Arbeitsbericht NAB 22-04

TBO Bachs-1-1: Data Report

Dossier X Petrophysical Log Analysis

August 2023

S. Marnat & J.K. Becker

National Cooperative
for the Disposal of
Radioactive Waste

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

nagra.ch

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S. Marnat[1] & J.K. Becker[2]

[1] Ad Terra Energyl
[2] Nagra

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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
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
DWK_ALKNA	Dry weight fraction potassium, ECS ALKNA closure model
DWK_MGWALK	Dry weight fraction potassium, ECS MGWALK closure model
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, 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
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
DWMG_MGWALK	Dry weight fraction magnesium, ECS MGWALK closure model
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
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 Micro imager
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
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
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
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
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
ECS 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 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 Bachs-1-1 borehole.

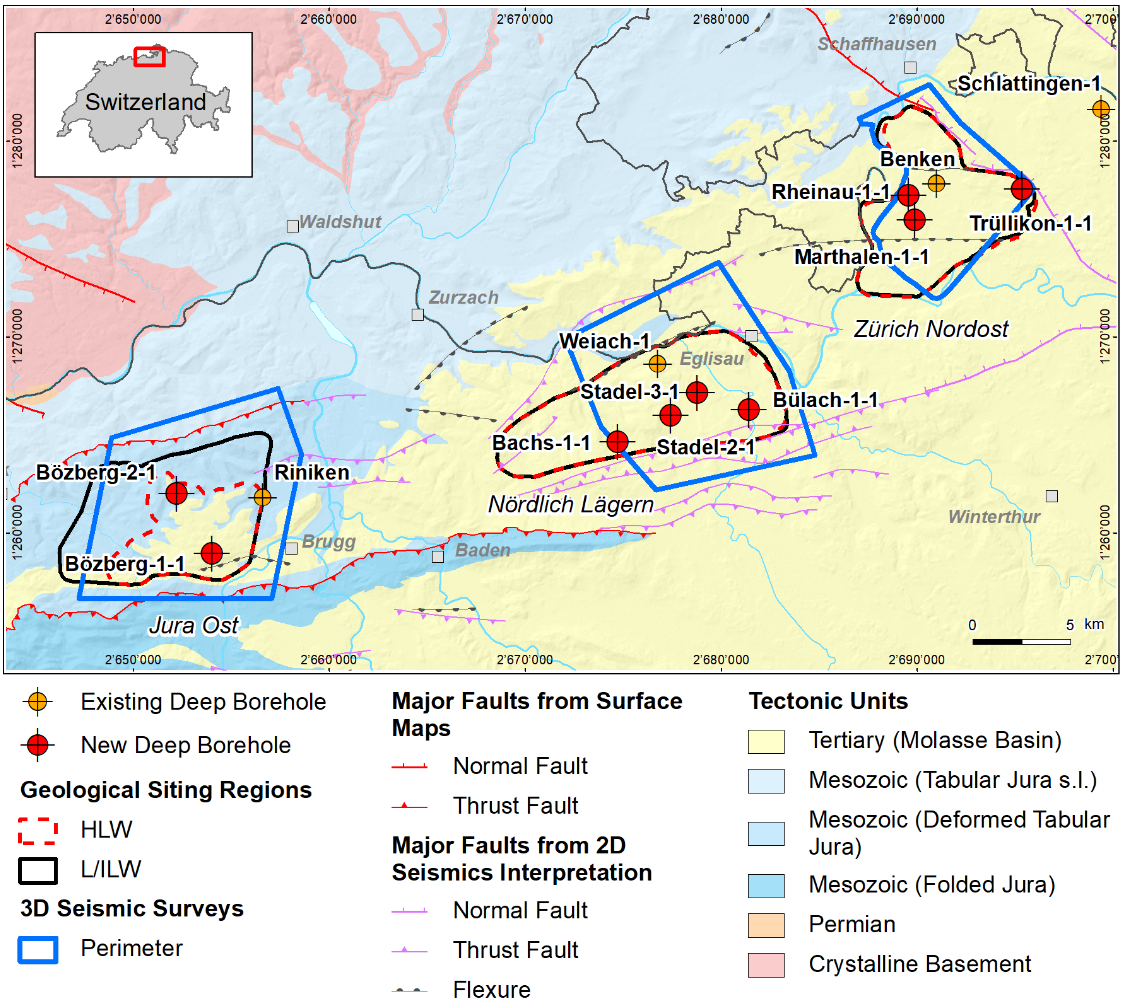

Fig. 1-1: Tectonic overview map with the three siting regions under investigation

1.2 Location and specifications of the borehole

The Bachs-1-1 (BAC1-1) exploratory borehole is the ninth (and last) borehole drilled within the framework of the TBO project. The drill site is located in the western part of the Nördlich Lägern siting region (Fig. 1-2). The vertical borehole reached a final depth of 1'306.26 m (MD)[1]. The borehole specifications are provided in Tab. 1-1.

Due to a loss of a measurement tool (dilatometer), the borehole was cemented up to 500 m MD and a sidetrack was initiated with a kickoff point (KOP) at about 600 m MD. This sidetrack was labelled Bachs-1-1B (BAC1-1B). BAC1-1B reached a final depth of 952 m MD but was abandoned during borehole reaming operations due to entering the original borehole BAC1-1. Therefore, the vertical borehole BAC1-1 was used again for the remaining investigations. For easier communication and labelling, the name BAC1-1 is generally used for this borehole, including the sidetrack, unless stated otherwise. A detailed description of all technical details about the drilling process can be found in Dossier I.

Tab. 1-1: General information about the BAC1-1 borehole

Siting region	Nördlich Lägern
Municipality	Bachs (Canton Zürich / ZH), Switzerland
Drill site	Bachs-1 (BAC1)
Borehole	Bachs-1-1 (BAC1-1) including sidetrack Bachs-1-1B (BAC1-1B)
Coordinates	LV95: 2'674'769.089 / 1'264'600.698
Elevation	Ground level = top of rig cellar: 450.35 m above sea level (asl)
Borehole depth	1'306.26 m measured depth (MD) below ground level (bgl)
Drilling period	10th September 2021 – 23rd April 2022 (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 – 700 m: Bentonite & polymers 700 – 1'057 m: Potassium silicate & polymers[3] 1'057 – 1'129 m: Water & polymers 1'129 – 1'306.26 m: Sodium chloride brine & polymers

The lithostratigraphic profile and the casing scheme are shown in Fig. 1-3. The comparison of the core versus log depth[4] of the main lithostratigraphic boundaries in the BAC1-1 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] Including side track.

[4] 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.

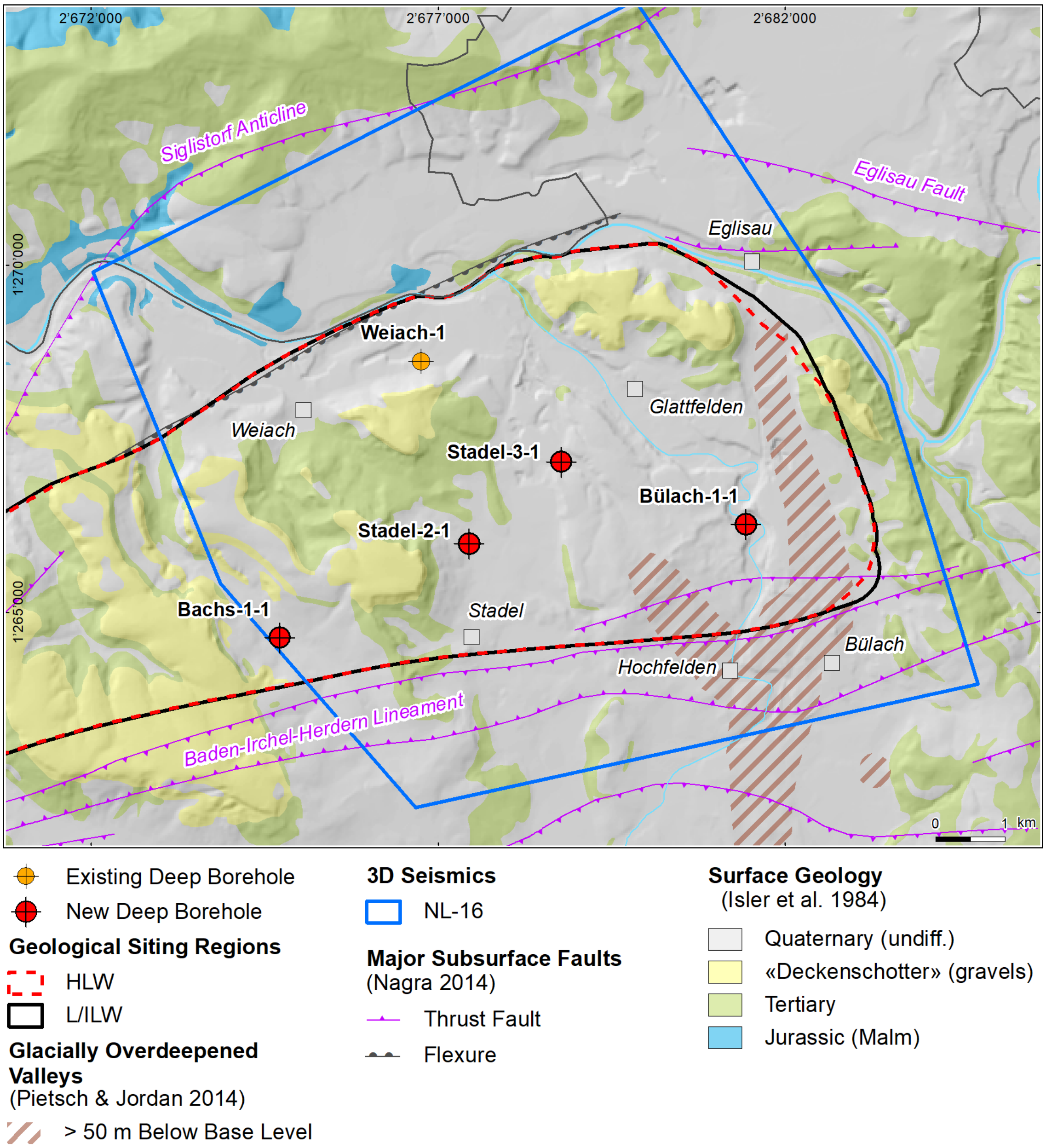

Fig. 1-2: Overview map of the investigation area in the Nördlich Lägern siting region with the location of the BAC1-1 borehole in relation to the boreholes Weiach-1, BUL1-1, STA3-1 and STA2-1

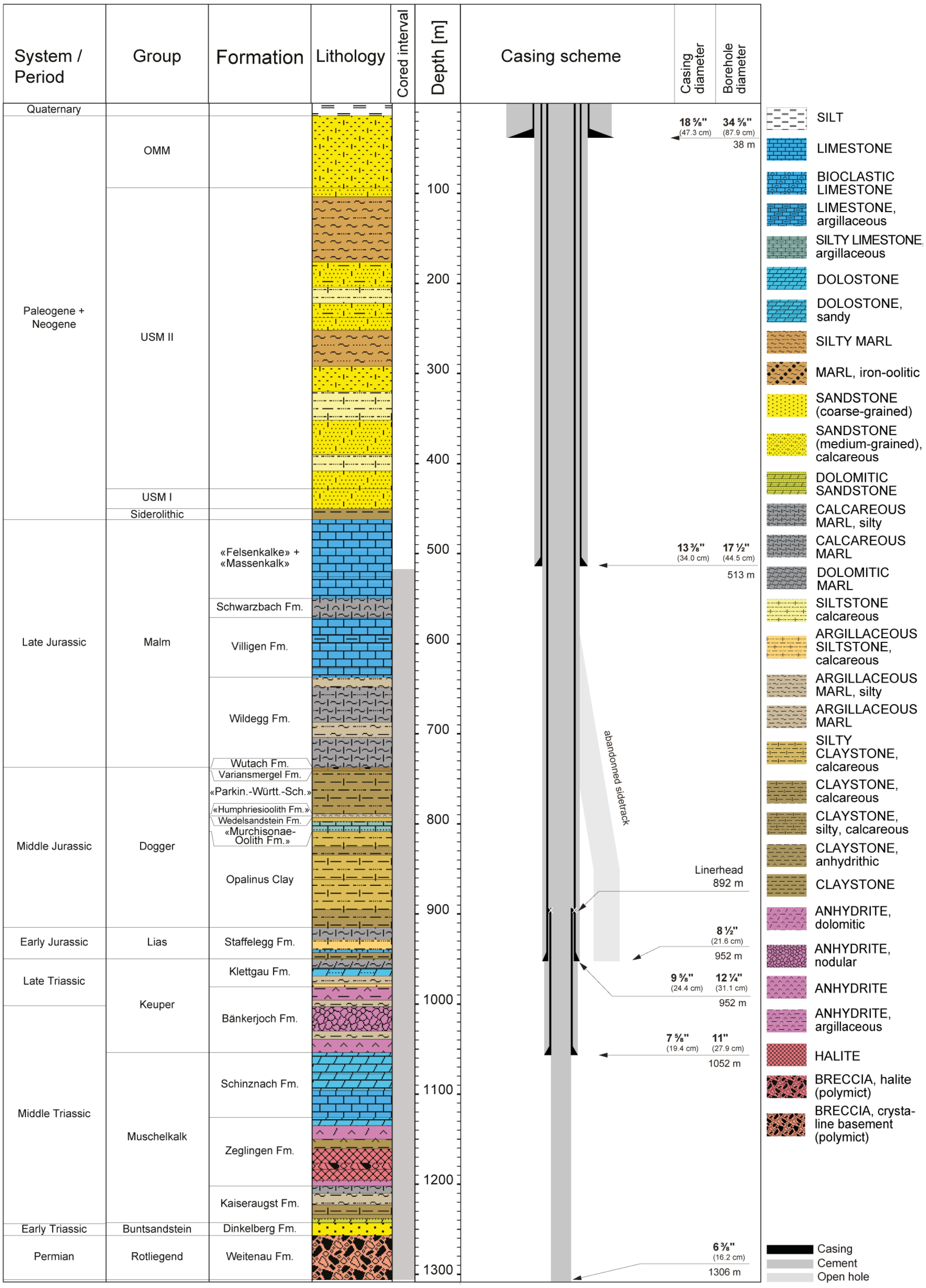

Fig. 1-3: Lithostratigraphic profile and casing scheme for the BAC1-1 borehole[5]

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

Tab. 1-2: Core and log depth for the main lithostratigraphic boundaries in the BAC1-1 borehole[6]

System / Period	Group	Formation	Core top depth in m (MD)	Log top depth in m (MD)
Quaternary				
Paleogene + Neogene	OMM		**14**	
	USM		94	
	Siderolithic		450	
Jurassic	Malm	«Felsenkalke» + «Massenkalk»	**462**	
		Schwarzbach Formation	549.69	550.03
		Villigen Formation	570.98	571.29
		Wildegg Formation	637.31	637.55
	Dogger	Wutach Formation	737.05	737.32
		Variansmergel Formation	738.81	739.08
		«Parkinsoni-Württembergica-Schichten»	741.22	741.47
		«Humphriesioolith Formation»	788.92	789.12
		Wedelsandstein Formation	791.05	791.25
		«Murchisonae-Oolith Formation»	793.11	793.31
		Opalinus Clay	808.34	808.57
	Lias	Staffelegg Formation	914.91	915.30
Triassic	Keuper	Klettgau Formation	**949.73**	**950.07**
		Bänkerjoch Formation	980.93	981.27
	Muschelkalk	Schinznach Formation	1053.90	1054.30
		Zeglingen Formation	1125.75	1126.20
		Kaiseraugst Formation	1202.03	1202.43
	Buntsandstein	Dinkelberg Formation	1242.82	1243.12
Permian	Rotliegend	Weitenau Formation	**1256.86**	**1257.26**
		final depth	1306.26	1306.77

[6] 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 BAC1-1 borehole

NAB 22-04 documents the majority of the investigations carried out in the BAC1-1 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 BAC1-1 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 22-04

Black indicates the dossier at hand.

Dossier	Title	Authors
I	TBO Bachs-1-1: Drilling	P. Hinterholzer-Reisegger
II	TBO Bachs-1-1: Core Photography	D. Kaehr, M. Stockhecke & Hp. Weber
III	TBO Bachs-1-1: Lithostratigraphy	P. Jordan, P. Schürch, M. Schwarz, T. Ibele, R. Felber, H. Naef & F. Casanova
IV	TBO Bachs-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 Bachs-1-1: Structural Geology	A. Ebert, E. Hägerstedt, S. Cioldi, L. Gregorczyk & F. Casanova
VI	TBO Bachs-1-1: Wireline Logging, Micro-hydraulic Fracturing and Pressure-meter Testing	J. Gonus, E. Bailey, J. Desroches & R. Garrard
VII	TBO Bachs-1-1: Hydraulic Packer Testing	R. Schwarz, R. Beauheim, L Schlicken-rieder, E. Manukyan & A. Pechstein
VIII	TBO Bachs-1-1: Rock Properties, Porewater Characterisation and Natural Tracer Profiles	E. Gaucher, L. Aschwanden, T. Gimmi, A. Jenni, M. Kiczka, M. Mazurek, P. Wersin, C. Zwahlen, U. Mäder & D. Traber
IX	*The geomechanical campaign in BAC-1-1 was limited to two oedometric tests. Hence, no dedicated Dossier IX was produced for NAB 22-04. The hydraulic conductivity values derived from the oedometric tests are documented in the Summary Plot.*	
X	TBO Bachs-1-1: Petrophysical Log Analysis	S. Marnat & J.K. Becker
	TBO Bachs-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 BAC-1 borehole. The detailed workflow for this analysis is described in a methodology report (Marnat & Becker, 2021). Though the general workflow as described Marnat & Becker (2021) is still followed, the results documented here also indirectly include information from other boreholes. Interpretation intervals and important parameters have been streamlined between the different boreholes wherever possible. Hence, results should be used for qualitative comparisons with previous work only. The general workflow is only shortly summarized here. Finally, comparable results for all boreholes will be documented in a separate report.

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 a same processing. For this reason, only the standard resolution version of the logs was input with a sampling rate of ½ foot (~ 15 cm).

For the Multimineral Log Analysis (abbrev. 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 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 composites of the petrophysical logs from the borehole BAC1-1 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 (ECGR_EDTC, 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 atomic electrons. The flux of gamma rays that reach 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 and DWCA_MGWALK (Ca), DWFE_ALKNA (Fe), DWSU_WALK2 and DWSU_ALKNA (S), DWAL_ALKNA (Al), DWK_ALKNA (K). The curves with MGWALK and ALKNA suffixes are obtained with additional closure models to the standard WALK2. 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 ALKNA closure model (DWFE_ALKNA) was preferred to the WALK2, as the results are closer to the XRF core measurements and are in better agreement with the core mineralogy in regional boreholes.

- 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 occured. 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 borehole BAC1-1 is given in the appendix and in Plate 1.

Usable log data were available for a MultiMin analysis from 518.77 to 1305.76 m (see Plate 1). Due to missing logs between drilling sections and cased hole sections (see borehole report, Dossier VI), a minor MultiMin interpretation gap, due to insufficient petrophysical logs coverage, remained in the following interval, as shown in Fig. 2-1:

- 949.6 – 952.0 m (between sections II and III)

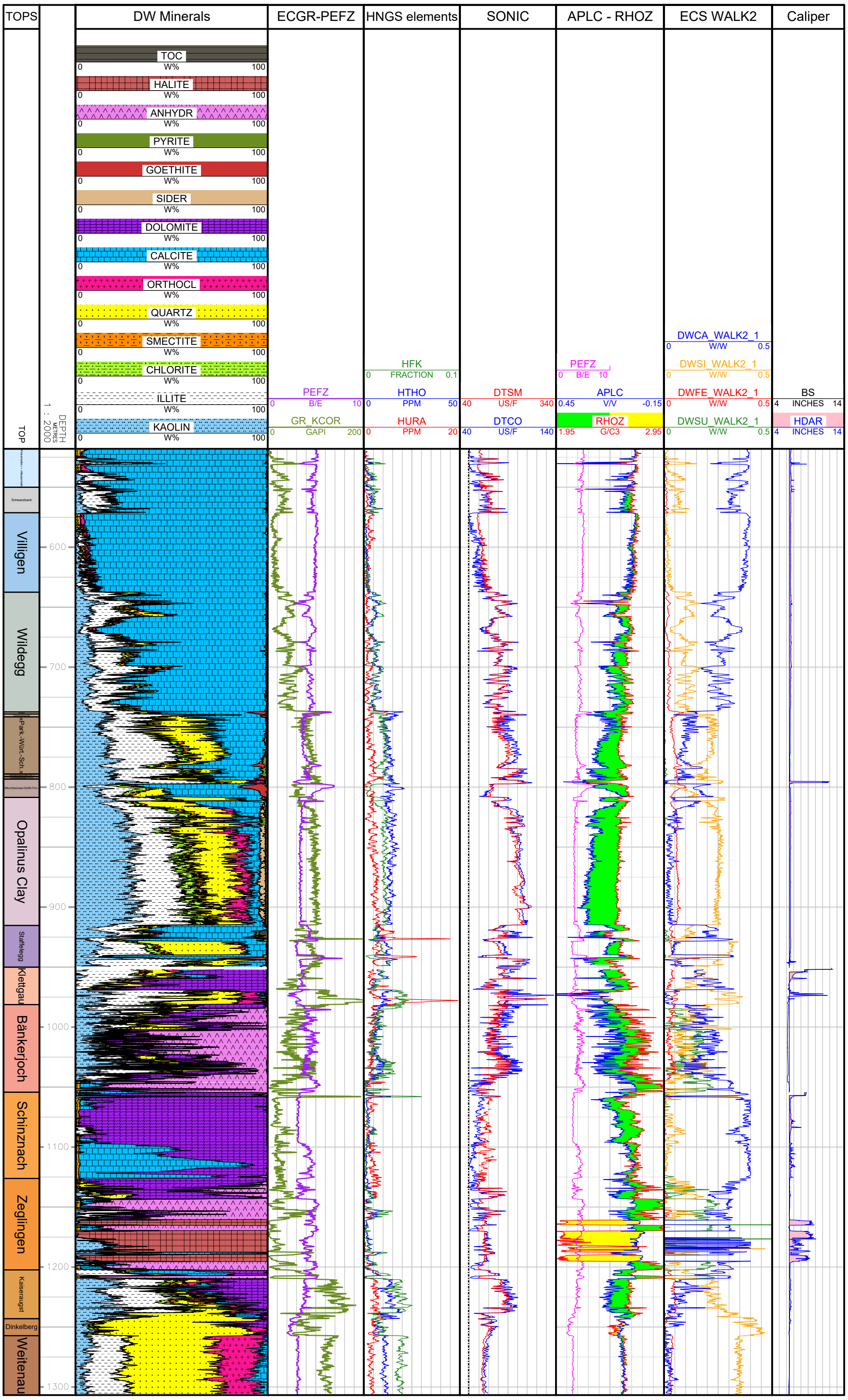

Fig. 2-1: Petrophysical log availability and gaps in the borehole BAC1-1

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.

A reduced wireline log suite was acquired in the upper interval (0 – 518.77 m), with gamma ray and sonic in a large hole (17½"). This did not allow a MultiMin processing in and above top Malm. The Molasse 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 (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 Plates 1 and 2). 84 core samples collected at depth ranging from 539.46 to 1126.88 m drillers depth were available, of which 75 were analysed for pycnometer total porosity, 81 for water loss total porosity, 74 for XRD mineralogy and 31 for clay types. The analysed minerals were quartz, K-feldspars, plagioclase, calcite, dolomite/ ankerite, magnesite, siderite, anhydrite, celestite, barite, pyrite, marcasite, goethite, maghemite, haematite, fluorite, clay minerals and organic carbon. The 31 samples analysed for clay typing (in the interval 651.68 – 971.8 m drillers depth) 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 (ed.) (2020).

The difference between core and log depth were taken from the correlation between FMI images and core images.

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

Core mineralogical measurements from four reference boreholes are implicitly used in this study: the TOC, smectite and chlorites content were computed through a clustering methodology (implemented in the Geolog Facimage module) trained on MAR1-1, BOZ1-1, BOZ2-1 and TRU1-1.

2.3 Multi-sensor Core Logger (MSCL) data

MSCL measurements from cores were available in the borehole BAC1-1 (from 725.58 to 981.90 m Drillers). 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 a gap. In these same intervals, no or limited 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 BAC1-1, the core logs were depth shifted using the Core to FMI depth shift table.

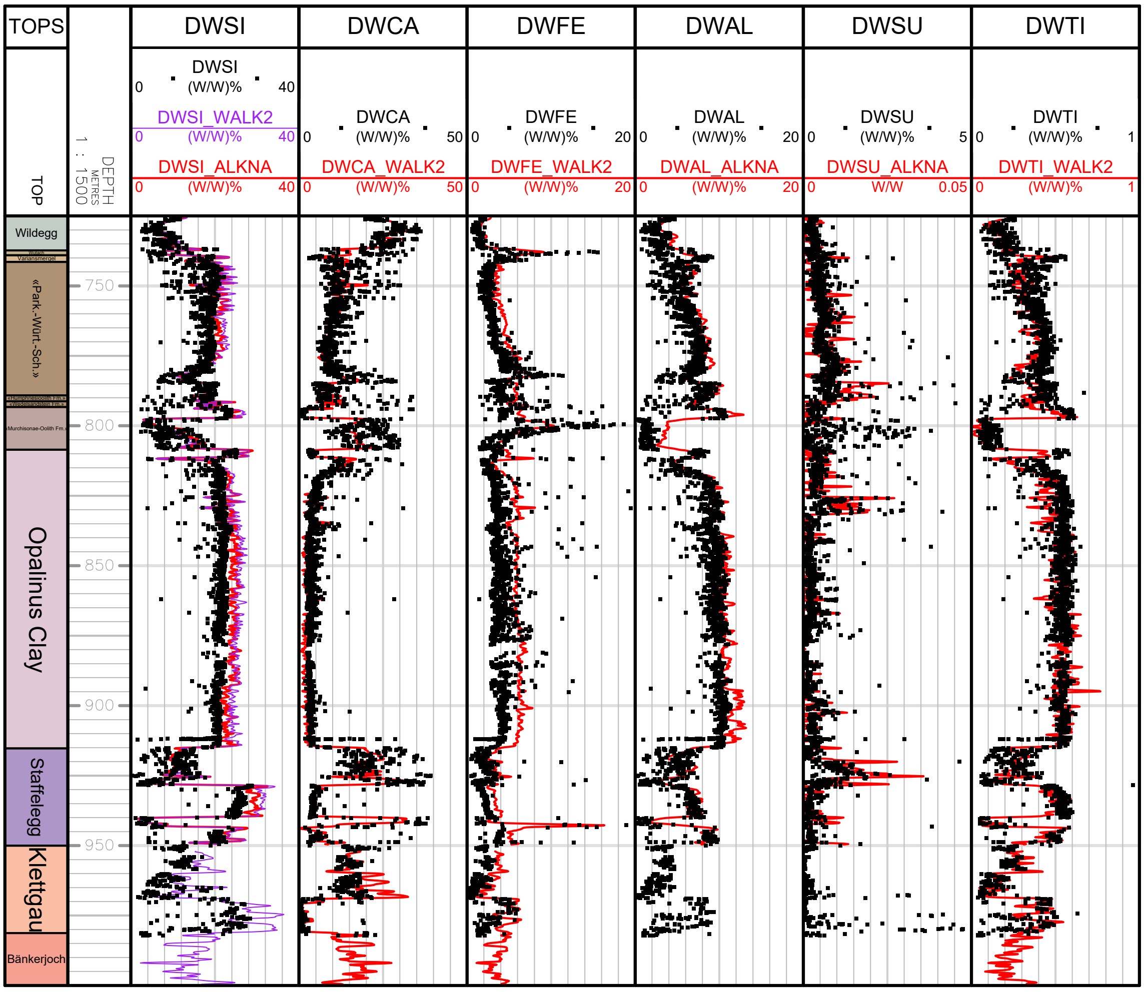

Fig. 2-2: XRF (black dots) and ECS (red and purple curves) elements comparison in BAC1-1

While the calcium, aluminium (from the ALKNA closure model) and titanium concentrations are almost similar, the XRF iron and silicon are slightly lower than ECS'.

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

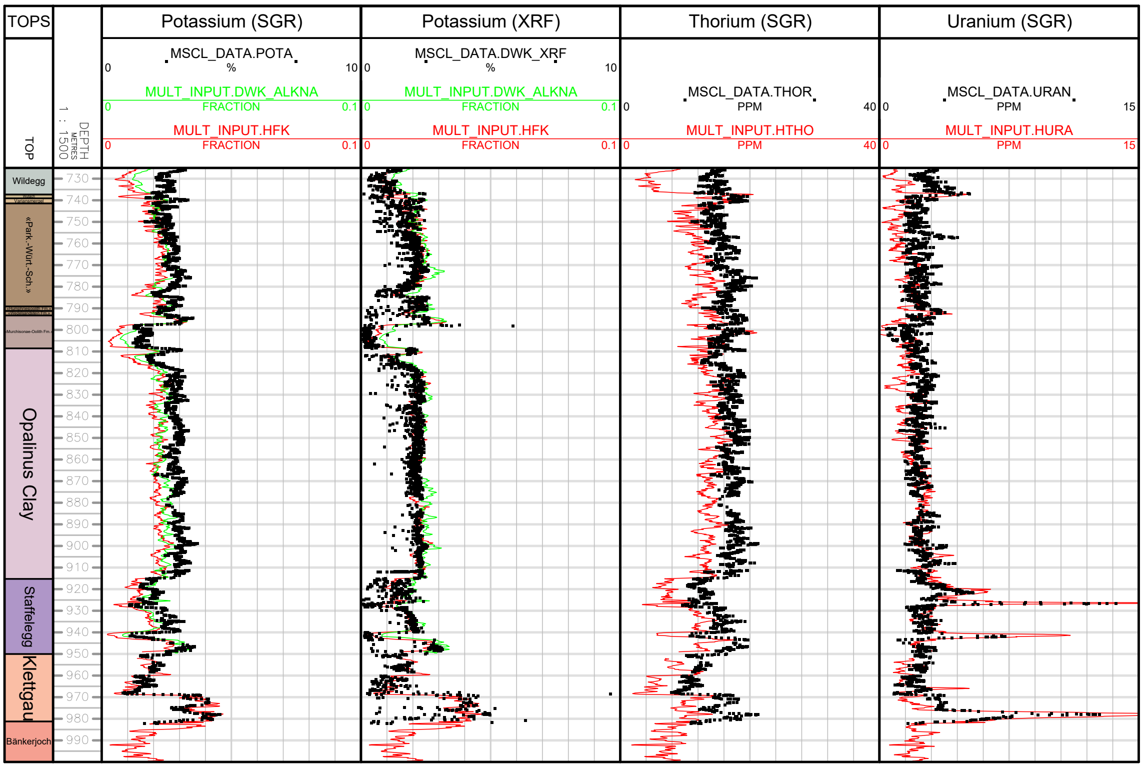

Fig. 2-3: Core (black dots: spectral gamma ray, and XRF poatssium) and wireline (red curves for HNGS, green curve ECS potassium) spectral gamma ray elements comparison

The thorium and potassium content from MSCL spectral GR are slightly higher than the HNGS wireline logs, while the XRF potassium is very close to the HFK and DWK_ALKNA curves. The MSCL uranium is close from HNGS HURA curve.

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.

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, four 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.

At the bottom of section II, the HNGS was not acquired below 493.2 m. As the ECS was run below this depth with the ALKNA closure model, the ECS potassium curve DWK_ALKNA was used instead. This curve was plotted against HFK in the same borehole section, and was corrected to HFK, as shown in Fig. 2-4 hereafter.

The HFK_DWK curve was generated as follows:

$$HFK\_DWK\ (\%) = 92.97 * DWK\_ALKNA\ (W/W) - 0.325586$$

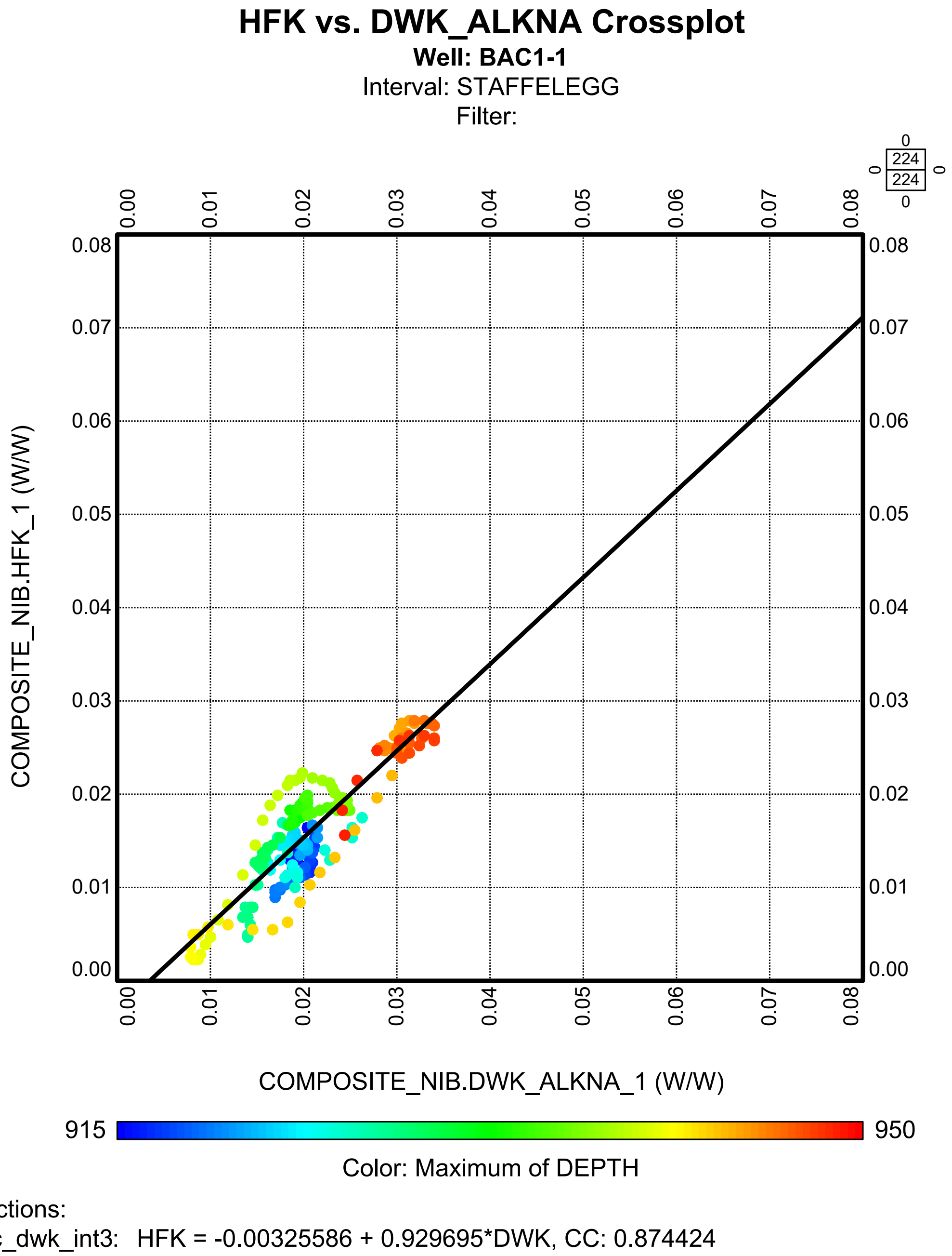

Fig. 2-4: HFK (from the SGR log) versus DWK_ALKNA (from the ECS log) in log-section II

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 2021). 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 the recent (Dossiers VIII of the respective borehole reports) and previous TBO boreholes core samples (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.
- Silicates: quartz, potassic feldspars, plagioclases
- Carbonates: calcite, siderite, dolomite/ankerite.
- Iron-rich minerals: goethite, pyrite.
- Evaporites: anhydrite.
- Organic carbon (kerogen, quantified by the TOC).

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 an example of 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 BAC1-1

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
518.8	529.0	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
529.0	529.7	MALM	00_malm_bac_dts	4.25	Badhole using DTSM
529.7	531.0	MALM	00_malm_bac_dtc	4.28	Badhole using DTCO
531.0	540.6	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
540.6	541.2	MALM	00_malm_bac_dts	4.25	Badhole using DTSM
541.2	543.6	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
543.6	544.4	MALM	00_malm_bac_dts	4.25	Badhole using DTSM
544.4	551.0	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
551.0	552.0	MALM	00_malm_bac_dtc	4.28	Badhole using DTCO
552.0	552.9	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
552.9	553.9	MALM	00_malm_bac_dtc	4.28	Badhole using DTCO
553.9	639.4	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
639.4	640.1	MALM	00_malm_bac_dtc	4.28	Badhole using DTCO
640.1	644.1	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
644.1	645.5	MALM	00_malm_bac_dtc	4.28	Badhole using DTCO
645.5	645.9	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
645.9	647.6	MALM	00_malm_bac_dtc	4.28	Badhole using DTCO
647.6	678.4	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
678.4	679.4	MALM	00_malm_bac_dtc	4.28	Badhole using DTCO
679.4	736.8	MALM	00_malm_al_rev	4.09	Malm with ECS ALKNA
736.8	808.2	BRAUNER DOGGER	00_bd_rev1	3.87	Brauner Dogger with ECS ALKNA
808.2	928.0	OPA - STAFFELEGG	opa_sta_rev	3.78	Opalinus & Staffelegg, ALKNA
928.0	941.7	STAFFELEGG	sta	3.74	Staffelegg with ALKNA
941.7	943.7	STAFFELEGG	00_sta_goeth	4.14	Iron hydroxide rich rocks
943.7	948.0	STAFFELEGG	sta_noct	3.74	No Ct curve
948.0	949.0	STAFFELEGG	sta_bac11_noaps	3.84	APS not acquired
949.0	949.7	STAFFELEGG	sta_bac11_nohngs	3.87	HNGS not acquired
949.7	952.0	STAFFELEGG-KLETTGAU	No model		Not enough logs
952.0	952.9	KLETTGAU	klet_w2_noct	3.59	No Ct curve
952.9	969.0	KLETTGAU	klet_w2	3.59	Klettgau, using ECS Walk2
969.0	970.5	KLETTGAU	klet_base	3.71	Base Klettgau, high K
970.5	974.3	KLETTGAU	klet_base_bh	3.98	Bad hole
974.3	981.8	KLETTGAU	klet_base	3.71	Base Klettgau, high K
981.8	1047.1	BSZ (*)	00_bsz_mgw	4.77	ECS MGWALK for dolomite
1047.1	1053.0	BSZ (*)	00_bsz_mgw_noct	4.66	No Ct curve
1053.0	1160.4	BSZ (*)	00_bsz_mgw	4.29	ECS MGWALK for dolomite
1160.4	1165.3	BSZ (*)	00_zeg_salt	1.77	Zeglingen halite
1165.3	1169.6	BSZ (*)	00_bsz_mgw	4.29	ECS MGWALK for dolomite
1169.6	1187.7	BSZ (*)	00_zeg_salt	1.77	Zeglingen halite
1187.7	1189.4	BSZ (*)	00_bsz_mgw	4.29	ECS MGWALK for dolomite
1189.4	1195.3	BSZ (*)	00_zeg_salt	1.77	Zeglingen halite
1195.3	1202.3	BSZ (*)	00_bsz_mgw	4.29	ECS MGWALK for dolomite
1202.3	1241.8	KAISERAUGST	00_kais_mg	3.92	ECS MGWALK, Kaiseraugst
1241.8	1257.2	DINKELBERG	00_dink_mg	3.90	ECS MGWALK, Dinkelberg
1257.2	1300.0	WEITENAU	weit_bac11	2.89	Weitenau
1300.0	1306.7	WEITENAU	weit_bac11_noct	2.89	No Ct curve
		BSZ (*): Bankerjoch, Schinznach, Zeglingen			

Mineral and fluid endpoints were manually optimised to both reduce the difference between measured and predicted logs and to 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 total gamma-ray and the electrical conductivities.

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

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. It is displayed in Fig. 3-1.
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 > 0.35 in.

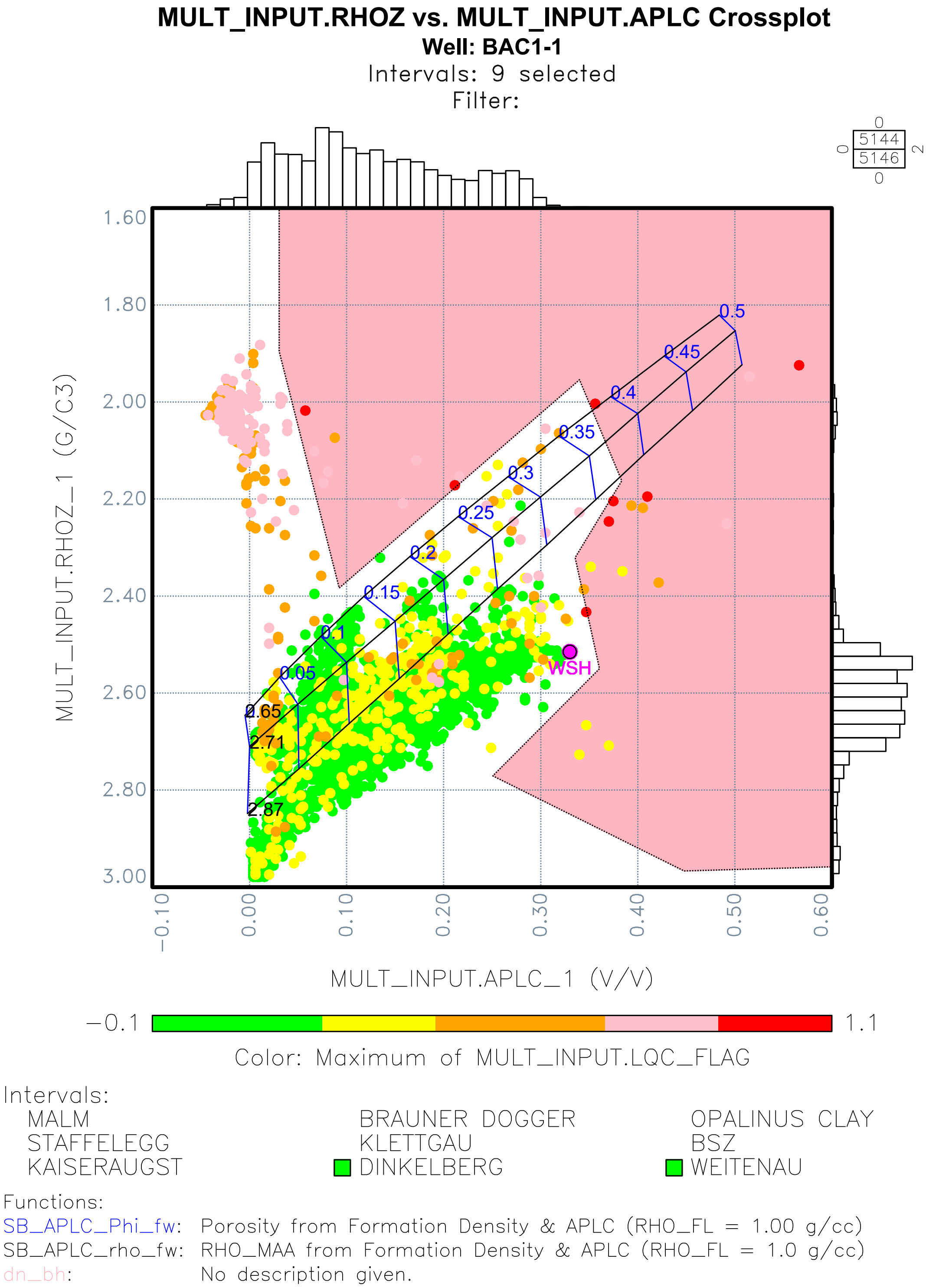

Fig. 3-1: Density-Neutron crossplot badhole indicator

The points displayed in the pink shading are flagged.

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

The 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_FLAG= (FLAG_BADHOLE_DN + FLAG_BADHOLE_OVERGAUGE +

FLAG_BADHOLE_RUGO + FLAG_BADHOLE_STOF) / 4

Hence, the value of the LQC_FLAG 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 said output.

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

MULT_QC

The MultiMin results were not edited in BAC1-1 (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, chlorites: non-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.

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 «Felsenkalke» + «Massenkalk» to the Weitenau Formation. The colour coding represents the formations, as per the attached legend.

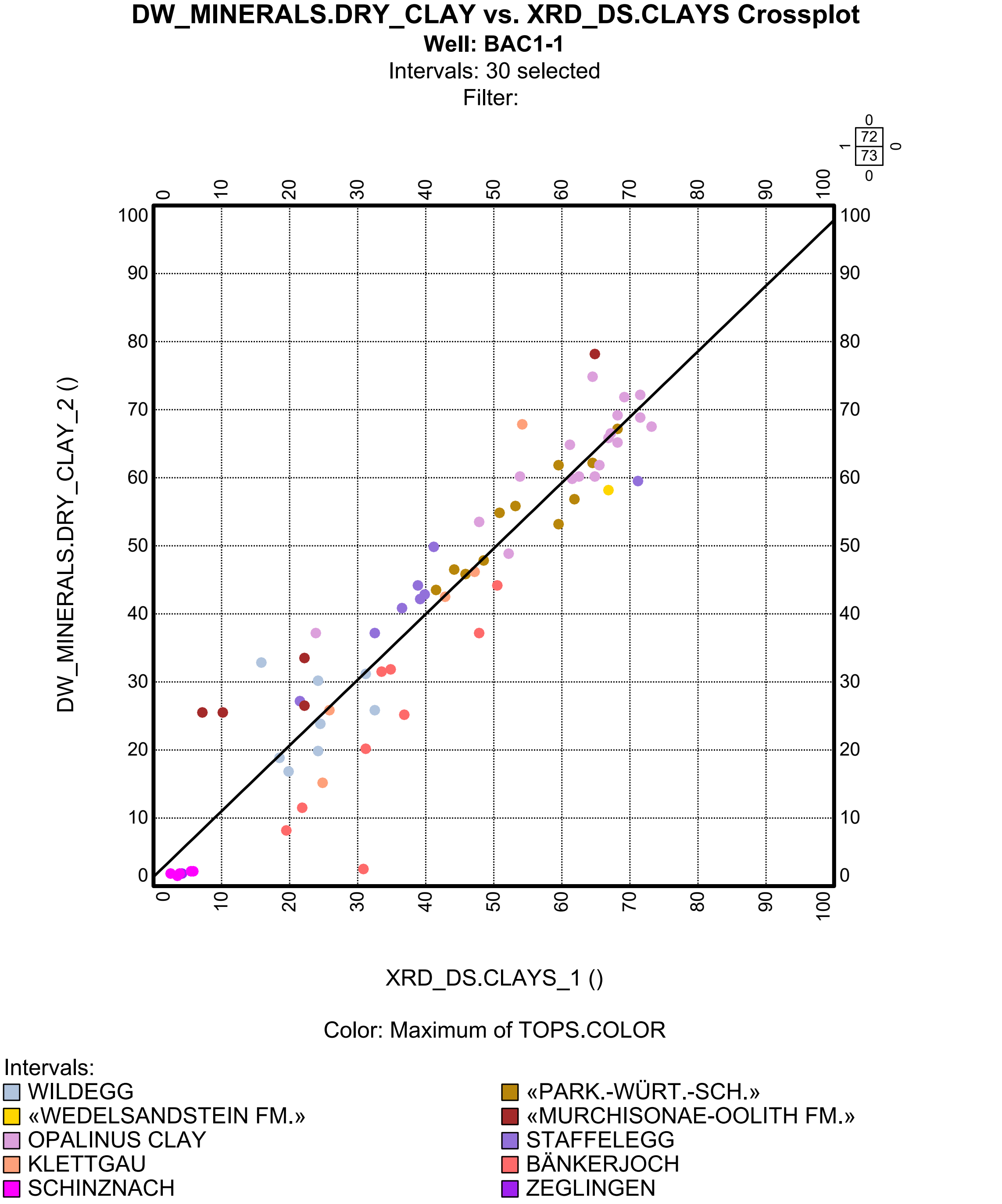

Fig. 4-1: Weight % of dry clay from MultiMin (y-axis) compared to core XRD data (x-axis), Wildegg to Zeglingen Formations

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

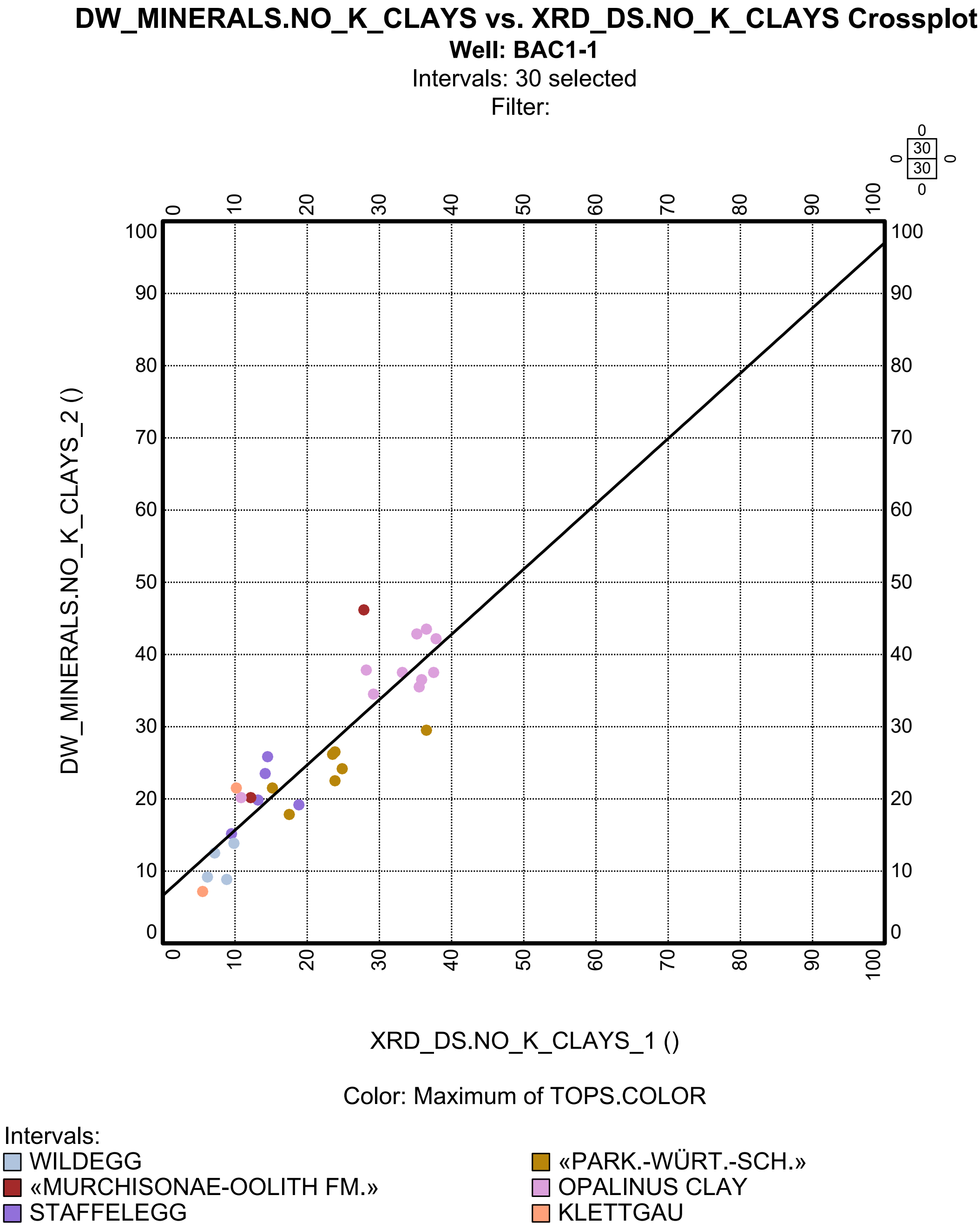

Fig. 4-2: Weight % of non-potassic dry clay from MultiMin (y-axis) compared to core XRD data (x-axis), Wildegg to Klettgau Formations

The XRD clay endmembers were not measured in all formations. The MultiMin non-potassic clay content is fairly correlated to the core XRD data (overall cc = 0.90).

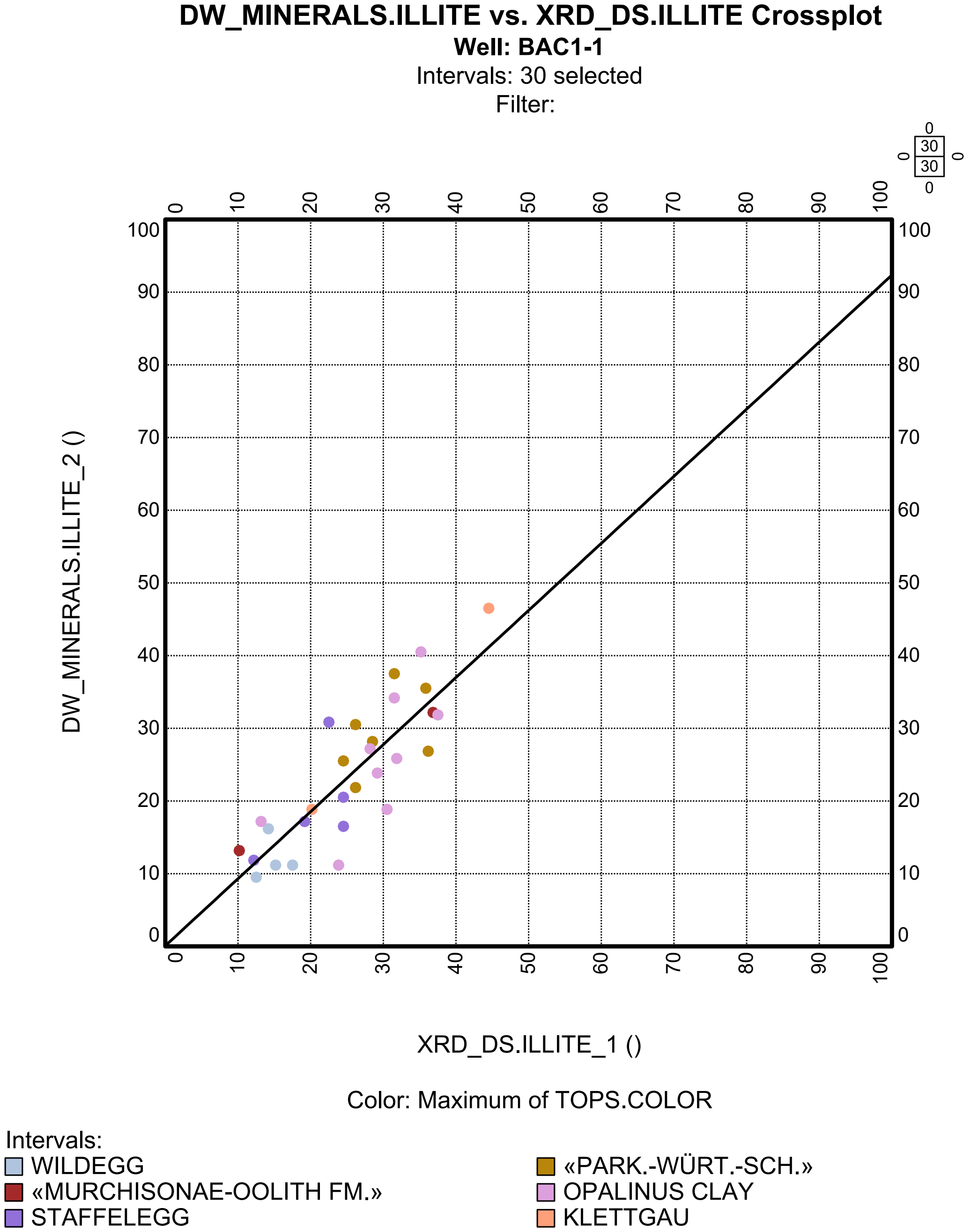

Fig. 4-3: Weight of illite from MultiMin (y-axis) compared to core XRD data (x-axis), Wildegg to Klettgau Formations

The XRD clay endmembers were not measured in all formations. The MultiMin illite content is fairly correlated to the core XRD data (cc = 0.84).

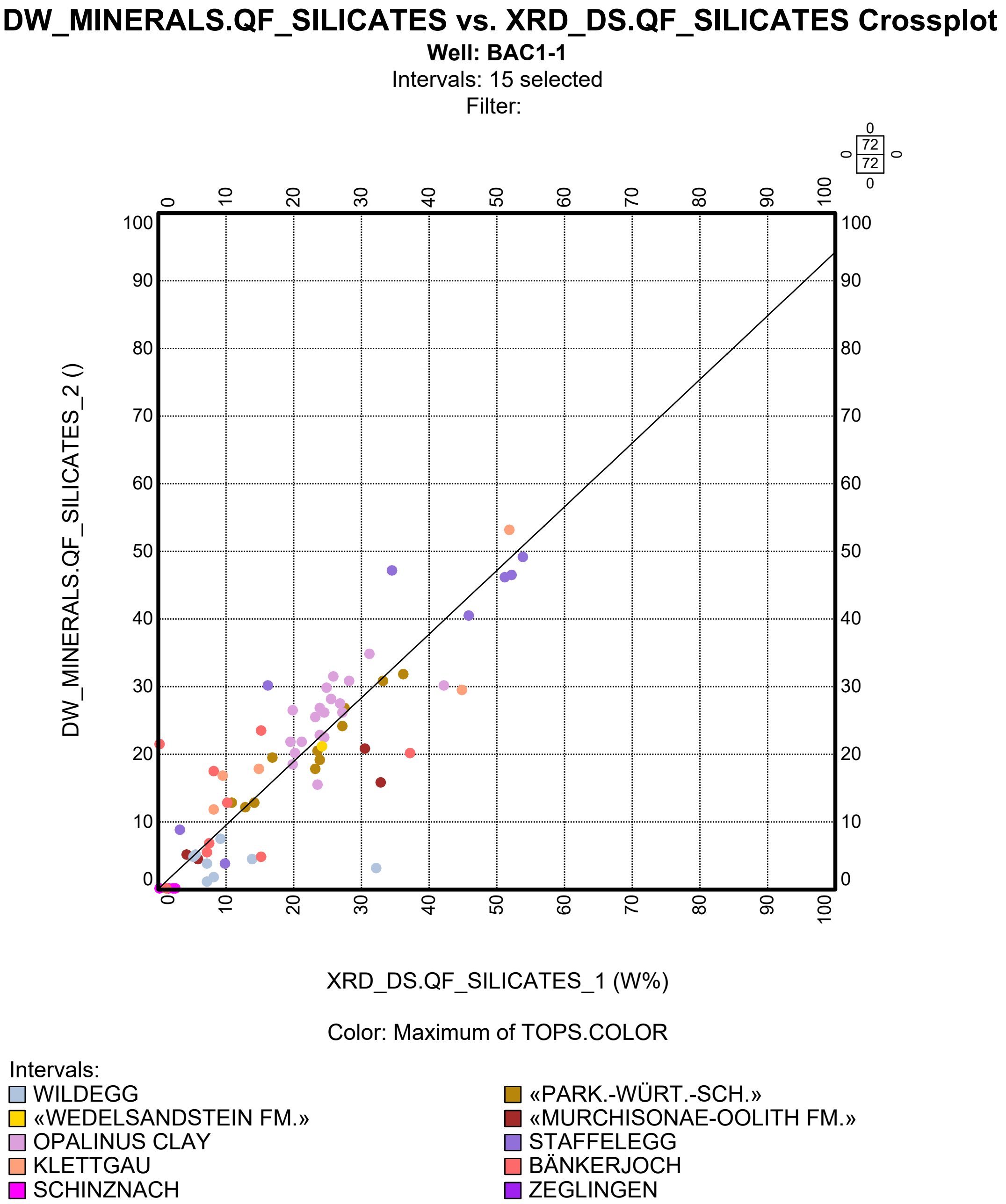

Fig. 4-4: Weight % of QF-silicates from MultiMin (y-axis) compared to core XRD data (x-axis), Wildegg to Zeglingen Formations

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

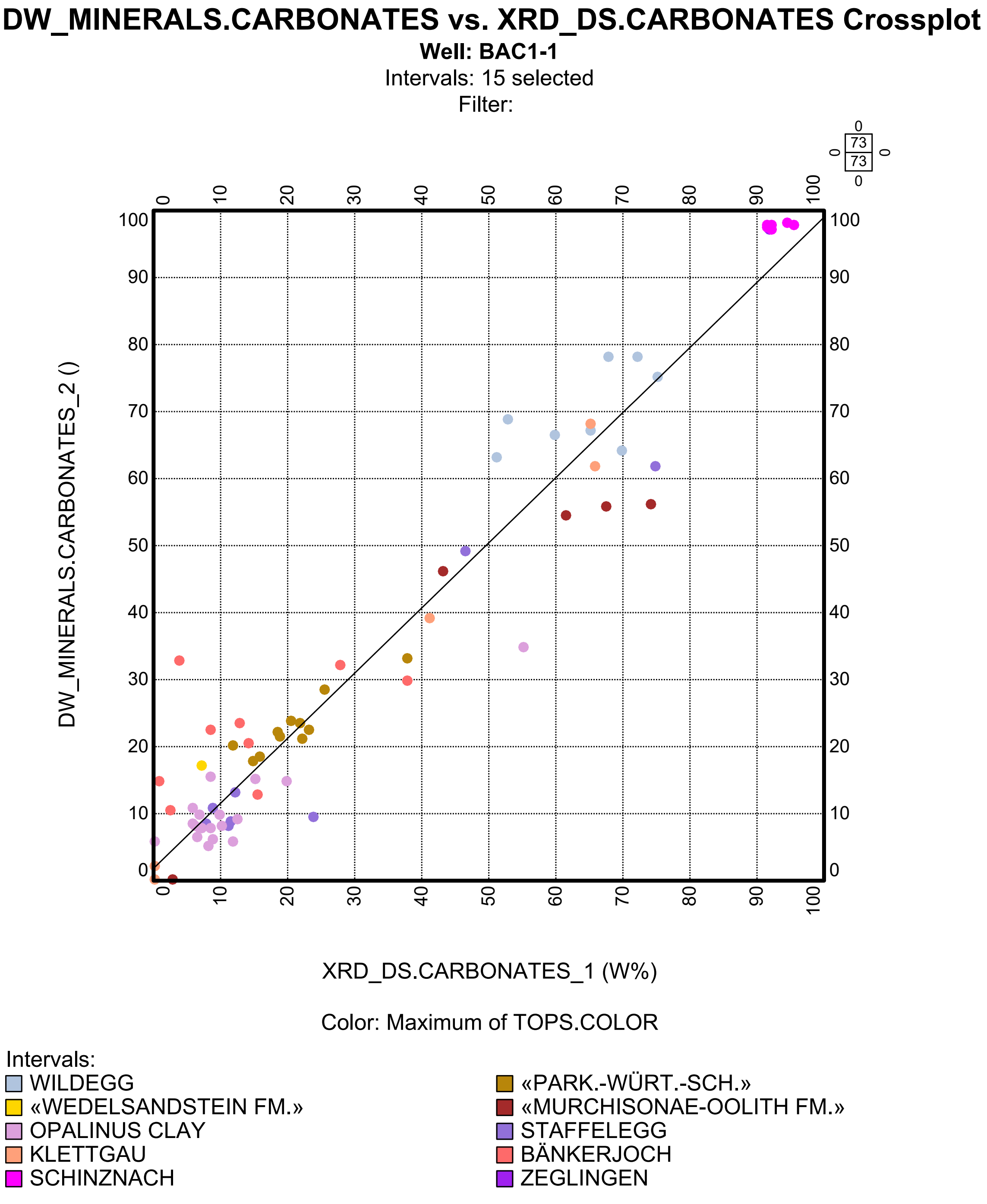

Fig. 4-5: Weight % of carbonates from MultiMin (y-axis) compared to core XRD data (x-axis), Wildegg to Zeglingen Formations

The carbonates include the calcite, dolomite and siderite content. The calibration to core XRD data is good (cc = 0.96), despite a few outliers and local heterogeneities.

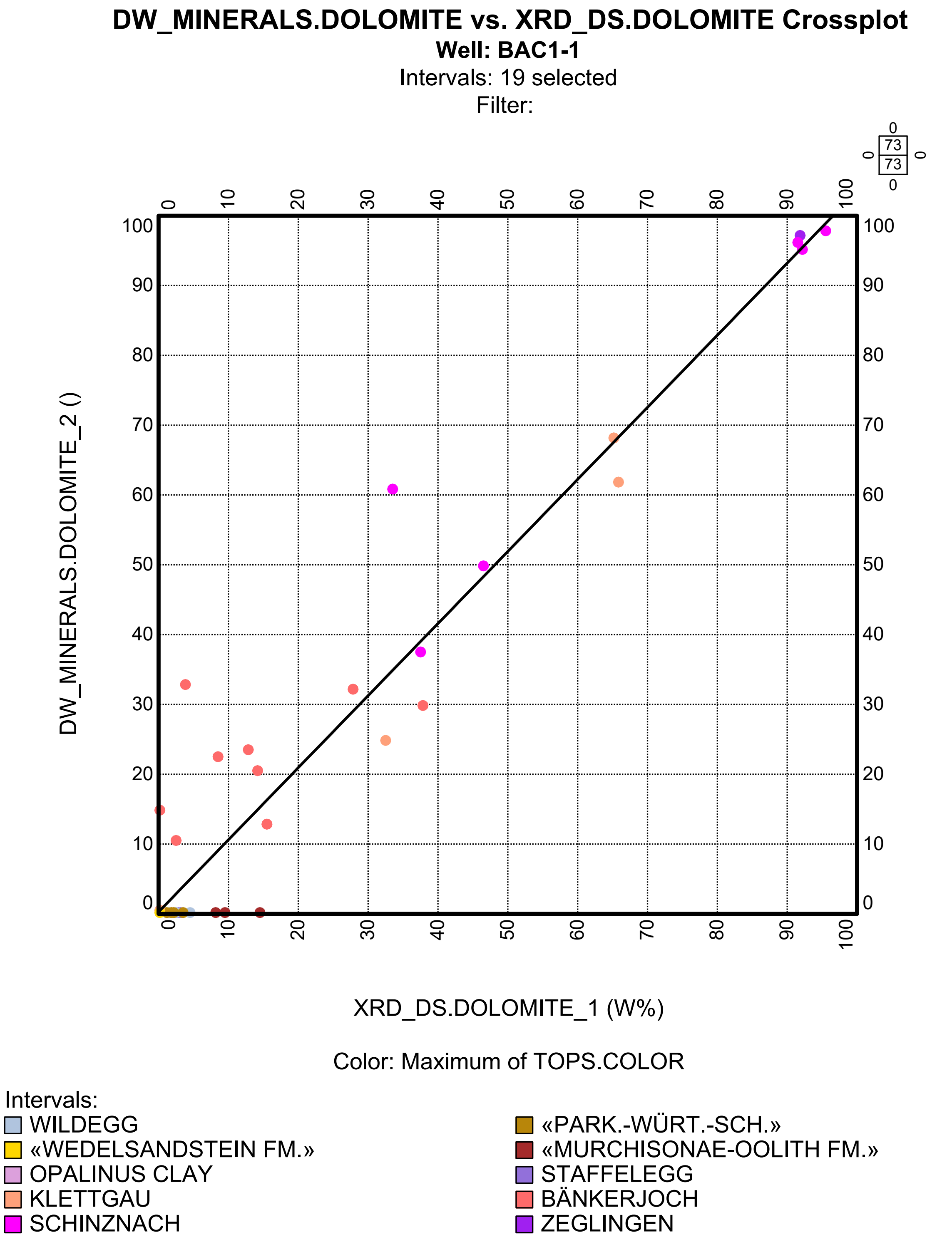

Fig. 4-6: Weight % of dolomite from MultiMin (y-axis) compared to core XRD data (x-axis), Wildegg to Zeglingen Formations

The dolomites are mostly located in the Triassic, within complex mineralogical settings including anhydrite. The calibration to core XRD data is good although the correlation coefficient is meaningless (cc = 0.95) due to low number of dolomitic samples.

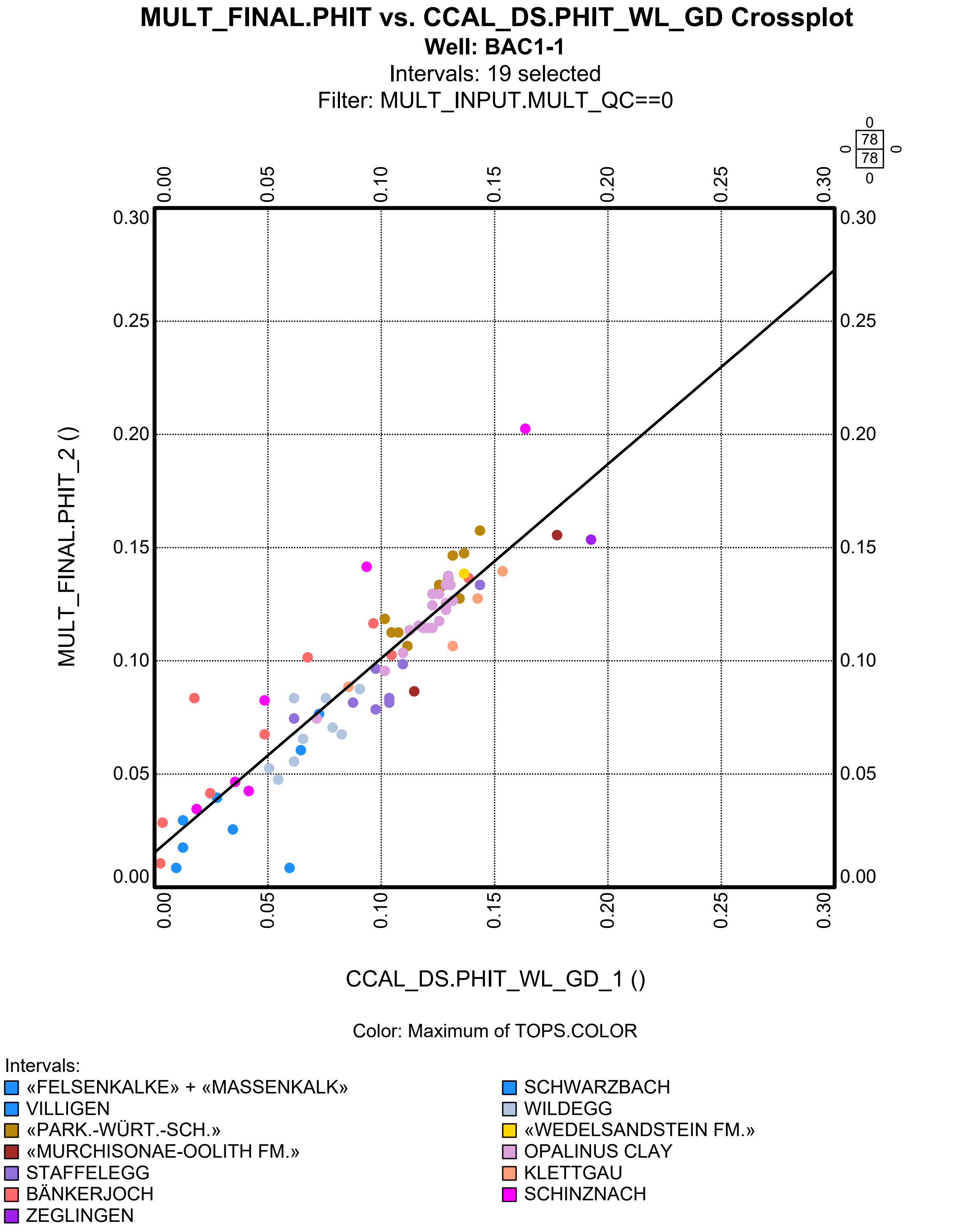

Fig. 4-7: Total porosity from MultiMin (v/v, y-axis) compared to core data (x-axis), «Felsenkalke» + «Massenkalk» to Zeglingen Formation

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 good (cc = 0.92).

4.2 Main results of the core-calibrated log analyses in the borehole BAC1-1

The main aim of the MultiMin interpretation were continuous curves of porosity and clay content of the borehole BAC1-1. 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 senso 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 (senso stricto) and feldspars.

Malm (462.0 – 737.32 m, «Felsenkalke» + «Massenkalk», Schwarzbach Formation, Villigen Formation and Wildegg Formation):

The top part of the «Felsenkalke» + «Massenkalk was logged in the first section of BAC1-1, during the technical logging. Only total gamma ray and sonic curves are available. The log data in the second section starts at 518.0 m, leaving a gap above with no MultiMin analysis.

As expected, carbonates are the main constituents in the formations of the Malm, the mean calcite content is 79.3 wt.-% (median of 81.1 wt.-%). Lithological changes (e.g. at group boundaries) are sometimes reflected in a sharp negative peak (i.e. decreasing carbonate content at the top Schwarzbach Fm. correlated to clay content increase), but, in general, variance of the carbonates in the Malm is low.

Generally, the clay content is low in the Malm, in BAC1-1 the clean top part could not be analysed. Consequently, the clay content mean is 16.8 wt.-% and the median 15.7 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 52.4 wt.-% with a mean and median of 26.2 and 26.6 wt.-%. In the Schwarzbach Formation, the maximum clay content is 35.9 wt.-% with a mean and median of 19.3 and 18.4 wt.-%.

Only more argillaceous and correlatively, the Schwarzbach and Wildegg Formations are less calcareous: respectively 78.9 wt.-% mean calcite in the Schwarzbach Formation and 68.6 wt.-% mean 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 4.4 wt.-% on core XRD data in the Villigen Formation). No siderite was measured on core XRD.

The QF-silicate content in the Malm is low (mean of 3.2 wt.-%, median of 2.3 wt.-%). The more clay-rich lithologies (Wildegg Formation) show a slightly increased QF-silicate content (mean/median Wildegg Formation: 4.4/3.5 wt.-%).

Total porosity in the Malm ranges between 0 and 14.7% (mean of 7.2%, median of 7.3%). The highest porosity (14.7%) is observed in the Wildegg Formation but must be treated with caution as they might represent artefacts due to a reduced data quality in these intervals; it was filtered with the MULT_QC flag.

Dogger (737.32 – 915.3 m, Wutach Formation, Variansmergel + «Parkinsoni-Württembergica-Schichten», «Herrenwis Unit», Wedelsandstein Formation, «Murchisonae-Oolith Formation», Opalinus Clay):

The boundary between the Malm and the Dogger is clearly marked by a sharp increase of iron content (DWFE_ALKNA up to 10.3 wt.-%), the clay content (characterized by a gamma ray peak, mostly thorium) 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 18.9 wt.-% and a median of 13.9 wt.-%. The carbonate content is dominated by the calcite above the Opalinus Clay (mean/median 30.1/26.9 wt.-%), and the calcite plus siderite in the Opalinus Clay (mean/median calcite 8.9/6.8 wt.-%; mean/median siderite 2.4/2.5 wt.-%). Moderate amounts of dolomite were measured with the core XRD in the «Murchinsonae-Oolith Formation», up to 14.34 wt.-%. This mineral was not modelled by MultiMin, as the ECS MGWALK closure model was not available.

The interval from 811 – 819 m at the top Opalinus Clay has a higher calcite content than the rest of the formation: mean 28.4 wt.-% and median 31.1 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 characterized due to the limited vertical resolution of the ECS tool.

The ECS iron contents (DWFE_WALK2 and DWFE_ALKNA) show high values in the Dogger, mostly in the Wutach Formation, at the base «Parkinsoni-Württembergica-Schichten» and at the base «Murchisonae-Oolith» Formations The XRD analysis on core samples identified several iron minerals and locally high concentration: siderite (mostly in the Opalinus Clay), goethite (up to 18.81 wt.-% in the «Murchisonae-Oolith Formation») and some pyrite.

The QF-Silicate content in the Dogger ranges between 0.8 and 40.0 wt.-%. The mean and median values (22.4 wt.-% and 23.9 wt.-%) are mostly related to the silicates content of the shaliest intervals like the Opalinus Clay.

The Opalinus Clay in the Dogger certainly is the formation with the highest clay content, ranging between 30.9 and 76.8 wt.-% (mean/median of 61.4/63.3 wt.-%). The clay content is high but variable in the formations above (minimum 22.4 wt.-%, maximum 81.4 wt.-%, mean/median of 49.3/48.9 wt.-%). Note that the maximum value is in a washout, and likely overestimated.

Total porosity of the Dogger also is different between the different units. PHIT is not very variable in the Opalinus Clay (minimum / maximum 6.3% / 14.2%, mean and median 11.7% and 12.0% with a low standard deviation 1.5%). It is more variable in the overlying Dogger formations (minimum / maximum 5.9% / 17.9%, mean / median 12.2% / 12.4% and a standard deviation 2.4%).

Lias (915.3 – 950.07 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 varies between the different members. It is high in the upper part, Gross Wolf down to Grünschholz/Breitenmatt/Rickenbach Members (maximum 79.8 wt.-%, mean/median 55.5/53.5 wt.-%) and in the Beggingen Member (maximum 82.5 wt.-%, mean/median 62.6/77.0 wt.-%). The Frick and Schambelen Members have a relatively lower carbonate content, respectively maximum 63.7 wt.-% and mean/median 12.6/10.8 wt.-%, and maximum 35.3 wt.-% and mean/median 15.2/15.8 wt.-%.

As in the previous groups, the carbonate content is dominated by calcite, low dolomite content was measured by cores XRD (up to 3.29 wt.-%) and no siderite. The dolomite was not modelled with MultiMin in the Staffelegg Formation.

The QF-silicate content is reversely correlated to the carbonate content. While the Gross Wolf down to Grünschholz/Breitenmatt/Rickenbach Members and the Beggingen Member show a moderate QF-silicate content (respectively mean/median 6.7/5.9 wt.-% and 1.9/0.8 wt.-%), the Frick and Schambelen Members show higher QF-silicate contents (respectively mean/median 44.2/45.0 wt.-% and 17.7/17.4 wt.-%).

The clay content follows a similar trend as the QF-silicates, moderate in Gross Wolf down to Grünschholz/Breitenmatt/Rickenbach Members and the Beggingen Member (respectively mean/median 33.6/35.1 wt.-% and 27.9/19.0 wt.-%) and higher in the Frick and Schambelen Members (respectively mean/median 42.4/43.4 wt.-% and 65.5 wt.-%).

The Staffelegg Formation is also characterised by high total organic carbon (TOC). The maximum TOC measured on cores was 5.37 wt.-%, while the maximum TOC MultiMin output was 6.6 wt.-%.

An iron-rich layer measured on the ECS DWFE_ALKNA (maximum 0.18 W/W in the Beggingen Member), high APLC was interpreted as an iron hydroxide mineral and modelled as goethite, although not thorium-rich.

The total porosity in the Staffelegg Formation ranges between 2.9 and 18.3%, mean/median 9.0/8.5% (filtered for the MULT_QC flag).

Keuper (950.07 – 1'054.3 m, Klettgau Formation, Bänkerjoch Formation):

The first meters of the Klettgau Formation could not be interpreted, as the wireline logs were missing between sections II and III. The transition between the Lias and the Keuper can therefore not be described in BAC1-1.

In the Keuper, the top part of the Klettgau Formation (Gruhalde to Gansingen Members) is characterised by a complex mineralogical mixture of carbonates (mostly dolomite) between 24.3 wt.-% and 86.3 wt.-%, mean/median 56.0/53.5 wt.-%, silicates (quartz and feldspars) between 7.8 wt.-% and 39.0 wt.-%, mean/median 15.7/14.9 wt.-%, and clays (dominant illite) between 5.0 wt.-% and 55.5 wt.-%, mean/median 27.9/28.4 wt.-%.

The base Klettgau Formation (Ergolz Member) is an argillaceous layer with up to 58.9 wt.-% QF-silicates, mean/median 35.4/33.5 wt.-%. The clay content is 55.2 wt.-% mean and 50.5 wt.-% median.

The underlying Bänkerjoch Formation is dominated by anhydritic deposits: 0 to 93.6 wt.-% (mean/median 41.1/39.4 wt.-%). In complement, carbonates (dolomite), clays and QF-silicates are well represented in this formation.

The Keuper total porosity ranges from 0 to 19.1% (mean 9.5% and median 9.7%). The lowest porosities correspond to the anhydrites, while the highest are located in the argillaceous layers.

The wireline log quality is often good in the Keuper, with a locally slightly enlarged caliper (in the Ergolz Member) and HDRA above 0 g/cc suggesting local wall rugosity. The MultiMin quality indicator is often above 1, indicating a limited log redundancy in a complex mineralogy setting.

Muschelkalk (1'054.3 – 1'243.12 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) and a correlated decrease of anhydrite. The Asp and Stamberg Members are mostly dolomitic (except for a thin peak of QF-silicate and clay content at base Asp Member), while the Liedertswil Member is a progressive transition from dolomites to dolomitic limestones at Leutschenberg/Kienberg Member bottom. The bottom part of the Leutschenberg/ Kienberg Member is again more dolomitic.

The carbonate content of the Schinznach Formation ranges from 0.1 to 98.2 wt.-% (mean 95.2 wt.-%, median 97.4 wt.-%): mean/median 90.0/94.2 wt.-% dolomite in the Asp and Stamberg Members at the top, 43.2/46.9 wt.-% dolomite and 54.1/51.0 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 Obere Sulfatzone Member is mostly anhydritic below 1'143.4 m.

The «Salzlager» Member is an intercalation of thick (up to 12.9 m) halite and anhydrite beds with low clay content. Washouts are observed in front of the halite beds, affecting log quality. A two-meter argillaceous limestone layer is noticed towards the base.

The «Untere Sulfatzone» is a massive anhydrite bed, with an increasing carbonate content at its base. The carbonate and clay content increase in the Kaiseraugst Formation, with a complex mineralogical mixture of carbonates, QF-silicates and clays: mean/median 28.8/26.8 wt.-% carbonates, 19.9/16.4 wt.-% QF-silicates and 45.8/51.7 wt.-% clays. A thin (2.5 m) anhydritic bed is seen at base Orbicularismergel Member, in the top part of the Kaiseraugst Formation.

Total porosity in the Muschelkalk is very variable and ranges between 0 and 26.7%. The highest values are located within the dolomites of the Stamberg Member at the top Schinznach Formation.

The lowest porosity rocks are the halite beds, anhydrites and the dolomitic limestones in the Liedertswil and Leutschenberg/Kienberg Members at the base Schinznach Formation.

Buntsandstein (1'243.12 – 1'257.26 m, Dinkelberg Formation):

The boundary from the Muschelkalk to the sandstones of the Buntsandstein is characterised by a progressive increase of the QF-silicate content and a correlative decrease of clay content.

The clay content is moderate (mean/median: 15.0/14.3 wt.-%, minimum 8.0 wt.-%, maximum 28.1 wt.-%). The QF-silicate content is high in the Buntsandstein (mean/median of 79.3/79.9 wt.-%, maximum 91.8 wt.-%).

A relatively high dolomite content is evidenced from the ECS elements (calcium and magnesium are measured with the MGWALK closure model) in the top half of the Dinkelberg Formation. The maximum carbonates content is 29.9 wt.-%, the mean/median 5.5/0.9 wt.-%.

The porosity seems to be reversely correlated to the carbonate content in the top half (possible carbonate cementation of the sandstone). Total porosity in the Buntsandstein ranges from 4.1 to 13.9% (mean 9.1%, median 8.8%).

Rotliegend (1'257.26 – 1'306.77 m, Weitenau Formation):

The main Weitenau Formation lithology is an argillaceous arkosic sandstone.

The dry clay content is moderate, maximum 32.8 wt.-%, mean/median 26.0/26.2 wt.-%. Correlatively, the QF-silicate content is high (mean and median: 68.9 and 69.0 wt.-%, maximum 76.7 wt.-%).

The carbonate content in the Weitenau Formation is low (mean/median 5.1/4.8 wt.-%, maximum 16.7 wt.-%).

The Weitenau Formation is a low total porosity formation: 2.4 to 7.7%, mean/median 4.1%.

4.3 Main results of the core-calibrated log analysis in the Opalinus Clay (808.57 – 915.3 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 4-15 show some general statistical values of the MultiMin analysis results within the Opalinus Clay.

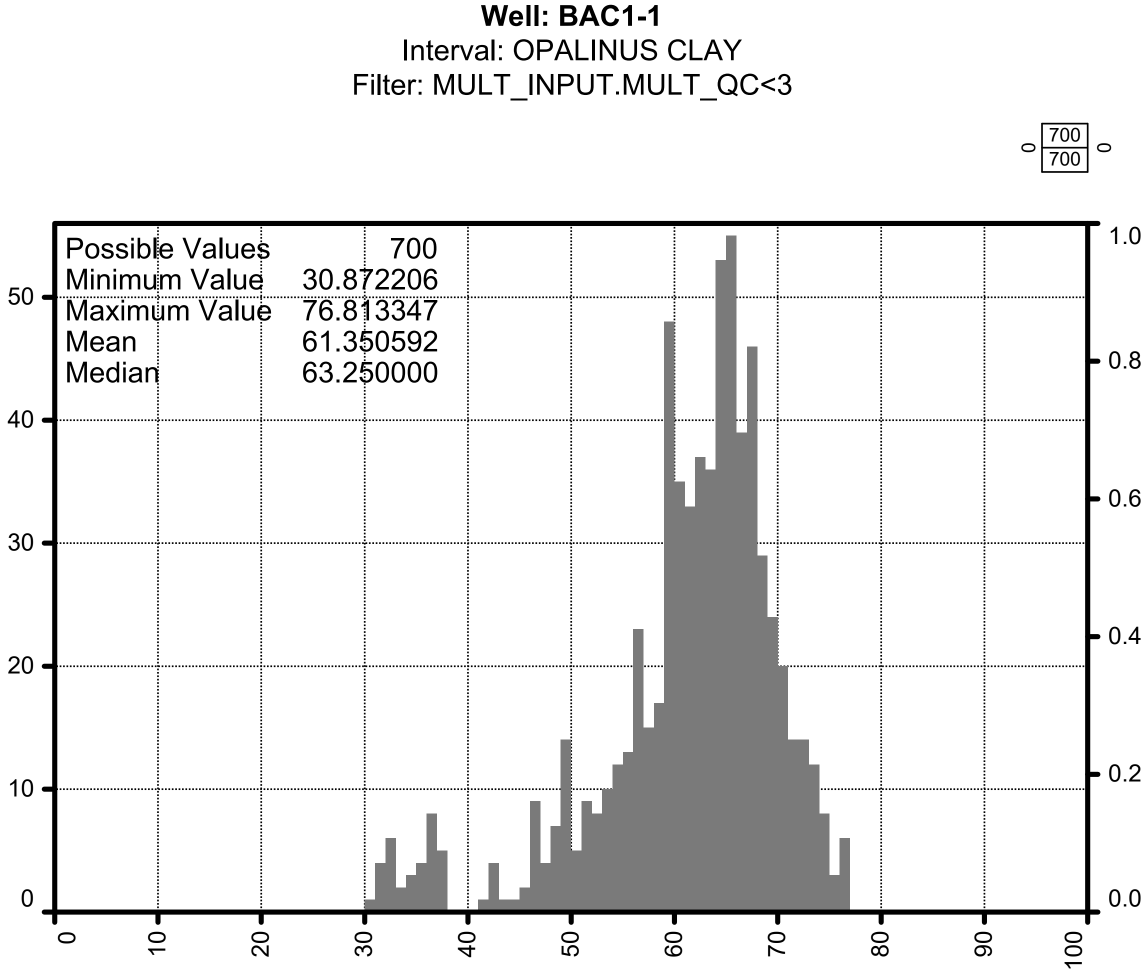

Fig. 4-8: Dry clay weight percentage frequency histogram in the Opalinus Clay

X-axis is the dry clay weight % 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 61.4 and 63.3 wt.-%. The lower part of the Opalinus Clay is more argillaceous than the top, as demonstrated in the two next figures.

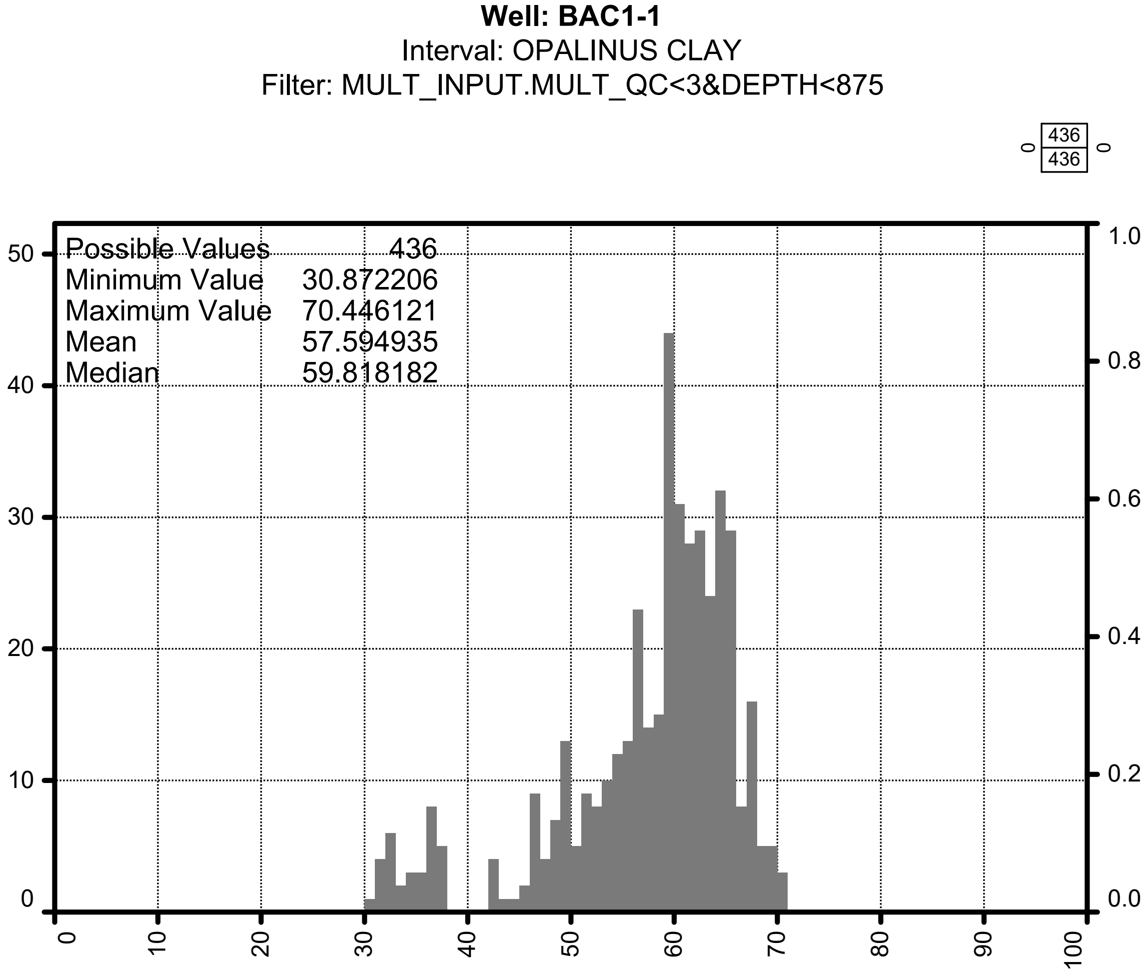

Fig. 4-9: Dry clay weight percentage frequency histogram in the upper section of the Opalinus Clay (above 875.0 m)

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

In the upper part of the Opalinus Clay (above 875.0 m), the mean and median dry clay contents are close to 57.6 and 59.8 wt.-%. The top part of the formation is less argillaceous than the bottom, see next figure.

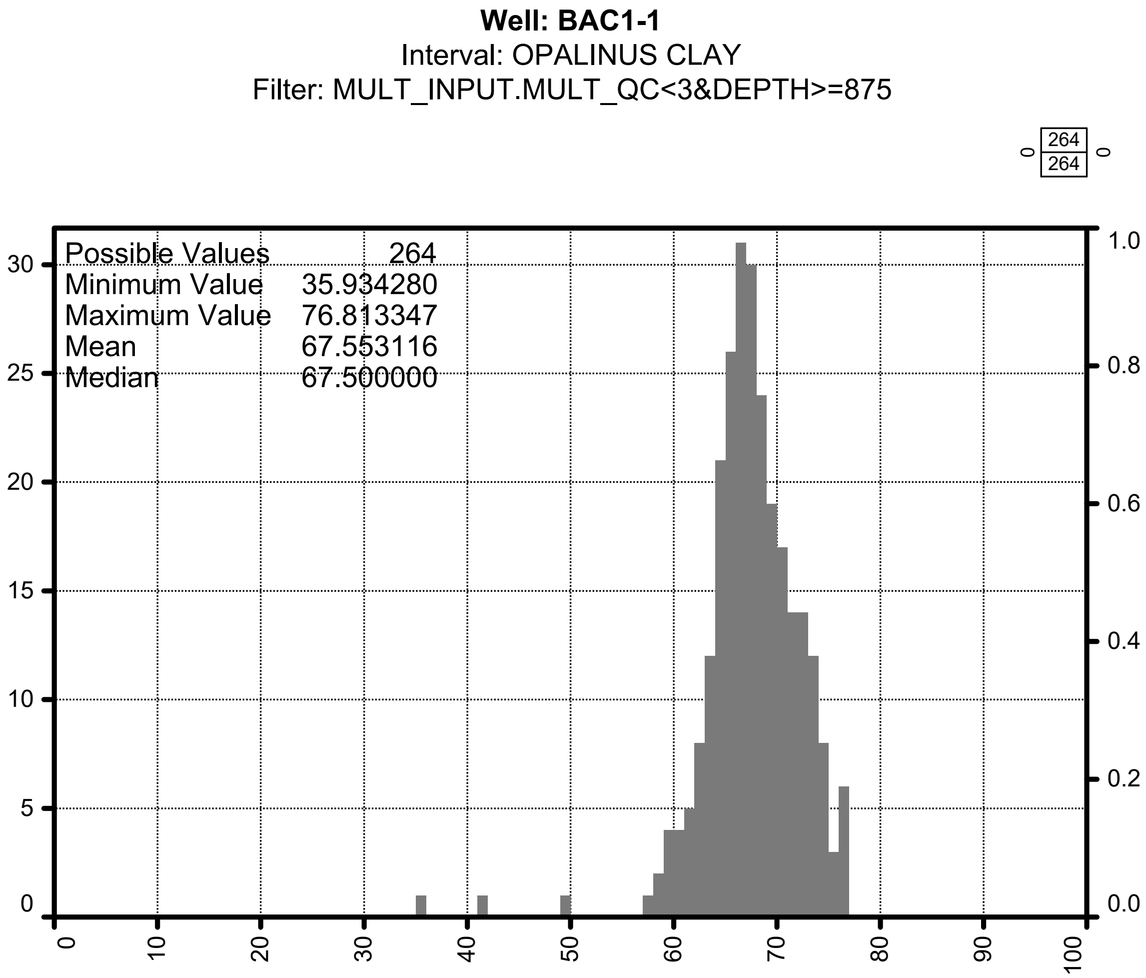

Fig. 4-10: Dry clay weight percentage frequency histogram in the lower section of the Opalinus Clay (below 875.0 m)

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

The bottom part of the Opalinus Clay (below 875.0 m), is more argillaceous: the mean and median dry clay content are close to 67.6 and 67.5 wt.-%.

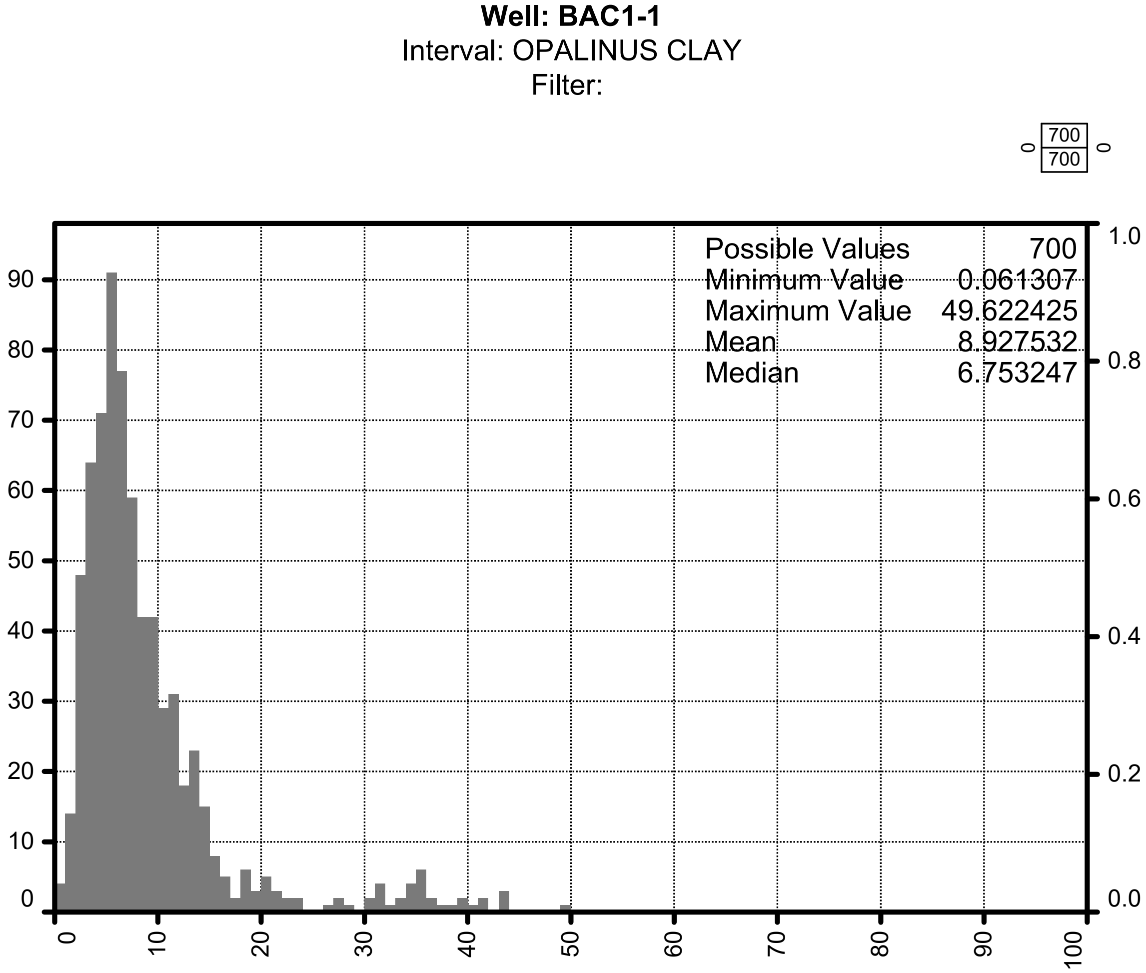

Fig. 4-11: Calcite weight percentage frequency histogram in the Opalinus Clay

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

The mean and median calcite content are close to 8.9 and 6.8 wt.-%. The maximum values are up to 49.6 wt.-%, i.e., corresponding to thin, calcite-rich layers. In case these layers are thinner than the log resolution, the maximum calcite content may be higher than computed by MultiMin.

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

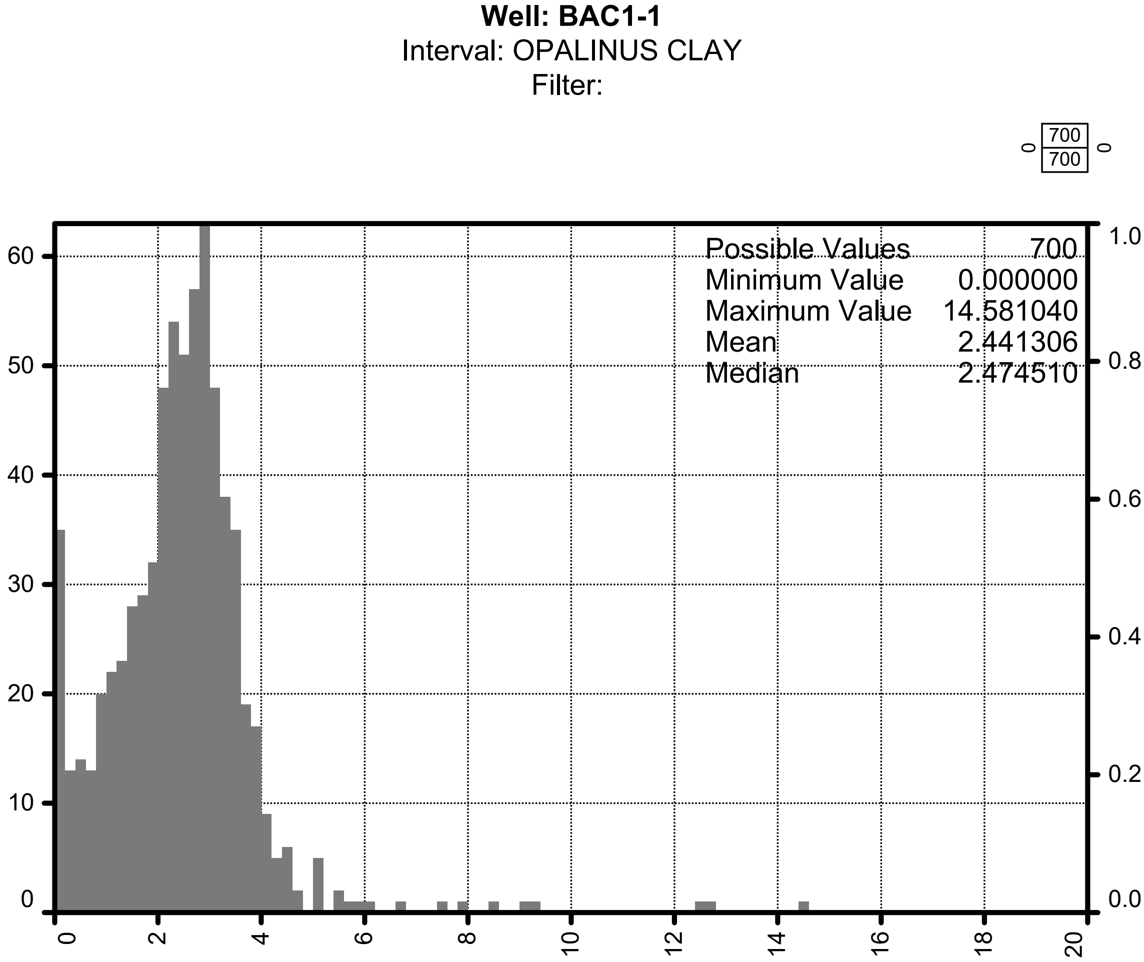

Fig. 4-12: Siderite weight percentage frequency histogram in the Opalinus Clay

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

The mean and median siderite content is close to 2.4 and 2.5 wt.-%, with a maximum value of 14.6 wt.-% and minimum values of 0 wt.-%. Please note that the siderite core calibration is less constrained than other minerals.

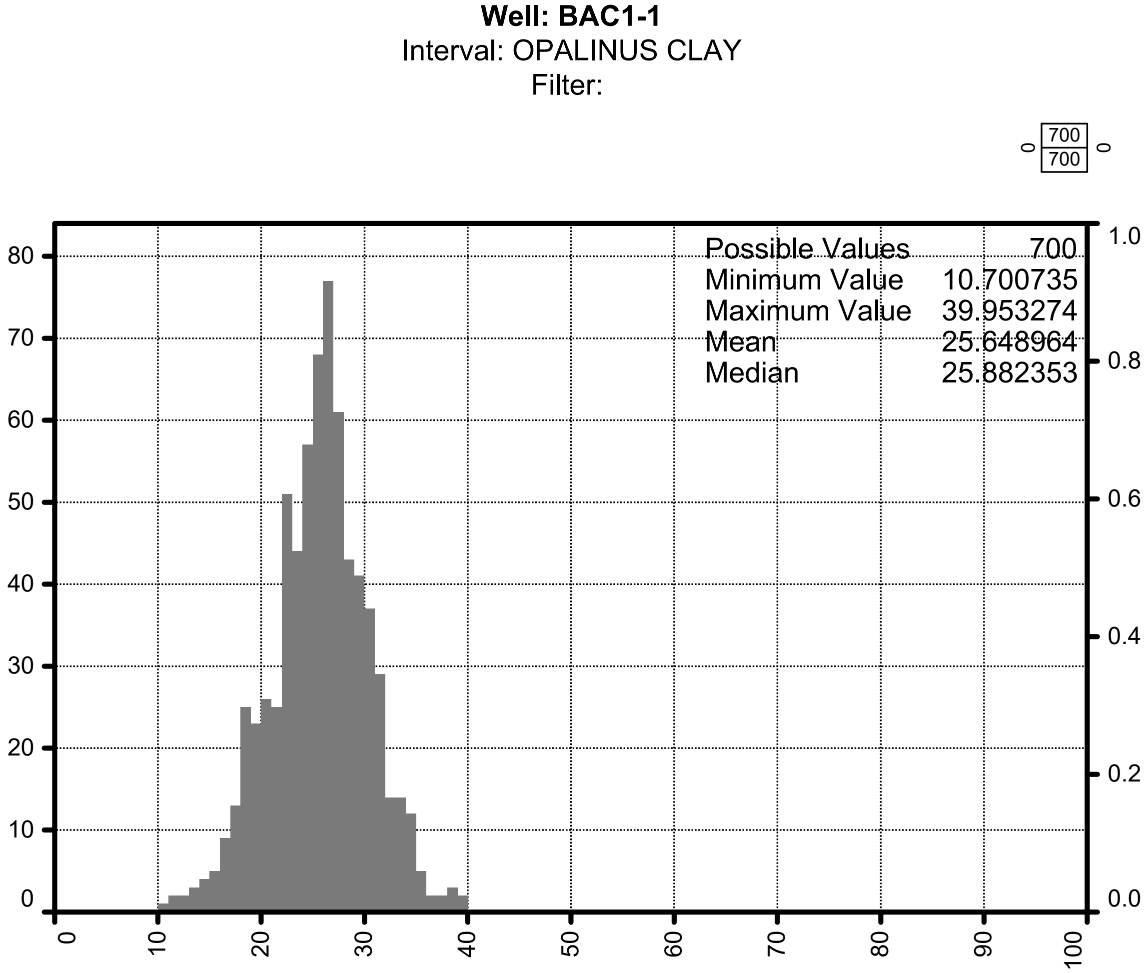

Fig. 4-13: QF-silicates (quartz and feldspars) weight percentage frequency histogram in the Opalinus Clay

X-axis is the QF-silicates weight % 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 25.6 and 25.9 wt.-%, much higher than the carbonates (calcite close to 8.9/6.8 wt.-%).

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

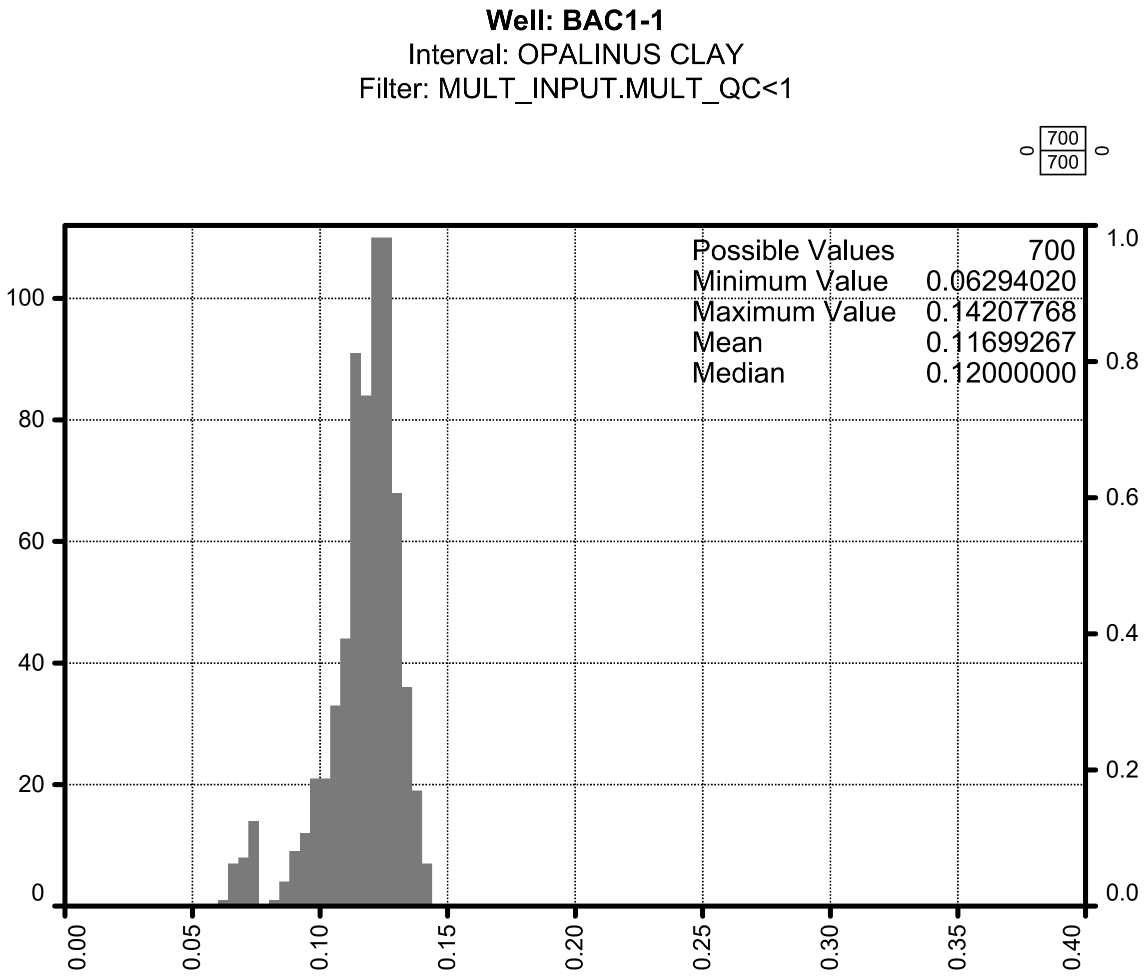

Fig. 4-14: Total porosity frequency histogram in the Opalinus Clay

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 close to 11.7 and 12.0%, with a range from 6.3 to 14.2%.

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

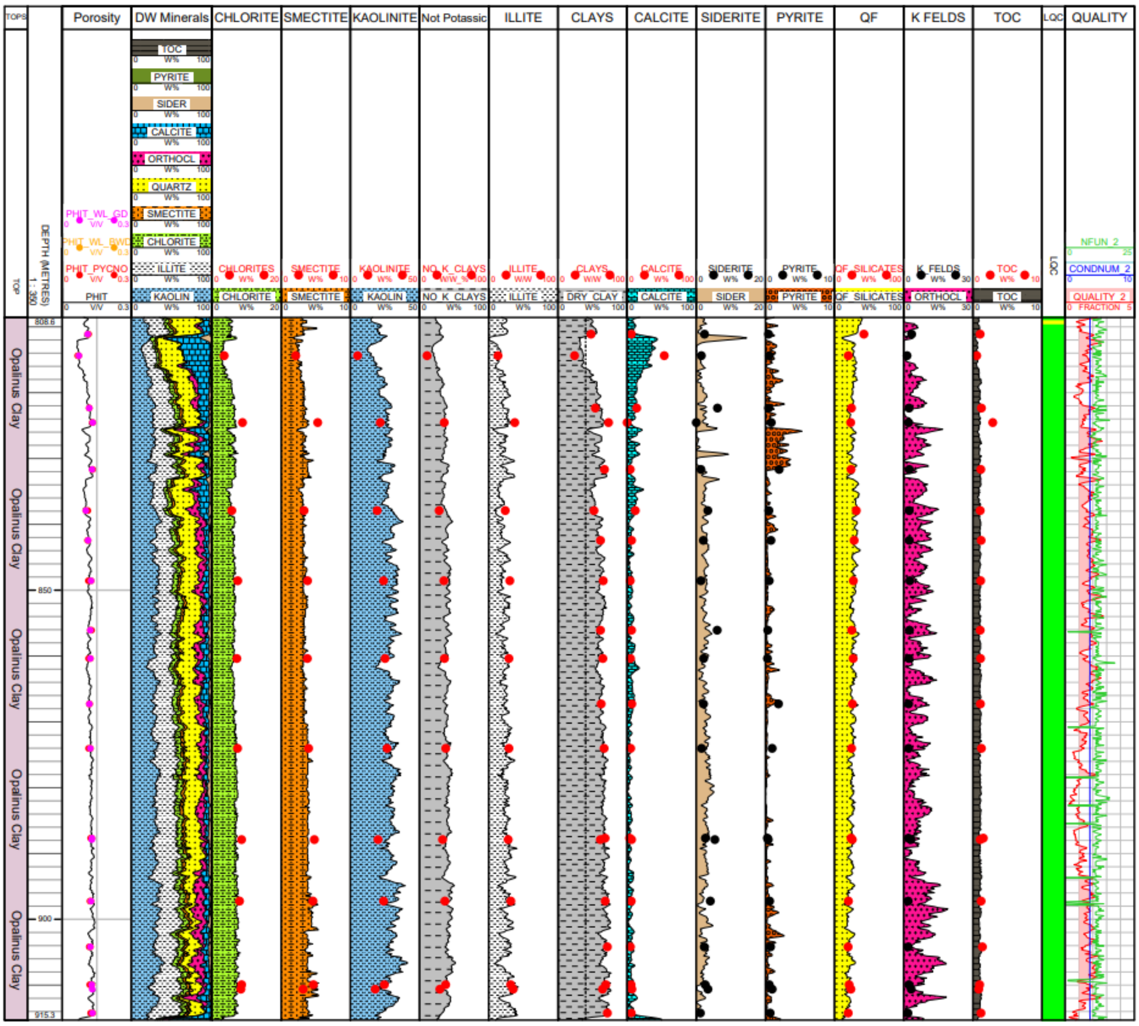

Fig. 4-15: Main MultiMin and core results in the Opalinus Clay

The back line in the "CLAYS" track represents a 40% baseline, circles represent lab measurements.

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 mineral dry weights, including clay endmembers, are well calibrated to the core measurements. The K-feldspars calibration is 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) except in the uppermost 20 m. A few carbonates streaks in the top part have a lower clay content.

5 Summary

The MultiMin interpretation was successfully applied in the borehole BAC1-1 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 calibration data 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 total porosity is well calibrated to core pycnometer and water-loss measurements.

The continuous curves from the MultiMin interpretation can be used to characterise the different formations (and hence members) occurring in BAC1-1. The Opalinus Clay shows a quite variable total clay content though in most locations it is well above 40 wt.-%, except in the uppermost 20 m. The lower third of the formation is 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 clays, QF-silicates and/or carbonate content. 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). The recent measurement of the magnesium content with the ECS tool (MGWALK closure model) greatly supported the calcite-dolomite characterisation in these formations. Similarly, the aluminium quantification with the ECS ALKNA closure model supported the clay content evaluation in the Malm and Dogger.

6 References

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