analysis performed in the BOZ2-1 borehole. The detailed workflow for this analysis is described in a methodology report (Marnat & Becker 2021, NAB 20-30). Here, only a very short summary is given. The lowest vertical resolution tools, such as ECS, Gamma Ray or Sonic, are limiting the resolution of the MultiMin analysis. High resolution and standard tools cannot be mixed in the same processing. For this reason, only the standard resolution version of the logs was used as input with a sampling rate of ½ foot (~ 15 cm).

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 measured log. Using optimisation techniques, the difference (i.e. the error) between calculated log responses and measured petrophysical logs is minimised by adjusting the assumed mineral content. Any deviation from this workflow is explained in this report.

The result of these analyses 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 composites of the petrophysical logs from the borehole BOZ2-1 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, Chapter 3.1. The petrophysical logs used for this study are listed below:

- **Caliper log** (EMS/PPC – Environmental Measurement Sonde/Powered Positioning Caliper). The caliper log uses several coupled pairs of mechanical arms (2 pairs with PPC, 3 pairs with EMS) to continuously measure the borehole shape in different orientations.
- **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** (APLC curve, from APS – Accelerator Porosity Sonde). The APS is a tool that can measure the neutron hydrogen index in water saturated formations.

  This measurement is corrected for environmental effect and normalized to limestone matrix. SLB refers to this corrected curve 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 an induced radiation tool that measures the bulk density of the formation and the photoelectric factor (PEF). It uses a radioactive source to emit gamma photons into the formation. The gamma rays undergo Compton scattering by interacting with the atomic electrons in the formation. Compton scattering reduces the energy of the gamma rays in a stepwise manner and scatters the gamma rays in all directions. When the energy of the gamma rays is less than 0.5 MeV, they can undergo photoelectric absorption by interacting with the electrons. The flux of gamma rays that reaches each of the detectors of the TLD is therefore attenuated by the formation, and the amount of attenuation is dependent upon the electronic density of the formation, which is related to its bulk density. In addition, the TLD provides the **photoelectric absorption index** (photoelectric factor – PEF), which represents the probability that a gamma photon will be photo-electrically absorbed per electron of the atoms that compose the material. The PEF characterises the mineralogy. The TLD tool is housed in the High-Resolution Mechanical Sonde that also includes the Micro-Cylindrically Focused Log (MCFL) sonde, that measures the micro-resistivity or alternatively, the resistivity very close to the borehole wall (RXOZ).
- **Element Spectroscopy** (ECS – Elemental Capture Spectroscopy). The ECS is also an induced radiation tool with a radioactive neutron source. The ECS measures the concentration of a series of elements in the formation by analyzing the spectrum of back scattered gamma rays. The following elements are used in this report: DWSI_WALK2 (Si), DWCA_WALK2 (Ca), DWFE_WALK2 (Fe), DWSU_WALK2 (S), DWTI_WALK2 (Ti). Special processing techniques allow under certain circumstances the measurement of supplementary elements

such as Mg (MGWALK closure model, DWMG _MGWALK curve); Al, K and Na (ALKNA closure model, with ALKNA suffix). The element spectroscopy measurements are provided in weight concentration.

During the QC process of the ECS acquisition, the DWMG_MGWALK response could be validated in the pure dolomites, reading close to the theoretical endpoint for dolomites: 0.132 W/W.

The iron concentration from the ECS WALK2 model was found systematically overestimating the XRF measurements on core samples. A correction was performed founded on the ECS and XRF results in MAR1-1 (see Section 2.3). The resulting iron concentration curve was called DWFE_CORR.

- **Resistivity** (HRLT – High Resolution Laterolog array Tool). The HRLT measures the formation electrical resistivities at different depths of investigation, providing a mud filtrate invasion profile, if any invasion. Processing allows the extrapolation of the resistivity measurements far into the formation (true formation resistivity), as well as close to the borehole wall (micro-resistivity). The resistivity is a function of the water content of the formation and its salinity.
- **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 BOZ2-1 borehole is given in Plate 1.

Usable log data were available for analysis from 102.8 to 713.0 m (see Plate 1). Due to gaps between drilling sections and cased hole sections (see Dossier I), two minor MultiMin interpretation gaps, due to insufficient petrophysical logs coverage, remained in the following intervals, as shown in Fig. 2-1:

- 367.9 – 370.1 m (between sections I and II)
- 613.4 – 614.4 m (between sections II and III)

In the upper interval (0 – 102.8 m drillers depth), only technical logging was performed which is not suitable for the log interpretation routines used here. The wireline logging in Chapter 3, below 615 m, was not sufficient for a detailed MultiMin analysis (no APS-TLD-ECS); the Multi Sensor Core Logger (MSCL) data were included in the input data.

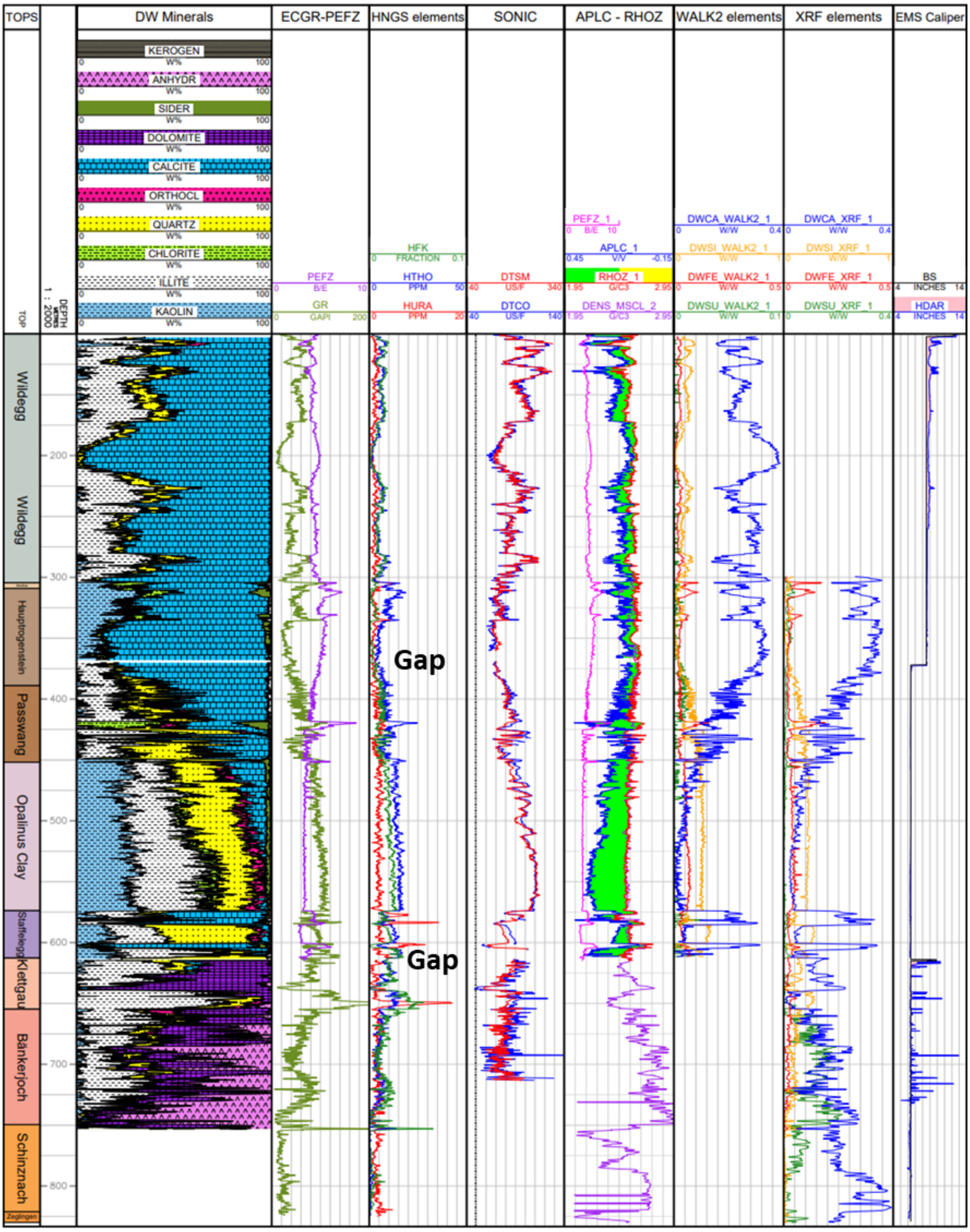

Fig. 2-1: Petrophysical log availability and gaps in the BOZ2-1 borehole

Please note that ECS elements are displayed as measured (in weight/weight, 0 – 1 w/w range) and are not converted to wt.-% (weight percentage) here.

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 (lab measurements of mineralogy, total 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). 62 core samples collected at depth ranging from 263.28 to 659.95 m were available, all were also analysed for total porosity (pycnometer, water-loss total porosity), 56 for XRD mineralogy and 7 for clay types. The analysed minerals were quartz, K-feldspars, plagioclase, calcite, dolomite/ankerite, siderite, magnesite, anhydrite, celestite, pyrite, clay minerals and organic carbon. The 7 samples analysed for clay typing (in the interval 443.71 – 597.83 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, the most relevant was selected compared to the MultiMin total porosity (PHIT 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. The shift ranges from 0.17 to 0.55 m in sections I and II, and is up to 1.35 m in section III. This shift was applied to the core data for an appropriate calibration.

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

2.3 Multi-sensor Core Logger (MSCL) data

MSCL measurements from cores were available for parts of the BOZ2-1 borehole (from 298.13 to 829.09 m). 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 a gap. In this same interval, no XRF data is available to fill the gaps.

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 (usually 0.05 m). This comparison is shown in Fig. 2.2 for BOZ2-1.

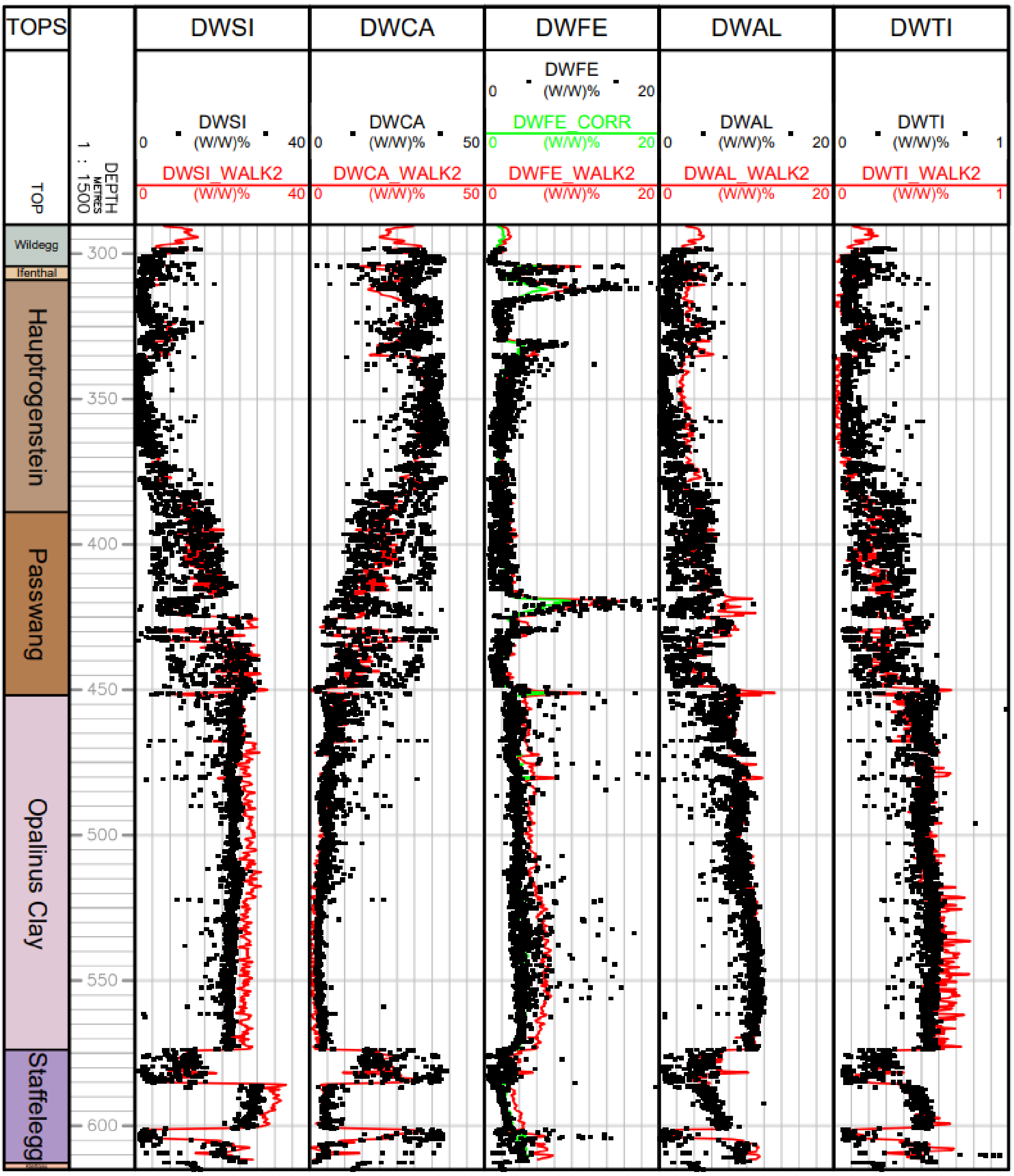

Fig. 2-2: XRF (black dots) and ECS WALK2 (red curves) elements comparison

While the calcium, aluminium and titanium concentrations are almost similar, the XRF iron and silicon are lower than ECS WALK2 closure model. The silicon content was not corrected, the minerals endpoints were adjusted accordingly.

The same bias on the iron content was already noticed in the recent MAR1-1 borehole, a correction was used based on the correlation between XRF iron and ECS DWFE_WALK2, using the following equation:

$$DWFE\_CORR = 0.0375+0.396*DWFE\_WALK2+4.882*DWFE\_WALK2^2$$

The DWFE_CORR curve was also plotted in Fig. 2-2 (green curve in the iron track), it is close to the XRF iron measurements in BOZ2-1. It was preferred to use the same amount of correction already performed in the recent boreholes.

The same check was done for the core and HNGS spectral gamma ray (see Fig. 2-3) in BOZ2-1.

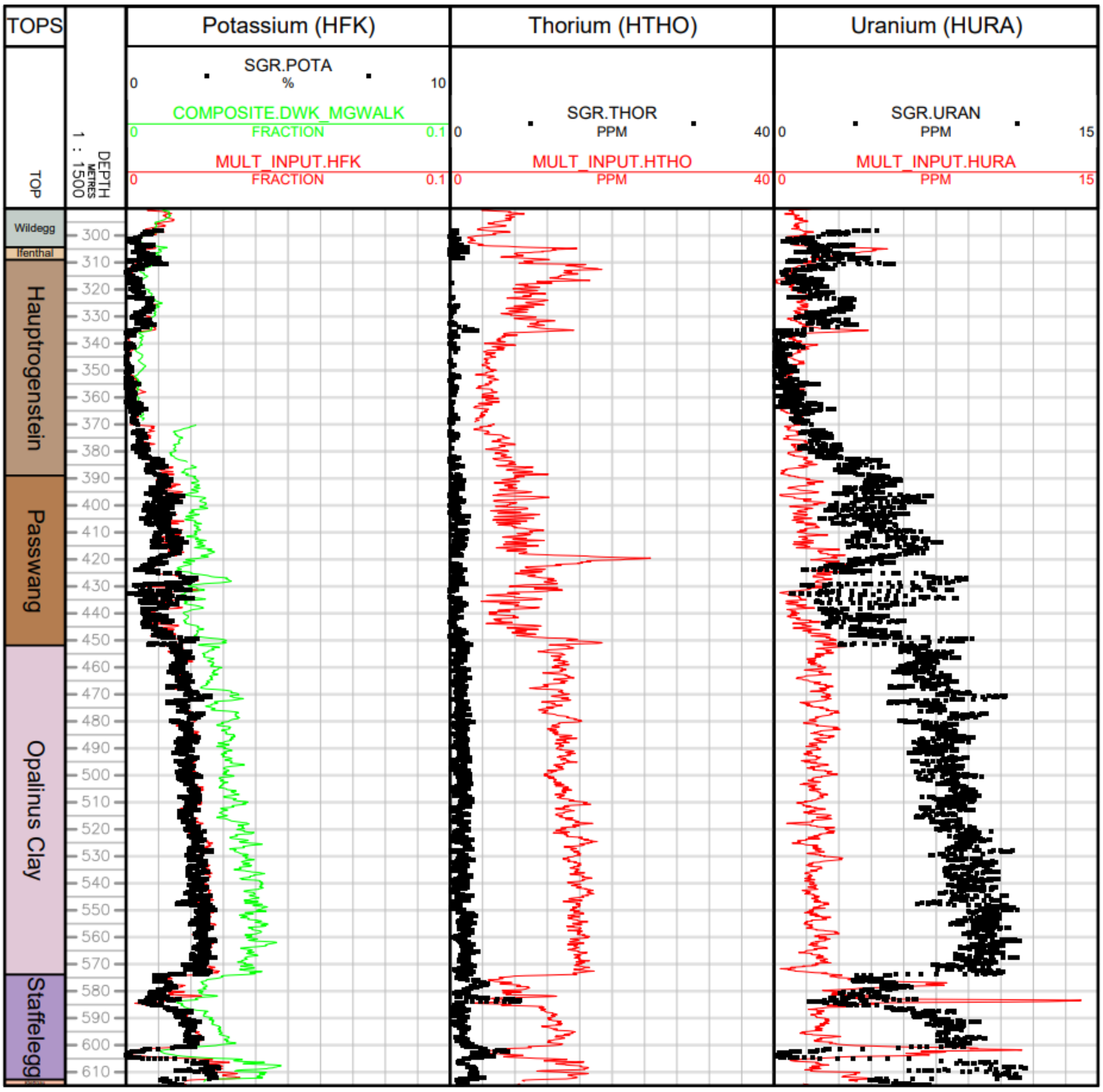

Fig. 2-3: Core (black dots: spectral gamma ray) and wireline HNGS (red curves) spectral gamma ray elements comparison

The potassium from MSCL is almost similar to HFK from HNGS (Fig. 2-3). Both MSCL uranium and thorium are inconsistent with HNGS curves. The potassium track shows in addition the DWK_MGWALK (green curve), potassium content from the ECS tool. It is well correlated to HFK but requires a correction to replace HFK where missing, usually at sections bottom. The HTHO from HNGS is often much higher than the thorium content measured with the MSCL. Hence, the MSCL data was used indirectly for a QC and subsequently to correct petrophysical log measurements, namely the iron content of the ECS measurements.

The MSCL logs (Bulk density, XRF elements) were used in the Keuper to replace the missing wireline logs (TLD, ECS).

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, two 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.

The ECS corrected iron content (DWFE_CORR) was used instead of DWFE_WALK2.

The wireline logging in section III, below 615 m, was not sufficient for a detailed MultiMin analysis (no APS-TLD-ECS); the MSCL data were included as input data. The MSCL data were upscaled to the wireline logs scale using a convolution product (see Section 3.1).

In the porous dolomites of the Schinznach Formation, the MSCL XRF sulphur concentration is up to 9.6 wt.-%, i.e. not compatible with the lab XRD anhydrite content, up to 6.5 wt.-%, most likely due to erroneous MSCL measurements. Therefore, no MultiMin analysis was performed below 753 m in BOZ2-1.

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 Tab. 2-1 and Appendix A.

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

Tab. 2-1: Precalc parameters used in BOZ2-1

Location	Mode	Comment	Unit	Name	100-368 m	368-615 m	615-829 m
Interval	In_Out	Option for formation temperature	ALPHA*8	OPT_FT	SONDE	SONDE	SONDE
Interval	In_Out	Option for reference	ALPHA*8	OPT_REF	DEPTH	DEPTH	DEPTH
Interval	In_Out	Option for resistivity mudcake calc	ALPHA*8	OPT_HMC_RES	SRT	SRT	SRT
Interval	In_Out	Option for salinity calculation	ALPHA*16	OPT_SAL	BATEMAN_KONEN	BATEMAN_KONEN	BATEMAN_KONEN
Interval	In_Out	Option for form'n/hydro pressure	ALPHA*8	OPT_FP	MUD_DENS	MUD_DENS	MUD_DENS
Interval	In_Out	Base of drilling mud	ALPHA*8	MUDBASE	WATER	WATER	WATER
Interval	In_Out	Drilling fluid density	LB/G	DFD	8.76	10.01	8.76
Interval	In_Out	Resistivity of mud sample	OHMM	RMS	1.23	0.16	3.14
Interval	In_Out	Mud sample temperature	DEGC	MST	17.3	13.7	10.1
Interval	In_Out	Resistivity of filtrate sample	OHMM	RMFS	1.16	0.12	2.71
Interval	In_Out	Mud filtrate sample temperature	DEGC	MFST	17.1	14.4	9.7
Interval	In_Out	Resistivity of mudcake sample	OHMM	RMCS	1.31	0.24	3.36
Interval	In_Out	Mudcake sample temperature	DEGC	MCST	17.2	13.2	10.2
Interval	In_Out	Drilling bit size	IN	BS	8.5	6.375	6.375
Interval	Output	Salinity of mud	PPM	SALM	PHASES.SALM	PHASES.SALM	PHASES.SALM
Interval	Output	Salinity of mud filtrate	PPM	SALMF	PHASES.SALMF	PHASES.SALMF	PHASES.SALMF
Log	Input	Depth	METRES	DEPTH	DEPTH	DEPTH	DEPTH
Log	Input	Mud temperature from sonde	DEGF	MTEM	FTEMP	FTEMP	FTEMP
Log	Input	Caliper from nuclear/porosity	IN	CALI_POR	HDAR	HDAR	HDAR
Log	Input	Caliper from resistivity/sonic	IN	CALI_RES	HDAR	HDAR	HDAR
Log	Input	Density log	G/C3	RHO	RHOZ	RHOZ	RHOZ
Log	Input	Photo-electric factor	B/E	PEF	PEFZ	PEFZ	PEFZ
Log	Input	True formation resistivity	OHMM	RT	RT_HRLT	RT_HRLT	RT_HRLT
Log	Input	Flushed zone resistivity	OHMM	RXO	RXOZ	RXOZ	RXOZ
Log	Output	Formation temperature	DEGF	FTEMP	FTEMP	FTEMP	FTEMP
Log	Output	Formation/hydrostatic pressure	PSI	FPRESS	FPRESS	FPRESS	FPRESS
Log	Output	Mud resistivity	OHMM	RM	RM	RM	RM
Log	Output	Mud filtrate resistivity	OHMM	RMF	RMF	RMF	RMF
Log	Output	Mudcake resistivity	OHMM	RMC	RMC	RMC	RMC
Log	Output	Mudcake from nuclear/porosity	IN	HMC_POR	HMC_POR	HMC_POR	HMC_POR
Log	Output	Mudcake from resistivity/sonic	IN	HMC_RES	HMC_RES	HMC_RES	HMC_RES
Log	Output	Photo-electric cross-section	B/C3	U	U	U	U
Log	Output	True formation conductivity	MH/M	CT	CT	CT	CT
Log	Output	Flushed zone conductivity	MH/M	CXO	CXO	CXO	CXO

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 2021). Many qualitatively good wireline logs were available down to the lower part 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 Bülach-1-1 and Trüllikon-1-1, Marthalen-1-1 etc. (see Dossier VIII of the respective borehole reports), 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
- 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_CORR values. Note that the problem would be even worse with the raw DWFE_WALK2 curve.
- 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 2021 for more details).

Tab. 3-1 shows the interpretation intervals, the available data and the MultiMin model names used in each interval. The intervals are defined based on their consistent 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 Appendix B.

Tab. 3-1: List of MultiMin models used in BOZ2-1

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 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/Comments
102.8	108.0	INT1_TOP	boz21_int1_top	4.38	Malm
108.0	109.8	INT1_TOP	boz21_int1_top_no_dts	4.36	Missing DTSM
109.8	304.2	INT1_TOP	boz21_int1_top	4.38	Malm
304.2	359.8	INT1_TOP	boz21_int1_top_bd	4.61	Brauner Dogger
359.8	365.9	INT1_TOP	boz21_int1_top_bd_no_dt	4.61	Missing Sonic
365.9	367.9	INT1_TOP	boz21_int1_top_bd_no_aps	4.14	Reduced logs dataset
367.9	370.1		No model		Not enough logs
370.1	372.5	INT1_BOT	boz21_int1_bot_no_ct	4.49	Missing CT
372.5	423.6	INT1_BOT	boz21_int1_bot	4.49	Brauner Dogger
423.6	424.1	INT1_BOT	boz21_int1_bot_no_ct	4.49	Missing CT
424.1	432.0	INT1_BOT	boz21_int1_bot	4.49	Brauner Dogger
432.0	432.4	INT1_BOT	boz21_int1_bot_no_ct	4.49	Missing CT
432.4	435.2	INT1_BOT	boz21_int1_bot	4.49	Brauner Dogger
435.2	435.6	INT1_BOT	boz21_int1_bot_no_ct	4.49	Missing CT
435.6	438.0	INT1_BOT	boz21_int1_bot	4.49	Brauner Dogger
438.0	438.3	INT1_BOT	boz21_int1_bot_no_ct	4.49	Missing CT
438.3	449.0	INT1_BOT	boz21_int1_bot	4.49	Brauner Dogger
449.0	579.4	INT2	boz21_int2	3.54	Opalinus and Staffelegg
579.4	580.0	INT2	boz21_int2_no_dt	3.54	Missing DTSM
580.0	581.7	INT2	boz21_int2	3.54	Opalinus and Staffelegg
581.7	582.0	INT2	boz21_int2_no_dt	3.54	Missing DTCO
582.0	585.4	INT2	boz21_int2	3.54	Opalinus and Staffelegg
585.4	601.0	INT3	boz21_int3	4.12	Staffelegg
601.0	601.4	INT3	boz21_int3_no_dt	3.58	Missing DTCO
601.4	603.9	INT3	boz21_int3	4.12	Staffelegg
603.9	605.1	INT3	boz21_int3_no_dt	3.58	Missing DTCO
605.1	605.6	INT3	boz21_int3	4.12	Staffelegg
605.6	611.5	INT3	boz21_int3_no_dt	3.58	Missing Sonic
611.5	613.4	INT3	boz21_int3_sta_base	2.53	Staffelegg
613.4	614.4		No model		Not enough logs

Tab. 3-1: (continued)

From (m)	To (m)	Interval name	Multimin Models	Cond Num	Description/Comments
614.4	614.9	INT3	boz21_int3_sta_base	**2.53**	Staffelegg
614.9	618.1	INT4_Top	boz21_int4_xrf	**3.28**	Using MSCL core data
618.1	618.9	INT4_Top	boz21_int4_xrf_nodens	**2.67**	Using MSCL core data
618.9	645.0	INT4_Top	boz21_int4_xrf	**3.28**	Using MSCL core data
645.0	646.1	INT4_Top	boz21_int4_xr_nodt	**3.33**	Using MSCL core data
646.1	671.0	INT4_Top	boz21_int4_xrf	**3.28**	Using MSCL core data
671.0	672.0	INT4_Top	boz21_int4_xr_nodt	**3.33**	Using MSCL core data
672.0	691.8	INT4_Top	boz21_int4_xrf	**3.28**	Using MSCL core data
691.8	693.1	INT4_Top	boz21_int4_xr_nodt	**3.33**	Using MSCL core data
693.1	711.4	INT4_Top	boz21_int4_xrf	**3.28**	Using MSCL core data
711.4	711.8	INT4_Top	boz21_int4_xr_nodt	**3.33**	Using MSCL core data
711.8	713.0	INT4_Top	boz21_int4_xrf	**3.28**	Using MSCL core data
713.0	721.3	INT4_Bot	boz21_int4_bot	**3.49**	Using MSCL core data
721.3	722.5	INT4_Bot	boz21_int4_nomg	**3.82**	Using MSCL core data
722.5	753.0	INT4_Bot	boz21_int4_bot	**3.49**	Using MSCL core data
753.0	830.0		No model		Not enough logs

Given the complexity of the MultiMin models applied to the BOZ2-1 wireline logging data, an inverse linear modelling of the MultiMin endpoints could not be attempted in BOZ2-1. 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 (2021).

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 2021). High uncertainty values often apply to the Sonic curves, the PEFZ (as PEFZ is already used for the U computation, Photo-electric cross-section) and the electrical conductivities.

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

Below 614.9 m, only a limited wireline log suite could be acquired (HNGS, HRLT and MSIP down to 713.0 m), limiting the ability to run a comprehensive MultiMin analysis. It was therefore decided to add the MSCL data measured on cores, i.e. the XRF elements and the bulk density, to the wireline dataset.

The MSCL data are discrete data acquired at a very short sampling rate, usually five centimetres.

The following curves were used:

Bulk density (Dens, g/cc)

- XRF elements in mass content: silicium, calcium, magnesium, iron, aluminium, sulphur, titanium, potassium
- Spectral gamma ray elements: potassium and thorium

The MSCL data were rescaled to the wireline log scale, i.e. a continuous logging with a longer vertical resolution.

The following steps were followed to generate the MSCL log dataset:

1. Depth shift of the MSCL dataset using the Core to FMI depth shift table
2. Interpolation of the MSCL data to a continuous log set with a regular sampling rate of five centimetres.
3. Use of the «Fill-Missing» tool in Geolog which linearly interpolates between the small gaps. The maximum fill parameter was set to ten samples.
4. Applying a convolution to all the curves with the following triangular operator:

   0 1 2 3 4 5 4 3 2 1 0
5. The remaining gaps were manually filled where high resolution data showed a clear continuity. Otherwise, they were kept unchanged.
6. The XRF elements were used directly as an input in the MultiMin models, the curves were not calibrated to the ECS elements.
7. The spectral gamma ray curves consistency with their equivalent HNGS logs was checked where both datasets were available (see here after)

The following correction was applied to the MSCL potassium (Fig. 3-1):

HFK (%) = 1.06043 * MSCL potassium

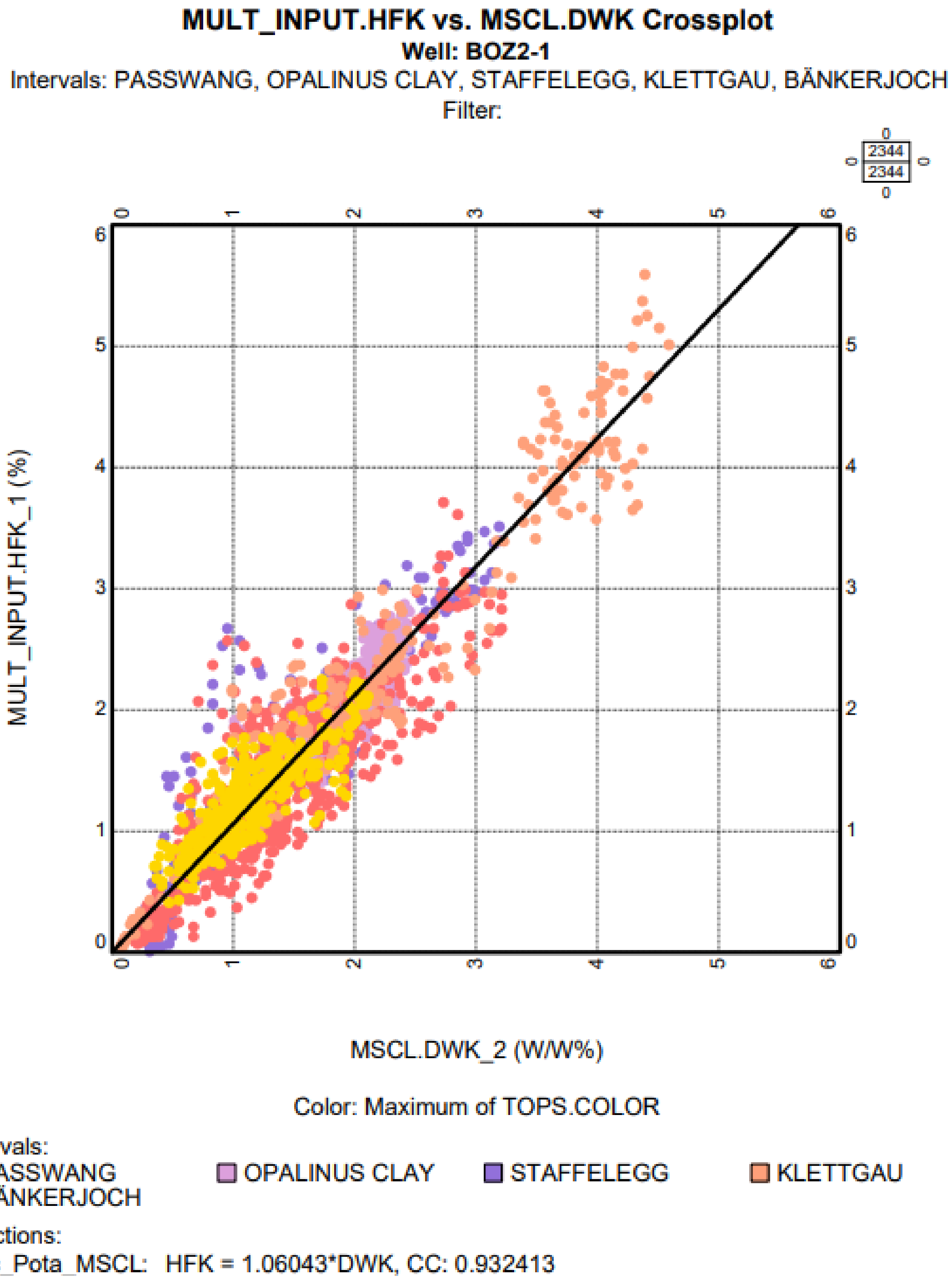

Fig. 3-1: HNGS potassium (HFK) versus MSCL potassium in BOZ2-1

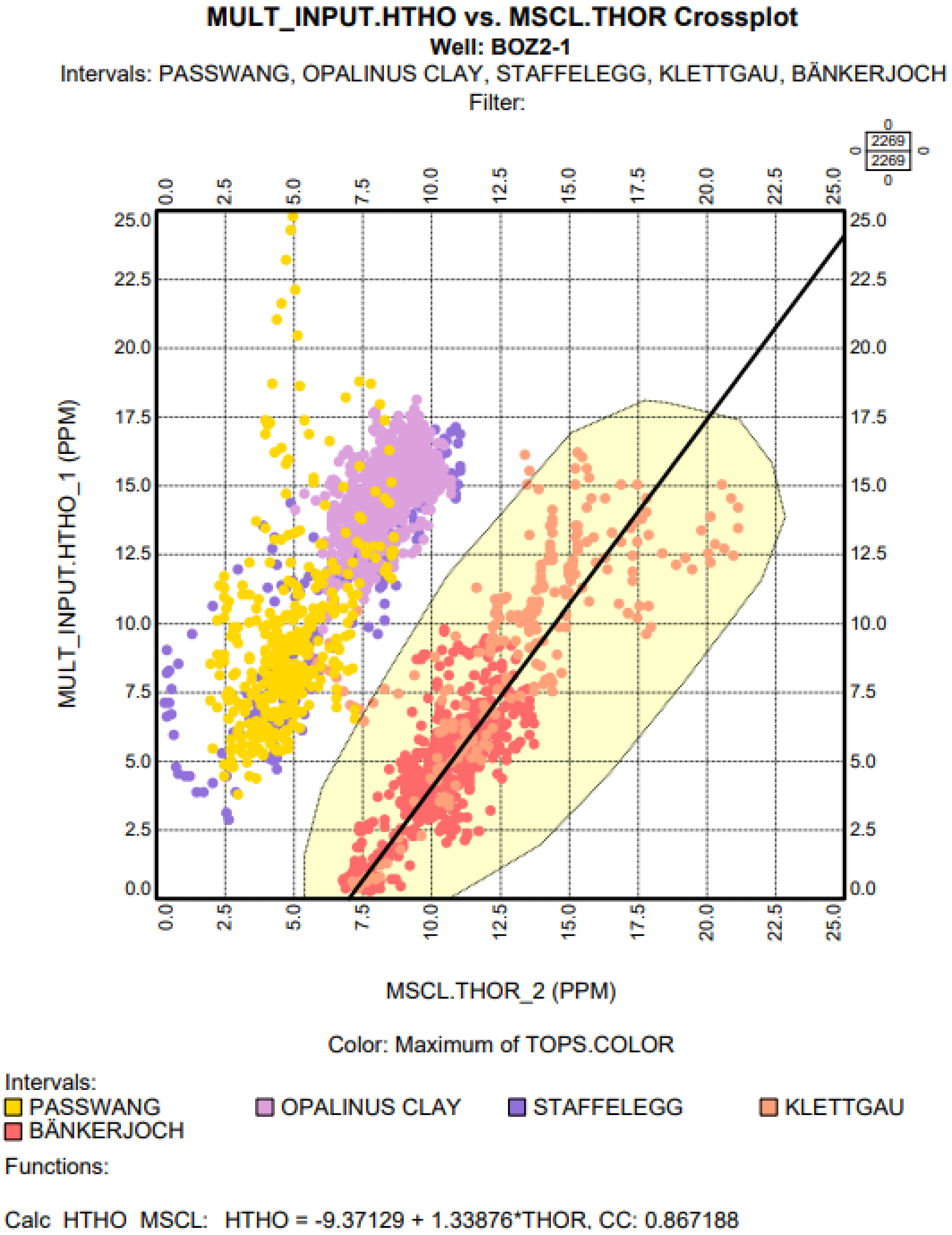

Fig. 3-2: HNGS thorium (HTHO) versus MSCL thorium in BOZ2-1

Two trends are visible in Fig. 3-2, one for the Dogger and Lias, and one for the Triassic. The latter was selected by the yellow polygon and used for the thorium content calibration in the Triassic (as for Lias and Dogger sufficient coverage of wireline logs was available):

$$\text{HTHO (ppm)} = 1.33876 * \text{MSCL Thorium} - 9.37129$$

The MSCL bulk density calibration to the TLD RHOZ curve was also checked (Fig. 3-3).

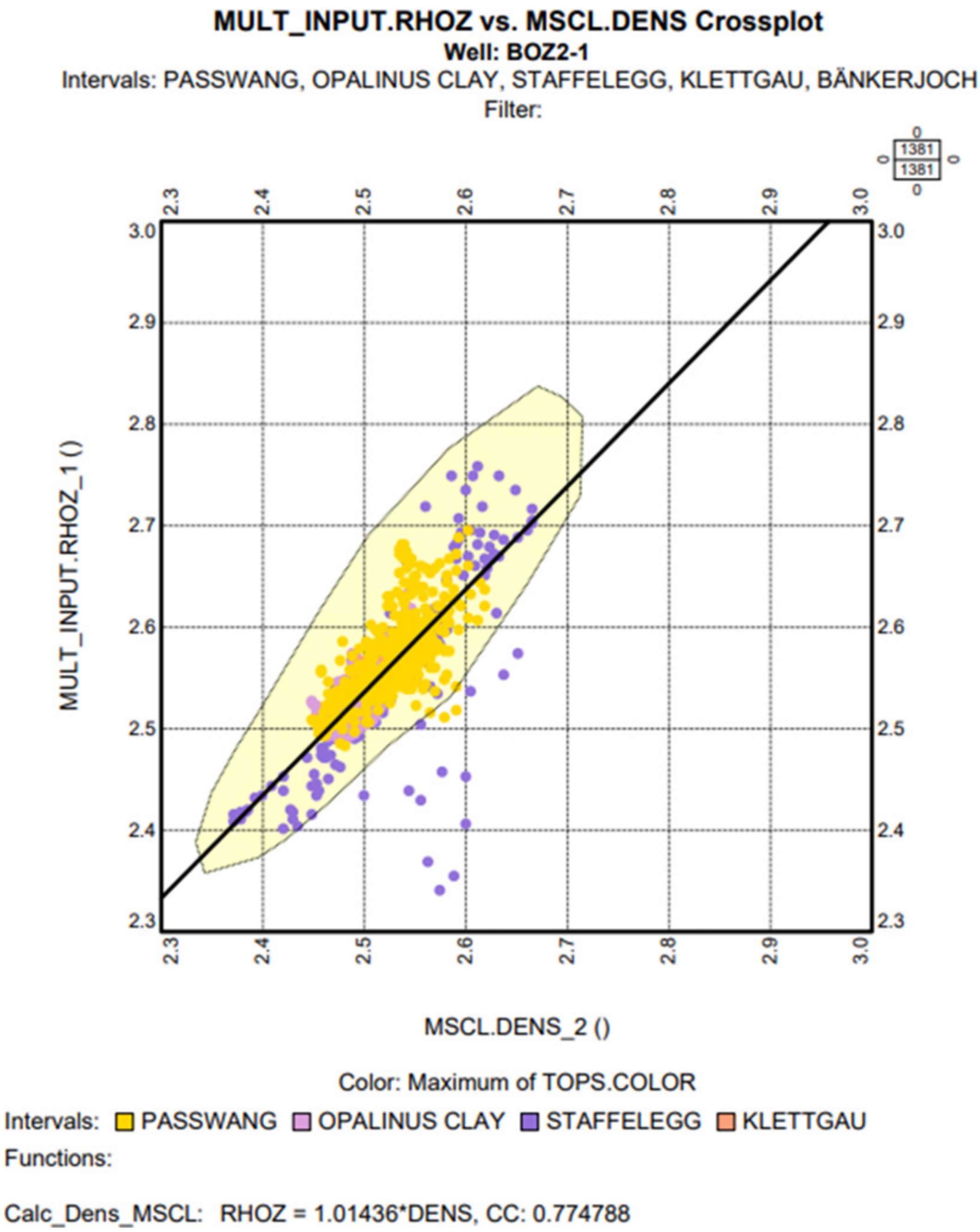

Fig. 3-3: TLD bulk density (RHOZ) versus MSCL bulk density in BOZ2-1

The following correction was applied to the MSCL density, determined using a linear regression in points selected by the yellow polygon, hence excluding a few outliers.:

RHOZ (g/cc) = 1.01436 * MSCL bulk density

Although this correlation is acceptable, the resulting bulk density in front of the Schinznach Formation is down to dubiously low values in mostly dolomitic rocks, close to 2.05 g/cc.

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)

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.

Four bad hole indicators, which can be used as a quality measure of the data, are calculated from some of the available wireline logs:

1. FLAG_UNFIT_ND: Neutron-Density crossplot, flagging bad hole and unusual mineralogical settings from expert picking in the density-neutron crossplot
2. FLAG_BADHOLE_OVERGAUGE: HDAR > 1.15 * Bit Size
3. FLAG_BADHOLE_RUGO: Borehole wall rugosity, HDRA > 0.025 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. FLAG_BADHOLE_STOF: APS Neutron standoff>0.35in

For detailed information about these four indicators, please refer to Dossier VI.

These four indicators have two possible values: 0 in good hole or 1 in bad hole. They were combined to generate a log quality control flag (LQC_INDEX) using the following equation:

LQC_INDEX = (FLAG_BADHOLE_DN + FLAG_BADHOLE_OVERGAUGE +

FLAG_BADHOLE_RUGO + FLAG_BADHOLE_STOF) / 4

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).

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 BOZ2-1 (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:

- Highly suspicious porosity spikes occur and usually are correlated to an LQC-Index above or equal to 0.5, the quality curve (displayed in Plates 1 and 2, see below) can show 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 a usually 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 indictor 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_CLAY).
- Comparable to the clay minerals, different carbonate minerals were also calculated (calcite, dolomite and siderite). In Plate 2, a track displays the total amount of carbonates (called CARBONATES). Next to it, two tracks show the calcite and dolomite content, as the latter two can be used to distinguish between some formations, especially below the Opalinus Clay.
- Below 614.4 m, only matrix and clay minerals could be computed, as APS-TLD-ECS could not be acquired. This section corresponds to the Keuper to Muschelkalk.

Figs. 4-1 to 4-5 show crossplots between mineral weight percentages from cores (X axis, from XRD lab analyses) and interpretation results from MultiMin (Y axis).

Fig. 4-6 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 Wildegg to the Klettgau Formations (data in the Bänkerjoch Formation should be regarded as semi-quantitative only). The color coding represents the formations, as per the attached legend.

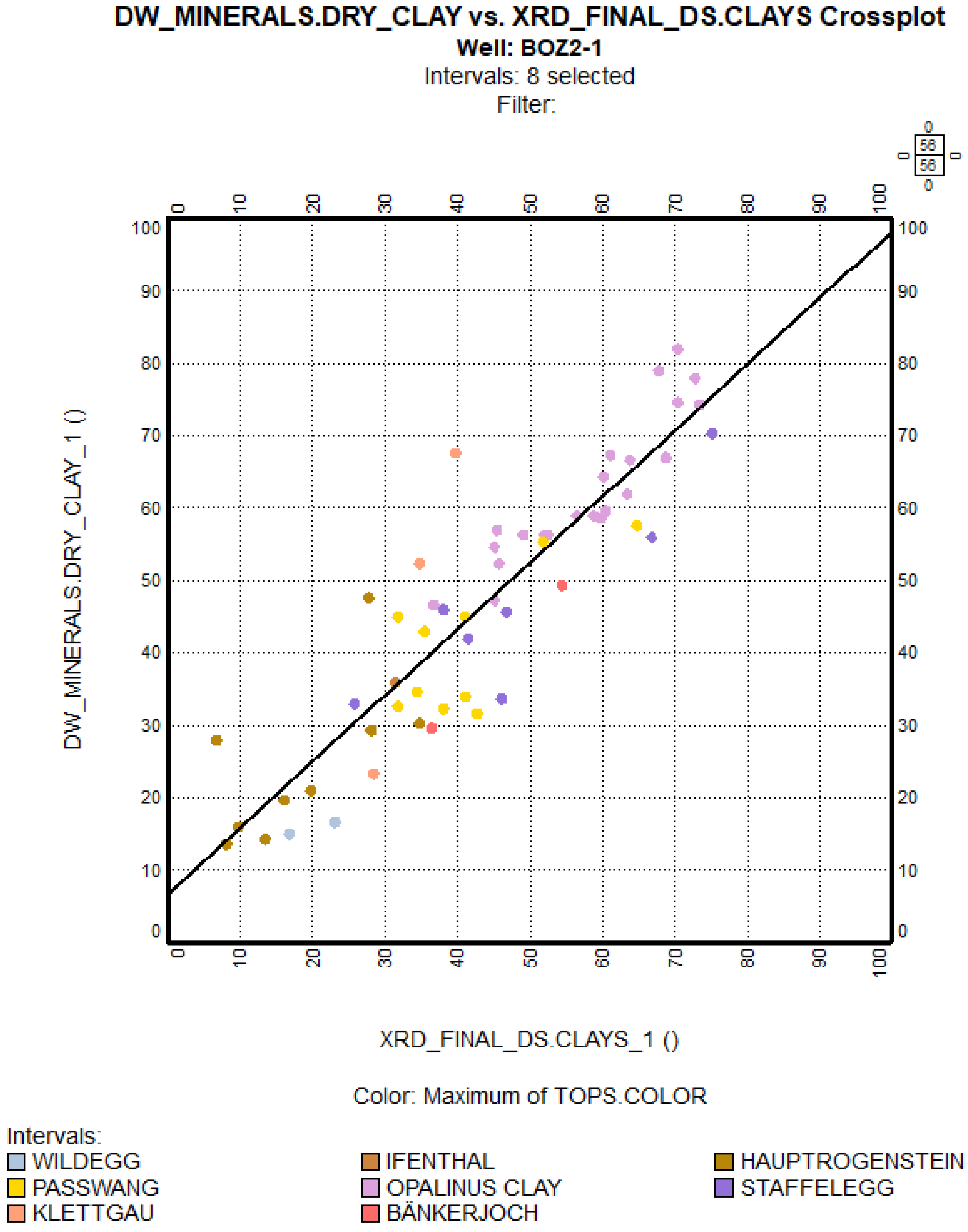

Fig. 4-1: Weight % of dry clay (y-axis) compared to core XRD data (x-axis), Wildegg to Bänkerjoch Formation

The MultiMin dry clay content is well correlated to the core XRD data (cc = 0.90).

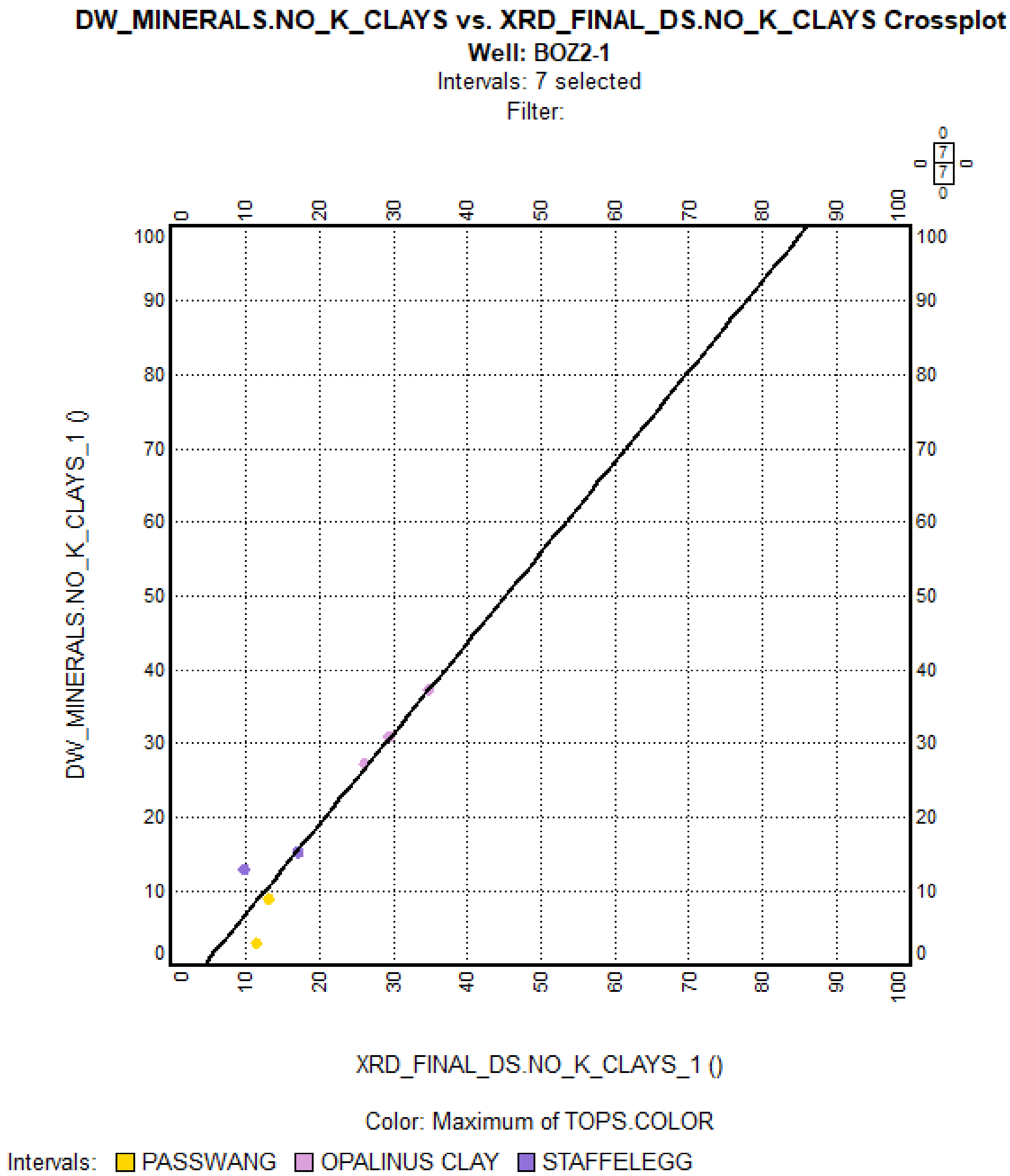

Fig. 4-2: Weight % of not potassic dry clay (y-axis) compared to core XRD data (x-axis) (XRD data in the Passwang to Staffelegg Formation)

The XRD clay endmembers were not measured in all formations, only 7 samples were analysed.

The MultiMin not potassic clay content is well correlated to the core XRD data (overall cc = 0.96), although not relevant with only seven samples.

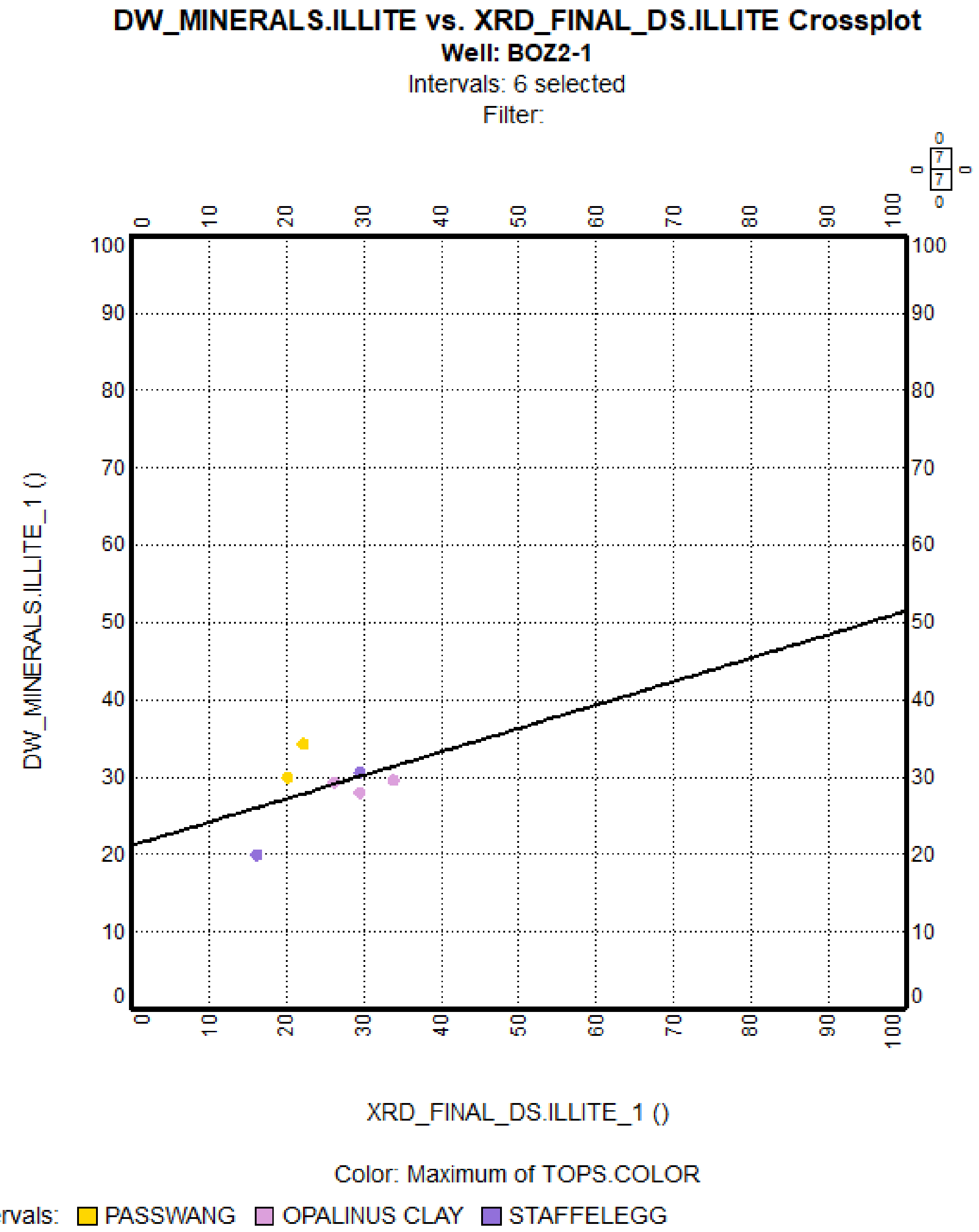

Fig. 4-3: Weight of illite (y axis) compared to core XRD data (x axis), XRD data in the Passwang to Staffelegg Formation)

The XRD clay endmembers were not measured in all formations.

The MultiMin illite content is close to the core XRD data but the correlation is not good due to the small number of core samples (cc = 0.46 with 7 samples).

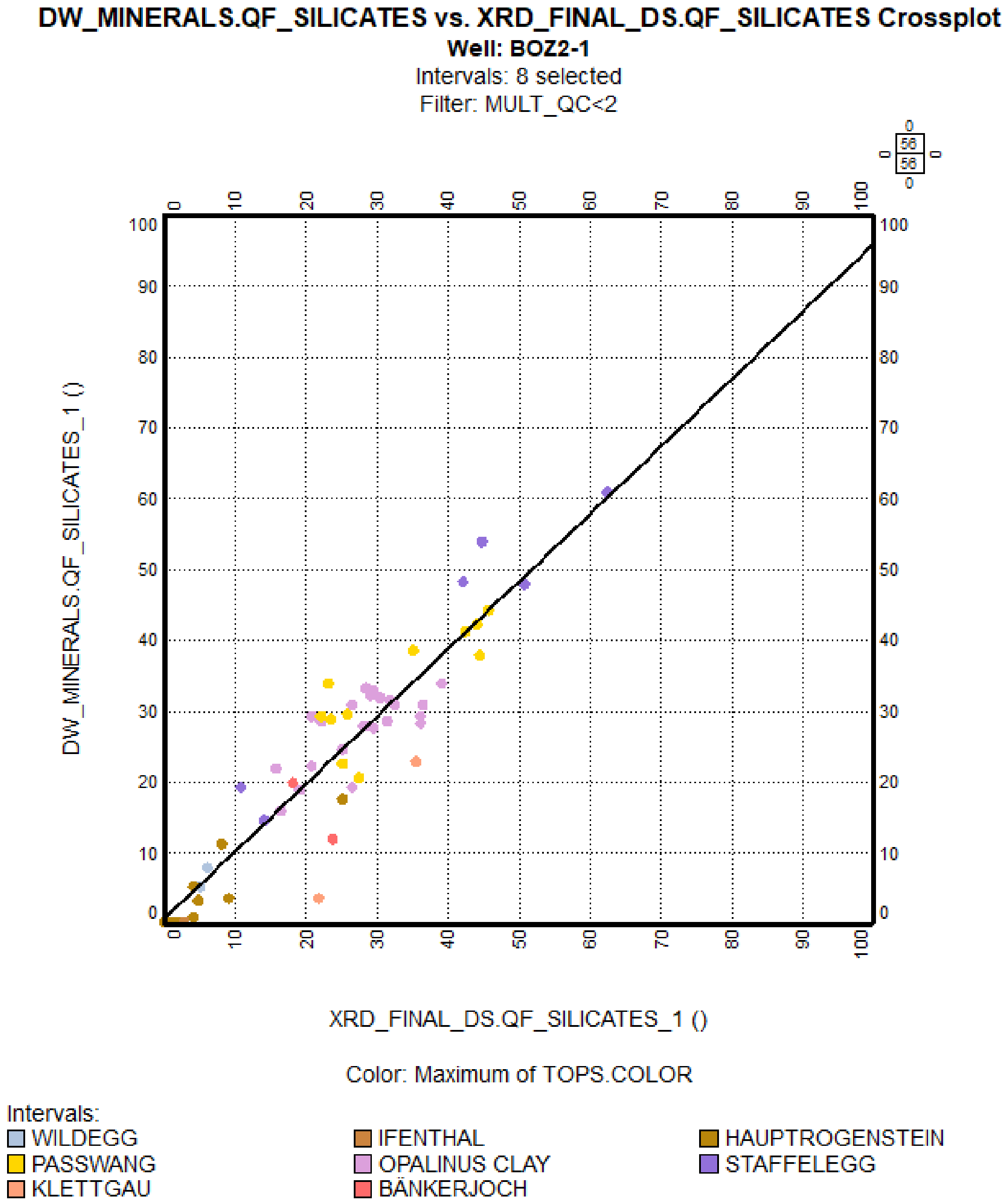

Fig. 4-4: Weight % of QF-silicates (y axis) compared to core XRD data (x axis), Wildegg to Bänkerjoch Formation

The QF-silicates are the sum of quartz and feldspars. The calibration to core XRD data is good (cc = 0.93).

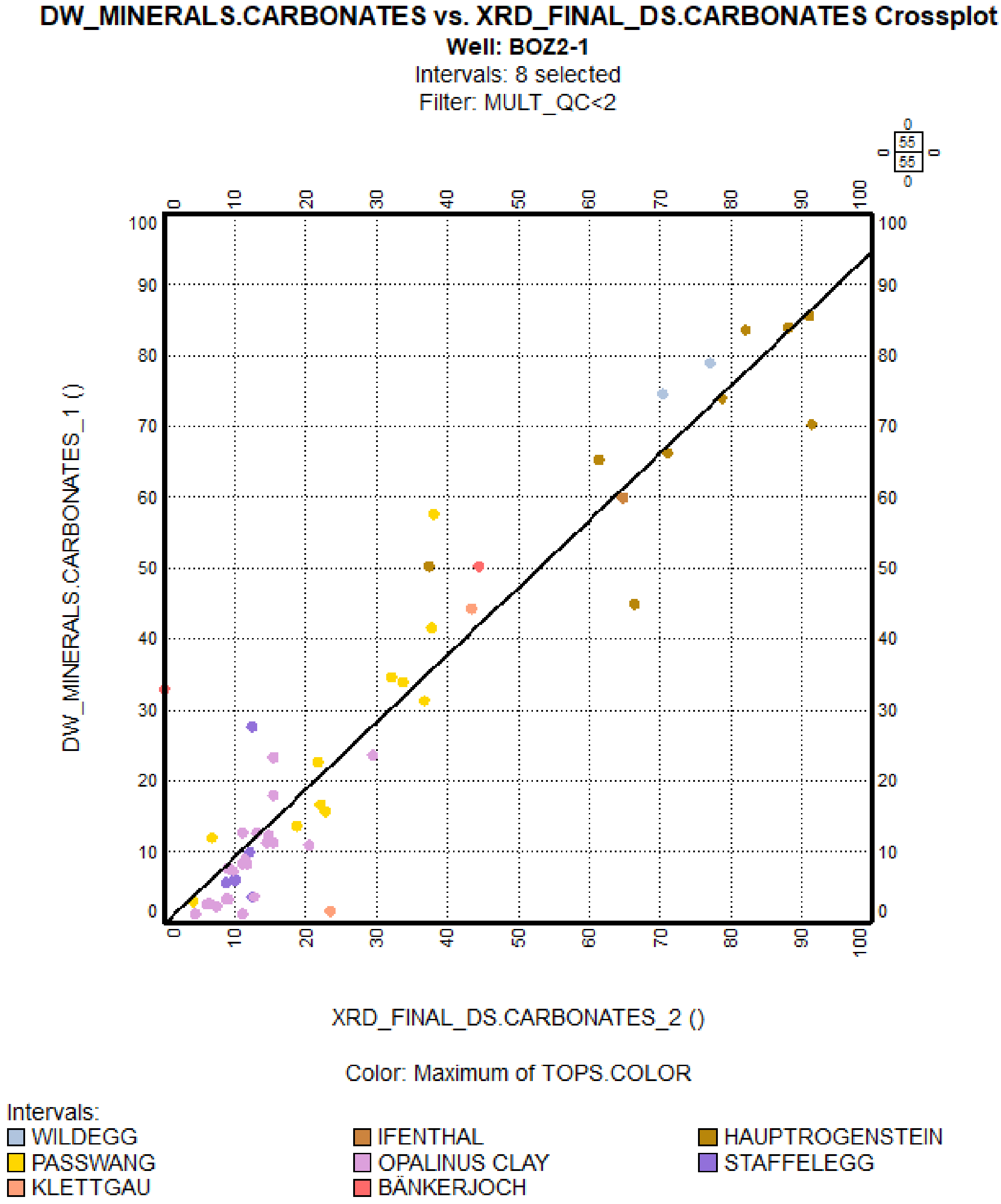

Fig. 4-5: Weight % of carbonates (y axis) compared to core XRD data (x axis), Wildegg to Bänkerjoch Formation

The carbonates include the calcite, dolomite and siderite content. The calibration to core XRD data is good (cc = 0.95).

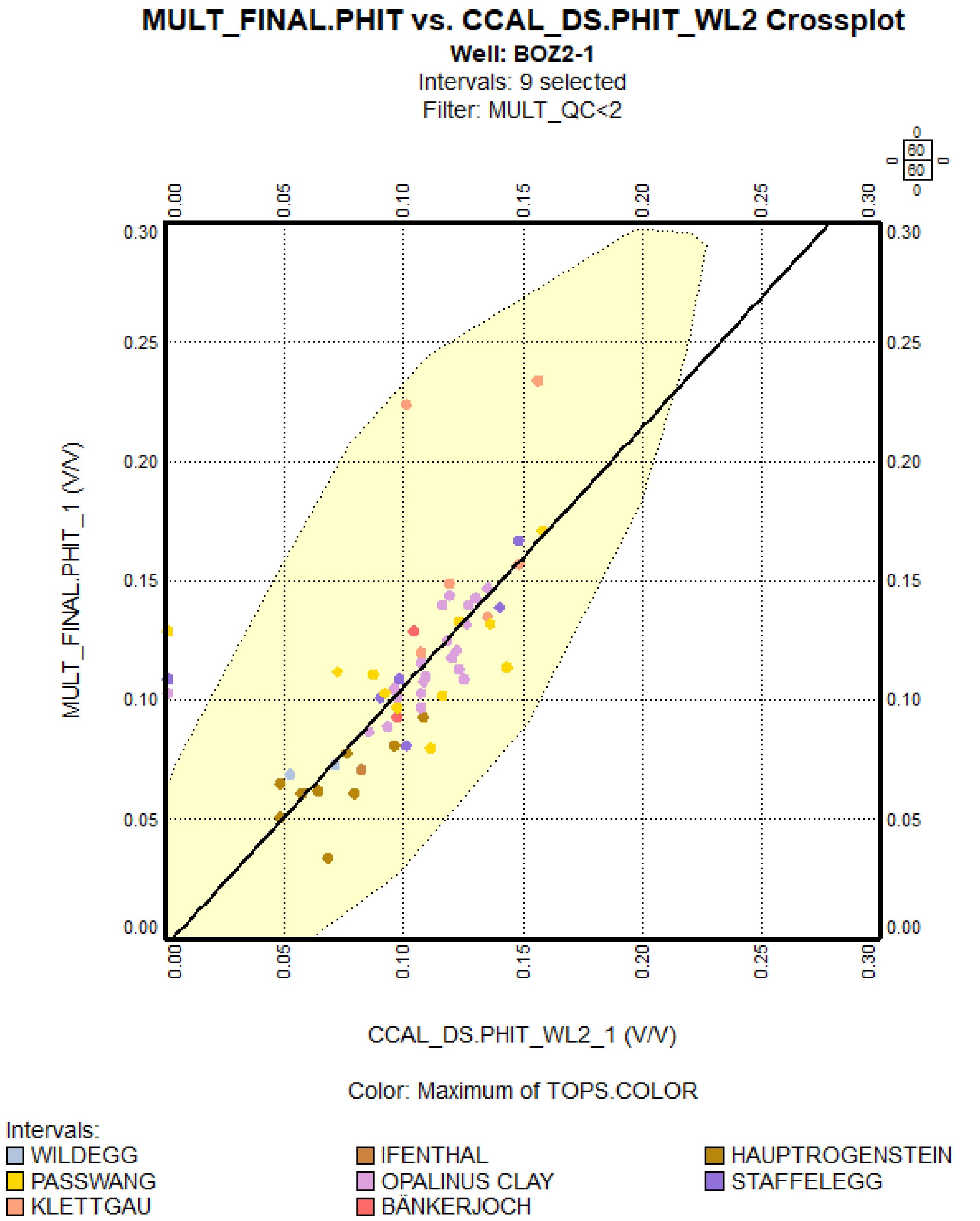

Fig. 4-6: Total porosity (v/v, y axis) compared to core data (x axis), Wildegg to Bänkerjoch Formation

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, core and log measurements are not fully equivalent as the logs evaluate in situ wet formations. Nevertheless, the correlation between MultiMin and lab porosity, is fair (cc = 0.77). Some dispersion can be noticed in the «Brauner Dogger», Hauptrogenstein Formation. The points inside the yellow polygon are used for the regression, excluding three data points in the Dogger showing inconsistent PHIT with zero values. The points outside near the y-axis are not well understood, with core PHIT close to 0%. Two data points in the Klettgau Formation are not well calibrated by the MultiMin model using MSCL data. The correlation is much better without these two points (cc = 0.87).

4.2 Main results of the core-calibrated log analyses in the BOZ2-1 borehole

The main aim of the MultiMin interpretation were continuous curves of porosity and clay content of BOZ2-1. 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, the clay content is used sensu lato meaning that the 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 (50.0 – 304.4 m, Wildegg Formation)

The first wireline logging data suitable for a MultiMin analysis start at 102.8 m. The top part of the Wildegg Formation (50 to 102.8 m) could therefore not be interpreted.

As expected, carbonates and clays are the main constituents in the Wildegg Formation. The mean dry clay content is 24.6 wt.-% (median of 25.0 wt.-%), while the mean calcite is 65.5 wt.-% (median 66.0 wt.%). The remaining is mostly quartz and feldspars, QF-silicate content is 8.9 wt.-% mean and 8.4 wt.-% median. The clays and matrix mineral proportions vary significantly in the Wildegg Fm., the clay content ranges from 0 to 51.1 wt.-%. The more clay-rich lithologies show a slightly increased QF-silicate content.

The carbonate content is dominated by calcite, as neither dolomite nor siderite was measured on core XRD.

Total porosity in the Wildegg Fm. ranges between 4.9 and 15.2% (mean of 9.3%, median of 9.0%), filtered by MULT_QC = 0.

Dogger (304.4 – 573.9 m, Ifenthal Formation, Hauptrogenstein, Passwang Formation, Opalinus Clay)

The boundary between the Malm and the Dogger is clearly marked by a sharp increase of the iron content (DWFE_CORR up to 7.2 wt.-%) and the clay content (characterised by a thorium peak).

The carbonate content in the Dogger is high in the Ifenthal Formation and the Hauptrogenstein, then decreases in the Passwang Formation and reaches low values at the base of the Opalinus Clay. The dry clays and QF-silicates increase accordingly and are highest in the lower third of the Opalinus Clay.

From the Ifenthal Formation to the Hauptrogenstein, the mean calcite content is 70.2 wt.-% (median 73.5 wt.-%), while the mean dry clay is 23.5 wt.-% (median 20.7 wt.-%) and the mean QF-silicates is 3.0 wt.-% (median 0.9 wt.-%).

In the Passwang Formation, the mean calcite content decreases to 37.5 wt.-% (median 37.6 wt.-%), while the mean dry clay content is 31.8 wt.-% (median 29.8 wt.-%) and the mean QF-silicate content is 27.4 wt.-% (median 25.0 wt.-%).

In the Opalinus Clay, the mean calcite content is down to 7.3 wt.-% (median 5.8 wt.-%), while the mean dry clay content is 62.4 wt.-% (median 62.4 wt.-%) and the mean QF-silicate content is 27.5 wt.-% (median 27.8 wt.-%). See more details in Section 4.3.

The Dogger carbonate content is dominated by calcite down to the middle of the Opalinus Clay and siderite (maximum 11.31 wt.-% on core XRD at 530.44 m) in the lower half of the Opalinus Clay. The mean siderite content is 1.9 wt.-% while the median is 1.6 wt.-%

When comparing the ECS iron content (corrected to XRF data, DWFE_CORR curve) with the XRD iron-rich minerals (siderite, pyrite) in the «Brauner Dogger», 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: iron oxides or hydroxides. This was modelled as iron oxide with MultiMin.

Total porosity of the Dogger also is contrasted between the different units. PHIT is not very variable in the Opalinus Clay (minimum / maximum 7.0 / 15.1%, mean 11.6% and median 11.5% with a low standard deviation 1.7%). PHIT is more variable in the overlying Dogger formations, strongly correlated with the clay content (clay bound water).

In the Passwang Formation, PHIT ranges from 3.4 to 17.4%, although this high value is dubious, related to high Fe content possibly poorly interpreted (with MULT-QC = 0). The mean PHIT is 9.6% and the median 9.3%.

In the Ifenthal Formation to the Hauptrogenstein, the mean porosity is 7.0% (median 6.8%), ranging from 3.1 to 11.8%.

Lias (573.9 – 612.8 m, Staffelegg Formation)

The formation boundary from the Opalinus Clay (Dogger) to the Staffelegg Formation (Lias) corresponds to 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 Gross Wolf Member down to Grünschholz and Beggingen Members have a relatively high carbonate content (calcite respectively mean/median 53.6 / 51.9 wt.-%, and 75.8 / 76.5 wt.-%), while the Frick and Schambelen Members have a significantly lower carbonate content (mean / median 5.2 / 4.6 wt.-% and 12.5 / 8.0 wt.-%). As in the previous groups, the carbonate content is dominated by calcite. As only a low dolomite content was measured from cores (maximum 3.19 wt.-% on XRD data), it was neglected in the MultiMin models. Although a significant sulphur content was measured by the ECS, no siderite and low pyrite (up to 4.6 wt.-%) content was measured from cores. MultiMin computed siderite from the excess iron, possibly in excessive amount.

The QF-silicate content shows the reverse of the carbonate content. While Gross Wolf down to Grünschholz and Beggingen Members show a relatively low QF-silicate content (respectively mean / median 10.3 / 9.4 wt.-% and 3.7 / 3.5 wt.-%), the Frick and Schambelen Members show higher QF-silicate contents (respectively mean / median 51.1 / 52.6 wt.-% and 23.5 / 20.0 wt.-%).

The clay content follows the same trend, moderate in the Gross Wolf down to Grünschholz and Beggingen Members (respectively mean / median 32.2 / 32.8 wt.-% and 11.4 / 11.5 wt.-%) and higher in the Frick and Schambelen Members (respectively mean / median 42.5 / 42.9 wt.-% and 62.1 / 61.0 wt.-%).

The Staffelegg formation is also characterised by high total organic carbon (TOC), not fully reconstructed by the MultiMin interpretation with the available wireline logs. The maximum TOC measured on cores was 2.68 wt.-% at 579.8 m. This miscalibration of the TOC most likely impacts the PHIT computation (overestimated in high-TOC intervals) and was flagged with the MULT_QC curve.

The total porosity in the Staffelegg Formation ranges between 0.1 and 24.1%, the highest values in the Rietheim Member possibly 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 18.3% in the Schambelen Member.

The mean / median PHIT in the Staffelegg Formation are 9.6 / 9.9% with MULT_QC = 0.

Keuper (612.8 – 749.52 m, Klettgau Formation, Bänkerjoch Formation):

As mentioned earlier in this Dossier, the MultiMin analysis was performed only in the Klettgau to Bänkerjoch Formations.

The Klettgau Formation is characterised by a high clay content (mean / median 47.7 / 49.0 wt.-%), a high carbonates content (mean / median 38.0 / 42.4 wt.-%) and a relatively low QF-silicate content (mean / median 12.8 / 9.9 wt.-%).

The Bänkerjoch Formation is less argillaceous (clays: mean / median 25.2 / 26.1 wt.-%), with a high carbonates content (mean / median 30.8 / 31.3 wt.-%) and high anhydrite (mean / median 34.8 / 32.6 wt.-%). The QF-silicate content is slightly lower, mean/median 9.1/8.7 wt.-%.

The total porosity is higher in the argillaceous Klettgau Formation (mean and median 14.8%) than in the anhydrite-rich Bänkerjoch Formation (mean / median 7.4 / 6.9%).

Muschelkalk (749.52 – 829.88 m, Schinznach Formation and Zeglingen Formation

Due to inconsistencies between MSCL and XRD data, this interval could not be evaluated, except from the top Schinznach Formation down to 753.3 m.

These few meters at top Schinznach Formation are porous dolomites, with PHIT up to 15.8%, just below the base Bänkerjoch Formation anhydrites.

4.3 Main results of the core-calibrated log analysis in the Opalinus Clay (451.9 – 573.89 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. 4-7 to 4-13 show some general statistical values of the MultiMin analysis results within the Opalinus Clay.

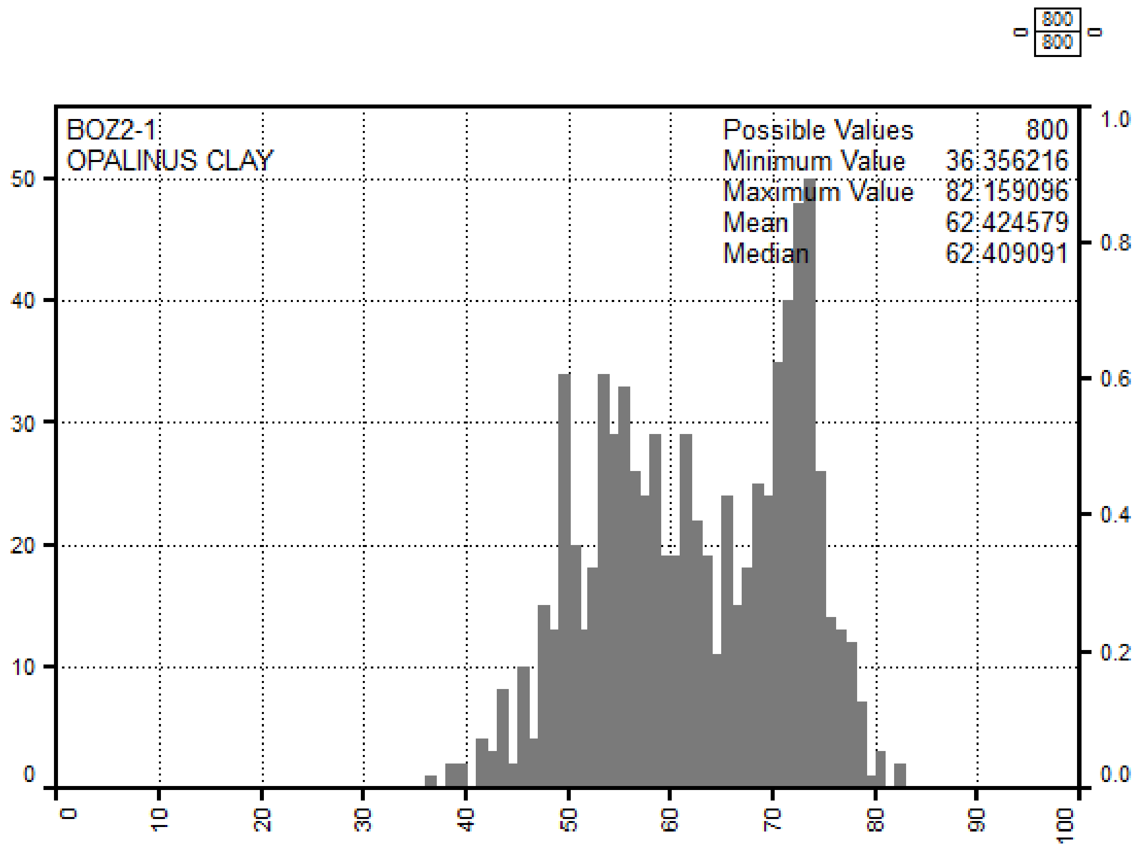

Fig. 4-7: Dry clay weight percentage frequency histogram in the Opalinus Clay

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 62.4 wt.-%. The distribution looks bimodal, with the lowest clay content in the shallowest part of the Opalinus Clay).

The two next frequency histograms (Figs. 4-8 and 4-9) show a split of the Opalinus Clay into an upper and lower part, showing that the latter is significantly more argillaceous.

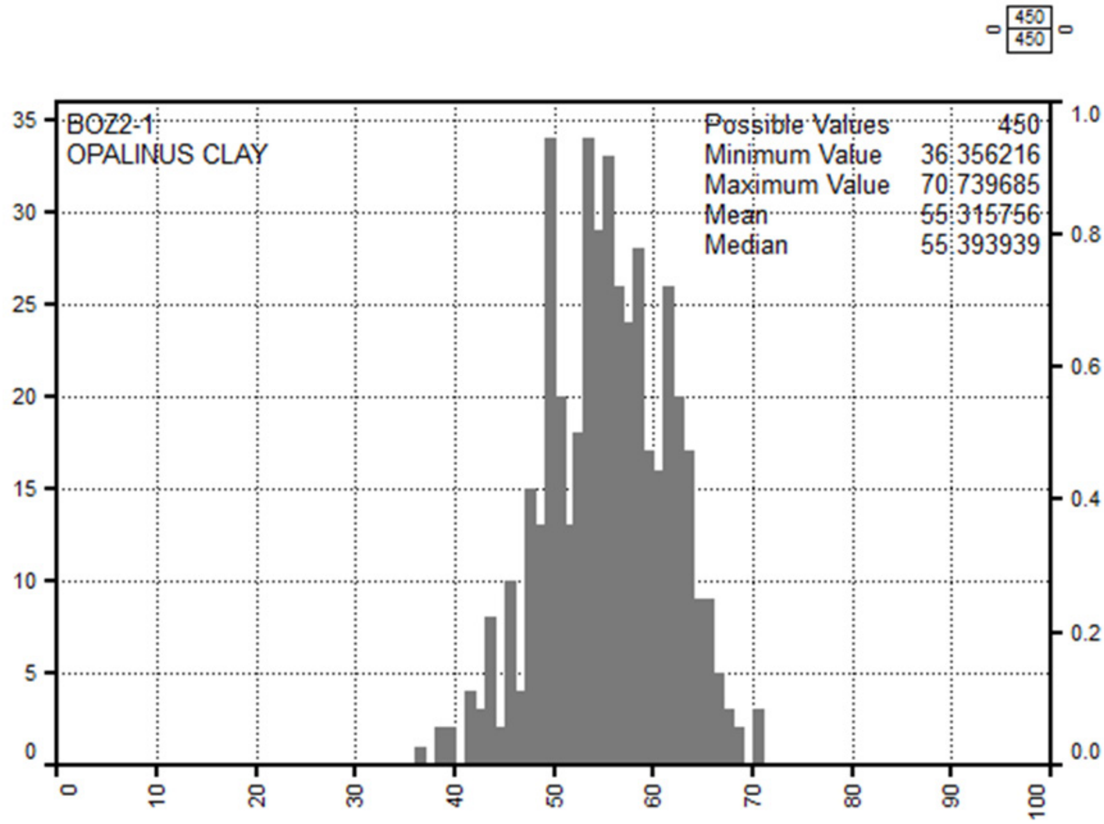

Fig. 4-8: Dry clay weight percentage frequency histogram in the upper section of the Opalinus Clay (above 520.5 m)

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 659 m), the mean and median dry clay content are close to 55.3 and 55.4 wt.-%. The top part of the formation is significantly less argillaceous than the bottom, see Fig. 4-9.

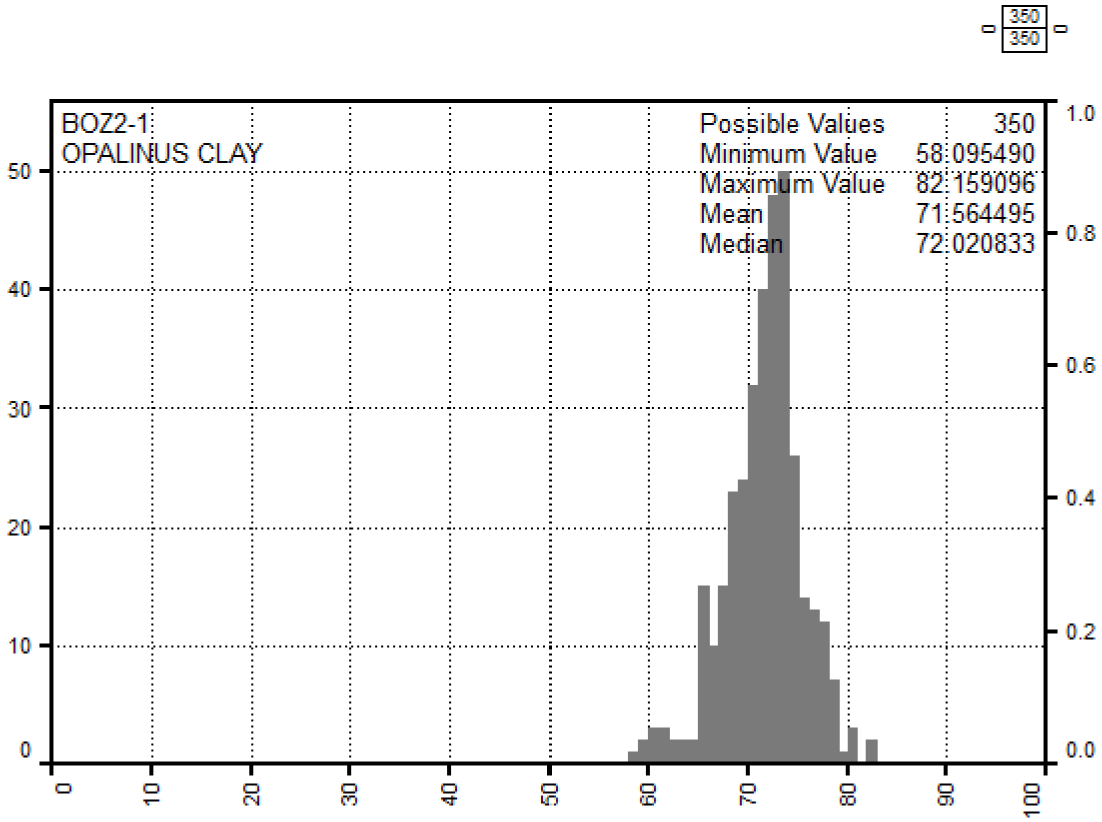

Fig. 4-9: Dry clay weight percentage frequency histogram in the lower section of the Opalinus Clay (below 520.5 m)

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 520.5 m) is more argillaceous: the mean and median dry clay content are close to 71.6 and 72.0 wt.-%.

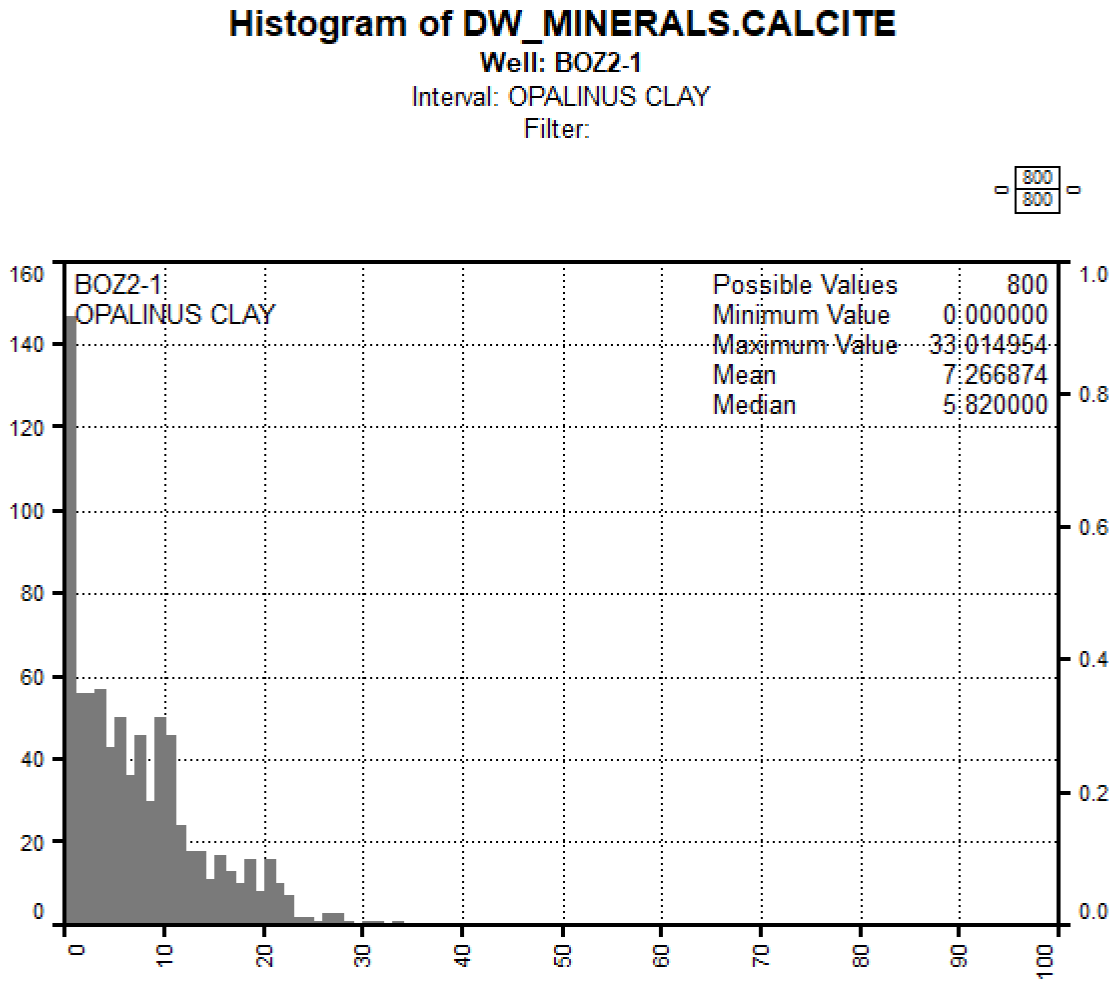

Fig. 4-10: Calcite weight percentage frequency histogram in the Opalinus Clay

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

The mean and median calcite content are close to 7.3 and 5.8 wt.-% (Fig. 4-10). The maximum values are up to 33.0 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.

The top part of the Opalinus Clay is more calcitic than the bottom (see Plates 1 and 2).

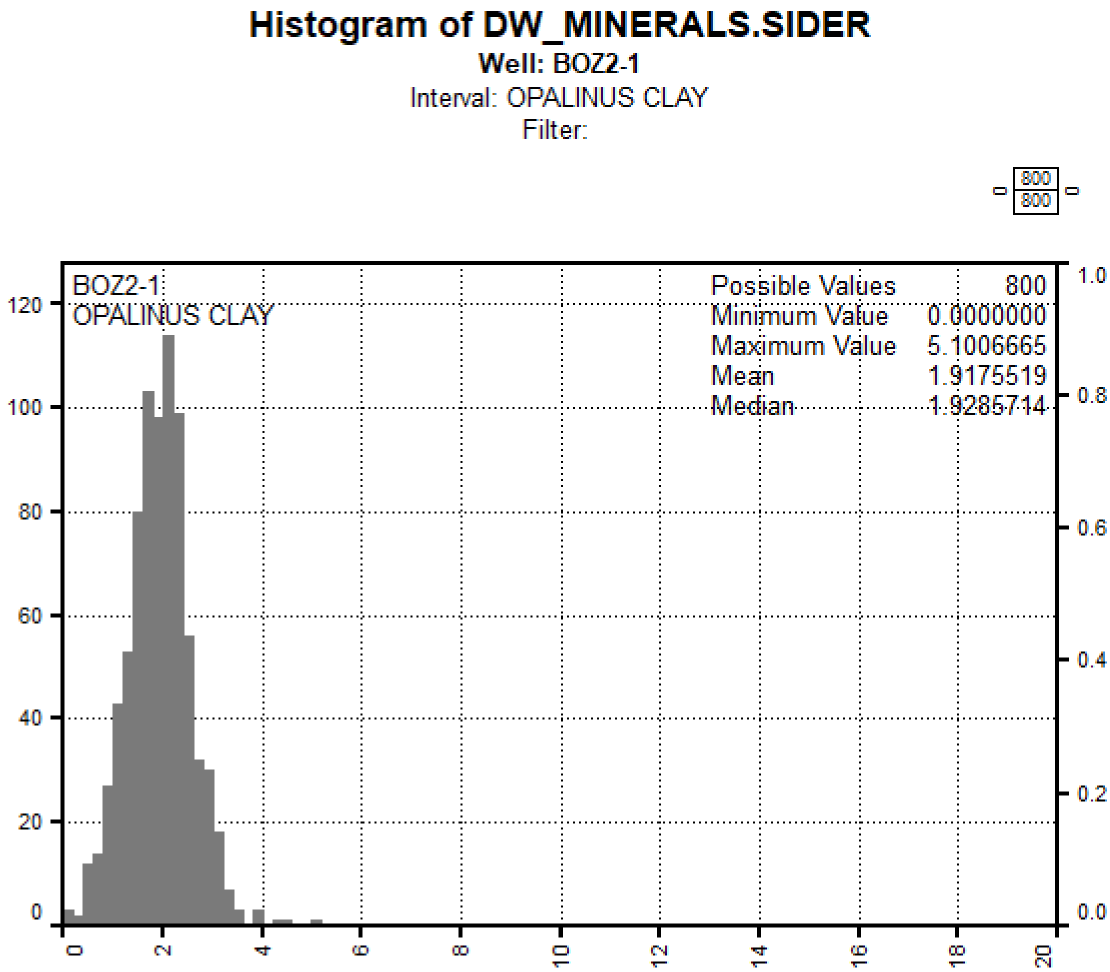

Fig. 4-11: Siderite weight percentage frequency histogram in the Opalinus Clay

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

The mean and median siderite content are close to 1.9 wt.-%, with a maximum value of 5.1 wt.-% and a minimum value of 0 wt.-% (Fig. 4-11). Please note that the siderite core calibration is less constrained than other minerals.

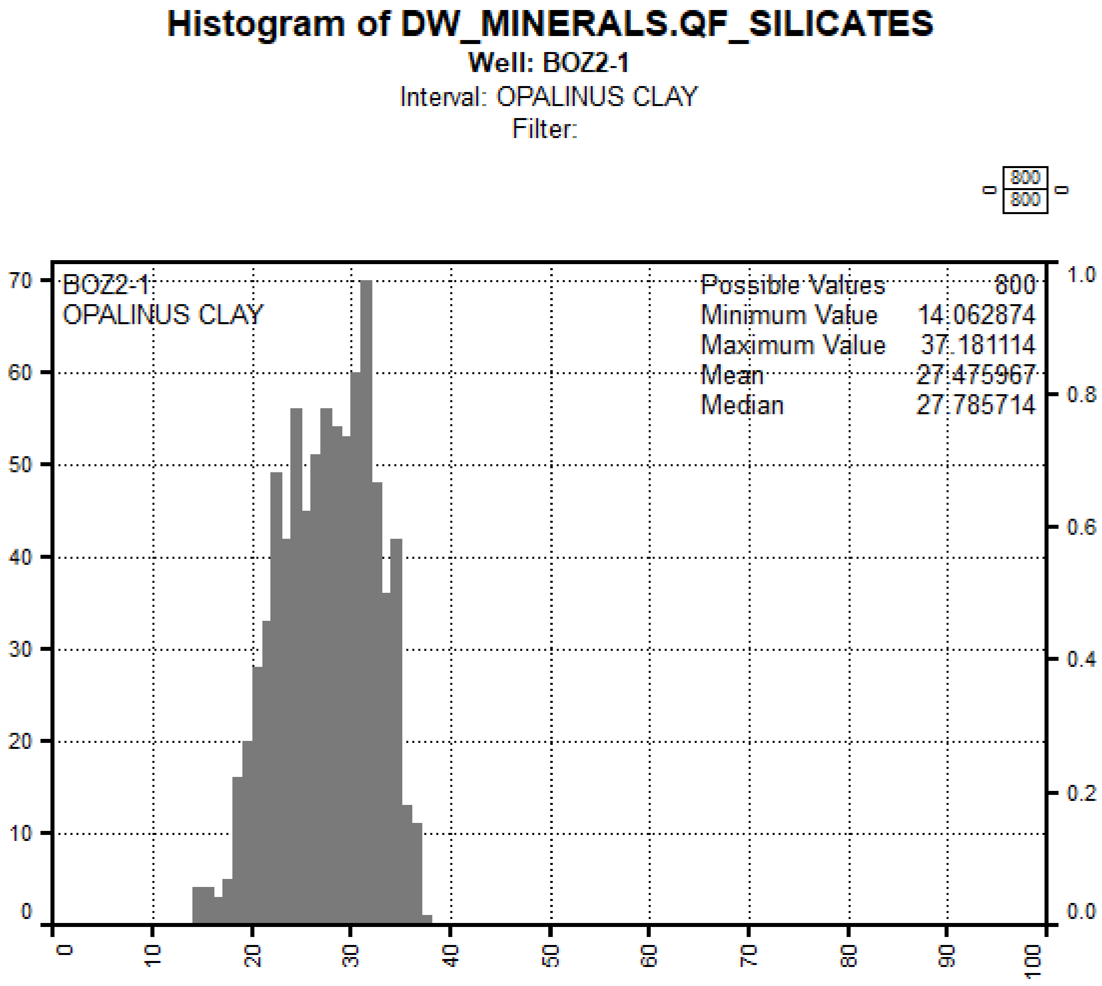

Fig. 4-12: QF-silicates (quartz and feldspars) weight percentage frequency histogram in the Opalinus Clay

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 27.5 and 27.8 wt.-% (Fig. 4-12), much higher than the carbonates (mean / median calcite close to 6 / 7 wt.-%).

From core XRD data, the quartz represents two thirds and feldspars the remaining third of the total QF-silicate content.

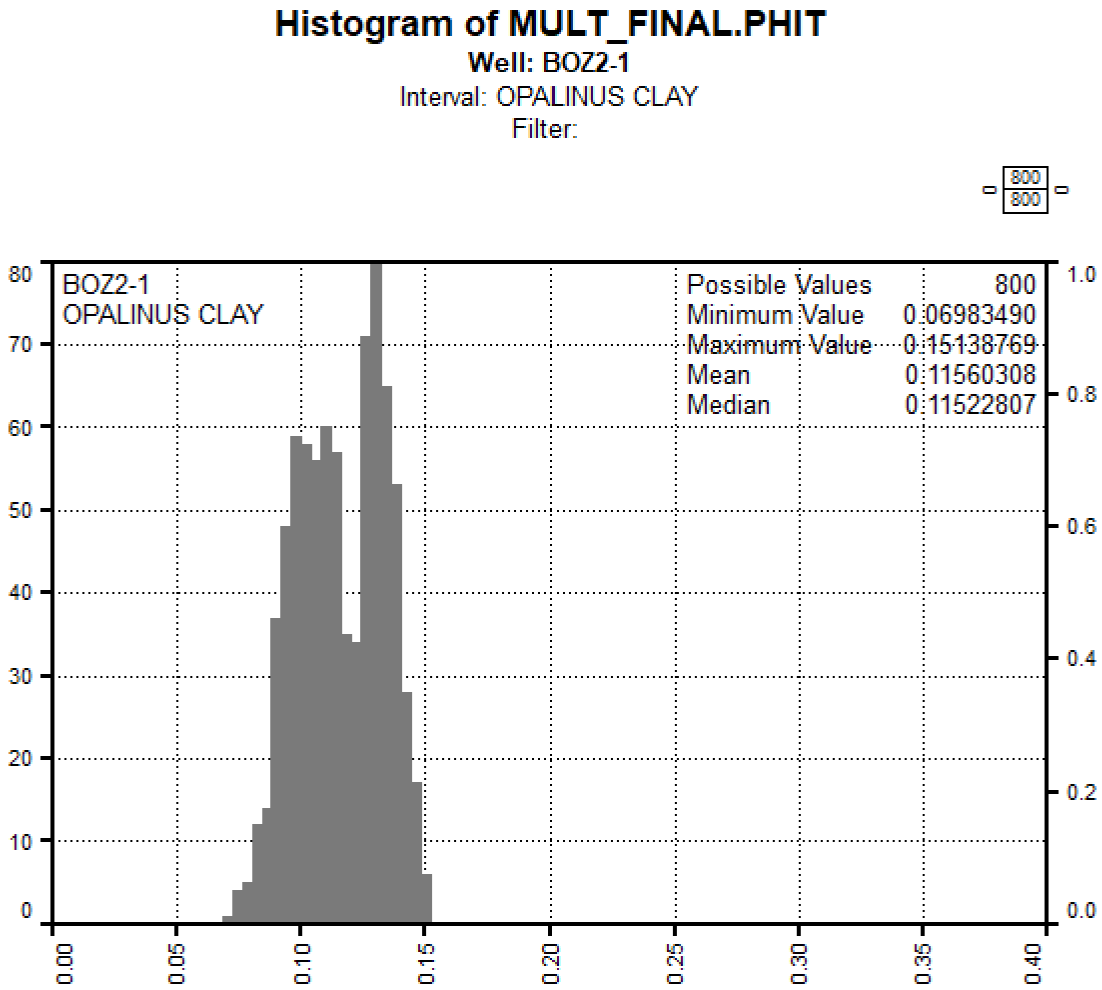

Fig. 4-13: Total porosity frequency histogram in the Opalinus Clay

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 close to 11.6% and 11.5%, with a range from 7.0 to 15.1% (Fig. 4-13). The distribution is bimodal, reflecting the distribution of the clay content.

Fig. 4-14 summarises the main results in the Opalinus Clay.

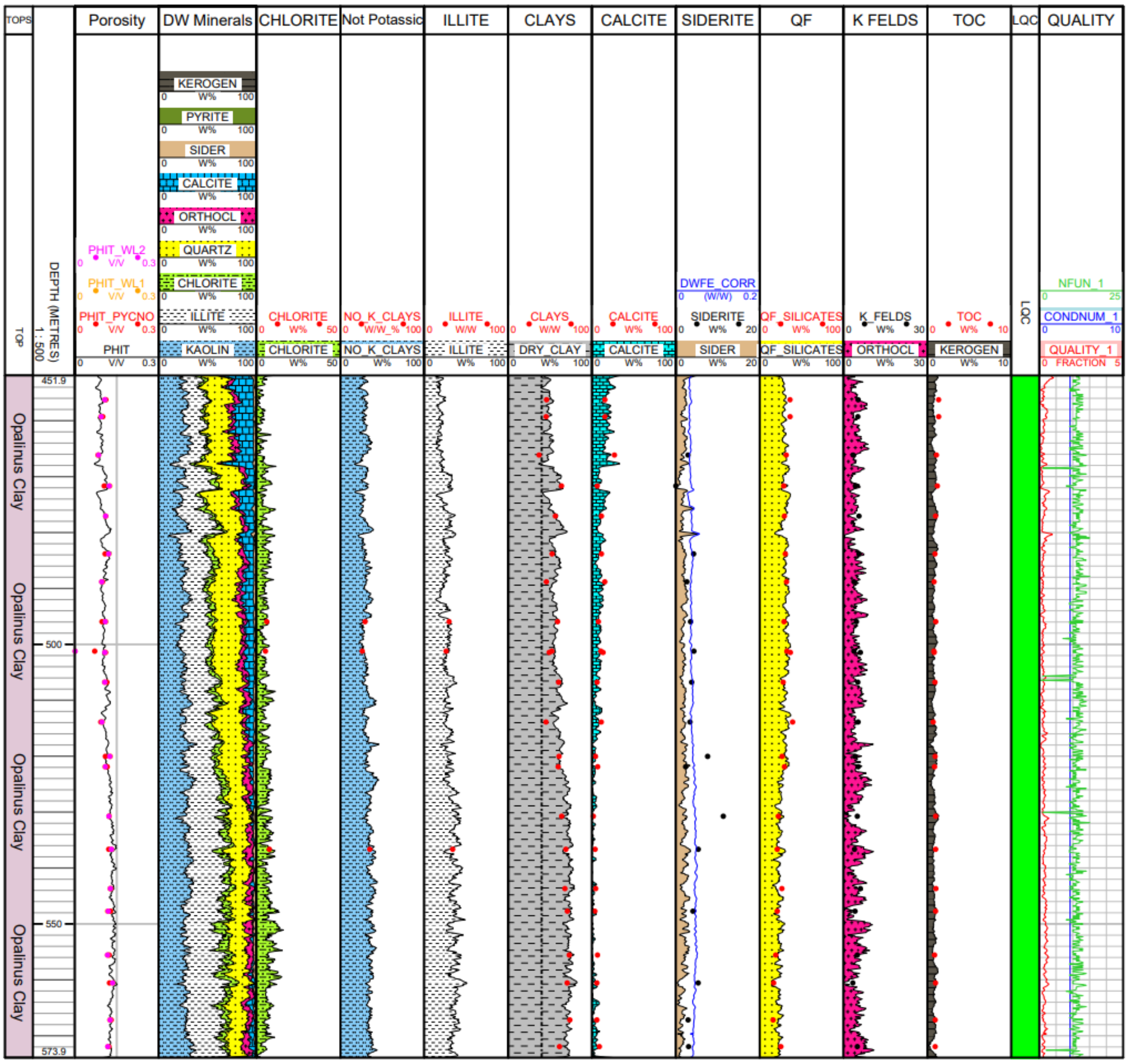

Fig. 4-14: Main log and core results in the Opalinus Clay

The back line in the all clay minerals track represents a 40% baseline.

The wireline log quality was good in all 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 calibration is less accurate, although the high XRD siderite is not reflected in the DWFE_CORR log (blue curve in the "Siderite" track), possibly due to local heterogeneities.

The whole Opalinus Clay is very argillaceous, almost always above the 40 wt% (black line in the "All Clay minerals" track in Fig. 4-14). A few carbonates streaks in the top third part have a lower clay content.

5 Summary

The MultiMin interpretation was successfully applied in the BOZ2-1 borehole using the Paradigm Geolog MultiMin software (see Plates 1 and 2). Based on available petrophysical logs and formation mineralogical contents, several specific MultiMin interpretation intervals were identified. 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), in organic-rich layers of the Staffelegg Formation and in the «Brauner Dogger» (core PHIT higher than MultiMin PHIT as core-derived bulk density is lower than logs).

The continuous curves from the MultiMin interpretation can be used to characterise the different formations (and hence members) occurring in BOZ2-1. The Opalinus Clay shows a quite variable total clay content, though in most locations it is well above 40 wt.-%. The lower third of the formation is significantly more argillaceous than the top, as already noticed in many regional locations.

In addition, boundaries between formations (and between members) are often clearly marked by a decrease or increase of clay, QF-silicate and/or carbonate contents.

The lowest section in the Triassic (Keuper and Muschelkalk) formations could not be fully logged, the TLD-APS-ECS services were not acquired. The MSCL data were successfully used as an input for the MultiMin models in the Keuper, however, due to the missing petrophysical logs, the results have a higher uncertainty than interpretations with a full coverage of petrophysical logs.

6 References

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