nagra.

Arbeitsbericht NAB 21-01

Determination of the Cation Exchange Capacities and Exchangeable Cations of deep Drilling Core Samples from the Siting Regions Jura Ost, Nördlich Lägern and Zürich Nordost

September 2022

National Cooperative
for the Disposal of
Radioactive Waste

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

www.nagra.ch

nagra.

Arbeitsbericht NAB 21-01

Determination of the Cation Exchange Capacities and Exchangeable Cations of deep Drilling Core Samples from the Siting Regions Jura Ost, Nördlich Lägern and Zürich Nordost

September 2022

B. Baeyens & M. M. Fernandes

PSI, Villigen

KEYWORDS

Siting regions, drill cores, argillaceous rocks, clay mineral content, cation exchange capacities, exchangeable cations

National Cooperative
for the Disposal of
Radioactive Waste

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

www.nagra.ch

Nagra Arbeitsberichte ("Working Reports") present the results of work in progress that have not necessarily been subject to a comprehensive review. They are intended to provide rapid dissemination of current information.
This report was prepared on behalf of Nagra. The viewpoints presented and conclusions reached are those of the author(s) and do not necessarily represent those of Nagra.

Table of Contents

List of Tables

List of Figures

1 Introduction

Opalinus Clay, an argillaceous sedimentary rock formation, is selected as the potential host rock for the deep geological disposal of radioactive Waste in Switzerland. In Stage 3 of the Sectoral Plan (Sachplan Geologisches Tiefenlager, Etappe 3) (Swiss Federal Office of Energy 2008), Nagra is thoroughly investigating the three remaining siting regions, namely Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO), where Opalinus Clay is present and meets the requirements related to its thickness and depth. In addition to 3D seismic measurements and quaternary boreholes, deep borehole investigations have the aim to complete the already existing overall picture of the underground geological environment in these regions. The outcome of these investigations and the safety-based comparison of the siting regions will contribute to guide Nagra's choice of the region best suited for a deep geological repository.

Site-specific physico-chemical rock data such as cation exchange capacities (CEC) and exchangeable cation occupancies are, amongst other geochemical and mineralogical parameters, part of the deep borehole investigations and are required for each potential region for the site selection procedure. This report focuses mainly on the CEC of the rock samples and on the cation occupancies of exchangeable alkaline and alkaline earth elements. The CEC is a measure of the total negative charge of the rock samples, resulting predominantly from the presence of 2:1 phyllosilicates on which cations adsorb on the planar sites via electrostatic bonding. CEC can also be defined as the sum of exchangeable cations at the clay mineral surfaces of the rock samples. The CEC is directly correlated to the content and type of clay minerals in the rock samples, and consequently to their adsorption properties towards radionuclides. Its variability is an excellent indicator for the homogeneity of the clay mineral content along the Opalinus Clay formation as well as to the upper and lower confining units for each borehole. The in-situ fractional occupancies of exchangeable cations, defined by the quantity of adsorbed cation (in meq/kg) divided by the CEC (in meq/kg) of the rock samples, can act as a “fingerprint” for the in-situ porewater compositions of the formation. In general, the composition of the porewater of rock formations consists essentially of solutes such as Cl resulting from the hydrologic evolution of the rock, and of solutes resulting from equilibrium with the minerals constituting the rock. In argillaceous rocks, the concentrations of dissolved cations are largely determined by cation exchange equilibria with the clay mineral fraction and by the equilibrium with carbonate and sulphide/sulphate minerals.

The objective of this work, mandated by Nagra, is to quantify the CEC and the pool of exchangeable cations of rock samples from 7 boreholes across the geological siting regions Jura Ost (JO), Nördlich Lägern (NL), and Zürich Nordost (ZNO). The samples were selected to represent the different lithologies of the natural barrier system, i.e., Opalinus Clay and the upper and lower confining units. 141 rock samples have been analysed with the focus on CEC and cation exchange occupancies. This report gives a detailed overview of the results obtained for the representative rock samples from Bözberg-1, Bözberg-2, Bülach-1, Stadel-2, Stadel-3, Trüllikon-1 and Marthalen-1.

2 Material and methodology

2.1 Material

The samples analysed in this study originated from the geological siting regions Jura Ost (JO), Nördlich Lägern (NL), and Zürich Nordost (ZNO) (Fig. 2-1), specifically from the cores recovered from the deep boreholes Bözberg-1-1 (BOZ1) and Bözberg-2-1 (BOZ2) from JO, Bülach-1-1 (BUL1), Stadel-2-1 (STA2) and Stadel-3-1 (STA3) from NL, and Trüllikon-1-1 (TRU1) and Marthalen-1-1 (MAR1) from ZNO (Fig. 2-1). The detailed descriptions (name, depth, geological formation, mineralogical composition) of the rock samples as provided by the University of Bern are given in Tab. A-1.

The mineralogical characterisation of the samples investigated in this study was performed by the Institute of Geological Sciences of the University of Bern. It should be noted that these analyses were carried out on sub-samples of the main core sample (same or close depth) and are not the identical samples used for the CEC measurements. In general, the sample selection was performed to ensure the determination of the physico-chemical parameters (CEC and cation occupancies) for the potential host rock (i.e., Opalinus Clay) as well as the upper and lower confining units.

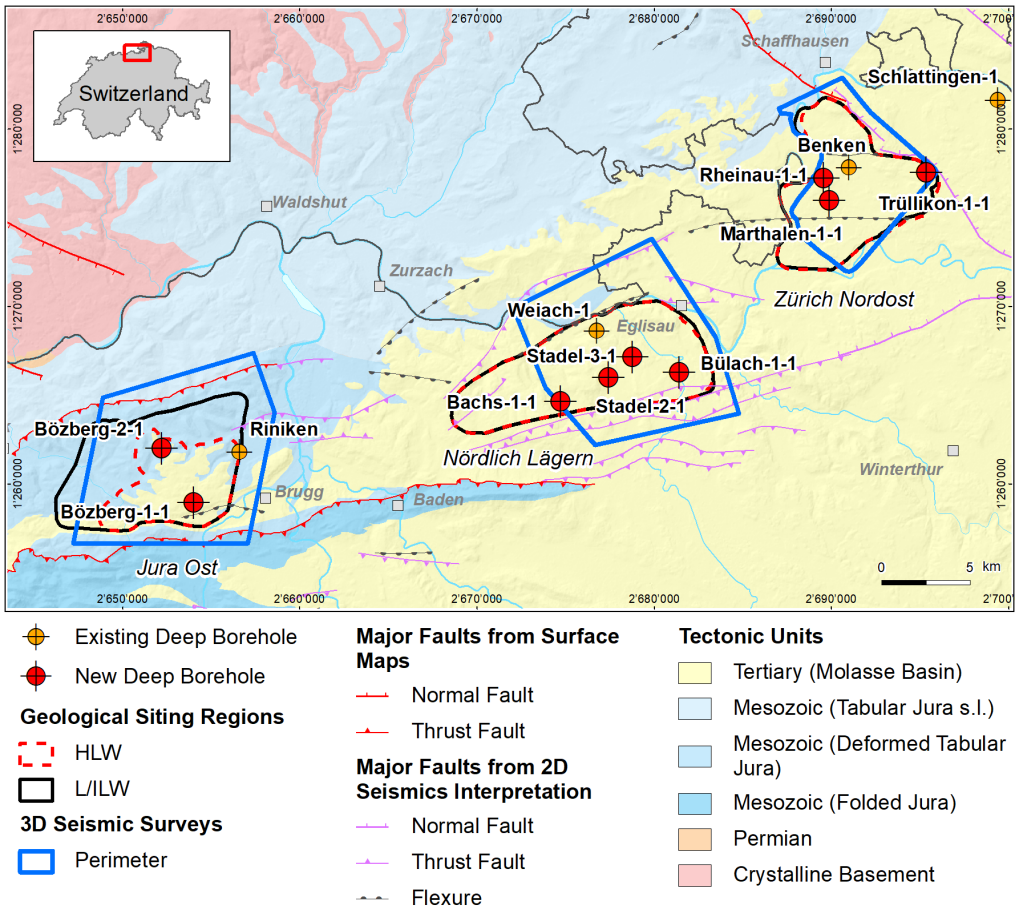

Fig. 2-1: Map illustrating the siting regions of the potential waste repositories, namely Jura Ost (JO), Nördlich Lägern (NL) and Zürich Nordost (ZNO), with details of the individual core locations Bözberg-1, Bözberg-2, Bülach-1, Stadel-2, Stadel-3, Trüllikon-1 and Marthalen-1

The samples (2 × 3 cm^3 cubes) were vacuum packed after preparation at the Institute of Geological Sciences (University of Bern). Once at PSI, the samples were transferred into a N_2 flooded glove box (O_2 < 1 ppm) for crushing and storage. All sample handling was done inside the glove box. The samples were first crushed by hand in an agate mortar to pieces < 1 cm^3. Subsequently, the samples were ground to a size < 1 mm in a Retsch mortar grinder. The grinder was cleaned after each sample to avoid cross-contamination. Samples were stored in the glove box in closed, well-labelled containers.

The core samples of the three siting regions were obtained from various depths (the range of the depths are given in parenthesis):

- 42 rock samples from the region JO were analysed, 32 samples from BOZ1 (266.75 to 808.61 m depth) and 10 samples from BOZ2 (402.15 to 606.13 m depth) (Tab. A-1).
- 68 samples from the region NL were analysed, 26 samples from BUL1 (734.45 to 1026.5 m depth), 20 samples from STA2 (734.53 to 960.43 m depth) and 22 samples from STA3 (700.77 to 924.15 m depth) (Tab. A-2).
- 31 samples from the region ZNO were analysed, 11 samples from TRU1 (722.66 to 951.78 m depth) and 20 samples from MAR1 (521.29 to 741.38 m depth) (Tab. A-3).

2.2 Experimental methodology

The physico-chemical parameters on all rock samples were derived from batch type experiments i.e., crushed rock suspension at low solid to liquid ratios. The water content of the crushed rock samples was determined by measuring the water loss when heated to 105 °C until constant weight was obtained in order to normalize the CEC and extraction data to the same sample dry weight.

A direct quantification of the CEC of the rock samples was carried out using the high selective divalent nickeltriethylenediamine (Ni-en) complex (Peigneur 1976).

The in-situ cation occupancies of Na, K, NH_4, Mg, Ca and Sr were determined by using the high selective Cs^+ index cation (Baeyens & Bradbury 2004). At sufficiently high concentration, this index cation is expected to completely displace and replace all cations present on the exchange sites of clay minerals. The main assumptions of the method are that (i) all cation exchange sites on the clay minerals arising from isomorphous substitution are occupied by the index cation, (ii) the exchange is rapid and reversible, and (iii) that no other site types existing on the surface of the clay mineral are involved. This approach allows the direct quantification of the CEC (consumption of the index cation) and the indirect quantification of the exchangeable cation occupancies (type and amount of cations released after correction for mineral and salt dissolution) of the rock samples.

2.2.1 Cation exchange capacity

In this study, four different approaches were used to determine the CEC of the argillaceous rock samples. Throughout the report CEC is expressed in milliequivalent per kilogram (meq/kg) rock sample. The four different approaches are described below.

Ni-CEC: The CEC of all rock samples was assessed by using the Ni-triethylenediamine (Ni-en) complex radiolabelled with ^{63}Ni. These measurements were carried out under ambient air conditions. For simplicity, the Ni-en CEC data reported in this report are denoted as “Ni-CEC”.

The procedure consists essentially of an adsorption experiment with ^{63}Ni labelled Ni-en. The high selectivity complex was prepared by the addition of uncharged ethylenediamine to a $Ni(NO_3)_2$ solution to obtain a stable Ni-triethylenediamine complex. 30 mL of the ^{63}Ni-en solution were

added to ~ 1 g of rock sample, pre-weighed into polypropylene centrifuge tubes, to give an solid to liquid (S:L) ratio of ~ 32 g·L^{-1}. The tubes were closed, shaken end-over-end for 1 day, centrifuged at 108'000 g (max), and the supernatant solutions were radio-assayed using a Packard Tri-Carb liquid scintillation counter. The pH of the supernatant was measured after phase separation.

The Ni-en adsorbed (Ni-en$_{ads}$) in meq/kg (equal to the CEC) is calculated from the redistribution of the radiotracer between the solid and liquid phases and is calculated from:

$$\text{Ni-en}_{ads} = \frac{A_{in}\text{-}A_{out}}{A_{in}} \cdot \text{Ni-en}_{in}$$

where A_{in} = initial ^{63}Ni activity (cpm); A_{out} = final ^{63}Ni activity (cpm) and Ni-en$_{in}$ = initial amount of Ni-en (in meq/kg). The average results of triplicate, respectively duplicate, experiments are summarized in the Tab. A-1 to Tab. A-3.

Cs-CEC: The CEC was also determined in the Cs-extraction/displacement experiments (see below) by quantifying the amount of equivalents Cs adsorbed per kg rock sample (similar to the quantification of amount of Ni-en$_{ads}$). The Cs-CEC values determined in this study, however, have a higher analytical uncertainty than the Ni-CEC values, because the excess of index cation was much larger for Cs compared to Ni-en. The Cs extraction experiments were carried out inside the glove box.

ΣCATIONS: Ideally, the sum of cations displaced from the exchange sites should correspond to the CEC of the rock samples if all exchangeable cations are displaced and quantified (see section 2.2.2).

CEC-Clay: The CEC of rock samples can also be estimated based on the detailed clay mineralogy by using the CEC values of the pure clay end-members present in the samples and scaled to their wt.-%. The estimated CEC-Clay values of the samples for which the detailed clay mineralogy was available are included in Tab. A-1 to Tab. A-3. The CEC values selected for the pure end-members in this study are: smectite: 870 meq/kg (Baeyens & Bradbury 1995), illite: 225 meq/kg (Baeyens & Bradbury 2004), kaolinite 28 meq/kg (Allard et al. 1983) and chlorite: 50 meq/kg (Allard et al. 1983). Note that these CEC values are not fixed parameters but are prone to variations depending on the selected source.

2.2.2 Extraction of exchangeable cations

Cs-extraction experiments: The major cations Na, K, Mg and Ca and two minor cations NH_4 and Sr were extracted by using the high selective Cs cation (Sawhney 1970). The experiments were performed in closed tubes in a N_2 flooded glove box (O_2 < 1 ppm) to avoid oxidation of the samples and the equilibration with CO_2. The exchangeable cations were displaced by using a fivefold equivalent excess of Cs with respect to CEC of the samples, determined prior by the Ni-en method. The 5-fold Cs excess was obtained by optimising the S:L ratio in the Cs extraction (Cs-ex) experiment. Each experiment was set up in duplicate. The tubes with the weighted amount of rock samples and the appropriate CsCl solution were shaken end-over-end for 1 day, centrifuged at 108'000 g (max), and the supernatant solutions were analysed for the cations Na, K, NH_4, Mg, Ca and Sr and the anions SO_4^{2-}/S and HCO_3^-/CO_3^{2-}. The pH of the supernatants was measured after phase separation.

The Cl^- inventories were determined in separate aqueous extraction (H_2O-ex) experiments (because CsCl was used in the Cs-ex experiments) by equilibrating weighted amounts of rock samples in de-ionised water at S:L ratios of ~ 30 g/L. Phase separation was as described above and the supernatant was analysed for Cl^-.

The concentrations of Na, K, Mg, Ca, Sr, S and Cs were determined by inductively coupled plasma optical emission spectrometry (ICP-OES). Cl^-, NH_4^+ and SO_4^{2-} were quantified by ion chromatography (IC). The analysis of total inorganic carbon (TIC) was carried out by a Dohrmann Carbon Analyser. The concentrations of extracted (exchangeable and dissolved) cations and of dissolved anions are summarized in Tab. A-1 to Tab. A-3.

Correction of the extracted cations: The cations extracted in the Cs-ex experiments, however, do not only arise from the cation exchange sites of the clay minerals in the rock samples but also from the dissolution of salts and minerals. The total extracted cations must therefore be corrected with the associated dissolved anions (including Cl which was extracted in a separate H_2O-ex experiment) to estimate the concentrations of displaced cations solely coming from the cation exchange sites (see e.g., Bradbury & Baeyens 1998, Hadi et al. 2019). The corrections were guided by detailed mineralogical compositions and the soluble salt content of the samples. Ideally, the total amount of exchangeable cations (expressed in meq/kg) should correspond to the CEC of the rock sample. However, for a complex rock system, this is not always the case since it implies that (i) all exchangeable cations are well identified and (ii) are recovered (and analysed) in the extract solution. It should also be noted that if the sum of the total extracted cations is similar to the sum of the total extracted anions (both expressed in an equivalent scale) no reliable analysis on cation loadings could be made. This is the case for rock samples where the clay mineral content is very low.

Calcite ($CaCO_3$) is the main reactive mineral phase as shown by the mineralogical composition of the rock samples given in Tab. A-1 to Tab. A-3. In some samples of the confining units, the calcite content is very high, such as in the BUL1-1-845.05 sample (98 wt.-%). In the Opalinus Clay formation of the three siting regions, the calcite content rarely exceeds 20 wt.-%. The Opalinus Clay in JO has calcite contents ranging from 3 to 14 wt.-%, in NL from 4.8 to 17 wt.-% (except for sample STA2-1-806.13, which contains 40.2 wt.-% calcite), and in ZNO from 3.4 to 20.4 wt.-%.

The content of dolomite/ankerite is generally below 5 wt.-% and is not present in all samples. In a few samples, the dolomite/ankerite content is high (19.9 wt.-% in BUL1-1-815.90; ~ 50 wt.-% in STA2-1-943.22, STA2-1-948.33 and STA2-1-955.62; 53.6 wt.-% in STA3-1-924.15, 37 wt.-% in BOZ1-1-694.72 and 32 wt.-% in BOZ1-1-723.97).

BOZ1-1-808.61 consists of almost pure (98 wt.-%) anhydrite/celestite minerals ($CaSO_4/SrSO_4$).

Siderite ($FeCO_3$) is present in amounts higher than 5 wt.-% in three samples (8 wt.-% in STA3-1-855.05, 10.5 wt.-% in STA3-1-866.67 and 8 wt.-% in BOZ2-1-519.74). Dissolved Fe, however, could not be quantified in the extraction experiments since it is expected to adsorb via surface complexation on the clay minerals. Pyrite content is generally very low. Saturation indices calculations of the extracted solution indicate that in most samples, TIC originates from the dissolution of calcite. In case of dolomite/ankerite-rich samples, TIC is also originating from equilibrium with these minerals. Anhydrite-rich samples are (over)saturated w.r.t. gypsum as supported by the high concentrations of extracted SO_4. Unless the mineralogy indicated the presence of anhydrite, Ca was corrected only by the amount of TIC measured in the Cs extraction solution. In case of anhydrite-rich samples, Ca was also corrected by the amount of SO_4 extracted. Since the intrusion of CO_2 was avoided during the experiments and degassed solutions were used, the dissolution of calcite generates one mole Ca and one mole CO_3^{2-}. If the concentrations of dissolved Fe and the exact content of dolomite and ankerite were available, it would be possible to distribute the amount of dissolved TIC more accurately among Ca, Fe and Mg. The approximation made in this study might lead to a slight underestimation of the Ca occupancies in favour of those of Mg (and Sr in a very few cases, extracted concentrations were generally very low), however, it does not affect the sum of exchangeable cations.

Na was corrected for Cl (one mole Na with one mole Cl) and SO_4^{2-} (two mole Na with one mole SO_4), assuming that Cl and SO_4 originate essentially from the dissolution of the NaCl and Na_2SO_4 salts, respectively. The release of SO_4 due to the oxidation of pyrite is assumed to be negligible because of the very low pyrite content in the samples. Furthermore, oxidation was avoided by preparing the rock samples (e.g., crushing) and by performing the experiments inside a glove box under N_2 conditions within very short equilibrium time (1 day).

The extracted concentrations of K, NH_4 (when analysed), Mg and Sr were not corrected. A detailed description of the correction method of the extraction data is given in each section.

Finally, the exchangeable occupancies of Na, K, NH_4, Mg, Ca and Sr of the rock samples (expressed in an equivalent scale) were calculated from the extracted cation concentrations after correction with the dissolved anionic species as described above, and then normalized to the dry weight of the rock samples. The equivalent fraction of each exchangeable cation ($N_B = N_{Na,} N_{K,} N_{NH4,} N_{Mg,} N_{Ca,} N_{Sr}$) or group of cations ($N_B = N_{K+NH4,} N_{Mg+Ca+Sr}$) is obtained by dividing the sum of each exchangeable cation or group of cations (in meq/kg) by the sum of all exchangeable cations ($\Sigma CATIONS$) (in meq/kg).

3 Results

The most important physico-chemical parameters determined on the drill core samples from the various boreholes of the three siting regions JO, NL and ZNO are summarised in Tab. A-3, respectively. Each rock sample is numbered in these tables and reference to the sample number is given rather than the corresponding full nomenclature to simplify the reading in the text and figures.

The tables contain the following information:

- Sample description: (i) sample number, (ii) identification nomenclature from the Rock-Water Interaction (RWI) group of the Institute of Geological Sciences of the University of Bern, (iii) depth of origin, (iv) geological formation and (v) geological group
- Detailed bulk and detailed clay mineralogical characterization (with few samples lacking data)
- CEC results: (i) Ni-CEC determined from the Ni-en consumption, (ii) CEC-Clay values calculated based on the detailed clay mineralogy (if available), (iii) Cs-CEC values determined from the Cs consumption in the Cs-ex experiments and (iv) CEC values calculated based on the sum of the displaced cations (ΣCATIONS)
- Total anion and cation extraction data: SO_4, S, TIC, Na, K, NH_4, Mg, Ca and Sr were obtained from the Cs-ex experiments whereas Cl is obtained from H_2O-ex experiments. These data are tabulated as analysed without any corrections (in a molar scale). The extraction data reveal in some cases an anomalous behaviour, which is treated in more detail for the individual samples concerned.
- Amount of exchangeable cations (in an equivalent scale) displaced by Cs after correction using the procedure described in Section 2.2.2. The sum of corrected cations (ΣCATIONS) is also included in the tables.
- Fractional occupancies (N_B values) defined by the equivalent of cation B (B = Na^+, K^+, NH_4^+, Mg^{2+}, Ca^{2+} or Sr^{2+}) adsorbed on the exchange complex divided by the equivalent of total cations (ΣCATIONS). The N_B values for (K^++NH_4^+) and (Mg^{2+}+Ca^{2+}+Sr^{2+}) are also given in the tables.

In the following sections, the parameters determined for each siting regions will be presented and discussed individually.

3.1 Jura Ost

3.1.1 CEC and clay mineralogy

The CEC of argillaceous rocks are related to the content and type of clay minerals, since other minerals present have no or limited cation exchange properties. In this study, the total clay content is available for all samples whereas the detailed mineralogical characterization of the clay fraction is only partially available. Ni-CEC values for JO were determined for 32 samples from Bözberg-1 (BOZ1) and 10 samples from Bözberg-2 (BOZ2). The detailed overview of Ni-CEC results is given in Tab. A-1.

The clay mineral content of the upper confining units (Wildegg, Hauptrogenstein and Passwang) of BOZ1 ranges from 6.8 wt.-% (sample 4) to 44.6 wt.-% (sample 16). The samples from the upper confining units Wildegg and Hauptrogenstein are dominated by calcite (from 46 to

77 wt.-%). In the lower confining units Staffelegg, Klettgau and Bänkerjoch, the clay mineral content ranges from 0 wt.-% (the anhydrite-rich, i.e. 97 wt.-%, sample 32) to 79 wt.-% (sample 28). The Ni-CEC from the lower and upper confining units varies from 3.5 for the anhydrite-rich unit to 164 meq/kg for sample 28. The clay mineral content in the Opalinus Clay ranges from 42 to 70 wt.-% and the associated Ni-CEC varies from 85 to 133 meq/kg.

For BOZ2, the clay mineral content ranges from 26 to 75.2 wt.-% in the upper and lower confining units, with Ni-CEC values ranging from 45.3 to 147.4 meq/kg. In the Opalinus Clay, the clay mineral content is relatively high and homogenous (59 to 70 wt.-%) with CEC values ranging from 110 to 127 meq/kg.

The measured Ni-CEC values and the total clay mineral content along the depth profile for the samples from BOZ1 and BOZ2 are illustrated in Fig. 3-1a and Fig 3-1b, respectively (sample 32 with 0 wt.-% clay minerals is not plotted). For most of the rock samples from JO, the Ni-CEC values and clay mineral content follow the same trend and confirm the correlation between these parameters. Slight deviations are observed (i.e., sample 9, 10 and 33), which could be due to:

(i) mineralogical heterogeneities of the rock samples and/or

(ii) the detailed clay mineralogical composition of the sample. For this comparative representation, only the total clay mineral content has been considered and not the detailed clay mineralogy (since that data was not consistently reported or analysed for all samples).

The CEC is a parameter which varies strongly and increases as follows depending on the type of clay minerals present in the rock samples: smectite > illite > chlorite > kaolinite. The ratio between the different clay mineral types is not constant for all samples, so the correlation between the CEC and the total clay mineral content cannot be constant and only allows the verification of the general trend. In addition, mixed clay minerals are difficult to evaluate and to quantify and thus may lead to differences in CEC properties of the samples. For cation correction problems, discussed in the next section, samples 9 and 10 will not be further considered.

The distribution of the Ni-CEC values of the samples from Opalinus Clay and confining units from JO is illustrated in Fig. 3-2 and reflects the much more homogenous distribution of the Ni-CEC values in the Opalinus Clay as in the confining units.

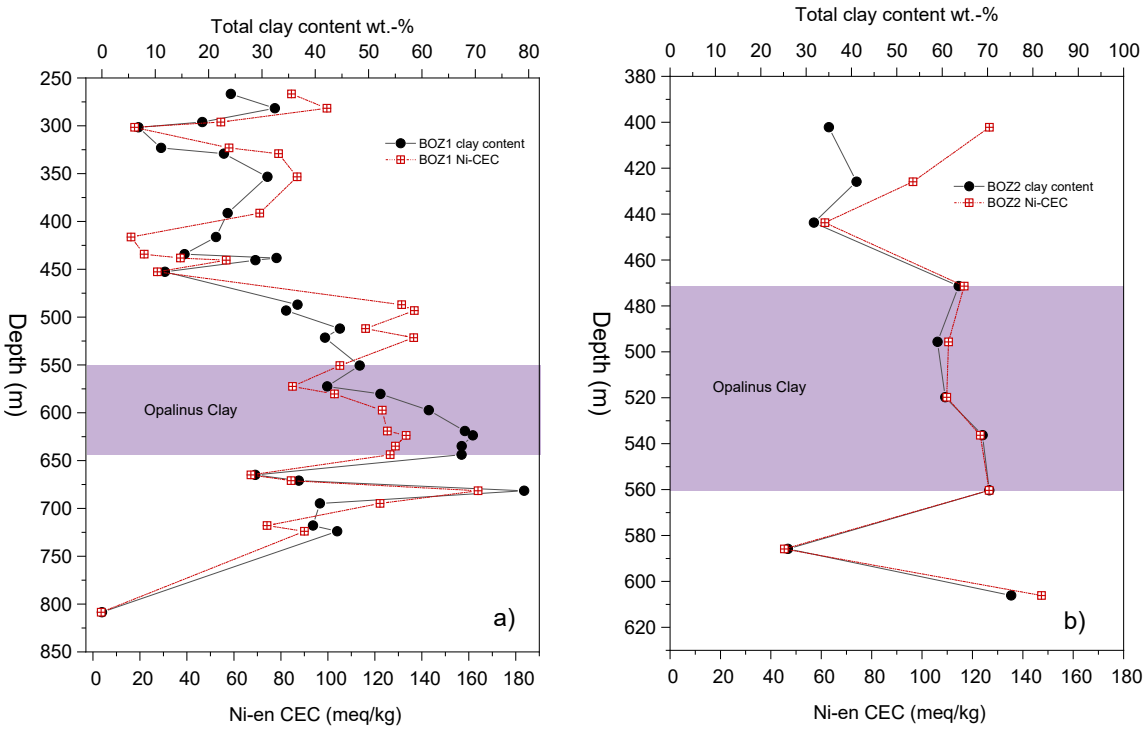

Fig. 3-1: Variation of the Ni-CEC along the depth profile as a function the total clay mineral content for the samples from the drill cores (a) BOZ1 (from 250 – 850 m depth) and (b) BOZ2 (from 380 – 620 m depth)

The lines are included to guide the eye.

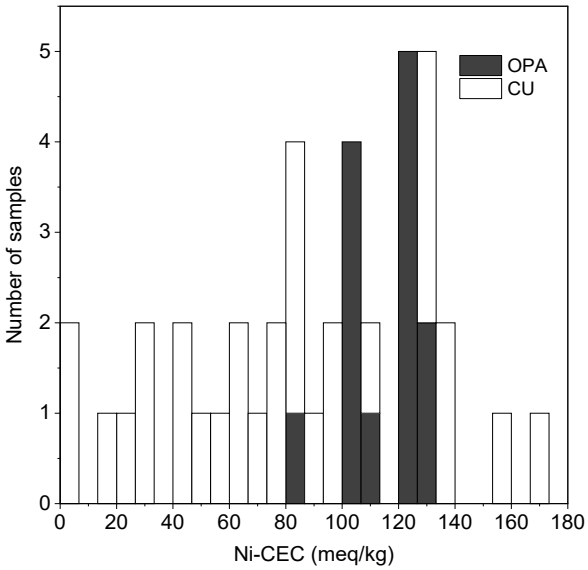

Fig. 3-2: Distribution of the Ni-CEC for the drill core samples of the Opalinus Clay (OPA) and the confining units (CU) from JO

3.1.2 Exchangeable cations

3.1.2.1 Correction of extracted cations

Since the total extracted cations originate not only from the exchangeable cations, but also from the dissolution of salts and minerals, the concentrations of the total extracted cations must be corrected with the dissolved anions to quantify the cations solely displaced from the cation exchange sites. It should be remembered that only Na and Ca are corrected with the dissolved anions. The concentrations of K, NH_4, Sr and Mg are not corrected to account for mineral/salt dissolution. Tab. A-1 indicates that the total extracted concentrations of NH_4 and Sr are very low compared to the other cations.

In the following two sections, the correction method for the rock samples from JO is discussed in detail. Based on the mineralogical composition some comments need to be made concerning a selected number of samples:

Sample 32 is essentially anhydrite. For this sample from the Bänkerjoch Formation (Keuper), the amount of released SO_4 (128.9 mmol/kg) is of same order than the amount of released Ca (135.2 mmol/kg) (see Tab. A-1). Obviously, the dissolution of anhydrite causes the high Ca and SO_4 concentrations in this extract. The measured Ca and SO_4 concentrations in the Cs extract are in line with the thermodynamic calculated solubility of anhydrite. Furthermore, the mineralogical analysis of this sample indicates that no clay minerals are present (see Tab. A-1), which is supported by the very low Ni-CEC determined for this sample (3.5 meq/kg). The cation occupancies for this rock sample cannot be reliable derived and is not further considered.

Tab. A-1indicates that samples 10, 15 and 33 exhibit higher amounts of Sr and SO_4 in the Cs extract compared to the other JO rock samples. The average Sr extraction of all JO samples (except samples 10, 15 and 33) is 0.35 ± 0.16 mmol/kg. It is assumed that this amount of Sr is displaced from the cation exchange sites. The excess Sr released in the Cs extract for samples 10, 15 and 33 equals to 5.25 mmol/kg, 1.75 mmol/kg and 3.75 mmol/kg, respectively. The average SO_4 extraction of all JO samples (except samples 10, 15, 32 and 33) is 2.6 ± 0.8 mmol/kg. The total SO_4 released in the Cs extract for samples 10, 15 and 33 are 11.4 mmol/kg, 6.7 mmol/kg and 6.3 mmol/kg, respectively. The excess Sr present in the Cs extract is likely arising from potential dissolution of celestite even so not expected based on the mineralogical data. The excess Sr released in the Cs extract can thus be associated with SO_4 through celestite dissolution. As a consequence, a pre-correction of SO_4 was carried out using the data given in Tab. A-1 in the following way:

- For sample 10, the total extracted SO_4 of 11.4 mmol/kg is reduced by the excess extracted Sr of 5.25 mmol/kg to yield a “Sr corrected” SO_4 value of 6.15 mmol/kg.
- For sample 15, the total extracted SO_4 of 6.7 mmol/kg is reduced by the excess extracted Sr of 1.75 mmol/kg to yield a “Sr corrected” SO_4 value of 4.95 mmol/kg.
- For sample 33, the total extracted SO_4 of 6.3 mmol/kg is reduced by the total extracted Sr of 3.75 mmol/kg to yield a “Sr corrected” SO_4 value of 2.55 mmol/kg.

These “Sr corrected” SO_4 values will be used to correct Na in Tab. A1. It should be noted that only these three samples (out of 141 rock samples from the three regions) have been treated this way.

Correction of extracted Na concentrations

As described in Section 2.2.2, the amount of Na extracted in Cs-ex experiments is assumed to consist of Na displaced from the cation exchange sites and from the dissolution of NaCl and Na_2SO_4 salts. As discussed in Hadi et al. (2019), the association of SO_4 with Na or Ca is difficult to quantify for most of the data obtained from these extraction experiments unless there is specific mineralogical evidence or high extracted Ca and SO_4 concentrations are measured simultaneously (e.g,. sample 32).

The total extracted quantities of Na, Cl and SO_4 expressed in meq/kg for BOZ1 and BOZ2 along the depth profile are shown in Fig. 3-3a and Fig. 3-3b, respectively. The aim of these graphs is to compare the total extracted Na with the total extracted Cl and SO_4.

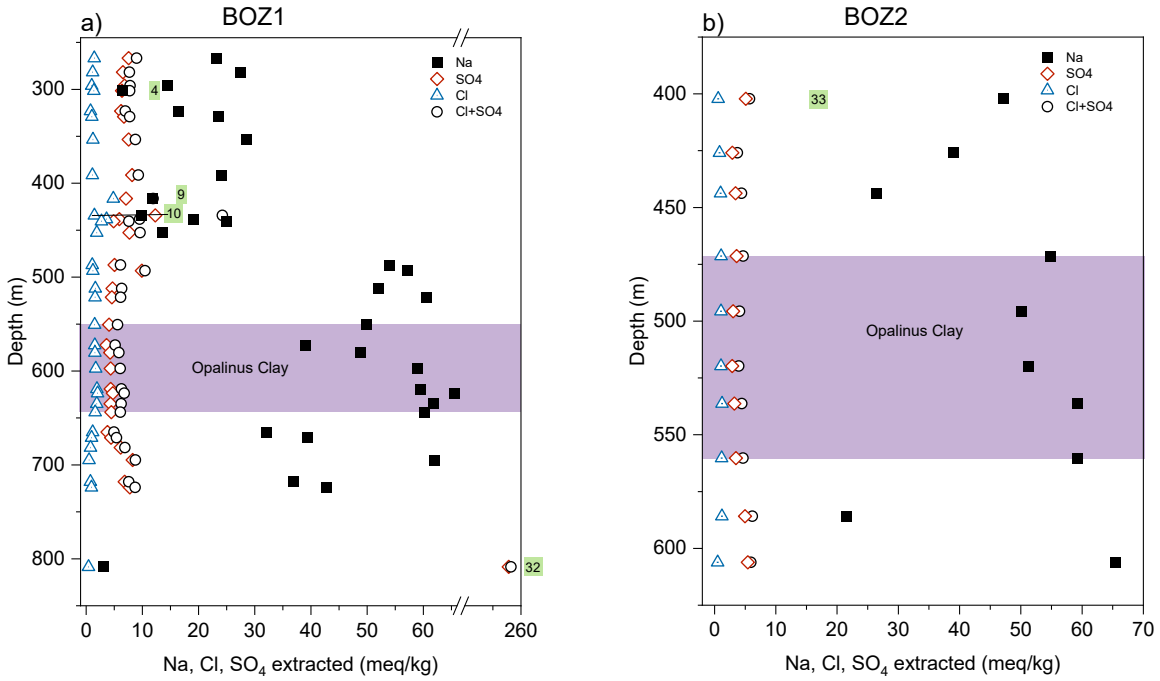

Fig. 3-3: Overview of the total extracted Na, Cl and SO_4 for (a) BOZ1 and (b) BOZ2. The sum of Cl and SO_4 (circles) represents the correction of Na arising from dissolved NaCl and Na_2SO_4 in the extraction solutions

For the samples 10, 15 and 33, the released SO_4 concentration is corrected for Sr.

The extent of correction of Na for Cl and SO_4 is illustrated in Fig. 3-3 by the white circles. These symbols represent the concentration of [Cl+SO_4] by which the extracted Na values have to be corrected to obtain the amount of Na displaced solely from cation exchange sites of the clay minerals. In most cases the total extracted Na is well above the extracted [Cl+SO_4] and the corrections are minimal. There are, however, some exceptions for the samples indicated in Fig. 3-3 by the green numbered squares.

- For the samples 4, 9 and 10, the correction of Na by [Cl+SO_4] results in negative Na loadings. In these cases, this correction cannot be applied and the correction of Ca with SO_4 will be considered (see next section).

- For sample 32 (anhydrite) the amount of released SO_4 (128.9 mmol/kg) is ~ 43 times higher than the amount of released Na (3 mmol/kg) (Fig. 3-3a) and of same order than the amount of released Ca concentration (135 mmol/kg). Na can obviously not be corrected with SO_4.

For the 38 remaining samples, the total extracted Na was corrected with [Cl+SO_4] and the results are given in Tab. A-1.

Correction of extracted Ca concentrations

As explained in Section 2.2.2, Ca is always corrected for TIC because of the ubiquity of calcite in almost all samples as shown in Tab. A-1. For samples with dolomite present, there will be also some contribution to the TIC originating essentially from the dissolution of this carbonate mineral. Consequently, a small fraction of TIC should be attributed to Mg. The same is valid for ankerite/siderite where Sr/Fe will be dissolved. However, the quantities of these elements are mostly small (except in samples 29 and 31), so that a meaningful and reliable correction cannot be carried out. The total extracted quantities of Ca and TIC expressed in mmol/kg for the rock samples from JO are illustrated in Fig. 3-4a and Fig. 3-4b.

For all samples, the extracted Ca values exceed the extracted TIC values. However, sample 4, 9 and 10, for which Ca is corrected for TIC and SO_4 yield very low (< 3 meq/kg) to negative Ca loadings. For these three samples, no reliable correction can be applied since SO_4 cannot be clearly assigned to neither Na nor Ca.

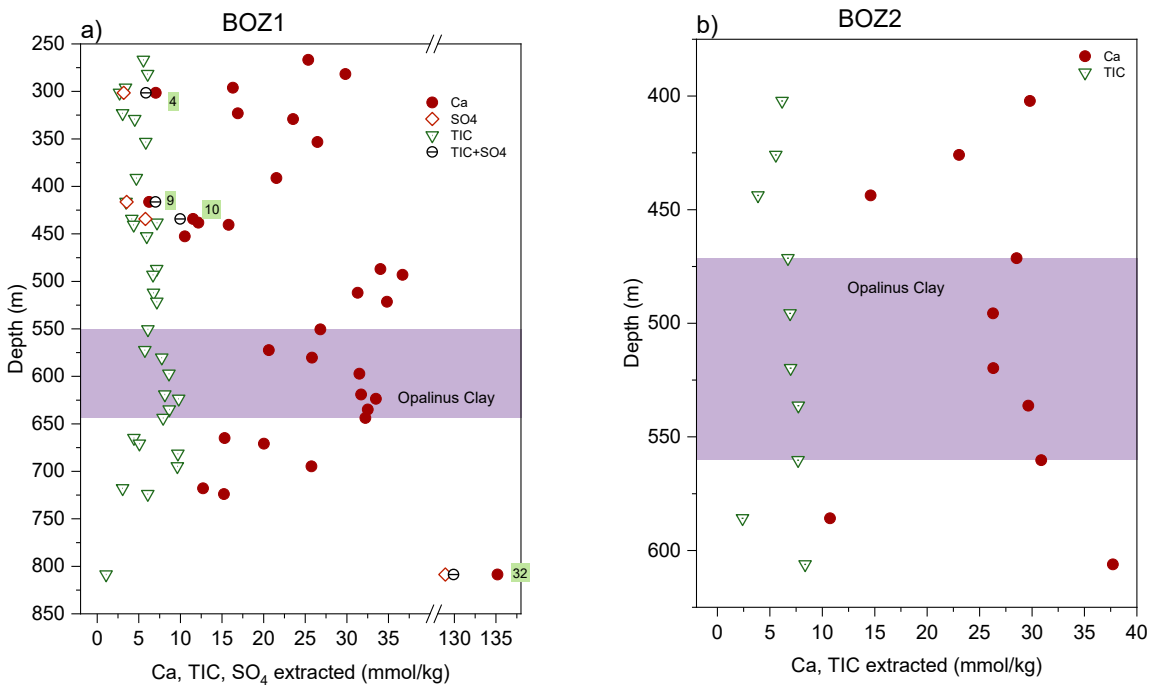

Fig. 3-4: Overview of the total extracted Ca and TIC analyses for (a) BOZ1 and (b) BOZ2

The samples for which SO_4 could not be associated with Na are also shown (green numbered squares). The sum of TIC and SO_4 (white circles) represent the correction for Ca arising from dissolved $CaCO_3$ and $CaSO_4$ in the extraction solutions. The SO_4 concentrations plotted for the samples 4, 9 and 10 are corrected for Sr.

3.1.2.2 Comparison of the CEC values obtained by the different approaches

The sum of the "corrected" extracted cation concentrations (ΣCATIONS) expressed in meq/kg given in Tab. A-1represents an indirect measurement of the CEC of the rock samples. For samples 4, 9, 10 and 32, no reliable correction could be carried out to differentiate the individual cation loadings, however, the overall ΣCATIONS can still be calculated from the total extracted cations minus the total dissolved anions. Fig. 3-12 shows the correlation between the Ni-CEC values and the CEC data obtained using the other three independent approaches, i.e.,

1. Cs consumption in the Cs-ex experiments (Cs-CEC)
2. Sum of corrected cations displaced in the Cs-ex experiments (ΣCations)
3. CEC values calculated from the clay mineralogy for the rock samples where detailed clay mineralogy data is available (CEC-Clay)

The correlation for all the methods is good and the general trend in the evaluated CEC data for all samples is as follows: Cs-CEC ≥ (ΣCATIONS) > Ni-CEC ~ CEC-Clay. The generally higher Cs-CEC values compared to the Ni-CEC values can be explained by the higher interlayer extraction yields of K^+ (and NH_4^+) due to the higher selectivity of Cs^+ compared to Ni-en^{2+} towards K^+ and NH_4^+ (De Preter 1990).

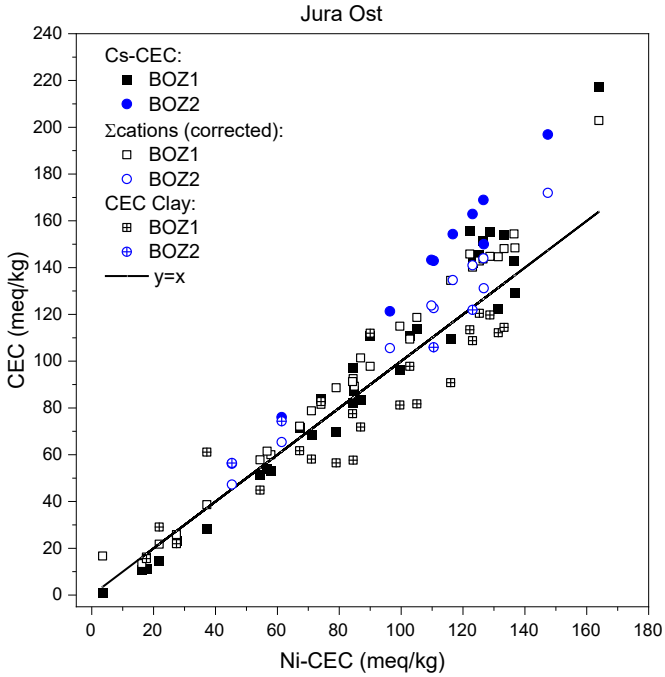

Fig. 3-5: Comparison of the Ni-CEC values with CEC data obtained from different measurements/approaches (Cs-CEC, ΣCations and CEC-Clay) for the drill core samples from JO

The solid line represents a correlation with slope equal 1.

3.1.2.3 Fractional occupancies of exchangeable cations

Fig. 3-6 shows the equivalent fractions of exchangeable Na, K, NH_4, Mg, Ca and Sr determined for all the samples from JO and their evolution along the depth profile. Na and Ca are mostly the dominant cations on the exchange sites followed by Mg and K. NH_4 and Sr are very low compared to the four major cations in all samples.

In the upper part of the BOZ1 drill core (from 266.75 m to 521.50 m depth), Ca is more dominant ($0.26 \leq N_{Ca} \leq 0.46$) compared with Na ($0.12 \leq N_{Na} \leq 0.35$). Mg also dominates over Na down to 391.30 m ($0.23 \leq N_{Mg} \leq 0.26$). The dominance of Ca and Mg, correlates very well with the general lower clay mineral content and the high Ca/Mg carbonate mineral content of these samples (dashed lines in Fig. 3-6). At depth below 521.50 m, Na becomes the dominant cation on the exchange sites ($0.35 \leq N_{Na} \leq 0.40$).

For the samples from BOZ2, the Na and Ca loadings ($0.31 \leq N_{Ca} \leq 0.36$; $0.32 \leq N_{Na} \leq 0.39$) are close and constant, except for the deepest sample (402.15 m depth) in this borehole.

The N_{Na}, N_{K+NH4} and $N_{Mg+Ca+Sr}$ values for all samples from JO are summarized in Tab. A-1 illustrated in a ternary plot in Fig. 3-7. In this graphical presentation, K and NH_4 have been grouped since their cation exchange behaviour is very similar and more selective on 2:1 clay minerals compared to Na (De Preter 1990). The alkaline-earth cations Mg, Ca and Sr are also grouped since their selectivity behaviour towards Na is also very similar (Bradbury & Baeyens 1998). The data in Fig. 3-7 clearly shows that the samples from the confining units are much more scatted than the samples from the Opalinus Clay formations. The Opalinus Clay samples from both boreholes are mostly concentrated in a very single narrow region (closed symbols), suggesting that the porewater composition of the Opalinus Clay formation in JO will be quite homogeneous (provided the Cl concentration in the porewater is constant). The N_B values in the confining units, particularly for BOZ1, are much more scattered suggesting more heterogeneous porewater compositions.

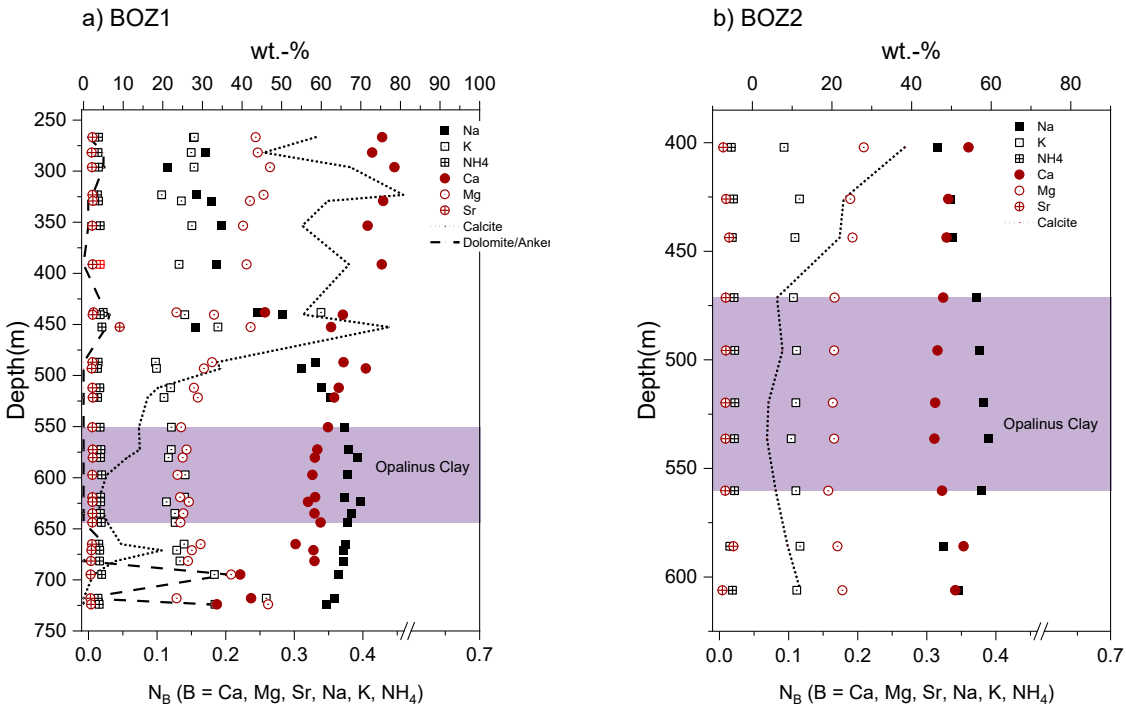

Fig. 3-6: Evolution of the N_B values (B = Na, K, NH_4, Mg, Ca or Sr) along the depth profile for the samples from (a) BOZ1 and (b) BOZ2

The lines indicate the mineralogical content of major minerals e.g. calcite in the investigated samples.

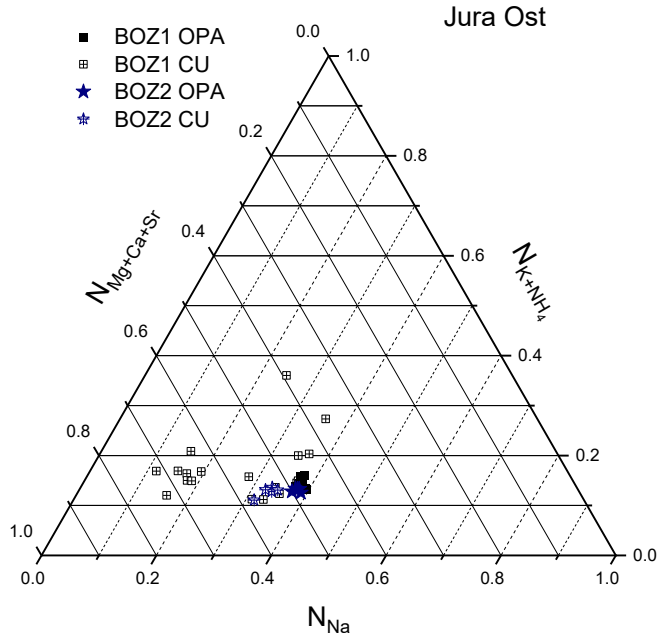

Fig. 3-7: N_{Na}, N_{K+NH_4} and $N_{Mg+Ca+Sr}$ data for all samples from JO

Closed symbols indicate the data for Opalinus Clay (OPA) and open symbols are for the confining units (CU).

3.2 Nördlich Lägern

3.2.1 CEC and clay mineralogy

Ni-CEC values were determined on 68 rock samples from NL, including 26 samples from Bülach-1 (BUL1), 20 samples from Stadel-2 (STA2) and 22 samples from Stadel-3 (STA3). An overview of the Ni-CEC results is given in Tab. A-1. xxx

As already mentioned in the previous Section 3.1.1, the CEC of argillaceous rocks are expected to correlate with the content and type of clay minerals, since other minerals present have no or limited cation exchange properties.

The clay mineral content of the upper confining units of BUL1 lies generally below 27.1 wt.-% except for the samples 5 (51.5 wt.-%), 11 (48.5 wt.-%) and 14 (63.3 wt.-%). In the lower confining units, the clay mineral content ranges from 10.1 to 46.2 wt.-%. The Ni-CEC values from the lower and upper confining units vary from 0 to 140 meq/kg. The clay mineral content in the Opalinus Clay ranges from 34.3 to 63.9 wt.-% and the associated the Ni-CEC varies from 64 to 101.2 meq/kg.

For STA2, the clay mineral content in the upper confining units is quite high and varies from 26.1 to 59.5 wt.-%, with Ni-CEC values ranging from 53.3 to 129.6 meq/kg. In the lower confining units the clay mineral content ranges from 0.4 to 49.5 wt.-% and the Ni-CEC values vary between 3.7 and 156.8 meq/kg. In the Opalinus Clay formation, the clay mineral content is relatively high and homogenous (26.3 to 69.4 wt.-%) with CEC values ranging from 45.2 to 127.3 meq/kg.

The clay mineral content of the STA3 samples is generally high, ranging from 8.8 to 60.1 wt.-% in the upper confining units, from 13.2 to 68.3 wt.-% in the lower confining units and from 42.2 to 64.7 wt.-% in the Opalinus Clay. The Ni-CEC values vary accordingly from 21.7 to 171 meq/kg in the upper and lower confining units and between 91.5 and 123.3 meq/kg in the Opalinus Clay.

The variation of the total clay mineral content along the depth profile of the drill cores from the three boreholes in NL is clearly reflected in the variation of the measured Ni-CEC values as illustrated in Fig. 3-8a, Fig. 3-8 and Fig. 3-8c for BUL1, STA2 and STA3, respectively. For the majority of the samples, the correlation between Ni-CEC and total clay mineral content is good. For one sample from the upper confining units (sample 50 (STA3-1-735.02)) and 3 samples from the lower confining units (sample 26 (BUL1-1-1026.50), sample 67 (STA3-1-913.19) and sample 68 (STA3-1-924.15) the correlation is poor.

- Samples 26 and 50 exhibit higher Ni-CEC values as expected from (the relationship with) the total clay mineral content. A reason may be a different composition of the clay mineral fraction (even though clay composition variability is fairly homogenous across the wells and units). Unfortunately, no detailed clay mineralogy is available for these samples.
- For the samples 67 and 68 similar Ni-CEC values were determined experimentally. However, based on the total clay mineral content of 68.3 wt.-% for sample 67, a much higher Ni-CEC would be expected whereas the opposite is expected for sample 68 with only 29.9 wt.-% clay mineral content (see Tab. A-2).

It should be noted that for these 4 samples the Ni-CEC values agree very well with CEC values determined by other different independent experimental approaches (i.e., Cs-CEC and $\Sigma_{CATIONS}$), confirming the reliability of the measured Ni-CEC values. Possible reasons for the poor correlation between the experimentally determined CEC and the clay mineral content of the outlier samples is discussed in Section 3.1.1.

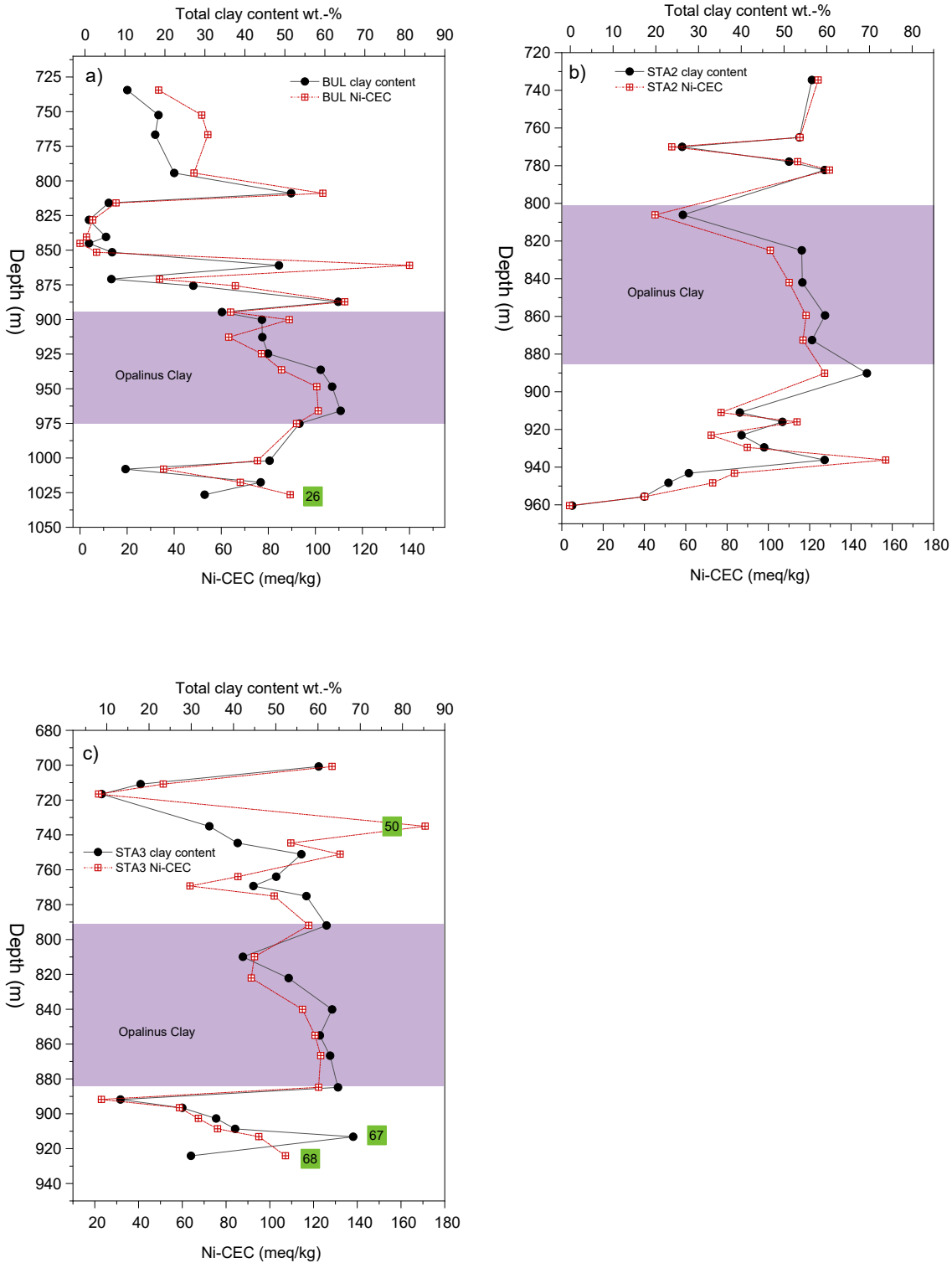

Fig. 3-8: Variation of the Ni-CEC and the total clay mineral content along the depth profile for the samples from NL for the drill cores (a) BUL1, (b) STA2 and (c) STA3

The lines are included to guide the eye.

The distribution of the Ni-CEC values of samples of Opalinus Clay and confining units from NL is illustrated in Fig. 3-9 and reflects the much more homogenous distribution of the Ni-CEC values in the Opalinus Clay as in the confining units.

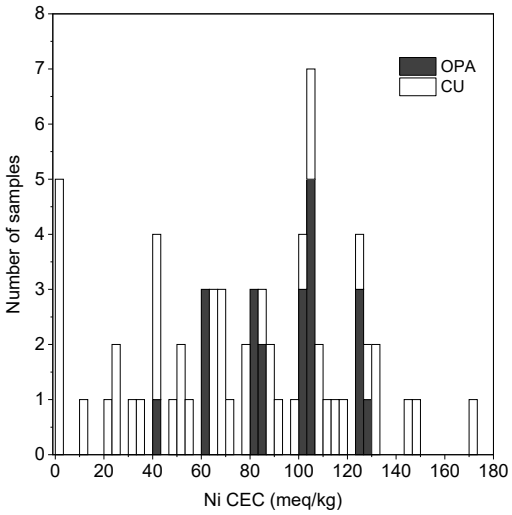

Fig. 3-9: Distribution of the Ni-CEC for the drill core samples from the Opalinus Clay (OPA) and the confining units (CU) from NL

3.2.2 Exchangeable cations

3.2.2.1 Correction of extracted cations

The dissolved cations (Na, K, NH_4, Mg, Ca and Sr) and the anions (TIC, SO_4/S) of the samples from NL were quantified in the Cs-ex and Cl was determined in H_2O-ex experiments (see section 2.2.2). The mineralogical analyses and the extracted concentrations normalized to the sample weight of the samples are summarized in Tab. A-2. As specified in Section 2.2.2, the concentrations of K, NH_4, Mg, and Sr were not corrected with dissolved anion concentrations. The total extracted concentrations of NH_4 and Sr are generally low compared to the other cations. The NH_4 concentrations are ≤ 3 mmol/kg except for sample 14 (BUL1-1-887.26), for which ~ 9.7 mmol/kg was measured. The Sr concentrations are ≤ 0.5 mmol/kg. In the following two sections, the corrections applied for the rock samples from NL are discussed in detail.

Correction of extracted Na

The correction procedure followed for the samples from NL is identical to the one described for the samples of JO in section 3.1.2.1 and follow the general procedure as outlined in Section 2.2.2.

The total extracted quantities of Na, Cl and SO_4 expressed in meq/kg for the samples from BUL1, STA2 and STA3 are shown in Fig. 3-10a, Fig. 3-10b and Fig. 3-10c, respectively. The aim of these graphs is to compare the total extracted Na with the total extracted Cl and SO_4 and to illustrate the significance of the corrections to be made to obtain the exchangeable Na on the planar sites of the clay minerals. The dissolved concentration of Cl and SO_4 are in almost all cases low and rather constant over the depth profile (< 10 meq/kg) in comparison with the extracted amount of Na (Fig. 3-10). The white circles in Fig. 3-10 represent the sum of Cl and SO_4

([$Cl+SO_4$]) to be subtracted from the total extracted Na concentrations in the correction procedure. For most of the samples from the three boreholes, the total extracted Na quantities (black squares in Fig. 3-10) are well above the extracted [$Cl+SO_4$] and the corrections are minimal.

There are, however, samples for which the correction of Na with SO_4 was not possible. These samples are shown in Fig. 3-10 by the green numbered squares. The clay mineral-poor samples 8 (5.3 wt.-%) and 9 (1 wt.-%) have released low Na concentrations and the correction yields negative Na loadings on the clay minerals (Tab. A-2).

For the clay mineral-poor sample 46 from the Klettgau Formation, high amounts of Ca (65.6 mmol/kg) and SO_4 (86 mmol/kg) were measured in the Cs-ex experiments, confirming the presence $CaSO_4$. The amount of SO_4 released (86 mmol/kg) is 7 times higher than the amount of Na released (12.2 mmol/kg). For this very clay mineral-poor sample, the methodology allows no reliable correction and therefore this sample is not further considered. (This sample resembles sample 32 from the Keuper Bänkerjoch formation from JO).

For the remaining 65 samples, the correction of Na for dissolved [$Cl+SO_4$] is applicable.

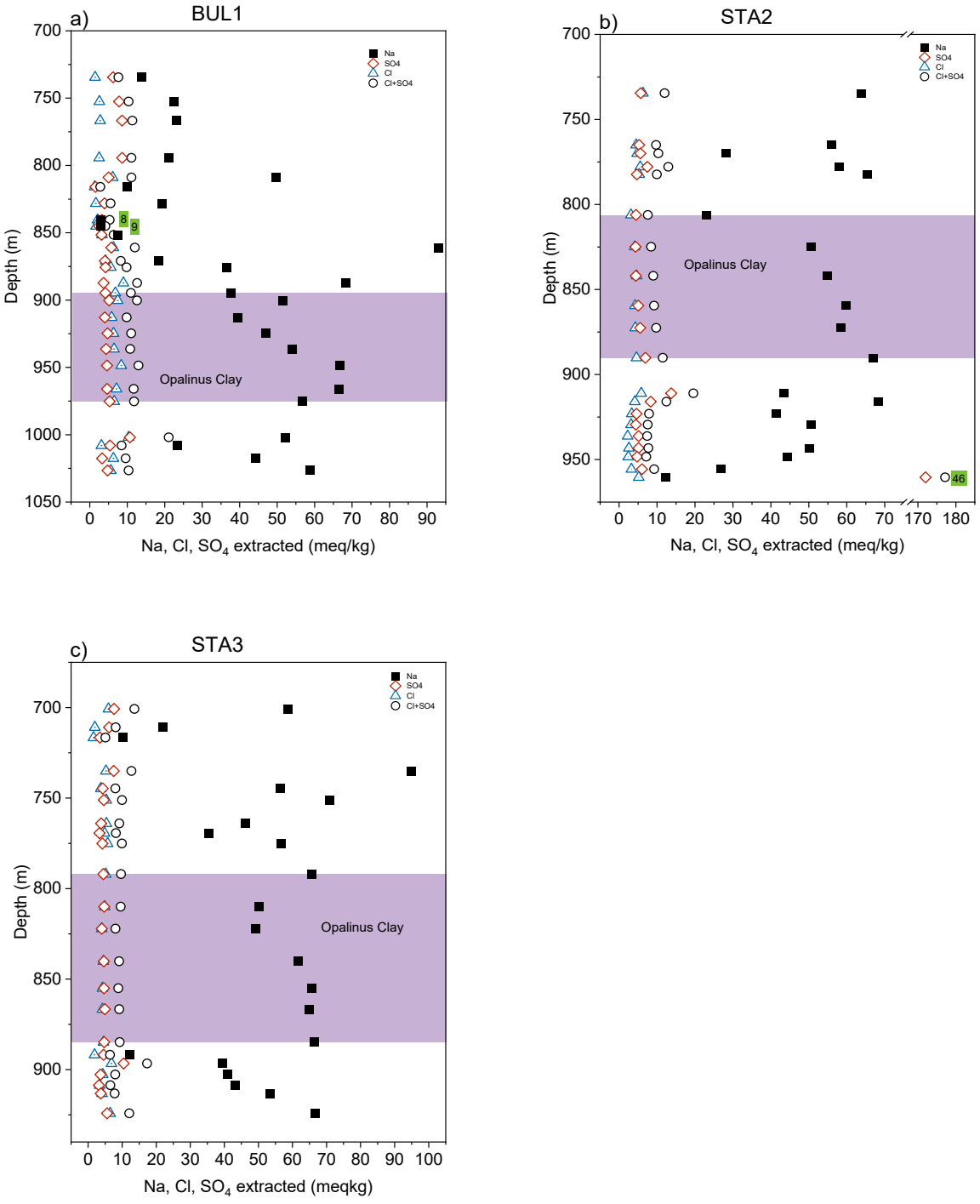

Fig. 3-10: Overview of the extracted concentrations of Na, Cl and SO_4 expressed in meq/kg for (a) BUL1, (b) STA2 and (c) STA3

The sum of Cl and SO_4 (circles) represents the correction of Na arising from dissolved NaCl and Na_2SO_4 in the extraction solutions.

Correction of extracted Ca

The procedure for correcting Ca only with TIC is discussed in section 2.2.2 and is applied for NL in a similar way as for JO (see section 3.2.2.1).

The total extracted quantities of Ca and TIC expressed in mmol/kg for the samples from BUL1, STA2 and STA3 are illustrated in Fig. 3-11a, Fig. 3-11b and Fig. 3-11c, respectively. As can be seen, in most cases, there is an excess of Ca compared to TIC and thus the correction can be made for these rock samples.

There are, however, a few exceptions. The clay mineral-poor (1.0 to 6.8 wt.-%) calcite-rich (74 to 97.7 wt.-%) samples 6, 7, 8, 9 and 10 from BUL1 (upper confining Herrenwis Unit), exhibit comparatively low concentrations of the major cations in the Cs extracts. For these samples the cation corrections could not reliably be applied and hence, these samples are not further considered.

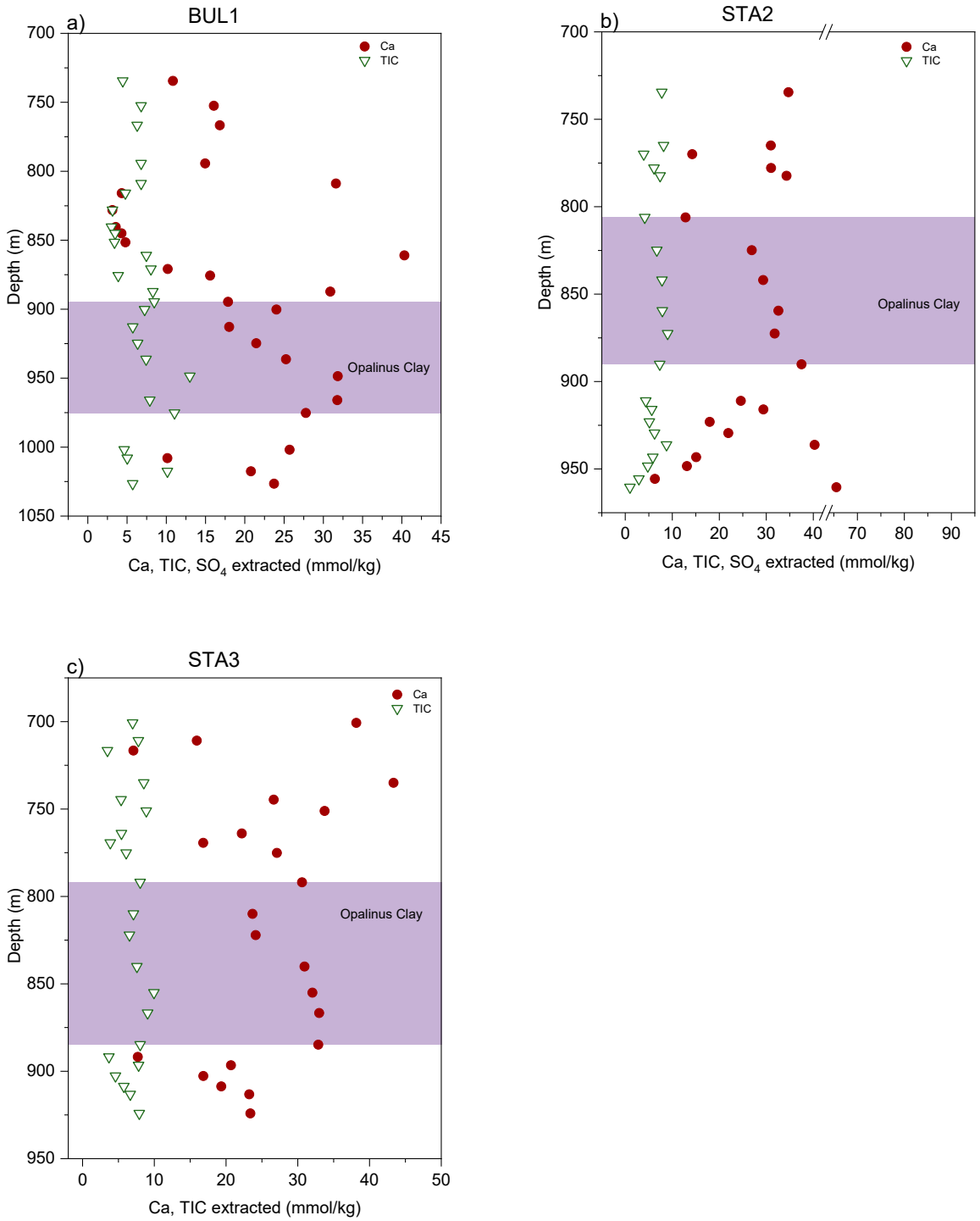

Fig. 3-11: Overview of the extracted Ca and TIC concentrations for (a) BUL1, (b) STA2 and (c) STA3

3.2.2.2 Comparison of the CEC values obtained by the different approaches

The correlation of the CEC values determined by the different approaches i.e., Cs consumption in the Cs-ex experiments (Cs-CEC), ΣCATIONS and estimate based on the clay mineralogy with the CEC values given in Section 2.2.1 (CEC-Clay) for the NL samples is shown in Fig. 3-5.

The results of ΣCATIONS representing an indirect measurement of the CEC of the rock samples are given in Tab. A-2. For the samples from the Herrenwis Unit, no reliable correction could be carried out to differentiate the individual cation loadings, however, ΣCATIONS can still be calculated from the total extracted cations minus the total dissolved anions. The cation correction was not possible for sample 46.

Fig. 3-12 shows the correlation of the Ni-CEC values with CEC data obtained by the other three independent approaches (Cs-CEC, ΣCATIONS and CEC-Clay).

The correlation for all the methods is good and the general trend in the evaluated CEC data for all samples is as follows: Cs-CEC ≥ (ΣCATIONS) > Ni-CEC ~ CEC-Clay and agrees with the observation made for the samples from JO. The Cs-CEC data for BUL1 samples deviate slightly more than the Cs-CEC data from STA2 and STA3.

The general good correlation between the Cs-CEC and sum of cations suggest that most of the major extractable cations were quantified.

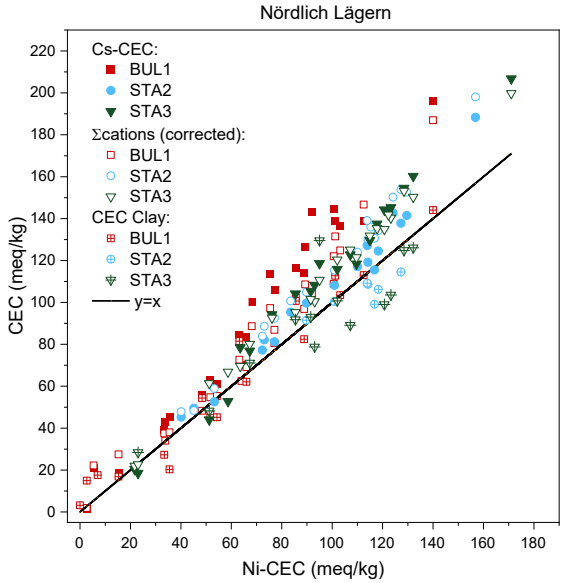

Fig. 3-12: Comparison of the Ni-CEC values with the CEC values obtained from different approaches (i.e. Cs-CEC, ΣCATIONS and CEC values calculated from the mineralogy, CEC-Clay) for the drill core samples from NL

The solid line represents a correlation with slope equal 1.

3.2.2.3 Fractional occupancies of exchangeable cations

Fig. 3-13 shows the equivalent fractions of exchangeable Na, K, NH_4, Mg, Ca and Sr determined for all the samples from NL and their evolution along the depth profile. The data for the samples from the Herrenwis Unit (green area in Fig. 3-13a) are not shown because N_B values could not be derived (low clay mineral/high carbonate samples).

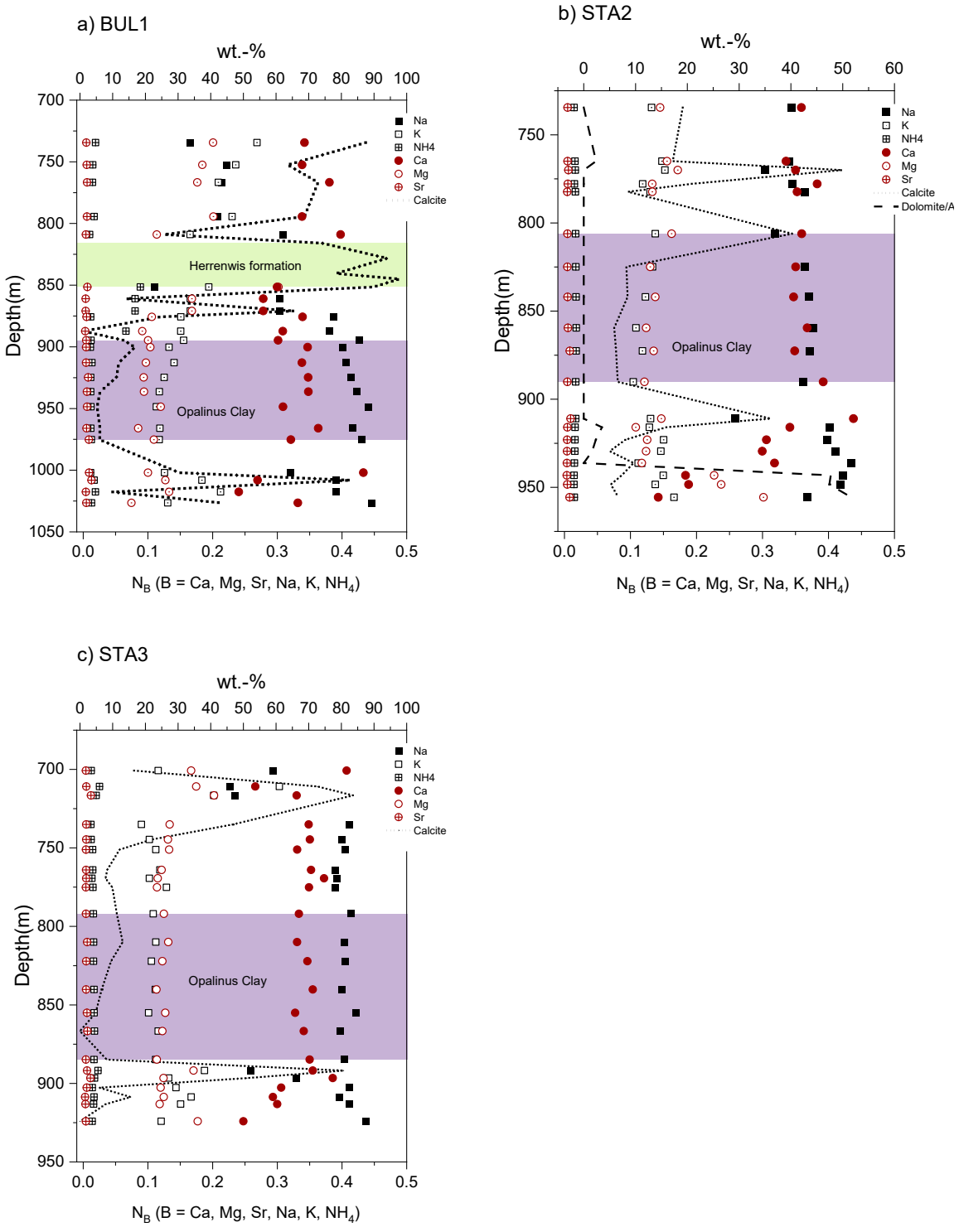

Fig. 3-13: Evolution of the N_B values (B = Na, K, NH_4, Mg, Ca or Sr) along the depth profile for the samples from (a) BUL1, (b) STA2 and (c) STA3

Dashed lines (to guide the eye) indicate the wt.-% of carbonate minerals in the given samples.

Similar to JO, Na and Ca are the dominant cations on the exchange sites followed by Mg and K. A few samples show higher N_B values for K and Mg. NH_4 and Sr are very low compared to the four major cations in all samples.

In the upper part of the BUL1 (from 734.53 m to 782.31 m depth), Ca is the dominant cation ($0.34 \leq N_{Ca} \leq 0.40$). The higher values for Ca and Mg seem to correlate with the general high Ca/Mg carbonate mineral content and the lower clay contents of the samples (illustrated by the dashed lines in Fig. 3-13a). At depth below 890.16 m, Na becomes the dominant cation on the exchange sites ($0.35 \leq N_{Na} \leq 0.40$). Na is the major cation in the Opalinus Clay and the N_{Na}/N_{Ca} ratio varies between 1.1 and 1.4.

For the samples from STA2, the N_B values for Na and Ca are close and rather constant down to 890.16 m depth. In the Opalinus Clay, N_{Na} and N_{Ca} are very close (0.32 – 0.39) and their ratio varies between 0.9 and 1.1. At a depth below 915.94 m, Na clearly dominates ($N_{Na} \sim 0.4$), Ca decreases and a noticeable increase of Mg is observed (up to $N_{Mg} \sim 0.3$) (in agreement with increased dolomite and low calcite contents).

Ca is the dominant exchangeable cation down to 716.58 m depth in STA3. In this upper part, the values obtained for K and Mg are also comparatively high. At depth below 735.02 m, Na clearly dominates ($N_{Na} \sim 0.4$), with exception for the calcite-rich samples at 891.81 m ($N_{Na} \sim 0.26$) and 896.60 m ($N_{Na} \sim 0.33$) depth. The N_{Na}/N_{Ca} ratio in the Opalinus Clay ~ 1.1 – 1.3.

For the three boreholes, the inversion from Na to Ca/Mg richer occupancies correlate well with increasing Ca/Mg carbonate minerals and decreasing clay mineral contents.

The N_B values are clearly much more scattered in the confining units compared to the Opalinus Clay. The N_B values are slightly more scattered in BUL1 compared to STA2 and STA3.

N_{Na}, N_{K+NH4} and $N_{Mg+Ca+Sr}$ determined for all samples from NL are summarized in Tab. A-2 and illustrated as a ternary plot in Fig. 3-14. With two exceptions (samples 15 and 32, both close to the upper confining units) all the Opalinus Clay samples (from the three boreholes) are concentrated in a narrow single region (closed symbols). The samples from the confining units are much more scattered compared to the samples from the Opalinus Clay. Providing that the ionic strength (given by the Cl content and the porosity) is homogeneous, it can be concluded from the N_B values that for NL, the porewater composition of the confining units will be less homogeneous compared to porewater compositions of the Opalinus Clay formation.

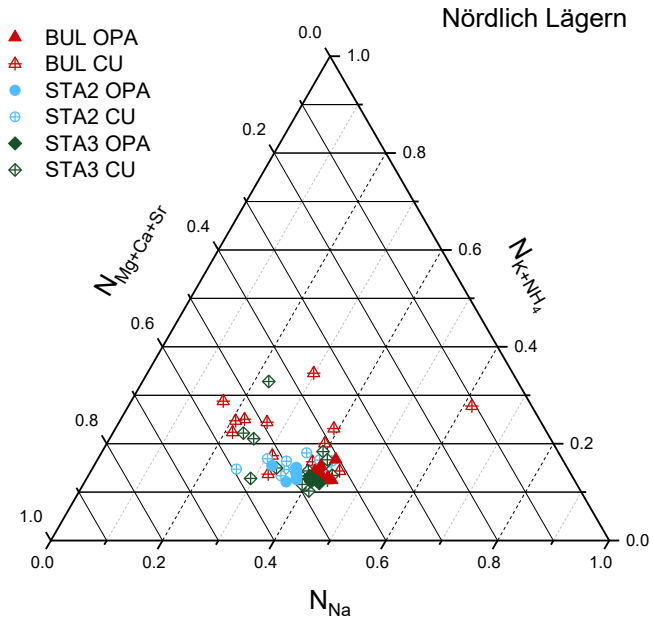

Fig. 3-14: N_{Na}, N_{K+NH_4} and $N_{Mg+Ca+Sr}$ data for all the samples from NL

Closed symbols are the data for Opalinus Clay (OPA) and open symbols are the data for the confining units (CU).

3.3 Zürich Nordost (ZNO)

3.3.1 CEC and clay mineralogy

For the ZNO region, Ni-CEC values were determined for 11 samples from Trüllikon-1 (TRU1) and 20 samples from Marthalen-1 (MAR1). The detailed overview of the measurements is given in Tab. A-3.

For TRU1, the clay mineral content and Ni-CEC of the samples from the confining units ranges from 11.1 to 67.8 wt.-% and 24.9 to 128.5 meq/kg, respectively. In the Opalinus Clay formation the clay mineral content and Ni-CEC ranges from 54.5 to 67.9 wt.-% and 89.4 to 114.1 meq/kg, respectively.

The MAR1 drill core samples from the confining units yield clay mineral contents ranging from 17.9 to 69.3 wt.-% and Ni-CEC values from 34.6 to 159.9 meq/kg. For the Opalinus Clay samples, the Ni-CEC values vary from 95.3 to 123.7 meq/kg and the clay mineral content vary from 43.3 to 69.8 wt.-%.

The measured Ni-CEC values and the total clay mineral content along the depth profile for the samples from TRU1 and MAR1 are shown in Fig. 3-15a and Fig. 3-15b, respectively. For the ZNO samples, the variation of the clay mineral content and the Ni-CEC values along the depth profile of the boreholes correlates very well. Small deviations may be caused by sample heterogeneity and clay mineralogical compositions (i.e., not fully representative of the specific sample investigated) as already discussed in previous sections.

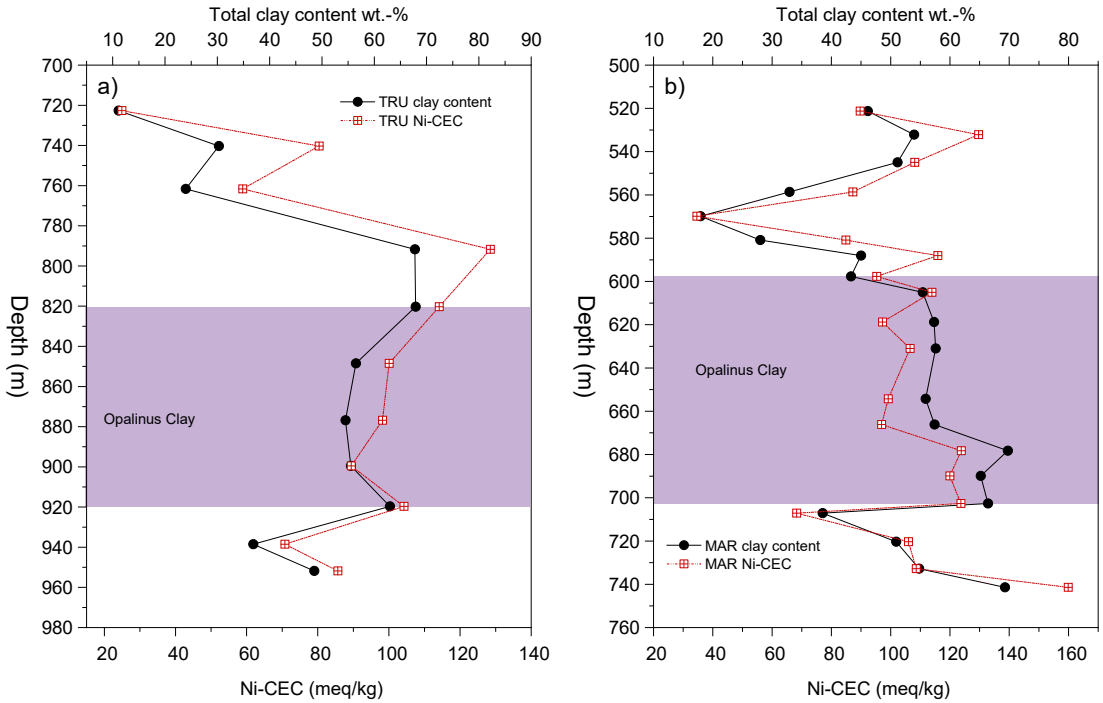

Fig. 3-15: Variation of the Ni-CEC along the depth profile as a function of the total clay mineral content for the samples from the cores (a) TRU1 and (b) MAR1

The lines are included to guide the eye.

Fig. 3-16 shows the distribution of the Ni-CEC values for the Opalinus Clay and for the confining units for the ZNO rock samples and illustrates the larger distribution of CEC values in the confining units compared to the Opalinus Clay.

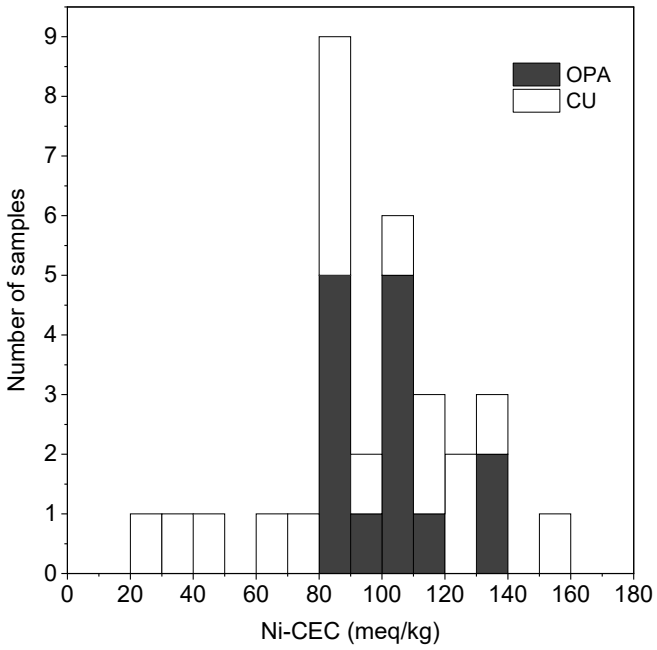

Fig. 3-16: Distribution of the Ni-CEC for the drill core samples of Opalinus Clay and confining units (CU) from ZNO

3.3.2 Exchangeable cations

3.3.2.1 Correction of extracted cations

The concentrations of the cations (Na, K, NH_4, Mg, Ca and Sr) and of the anions (TIC and SO_4/S) were quantified in the Cs-ex experiments for the 31 samples from ZNO. The amount of dissolved Cl was determined separately in H_2O-ex experiments. The results are summarized in Tab. A-3. The same procedure as for the samples of JO and NL is applied to the samples of ZNO to quantify the exchangeable cation occupancies. The total extracted concentrations of K, NH_4, Mg and Sr are not corrected for salt or mineral dissolution.

In the following 2 sections the corrections applied to Na and Ca for the rock samples from ZNO are discussed in detail.

Correction of extracted Na

The extracted Na concentrations are corrected by associating Na with Cl and SO_4 originating from the dissolution of NaCl and Na_2SO_4 salts. The mineralogical analyses presented in Tab. A-3 show that none of the samples contain significant amounts of sulphate minerals, so the association of Ca with SO_4 is not expected.

The extracted quantities of Na, Cl and SO_4 for the samples from TRU1 and MAR1 are shown in Fig. 3-17a and Fig. 3-17b, respectively. In all cases there is an excess of Na compared to the amount of [Cl+SO_4] and hence, the correction of Na for dissolved Cl and SO_4 is applicable to all samples from ZNO. It should be noted that none of the ZNO samples contains very little clay mineral contents (sample 1 exhibits the lowest clay mineral content of 11.1 wt.-%).

For sample 16 from the Wedelsandstein Formation of MAR1 high Cl (11.1 mmol/kg) and low Na (22.1 mmol/kg) concentrations were measured in comparison to the other samples.

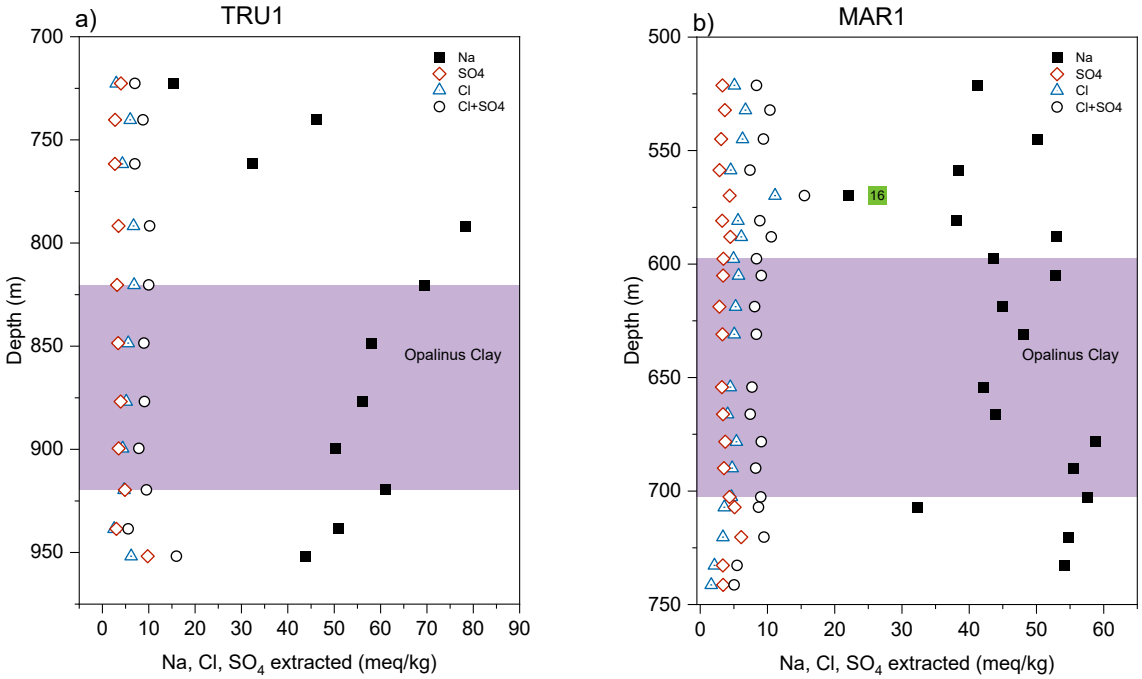

Fig. 3-17: Overview of the extracted concentrations of Na, Cl and SO_4 expressed in meq/kg for (a) TRU1 and (b) MAR1

The sum of Cl and SO_4 (circles) represents the correction of Na arising from dissolved NaCl and Na_2SO_4 in the extraction solutions.

Correction of extracted Ca

As already discussed in Section 2.2.2 and applied to the JO and NL samples, Ca is corrected with the TIC concentrations released in the Cs-ex experiments. Fig. 3-18 shows the extracted amounts of Ca and TIC (representative of the correction) expressed in mmol/kg. For all samples of ZNO, the amount of Ca extracted is sufficiently high and can be corrected with TIC.

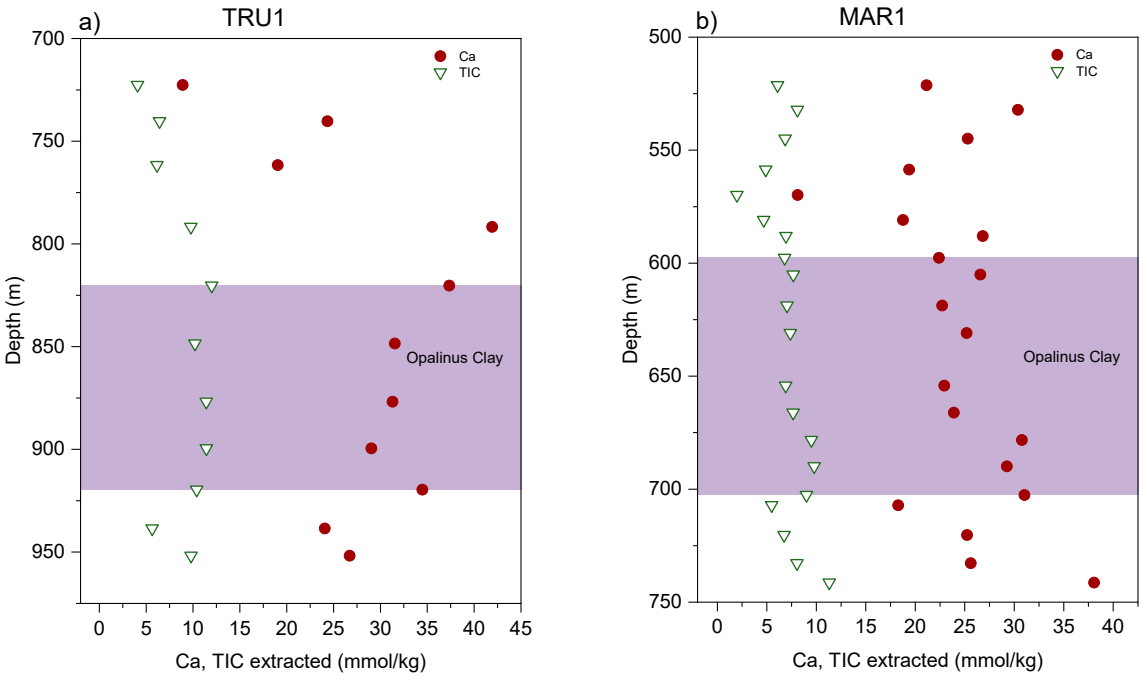

Fig. 3-18: Overview of the extracted Ca and TIC concentrations for (a) TRU1 and (b) MAR1

3.3.2.2 Comparison of the CEC values obtained by the different approaches

Fig. 3-19 shows the correlation of the Ni-CEC data of the ZNO samples with CEC values obtained by the different approaches, i.e., Cs-CEC, ΣCATIONS and CEC-Clay. Cs-CEC and Ni-CEC values correlate well for the samples from both boreholes. The ΣCATIONS determined for MAR1 samples deviates most, particularly for the three samples with highest clay content. The reason for the discrepancy is not clear.

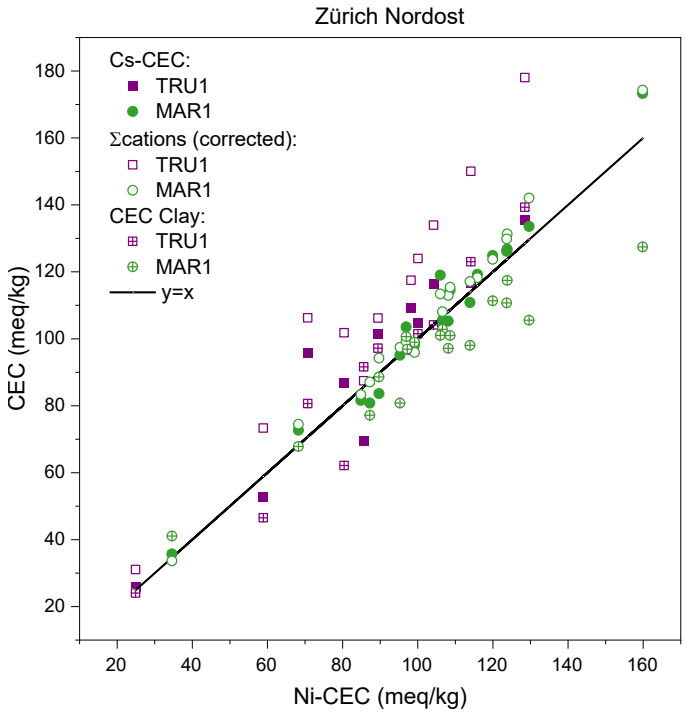

Fig. 3-19: Comparison of the Ni-CEC values with the CEC values obtained from different measurements/approaches (i.e., Cs-CEC, ΣCATIONS and CEC values calculated from the clay mineralogy) for the drill core samples from ZNO.

The solid line represents the correlation with slope equal 1.

3.3.2.3 Fractional occupancies of exchangeable cations

The fractional occupancies of Na, K, NH_4, Mg, Ca and Sr in the different samples from ZNO along the depth profile are shown in Fig. 3-20. For most samples from both boreholes, Na and Ca are the major exchangeable cations (30 – 40%), with Na slightly higher as Ca, followed by Mg (13 – 24%) and K (~ 10%). NH_4 and Sr loadings are very low compared to the four major cations in all samples.

For the TRU1 borehole samples Na and Ca are the dominant cations with similar N_B values ($0.27 \leq N_{Na} \leq 0.43$; $0.31 \leq N_{Ca} \leq 0.39$). The N_{Na}/N_{Ca} ratio is equal to 1.2 for the four samples in the Opalinus Clay.

In MAR1, Na and Ca are also the dominant exchangeable cations ($0.27 \leq N_{Na} \leq 0.43$; $0.31 \leq N_{Ca} \leq 0.39$), except for sample 16. As mentioned before, the measured Cl, Na, Mg, and Ca extraction values of this sample deviate from the other samples, resulting in particular very low N_{Na} value of 0.2. In the Opalinus Clay, the N_{Na}/N_{Ca} ratio varies between 1.1 and 1.2.

Fig. 3-20 illustrates that the N_B values of the major exchangeable cations are very homogenous over the entire depth for the samples from ZNO.

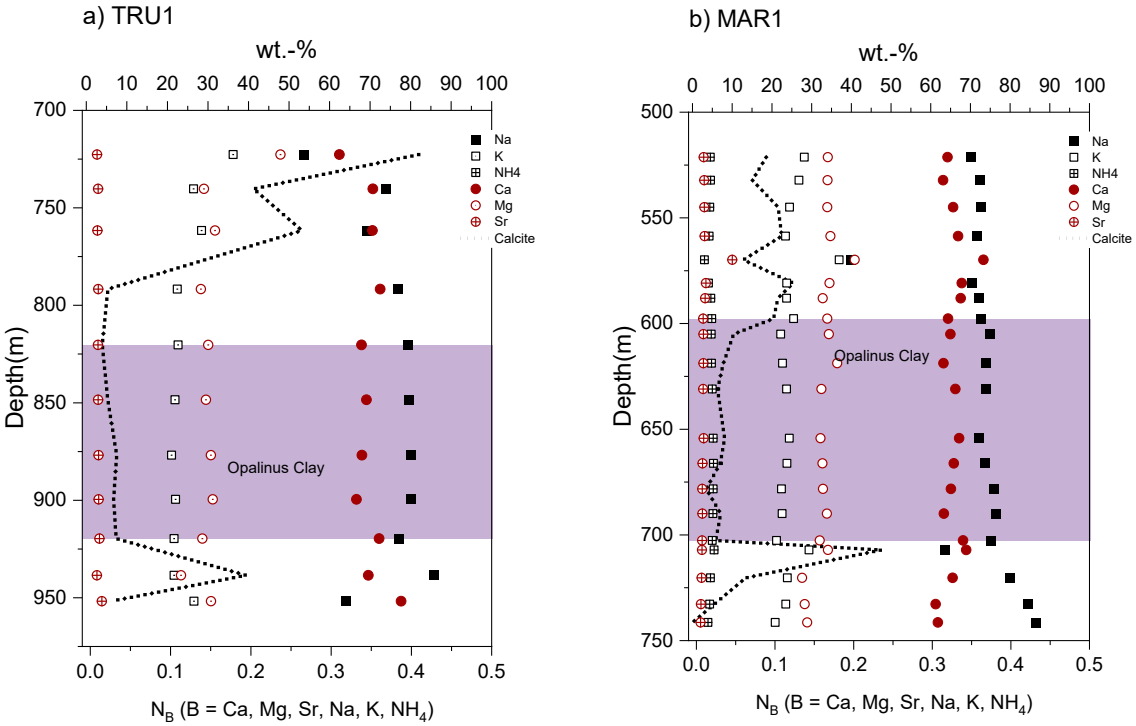

Fig. 3-20: Evolution of the N_B values (B = Na, K, NH_4, Mg, Ca or Sr) along the depth profile for the samples from (a) TRU1 and (b) MAR1

Dashed lines (to guide the eye) indicate the wt.-% of major reactive minerals other than clay minerals.

The N_{Na}, N_{K+NH4} and $N_{Mg+Ca+Sr}$ values determined for all samples from ZNO are summarized in Tab. A-3 and illustrated in the ternary graph in Fig. 3-21. As observed for the JO and NL samples, all Opalinus Clay samples within a drill core are concentrated in a single narrow region (closed coloured triangles). The samples from the confining units are more scattered with sample 16 from MAR1 being an outliner. In comparison to the samples from the confining units from NL and JO (see Fig. 3-14 and Fig. 3-7) the samples from ZNO are much less scattered.

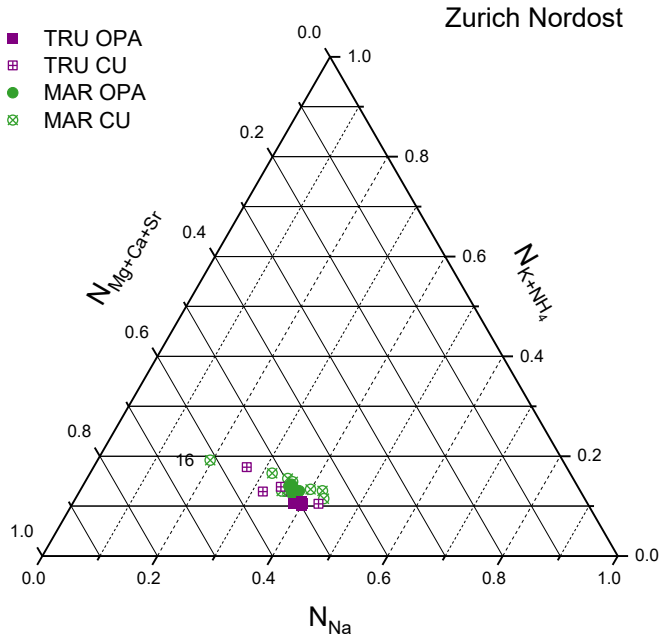

Fig. 3-21: N_{Na}, N_{K+NH_4} and $N_{Mg+Ca+Sr}$ data for all the samples from ZNO

Closed symbols are the data for Opalinus Clay (OPA) and open symbols are for the confining units (CU).

4 Comparison of the geochemical data for JO, NL and ZNO

4.1 Compilation of CEC results

An important physico-chemical parameter for the geodatabase is the cation exchange capacity (CEC) of rock samples originating from different boreholes from the three regions (JO, NL, ZNO) considered as potential repository sites for radioactive waste. Different methods have been applied in this study to determine the CEC on 141 deep drill core samples.

The use of a high selective index cation (Cs^+) or index complex (Ni-en^{2+}) in concentrations high enough to saturate the cation exchange sites of the rock samples directly determine the CEC by measuring the consumption of the index cation or index complex. Fig. 4-1a shows the correlation the CEC data obtained by this method for the two different index cations (Cs-CEC and Ni-CEC) for all rock samples from the three regions. The correlation between both independent methods is good. The Cs index cation, however, yields consistently higher values compared with the Ni-en index complex (slope = 1.2), partly due to the more selective displacement of K and NH_4 from illite by Cs.

The Cs extraction method allows determining the CEC of the rock samples indirectly by quantifying the cations displaced from the exchangeable sites. The dissolved salts and minerals are quantified by the anions detected in the Cs-ex and H_2O-ex experiments. The CEC (denoted as ΣCATIONS) is obtained from the sum of the corrected cations (total extracted cations minus dissolved anions). Fig. 4-1b shows the correlation between Ni-CEC and ΣCATIONS. The values obtained by these methods correlate very well, which increases the confidence in the applicability and reliability of these methods for determining cation occupancies. Similar as for the Cs-CEC method, consistently higher values are obtained compared to the Ni-CEC data.

Finally, the CEC of the rock samples can also be estimated from the clay mineralogical composition assuming reference CEC values for the clay mineral end-members and their wt.-% in the bulk rock sample. Fig. 4-1c shows the correlation between the Ni-CEC and the CEC-Clay (for the samples where the detailed clay mineralogy is available). With the exception of three data points from ZNO, the correlation can be regarded as good. This method, however, relies on the transferability of the determined clay mineralogy of the rock samples on which the CEC measurements were performed. In the present case, this cannot be fully guaranteed since the samples on which the clay mineralogy was determined are not identical to the samples on which the Ni-CEC was measured.

An important observation is that there are no clear trends seen in the CEC correlations for the rock samples originating neither from different borehole nor from different siting regions.

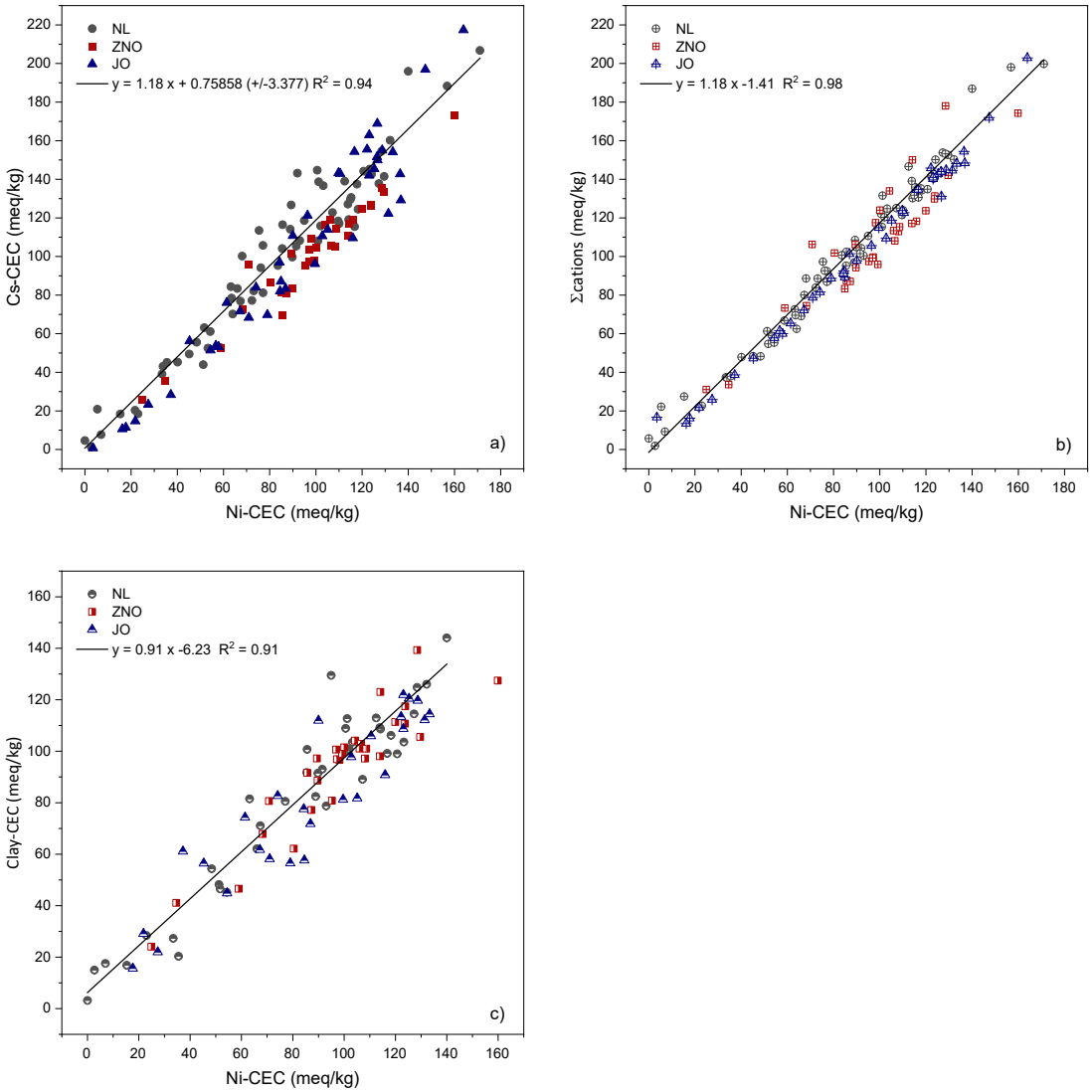

Fig. 4-1: Correlation between the Ni-CEC and (a) Cs-CEC, (b) ΣCATIONS and (c) CEC-Clay data determined for the drill core samples from the three siting regions

4.2 Compilation of the fractional occupancies of exchangeable cations

Fig. 4-2a, Fig. 4-2b and Fig. 4-2c show the N_B values derived for the major (Na, K, Mg and Ca) and minor (NH_4 and Sr) exchangeable cations for the samples from JO, NL and ZNO, respectively. The following trend in the N_B values is generally observed: $N_{Na} > N_{Ca} >> N_{Mg} \sim N_K >> N_{NH4} \sim N_{Sr}$. There are some deviations (and outliers) in the upper confining units in JO (at depth between 250 m and 400 m) and NL (at 700 m depth) and some single data points in the lower confining units for all three regions.

The scatter in the N_B values is the most pronounced in NL, whereas this is much less for JO and ZNO. Further, the data scatter for samples from the confining units is higher compared to the samples from the Opalinus Clay. This is more clearly illustrated in Fig. 4-3 where the N_B values for all the rock samples are presented in ternary plots for the confining units and the Opalinus Clay.

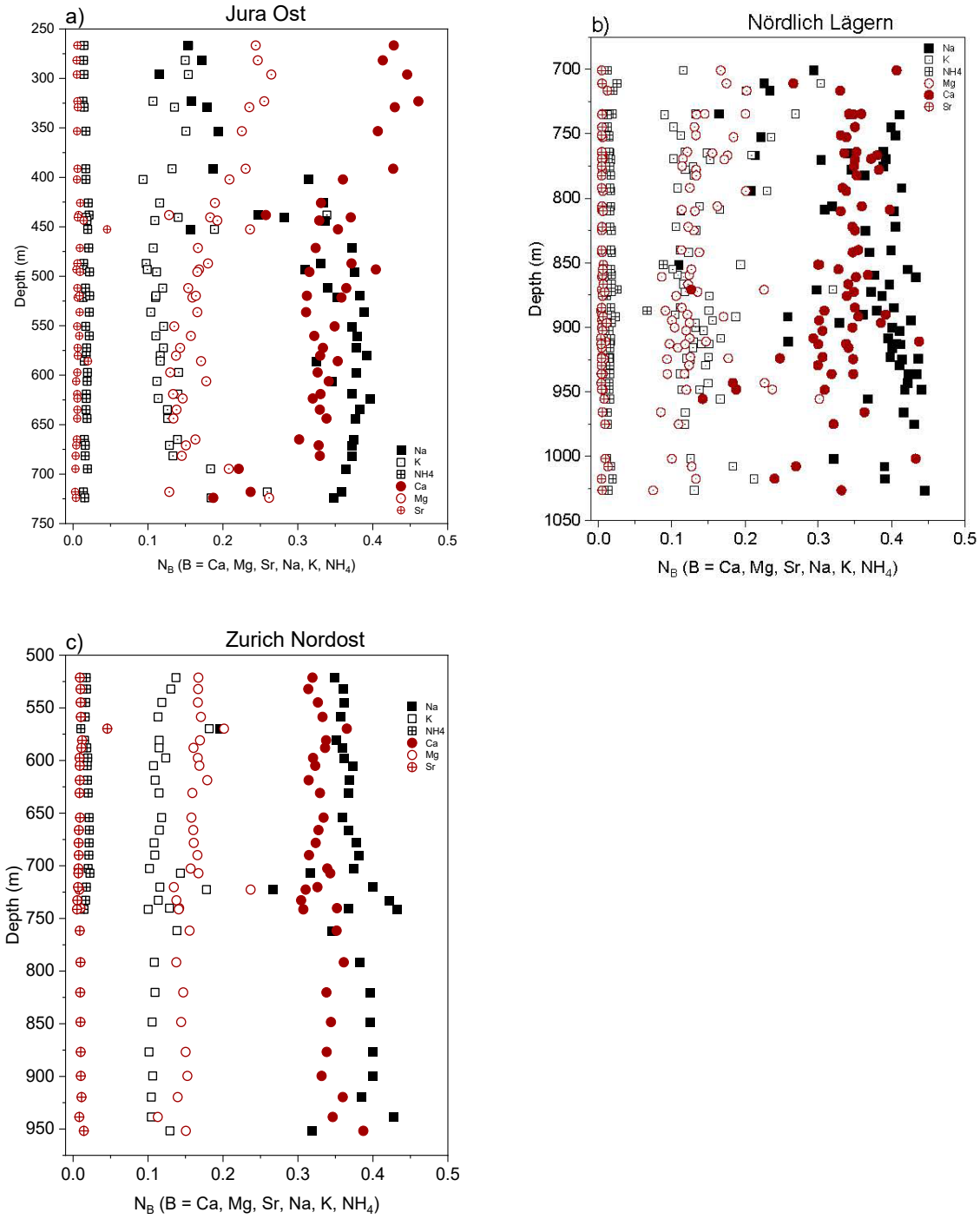

Fig. 4-2: Fractional occupancies of Na, K, NH_4, Mg, Ca and Sr for the deep drill core samples from (a) JO, (b) NL and (c) ZNO

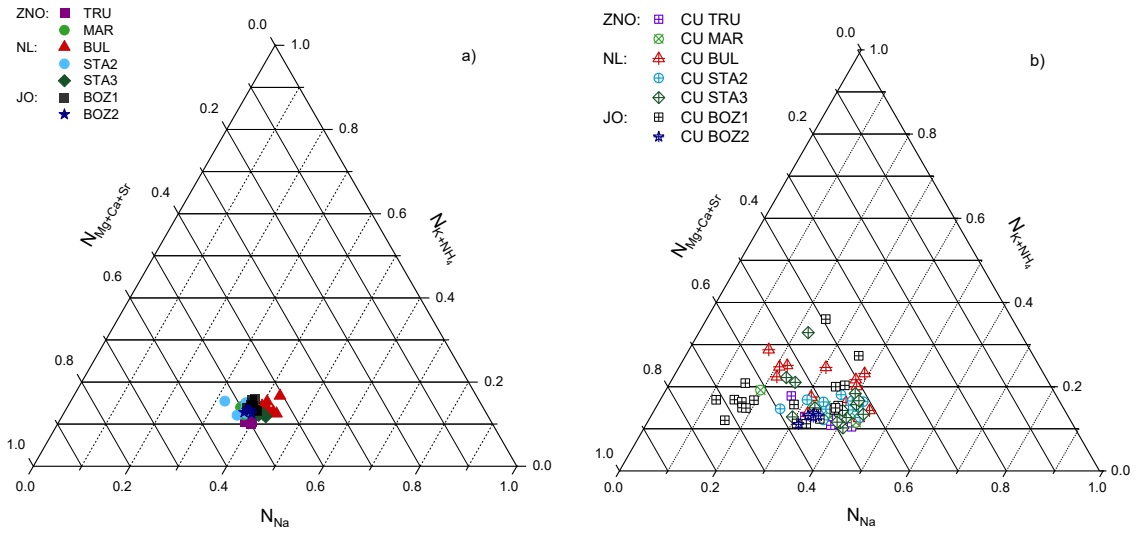

Fig. 4-3: Ternary representation of N_{Na}, $N_{Mg+Ca+Sr}$ and N_{K+NH4} determined for the samples from (a) Opalinus Clay and (b) the confining units for the samples from JO, NL and ZNO

4.3 Physico-chemical parameters for the Opalinus Clay data from JO, NL and ZNO

The compilation of the fractional cation occupancies, presented in section 4.2, clearly shows that the N_B values for Na, [K+NH_4] and [Mg+Ca+Sr] in the Opalinus Clay samples for JO, NL and ZNO (Fig. 4-3a) are very similar. In other words, the "fingerprint" of the exchangeable cations of the argillaceous rock samples originating from 7 different boreholes from 3 different siting regions is almost constant. This is clearly not the case for the samples originating from the confining units of all three siting regions (see Fig. 4-3b).

Cl and SO_4 inventories of the samples are two further key parameters, which were also obtained in this study in the H_2O-ex and Cs-ex experiments, respectively. Fig. 4-4a and Fig. 4-4b show for the 32 samples from Opalinus Clay from JO, NL and ZNO the Cl and SO4 inventories, respectively.

The Cl inventories along the depth profile for JO scatter very little and are low (< 2 mmol/kg). For the samples from the two boreholes from ZNO, the Cl inventories are also similar, however, slightly more scattered and higher than for JO (4 - 6 mmol/kg) except for one sample of TRU1 at 820.28 m depth. The Cl inventories are less homogenous in NL. For STA2 and STA3 the Cl inventories (4 – 5 mmol/kg) are similar and in agreement with the data determined for ZNO. The samples from BUL1 from NL show the highest Cl inventories (5.8 – 8.4 mmol/kg) and exhibit the highest scatter.

The SO_4 inventories for the Opalinus Clay samples are very low (1.5 to 2.5 mmol/kg), similar and homogenous independently of the siting regions. One sample from STA2 at a depth of 870 m showed a higher SO_4 inventory (3.5 mmol/kg).

The Cl and SO_4 inventories combined with the anion accessible porosities will allow calculating the Cl and SO_4 concentrations of the in-situ porewater compositions.

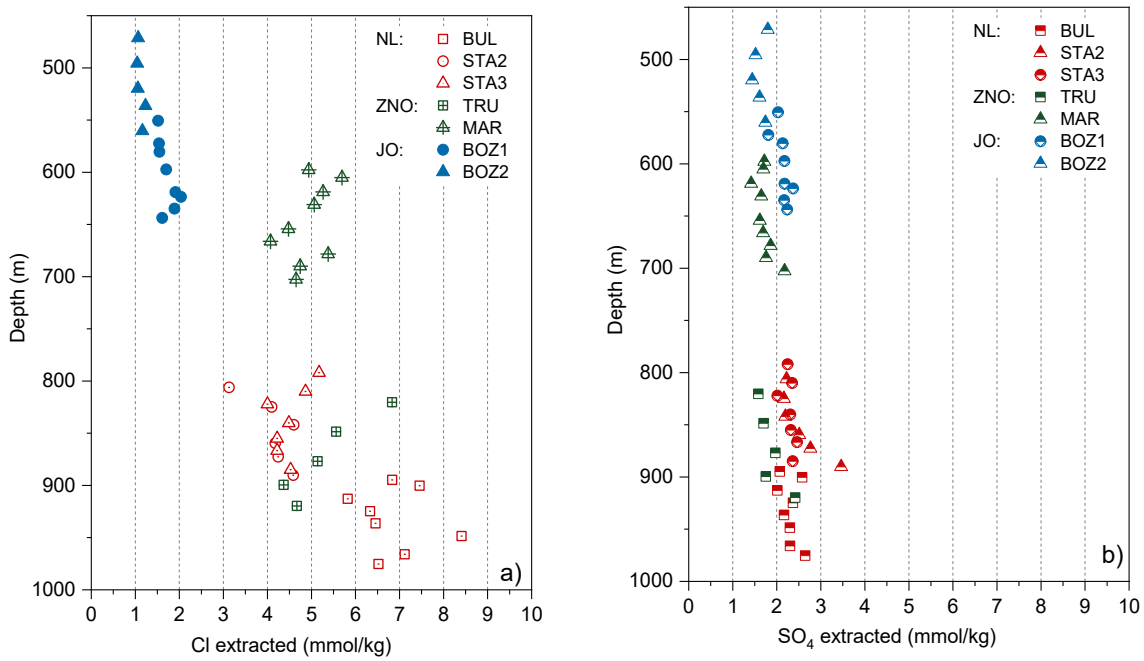

Fig. 4-4: Inventory of (a) Cl and (b) SO_4 determined for the Opalinus Clay samples from the different regions along the depth profile

The site-specific physico-chemical parameters obtained in this study are key parameters required for the modelling of in-situ porewaters of the Opalinus Clay formations representative for the three different siting regions. The knowledge of the in-situ porewater compositions is very important since it is critical for the prediction radionuclide solubilities and the development of sorption databases, and hence to repository safety studies.

In order to model porewater composition by considering cation exchange reaction with the clay minerals and thermodynamic equilibria with the mineral phases as shown by various studies (Bradbury & Baeyens 1998, Bradbury & Baeyens 2003, Gaucher et al. 2006, Wersin et al. 2022) following parameters are required:

- cation exchange capacity (CEC)
- mineralogical composition
- exchangeable cation occupancies
- Cl inventories and accessible porosity data (free water)
- in-situ pCO_2 (controlled by carbonate minerals)
- in-situ pε (Fe^{2+}/Fe^{3+} controlled by equilibrium with iron minerals pyrite-siderite)
- exchangeable cation occupancies (fingerprint)
- cation exchange selectivity coefficients

A number of these key parameters are provided in this report for rock samples originating from 7 boreholes from the three different siting regions.

5 Summary

The site-specific geochemical rock parameters, i.e., CEC and exchangeable cation occupancies, were determined by different experimental approaches using highly selective index cations (Ni-en and Cs) for 141 rock samples originating from the siting regions Jura Ost, Nördlich Lägern, and Zürich Nordost. In case of extremely clay mineral poor samples where the quantity of dissolved salts/minerals exceed the pool of total displaced cations these parameters cannot be determined reliably and hence, the methodology is not applicable.

CEC values were derived by different and independent methods/approaches and for most samples the agreement between these different methods is good. Generally, the Cs-CEC values derived from the Cs-ex experiments (by Cs consumption or by determination of the exchangeable cation loadings) are up to max. ~ 25 % higher than the Ni-CEC data obtained using the Ni-en complex as index cation.

With a few exceptions, the CEC values and total clay mineral content of the rock samples follow similar trends, confirming existing knowledge that the CEC is related to the clay mineral composition and content. This trend, however, could be improved if the measured CEC and the calculated CEC-Clay (using the detailed clay mineralogy) was determined on exactly the same rock samples used in the experiments (to avoid sample heterogeneity).

The exchangeable cations (Na, Ca, Mg, Sr, K and NH_4) of the rock samples were derived in the Cs-ex and H_2O-ex experiments after correction with the released anions (Cl, TIC, SO_4), to account for salt and mineral dissolution. In most cases, the correction of Na with Cl (NaCl) and SO_4 (Na_2SO_4) and Ca with TIC ($CaCO_3$) could be applied well. For a few samples, the presence of $CaSO_4$ or $SrSO_4$ was either indicated by the mineralogical compositions of the samples or suggested by the increased released amounts of Ca, Sr and SO_4 in the extraction solutions. In these cases, corrections were done accordingly.

The physico-chemical parameters obtained in this study on rock samples from 7 different boreholes from three different siting regions (JO, NL and ZNO) consist of CEC and exchangeable cation occupancies. In addition, Cl and SO_4 inventories for each rock sample have been determined. Additional important data such as bulk and detailed clay mineralogy (provided by UniBern) are provided in this report. Ternary representations visualize extremely homogeneous fractional occupancies for Na, K+NH_4 and Mg+Ca+Sr in the Opalinus Clay samples. These physico-chemical parameters are important rock parameters required for the determination of the in-situ porewater compositions of the formations under consideration for the safety analysis.

6 References

Allard, B., Karlsson, F., Tullborg, E.L. & Larson, S. (1983): Ion exchange capacities and surface areas of some major components and common fracture filling materials of igneous rocks. SKB TR-83-64, Svensk Kärnbränslehantering AB

Baeyens, B. & Bradbury, M.H. (1995): A Quantitative Mechanistic Description of Ni, Zn and Ca Sorption on Na- Montmorillonite. Part I: Physico-Chemical Characterisation and Titration Measurements. Nagra Technical Report NTB 95-04

Baeyens, B. & Bradbury, M.H. (2004): Cation exchange capacity measurements of illite using the sodium and cesium isotope dilution technique: Effects of the index-cation, electrolyte concentration and competition: Modeling. Clays and Clay Minerals 52, 421-431

Bradbury, M.H. & Baeyens, B. (1998): A physicochemical characterisation and geochemical modelling approach for determining porewater chemistries in argillaceous rocks. Geochimica et Cosmochimica Acta 62, 783-795

Bradbury, M.H. & Baeyens, B. (2003): Porewater chemistry in compacted re-saturated MX-80 bentonite. Journal of Contaminant Hydrology 61, 329-338

Gaucher, É.C., Blanc. P., Bardot. F., Braibant. G., Buschaert, S., Crouzet, C., Gautier, A., Girard, J.-P., Jacquot, E., Lassin, A., Negrel, G., Tournassat, C., Vinsot, A. & Altmann, S. (2006): Modelling the porewater chemistry of the Callovian-Oxfordian formation at a regional scale. Comptes Rendus Geoscience 338, 917-930

Hadi. J., Wersin. P., Mazurek. M., Waber. H.N., Marques Fernandes. M., Baeyens. B., Honty, M., De Craen, M., Frederickx, L., Dohrmann, R. & Fernandez, A.M. (2019): Intercomparison of CEC Method within the GD Project, in: M. T. T. R. T. 2017-06 (Ed.)

Peigneur, P. (1976): Stability and adsorption affinity of some transition metal-amine complexes in aluminosilicates. Ph.D Thesis, Univ. Leuven, Belgium

Sawhney, B.L. (1970): Potassium and Cesium Ion Selectivity in Relation to Clay Mineral Structure. Clays and Clay Minerals 18, 47-52

Swiss Federal Office of Energy (2008): Sectoral plan for deep geological repositories. Conceptual part. Federal Department of the Environment, Transport, Energy and Communications DETEC, Bern

Wersin, P., Mazurek, M. & Gimmi, T. (2022): Porewater chemistry of Opalinus Clay revisited: Findings from 25 years of data collection at the Mont Terri Rock Laboratory. Applied Geochemistry 138, 105234

App. A

Tab. A-1: Summary of the geochemical parameters for the samples from the siting region Jura Ost

Samples					Mineralogy								Clay mineralogy					CEC				Total anion & cation exactions									Exchangeable cations (corrected)						Fractional occupancies								
Nr	ID (RWI)	Depth	Group	Formation	Plagioclase	K-feldspar	Quartz	Calcite	Dol/Ank	Siderite	Pyrite	Anhydrite / Celestite	Illite EM	Smectite EM	Kaolinite EM	Chlorite EM	Total clay minerals	CEC-Clay	N-CEC	Cs-CEC	∑cations	Cl	SO_4	TIC	Na	K	NH_4	Mg	Ca	Sr	Na	K	NH_4	Mg	Ca	Sr	N_{Na}	N_K	N_{NH4}	N_{Mg}	N_{Ca}	N_{Sr}	N_{Na}	N_{K+NH4}	$N_{Mg+Ca+Sr}$
		[m]			[wt.-%]													[meq/kg]				[mmol/kg]									[meq/kg]						[-]								
1	BOZ1-1-266.75-DI	266.75	Malm	Wildegg	1.0	4.0	10.0	58.6	1.2		0.5		17.4	1.9	3.1	1.7	24.2	57.7	84.5	82.0	92.6	1.4	3.8	5.5	23.2	14.3	1.4	11.3	25.4	0.3	14.2	14.3	1.4	22.6	39.6	0.5	0.15	0.15	0.01	0.24	0.43	0.01	0.15	0.17	0.68
2	BOZ1-1-281.72-DI	281.72	Malm	Wildegg	1.0	4.0	11.0	45.5	5.1		0.4		24.0	2.9	4.5	1.3	32.4	81.2	99.6	96.2	114.9	1.2	3.3	6.1	27.4	17.2	1.6	14.2	29.8	0.3	19.7	17.2	1.6	28.3	47.5	0.6	0.17	0.15	0.01	0.25	0.41	0.00	0.17	0.16	0.67
3	BOZ1-1-296.08-DI	296.08	Malm	Wildegg		2.0	6.0	67.4	5.0		0.4		13.5	1.5	2.6	1.1	18.8	44.9	54.4	51.5	57.8	1.0	3.4	3.4	14.5	8.9	0.9	7.7	16.3	0.1	6.7	8.9	0.9	15.3	25.8	0.3	0.12	0.15	0.01	0.26	0.45	0.01	0.12	0.17	0.72
4	BOZ1-1-301.54-DI	301.54	Malm	Wildegg			2.0	89.8	1.0		<0.1		4.5	0.5	1.2	0.7	6.8	15.6	17.7	11.4	16.2	1.4	3.2	2.7	6.5	3.9	0.3	2.1	7.0	0.1	-1.3	3.9	0.3	4.3	8.7	0.3									
5	BOZ1-1-323.16-DI	323.16	Malm	Wildegg		2.0	3.0	80.7	2.3		0.6						11.1		57.9	53.2	60.0	0.8	3.1	3.1	16.4	6.4	0.8	7.7	16.9	0.2	9.5	6.4	0.8	15.3	27.7	0.4	0.16	0.11	0.01	0.26	0.46	0.01	0.16	0.12	0.72
6	BOZ1-1-329.10-DI	329.10	Malm	Wildegg		3.0	10.0	61.7	1.2		0.8		16.5	2.1	2.7	1.6	22.9	56.5	79.0	69.8	88.7	1.0	3.4	4.5	23.6	12.0	1.3	10.4	23.5	0.3	15.8	12.0	1.3	20.9	38.1	0.6	0.18	0.14	0.01	0.24	0.43	0.01	0.18	0.15	0.67
7	BOZ1-1-353.36-DI	353.36	Malm	Wildegg		4.0	8.0	55.2	1.2		0.2		19.8	2.8	5.9	2.5	31.0	71.8	86.9	83.4	101.4	1.2	3.8	5.8	28.5	15.3	1.7	11.4	26.5	0.3	19.7	15.3	1.7	22.8	41.3	0.6	0.19	0.15	0.02	0.23	0.41	0.01	0.19	0.17	0.64
8	BOZ1-1-391.30-DI	391.30	Malm	Wildegg		3.0	6.0	67.0			<0.1		13.9	2.8	5.2	1.6	23.6	58.1	71.0	68.4	78.8	1.1	4.1	4.7	24.0	10.4	1.3	9.1	21.5	0.2	14.7	10.4	1.3	18.2	33.7	0.5	0.19	0.13	0.02	0.23	0.43	0.01	0.19	0.15	0.66
9	BOZ1-1-416.35-DI	416.35	Dogger	Ifenthal		1.0	2.0	69.4	6.0		<0.1						21.4		16.2	10.6	13.5	4.8	3.5	3.5	11.8	4.6	0.2	1.5	6.2	0.1	-0.1	4.6	0.2	3.1	5.5	0.2									
10	BOZ1-1-434.29-DI	434.29	Dogger	Hauptrogenstein		2.0	4.0	73.8	4.3		0.1		8.4	0.9	4.3	2.0	15.5	29.1	21.8	14.7	21.8	1.5	11.4	4.2	9.8	4.5	0.5	2.7	11.5	5.6	-4.0	4.5	0.5	5.4	14.7	0.7									
11	BOZ1-1-438.20-DI	438.20	Dogger	Hauptrogenstein		1.0	4.0	55.8	5.6		0.5		17.0	2.0	5.9	8.2	32.7	61.1	37.2	28.4	38.7	3.6	3.0	7.2	19.1	13.1	0.8	2.5	12.2	0.1	9.5	13.1	0.8	5.0	9.9	0.3	0.25	0.34	0.02	0.13	0.26	0.01	0.25	0.36	0.39
12	BOZ1-1-440.55-DI	440.55	Dogger	Hauptrogenstein		2.0	6.0	55.7	6.6		0.6						28.8		56.7	53.8	61.5	2.7	2.4	4.4	25.0	8.6	1.1	5.6	15.8	0.2	17.4	8.6	1.1	11.3	22.8	0.4	0.28	0.14	0.02	0.18	0.37	0.01	0.28	0.16	0.56
13	BOZ1-1-452.61-DI	452.61	Dogger	Hauptrogenstein		1.0	4.0	77.1	5.8		<0.1		6.3	0.7	2.8	1.9	11.8	22.0	27.4	23.3	25.9	1.9	3.8	6.0	13.6	4.9	0.5	3.1	10.5	0.6	4.0	4.9	0.5	6.1	9.2	1.2	0.16	0.19	0.02	0.24	0.35	0.05	0.16	0.21	0.64
14	BOZ1-1-487.01-DI	487.01	Dogger	Passwang	3.0	5.0	20.0	33.6			1.1		26.4	5.9	1.8	2.6	36.6	112.2	131.4	122.2	144.6	1.1	2.5	7.2	53.9	14.1	2.1	13.0	34.0	0.4	47.8	14.1	2.1	26.1	53.8	0.9	0.33	0.10	0.01	0.18	0.37	0.01	0.33	0.11	0.56
15	BOZ1-1-493.15-DI	493.15	Dogger	Passwang	2.0	5.0	22.0	34.6			1.2						34.5		136.8	129.2	148.4	1.2	6.7	6.7	57.2	14.7	2.0	12.5	36.7	2.1	46.0	14.7	2.0	25.0	60.0	0.7	0.31	0.10	0.01	0.17	0.40	0.00	0.31	0.11	0.58
16	BOZ1-1-512.03-DI	512.03	Dogger	Passwang	3.0	5.0	27.0	18.8			1.1		25.9	3.1	10.7	4.9	44.6	90.8	116.0	109.6	134.5	1.6	2.3	6.8	52.0	16.1	2.2	10.3	31.3	0.4	45.6	16.1	2.2	20.7	49.1	0.8	0.34	0.12	0.02	0.15	0.36	0.01	0.34	0.14	0.52
17	BOZ1-1-521.50-DI	521.50	Dogger	Passwang	4.0	5.0	31.0	16.2			1.4						41.8		136.5	142.7	154.4	1.6	2.3	7.2	60.6	17.0	2.1	12.3	34.8	0.5	54.4	17.0	2.1	24.6	55.3	1.0	0.35	0.11	0.01	0.16	0.36	0.01	0.35	0.12	0.52
18	BOZ1-1-550.63-DI	550.63	Dogger	Opalinus Clay	3.0	4.0	28.0	14.0			1.9		23.7	2.4	16.4	5.8	48.3	81.8	105.1	114.0	118.7	1.5	2.0	6.1	49.8	14.4	2.0	8.0	26.8	0.3	44.2	14.4	2.0	16.0	41.4	0.7	0.37	0.12	0.02	0.14	0.35	0.01	0.37	0.14	0.49
19	BOZ1-1-572.43-DI	572.43	Dogger	Opalinus Clay	3.0	5.0	31.0	14.2		3.3	0.6						42.2		84.9	87.1	89.3	1.5	1.8	5.7	38.9	10.8	1.6	6.4	20.6	0.3	33.8	10.8	1.6	12.8	29.8	0.6	0.38	0.12	0.02	0.14	0.33	0.01	0.38	0.14	0.48
20	BOZ1-1-580.34-DI	580.34	Dogger	Opalinus Clay	3.0	4.0	25.0	11.0		3.7	0.5		28.2	3.1	15.1	5.7	52.2	97.8	102.8	110.6	109.4	1.5	2.1	7.8	48.7	12.8	1.9	7.5	25.8	0.3	42.9	12.8	1.9	15.0	36.1	0.7	0.39	0.12	0.02	0.14	0.33	0.01	0.39	0.13	0.47
21	BOZ1-1-597.28-DI	597.28	Dogger	Opalinus Clay	3.0	4.0	20.0	5.9		3.9	1.1		30.0	3.7	22.1	6.1	61.3	108.8	123.1	142.0	140.2	1.7	2.2	8.6	59.0	19.8	2.7	9.1	31.5	0.4	53.0	19.8	2.7	18.2	45.8	0.8	0.38	0.14	0.02	0.13	0.33	0.01	0.38	0.16	0.46
22	BOZ1-1-619.10-DI	619.10	Dogger	Opalinus Clay	3.0	5.0	16.0	4.0		3.0	0.1		36.1	3.4	19.0	8.8	68.0	120.5	125.3	145.4	142.8	1.9	2.2	8.1	59.5	20.0	2.5	9.5	31.7	0.4	53.2	20.0	2.5	19.1	47.2	0.8	0.37	0.14	0.02	0.13	0.33	0.01	0.37	0.16	0.47
23	BOZ1-1-623.60-DI	623.60	Dogger	Opalinus Clay	3.0	4.0	16.0	3.1		3.1	0.3		32.7	3.5	25.7	7.0	69.5	114.5	133.3	154.1	148.1	2.0	2.4	9.8	65.5	16.8	2.6	10.8	33.5	0.4	58.7	16.8	2.6	21.7	47.4	0.9	0.40	0.11	0.02	0.15	0.32	0.01	0.40	0.13	0.47
24	BOZ1-1-634.90-DI	634.90	Dogger	Opalinus Clay	3.0	5.0	14.0	5.0		4.0	0.6		33.0	4.0	24.3	6.7	67.4	119.7	128.7	155.1	144.8	1.9	2.2	8.7	61.7	18.2	2.5	10.0	32.5	0.4	55.5	18.2	2.5	20.0	47.7	0.8	0.38	0.13	0.02	0.14	0.33	0.01	0.38	0.14	0.47
25	BOZ1-1-643.80-DI	643.80	Dogger	Opalinus Clay	2.0	4.0	15.0	6.0		3.6	1.1						67.4		126.5	151.6	143.7	1.6	2.2	7.9	60.2	18.1	2.7	9.6	32.2	0.4	54.2	18.1	2.7	19.3	48.6	0.8	0.38	0.13	0.02	0.13	0.34	0.01	0.38	0.14	0.48
26	BOZ1-1-665.00-DI	665.00	Lias	Staffelegg	3.0	6.0	44.0	9.5	5.4		2.9		18.4	2.0	6.0	2.3	28.7	61.7	67.2	71.7	72.2	1.2	1.9	4.4	32.0	10.1	1.1	5.9	15.3	0.2	27.1	10.1	1.1	11.8	21.8	0.4	0.37	0.14	0.02	0.16	0.30	0.01	0.37	0.15	0.47
27	BOZ1-1-670.95-DI	670.95	Lias	Staffelegg	2.0	6.0	31.0	19.8	2.5		1.1		24.3	2.2	7.4	3.0	36.9	77.6	84.3	97.0	91.3	1.0	2.2	5.1	39.3	11.7	1.5	6.9	20.0	0.2	33.9	11.7	1.5	13.8	29.9	0.4	0.37	0.13	0.02	0.15	0.33	0.00	0.37	0.15	0.48
28	BOZ1-1-681.57-DI	681.57	Lias	Staffelegg	0.0	0.0	9.0	8.0			3.0						79.2		163.9	217.3	202.9	0.8	3.1	9.7	82.4	27.1	3.3	14.7	43.1	0.4	75.5	27.1	3.3	29.4	66.8	0.7	0.37	0.13	0.02	0.15	0.33	0.00	0.37	0.15	0.48
29	BOZ1-1-694.72-DI	694.72	Keuper	Klettgau	4.0	7.0	9.0	2.4	36.6		<0.1		36.0	3.7	0.4	0.8	40.9	113.4	122.2	155.5	145.8	0.5	4.1	9.6	61.9	26.8	2.8	15.2	25.8	0.2	53.2	26.8	2.8	30.3	32.3	0.5	0.36	0.18	0.02	0.21	0.22	0.00	0.36	0.20	0.43
30	BOZ1-1-717.96-DI	717.96	Keuper	Klettgau	12.0	19.0	29.0	0.0			<0.1		27.3	2.0	4.0	5.9	39.6	82.7	74.1	84.0	81.6	0.7	3.4	3.1	36.8	21.2	1.1	5.2	12.7	0.1	29.2	21.2	1.1	10.5	19.3	0.2	0.36	0.26	0.01	0.13	0.24	0.00	0.36	0.27	0.37
31	BOZ1-1-723.97-DI	723.97	Keuper	Bänkerjoch	4.0	8.0	11.0	0.0	32.0		0.6		34.8	3.5	0.0	5.7	44.1	111.9	90.0	110.8	97.8	0.9	3.9	6.1	42.7	18.0	1.5	12.8	15.2	0.2	34.0	18.0	1.5	25.6	18.3	0.4	0.35	0.18	0.02	0.26	0.19	0.00	0.35	0.20	0.45
32	BOZ1-1-808.61-DI	808.61	Keuper	Bänkerjoch					2.7		0.0	97.2					0.0		3.5	0.8	16.7	0.4	128.9	1.1	3.0	0.9	0.0	0.8	135.2	0.5															
33	BOZ2-1-402.15-PW	402.15	Dogger	Passwang Fm.	2.1	4.2	21.1	38.3									35.0		126.7	150.0	131.2	0.6	6.3	6.2	47.1	12.3	2.3	13.7	29.8	4.1	41.3	12.3	2.3	27.4	47.3	0.7	0.31	0.09	0.02	0.21	0.36	0.01	0.31	0.11	0.57
34	BOZ2-1-425.92-PW	425.92	Dogger	Passwang Fm.	1.8	4.4	29.1	22.9			0.1						41.1		96.4	121.3	105.6	0.8	1.5	5.6	39.0	12.2	2.2	10.0	23.1	0.5	35.2	12.2	2.2	20.0	35.0	1.0	0.33	0.12	0.02	0.19	0.33	0.01	0.33	0.14	0.53
35	BOZ2-1-443.71-PW	443.71	Dogger	Passwang Fm.	3.5	5.0	37.4	21.9			0.1		20.3	2.9	3.2	5.3	31.7	74.3	61.4	76.1	65.4	1.0	1.7	3.9	26.4	7.1	1.2	6.3	14.6	0.5	22.0	7.1	1.2	12.6	21.5	0.9	0.34	0.11	0.02	0.19	0.33	0.01	0.34	0.13	0.54
36	BOZ2-1-471.37-PW	471.37	Dogger	Opalinus Clay	2.7	4.2	21.7	6.2			0.4						63.6		116.7	154.3	134.7	1.1	1.8	6.7	54.8	14.4	2.8	11.2	28.5	0.6	50.1	14.4	2.8	22.5	43.6	1.2	0.37	0.11	0.02	0.17	0.32	0.01	0.37	0.13	0.50
37	BOZ2-1-495.66-PW	495.66	Dogger	Opalinus Clay	2.6	4.6	21.8	7.6		3.5	<0.1		29.6	3.5	19.7	6.1	58.9	105.9	110.5	142.9	122.7	1.0	1.5	6.9	50.1	13.7	2.7	10.2	26.3	0.6	46.1	13.7	2.7	20.4	38.7	1.1	0.38	0.11	0.02	0.17	0.32	0.01	0.38	0.13	0.49
38	BOZ2-1-519.74-PW	519.74	Dogger	Opalinus Clay	2.6	4.1	19.9	4.0		7.6	0.2						60.6		109.8	143.3	123.8	1.1	1.4	7.0	51.3	13.7	2.8	10.2	26.3	0.5	47.3	13.7	2.8	20.3	38.6	1.1	0.38	0.11	0.02	0.16	0.31	0.01	0.38	0.13	0.48
39	BOZ2-1-536.30-PW	536.30	Dogger	Opalinus Clay	2.3	3.9	14.7	3.7		5.4	0.2		33.9	4.1	23.4	7.6	68.9	121.9	123.1	162.9	141.0	1.2	1.6	7.7	59.3	14.6	3.1	11.7	29.6	0.6	54.8	14.6	3.1	23.4	43.8	1.2	0.39	0.10	0.02	0.17	0.31	0.01	0.39	0.13	0.49
40	BOZ2-1-560.29-PW	560.29	Dogger	Opalinus Clay	1.8	3.3	11.5	5.8		5.3	0.9						70.4		126.6	168.9	144.0	1.2	1.7	7.7	59.3	15.9	3.1	11.3	30.9	0.6	54.7	15.9	3.1	22.7	46.4	1.2	0.38	0.11	0.02	0.16	0.32	0.01	0.38	0.13	0.49
41	BOZ2-1-585.84-PW	585.84	Lias	Staffelegg Fm.	2.8	5.7	54.1	8.9			2.0		16.1	2.0	5.1	2.8	26.0	56.5	45.3	56.2	47.3	1.2	2.5	2.4	21.5	5.5	0.7	4.0	10.7	0.5	15.3	5.5	0.7	8.1	16.7	1.0	0.32	0.12	0.01	0.17	0.35	0.02	0.32	0.13	0.54
42	BOZ2-1-606.13-PW	606.13	Lias	Staffelegg Fm.		2.5	8.3	12.0			1.1						75.2		147.4	196.9	172.0	0.5	2.7	8.4	65.4	19.2	3.2	15.3	37.7	0.4	59.5	19.2	3.2	30.6	58.7	0.7	0.35	0.11	0.02	0.18	0.34	0.00	0.35	0.13	0.52

Tab. A-2: Summary of all the geochemical parameters for the samples from the siting region Nördlich Lägern

Samples					Mineralogy [wt.-%]								Clay mineralogy [wt.-%]				
Nr	ID (RWI)	Depth [m]	Group	Formation	Plagioclase	K-feldspat	Quartz	Calcite	Dol/Ank	Siderite	Pyrite	Anhydrite / Celestite	Illite EM	Smectite EM	Kaolinite EM	Chlorite EM	Total clay minerals
1	BUL1-1-734.45-DI	734.45	Malm	Villigen Fm.			1.6	87.4			0.1		7.4	1.1	1.4	0.6	10.6
2	BUL1-1-752.48-DI	752.48	Malm	Wildegg Fm.		3.0	7.5	63.6	7.1		0.3		14.5	1.5	1.3	1.1	18.4
3	BUL1-1-766.65-DI	766.65	Malm	Wildegg Fm.		2.5	5.4	72.9	1.3		0.1		12.4	1.9	2.5	0.9	17.6
4	BUL1-1-794.35-DI	794.35	Malm	Wildegg Fm.		3.3	5.5	68.7					15.8	2.0	2.7	1.8	22.3
5	BUL1-1-808.92-DI	808.92	Dogger	Parkinsoni-Württ.'	1.5	4.9	14.6	25.8			1.2		29.8	3.5	14.2	4.0	51.5
6	BUL1-1-815.90-DI	815.90	Dogger	'Herrenwis Unit'				74.0	19.9				4.8	0.7		0.5	5.9
7	BUL1-1-828.17-DI	828.17	Dogger	'Herrenwis Unit'			4.0	94.0			0.1						1.0
8	BUL1-1-840.45-DI	840.45	Dogger	'Herrenwis Unit'		1.5	10.1	78.4	4.3		0.3		4.1	0.6	0.0	0.5	5.3
9	BUL1-1-845.05-DI	845.05	Dogger	'Herrenwis Unit'			1.2	97.7					0.7	0.2	0.0	0.1	1.0
10	BUL1-1-851.50-DI	851.50	Dogger	'Herrenwis Unit'			3.1	89.9			0.2		5.4	0.6	0.4	0.4	6.8
11	BUL1-1-861.00-DI	861.00	Dogger	Wedelsandstein	3.3	5.6	26.6	14.2			1.1		36.9	6.8	2.7	2.1	48.5
12	BUL1-1-870.91-PW	870.91	Dogger	Wedelsandstein	1.6	3.6	22.6	65.5									6.6
13	BUL1-1-875.69-PW	875.69	Dogger	Wedelsandstein	4.2	6.2	36.6	24.6			1.0		17.2	2.4	4.5	2.9	27.1
14	BUL1-1-887.26-PW	887.26	Dogger	Murchiso-Oolit.'	3.4	5.8	23.3	1.0		0.5	1.7		30.1	4.1	22.1	7.1	63.3
15	BUL1-1-894.68-PW	894.68	Dogger	Opalinus Clay	3.1	7.0	39.1	13.4		1.7	0.7						34.3
16	BUL1-1-900.26-PW	900.26	Dogger	Opalinus Clay	2.9	5.1	27.0	16.8		1.8	1.2		23.6	2.7	13.6	4.4	44.3
17	BUL1-1-912.84-PW	912.84	Dogger	Opalinus Clay	3.5	5.3	31.2	11.8		2.1	1.0		22.2	2.9	13.9	5.4	44.4
18	BUL1-1-924.73-PW	924.73	Dogger	Opalinus Clay	3.0	5.5	31.0	11.1		2.5	0.4		22.7	2.6	16.9	3.5	45.8
19	BUL1-1-936.36-PW	936.36	Dogger	Opalinus Clay	3.3	5.0	22.7	6.1		2.6	0.4		28.7	3.1	20.8	6.3	58.9
20	BUL1-1-948.58-PW	948.58	Dogger	Opalinus Clay	3.7	5.7	18.2	5.2		4.1	0.3		30.0	3.7	21.5	6.6	61.8
21	BUL1-1-965.98-PW	965.98	Dogger	Opalinus Clay	3.3	5.2	17.1	6.1		2.4	1.1		28.9	4.3	22.7	8.0	63.9
22	BUL1-1-975.25-PW	975.25	Dogger	Opalinus Clay	3.2	5.0	26.4	6.0		4.6	0.2		23.7	3.1	21.4	5.4	53.6
23	BUL1-1-1001.96-RP	1001.96	Lias	Staffelegg Fm.	1.6	3.6	10.1	30.4			3.4						46.2
24	BUL1-1-1008.04-PW	1008.04	Lias	Staffelegg Fm.		1.8	3.7	82.7	1.4				5.8	0.7	2.8	0.8	10.1
25	BUL1-1-1017.56-RP	1017.56	Lias	Staffelegg Fm.	3.1	4.8	33.2	9.9	1.8	1.3	1.1						43.9
26	BUL1-1-1026.50-PW	1026.50	Lias	Staffelegg Fm.		3.8	22.1	43.3			0.4						29.9
27	STA2-1-734.53-PW	734.53	Dogger	Variansmergel Fm.	2.0	5.4	15.4	19.1			1.1						56.5
28	STA2-1-764.99-PW	764.99	Dogger	Parkinsoni-Würt.'	2.9	6.3	15.8	17.2	2.4		1.1						53.6
29	STA2-1-770.01-PW	770.01	Dogger	'Herrenwis Unit'	2.0	4.6	16.6	49.9			0.3						26.1
30	STA2-1-777.85-PW	777.85	Dogger	'Humphriesioolith Fm.'	2.8	5.0	18.6	20.7			1.1		28.4	4.3	10.8	7.5	51.2
31	STA2-1-782.31-PW	782.31	Dogger	Wedelsandstein Fm.	3.0	5.9	21.5	8.6			0.7						59.5
32	STA2-1-806.13-PW	806.13	Dogger	Opalinus Clay	2.0	3.8	25.0	40.2		1.9	0.2						26.3
33	STA2-1-824.92-PW	824.92	Dogger	Opalinus Clay	3.4	5.2	23.8	8.2		2.7	1.6		28.2	3.4	15.9	6.6	54.1
34	STA2-1-841.98-PW	841.98	Dogger	Opalinus Clay	3.2	5.5	22.7	8.5		4.9	0.1						54.3
35	STA2-1-859.51-PW	859.51	Dogger	Opalinus Clay	3.5	5.0	20.4	5.9		4.3	0.6		27.4	4.1	21.3	6.9	59.6
36	STA2-1-872.57-PW	872.57	Dogger	Opalinus Clay	2.8	5.5	21.2	6.2		6.4	0.4		25.5	3.8	21.9	5.4	56.5
37	STA2-1-890.16-PW	890.16	Dogger	Opalinus Clay	2.0	5.3	12.4	6.6		1.6	1.7		31.6	3.7	25.5	8.7	69.4
38	STA2-1-911.03-PW	911.03	Lias	Staffelegg Fm.	3.0	4.2	9.7	36.1			2.6						39.7
39	STA2-1-915.94-PW	915.94	Lias	Staffelegg Fm.	4.1	4.8	13.2	15.9	3.5		2.6		31.4	3.8	9.0	5.1	49.6
40	STA2-1-923.05-PW	923.05	Lias	Staffelegg Fm.	3.2	5.6	39.8	8.0	2.3		0.5						40.0
41	STA2-1-929.50-PW	929.50	Lias	Staffelegg Fm.	3.1	5.1	38.5	5.0	1.6		0.5		25.1	3.3	10.6	6.3	45.4
42	STA2-1-939.20-PW	939.20	Lias	Staffelegg Fm.	2.8	6.0	20.7	9.6			1.0						59.5
43	STA2-1-943.22-PW	943.22	Keuper	Klettgau Fm.	2.8	4.8	9.5	7.3	47.7		0.1						27.7
44	STA2-1-948.33-PW	948.33	Keuper	Klettgau Fm.	4.3	6.1	13.9	5.2	47.4		<0.1						22.9
45	STA2-1-955.63-PW	955.63	Keuper	Klettgau Fm.	1.2	5.2	17.8	6.7	51.7		0.1						17.3
46	STA2-1-960.43-PW	960.43	Keuper	Klettgau Fm.	0.6	1.4	2.9		88.5			6.0					0.4
47	STA3-1-700.77-PW	700.77	Dogger	Variansmergel Fm.	1.2	4.9	15.3	16.5			1.4		36.5	4.1	14.6	4.9	60.1
48	STA3-1-710.87-PW	710.87	Dogger	Herrenwies Fm.		1.9	4.1	72.7	3.0		<0.1		14.7	1.6	0.0	1.6	18.0
49	STA3-1-716.58-PW	716.58	Dogger	Herrenwies Fm.		1.4	2.5	83.6	3.6		<0.1						8.8
50	STA3-1-735.02-PW	735.02	Dogger	Herrenwies Fm.	1.9	4.2	12.1	46.7			0.4						34.3
51	STA3-1-744.66-PW	744.66	Dogger	Wedelsandstein Fm.	3.0	4.6	28.6	21.9			0.4						41.0
52	STA3-1-751.10-PW	751.10	Dogger	Wedelsandstein Fm.	2.4	5.3	21.7	12.1		1.8	<0.1		34.0	5.0	13.3	3.8	56.1
53	STA3-1-764.00-PW	764.00	Dogger	Wedelsandstein Fm.	2.9	5.6	31.7	8.3			0.9		25.0	3.2	15.6	6.2	50.1
54	STA3-1-769.35-PW	769.35	Dogger	Murchisonae-Oolith Fm.	2.5	4.2	39.4	7.8			0.9						44.7
55	STA3-1-775.10-PW	775.10	Dogger	Murchisonae-Oolith Fm.	2.5	4.5	22.4	9.9		2.2	0.7		28.1	3.3	19.5	6.3	57.2
56	STA3-1-791.96-PW	791.96	Dogger	Opalinus Clay	2.2	2.7	17.8	11.3		1.8	1.3						62.0
57	STA3-1-809.87-PW	809.97	Dogger	Opalinus Clay	3.7	5.5	30.9	13.0		3.3	0.5		21.1	2.9	14.2	4.1	42.2
58	STA3-1-822.13-PW	822.13	Dogger	Opalinus Clay	2.7	4.9	24.7	9.5		3.6	0.6		25.9	3.1	18.8	5.3	53.0
59	STA3-1-840.14-PW	840.14	Dogger	Opalinus Clay	2.4	4.7	17.4	6.6		2.1	2.4						63.3
60	STA3-1-855.05-PW	855.05	Dogger	Opalinus Clay	3.0	4.9	17.5	4.8		8.0	0.4		27.0	3.3	23.7	6.4	60.4
61	STA3-1-866.67-PW	866.67	Dogger	Opalinus Clay	3.2	5.1	16.9			10.5	0.4		28.4	3.4	24.3	6.7	62.8
62	STA3-1-884.83-PW	884.83	Dogger	Opalinus Clay	2.8	4.8	14.5	8.2		3.4	0.8						64.7
63	STA3-1-891.81-PW	891.81	Lias	Steffelegg Fm.		2.0	3.8	80.7			0.1		8.4	0.9	2.1	1.8	13.2
64	STA3-1-896.60-PW	896.60	Lias	Steffelegg Fm.	1.2	2.8	8.2	51.0			2.7						27.9
65	STA3-1-902.70-PW	902.70	Lias	Steffelegg Fm.	3.1	5.7	46.3	5.9	1.8		0.7		19.7	2.5	9.2	4.5	35.9
66	STA3-1-908.65-PW	908.65	Lias	Steffelegg Fm.	2.8	4.4	35.6	15.5			0.6						40.4
67	STA3-1-913.19-PW	913.19	Lias	Steffelegg Fm.	1.9	4.0	16.2	7.9			0.8		36.7	4.3	18.9	8.4	68.3
68	STA3-1-924.15-PW	924.15	Keuper	Klettgau Fm.	2.6	5.6	7.9		53.6		0.2		23.8	4.0	0.4	1.8	29.9

	CEC [meq/kg]				Total anion & cation exactions [mmol/kg]								
Nr	CEC-Clay	Ni-CEC	Cs-CEC	Σcations	Cl	SO_4	TIC	Na	K	NH_4	Mg	Ca	Sr
1	27.3	33.4	39.1	37.4	1.4	3.1	4.4	13.8	10.1	0.7	3.8	10.8	0.1
2	46.5	51.7	63.2	54.7	2.5	3.9	6.8	22.5	12.9	0.8	5.0	16.1	0.1
3	45.2	54.3	61.1	55.3	2.8	4.3	6.3	23.2	11.6	0.8	4.9	16.8	0.2
4	54.3	48.4	55.6	48.3	2.5	4.3	6.8	21.2	11.1	0.8	4.9	15.0	0.1
5	103.5	103.2	136.7	124.8	6.1	2.5	6.8	49.7	20.6	1.2	7.1	31.6	0.3
6	16.8	15.3	18.4	27.5	1.3	0.8	4.8	10.1	6.2	0.5	7.2	4.3	0.0
7		5.4	20.9	22.2	1.6	2.0	3.1	19.2	6.1	0.1	1.2	3.1	0.0
8	15.0	2.7	1.3	1.9	2.1	1.6	3.0	2.9	1.0	0.1	1.0	3.6	0.1
9	3.2	0.0	4.6	5.7	1.7	1.3	3.5	3.0	2.1	0.8	1.1	4.3	0.1
10	17.5	7.0	7.7	9.3	3.2	1.6	3.4	7.4	1.8	0.8	1.4	4.8	0.0
11	144.1	140.0	196.0	187.0	6.3	2.9	7.5	93.0	21.8	1.6	8.0	40.3	0.4
12		33.8	43.1	37.2	4.2	2.0	5.8	19.6	6.2	3.0	3.1	11.0	0.1
13	62.1	66.0	83.4	69.1	5.6	2.1	3.9	36.6	10.4	0.8	3.7	15.6	0.2
14	113.0	112.5	139.0	146.7	9.0	1.8	8.3	68.4	22.1	9.7	6.7	30.9	0.2
15		64.0	70.2	62.5	6.8	2.1	8.5	37.6	9.7	0.8	3.1	17.9	0.1
16	82.4	88.9	114.1	96.9	7.5	2.6	7.2	51.5	12.8	1.1	5.0	24.0	0.2
17	81.5	63.2	84.3	72.6	5.8	2.0	5.7	39.4	10.2	1.0	3.5	18.0	0.2
18	80.5	77.1	105.7	86.9	6.3	2.4	6.3	47.1	10.9	1.0	4.1	21.5	0.3
19	100.7	85.6	116.4	102.5	6.5	2.2	7.4	54.1	12.1	1.2	4.8	25.3	0.3
20	108.9	100.6	144.7	122.1	8.4	2.3	13.0	66.8	13.8	1.4	7.3	31.8	0.4
21	112.7	101.2	138.7	131.5	7.1	2.3	7.9	66.5	15.6	1.6	5.6	31.8	0.3
22		92.0	143.2	104.3	6.5	2.6	11.0	56.8	12.3	1.3	5.7	27.8	0.5
23		75.4	113.5	97.3	10.4	5.3	4.6	52.3	12.2	1.1	4.9	25.7	0.4
24	20.3	35.5	45.2	38.0	3.1	2.7	5.0	23.3	7.0	0.6	2.4	10.1	0.2
25		68.1	100.2	88.6	6.3	1.6	10.1	44.3	18.8	1.7	5.9	20.8	0.2
26		89.3	126.7	108.6	5.6	2.4	5.7	58.7	14.2	1.4	4.0	23.7	0.3
27		124.1	142.7	150.2	6.3	2.8	7.8	63.7	19.8	2.2	10.9	34.7	0.4
28		115.3	130.6	136.0	4.5	2.6	8.2	56.0	20.1	2.2	10.6	31.0	0.3
29		53.3	52.5	58.9	4.8	2.8	3.9	28.2	9.0	1.0	5.1	14.3	0.2
30	108.6	114.2	119.2	130.2	5.6	3.7	6.1	57.9	15.4	2.0	8.7	31.0	0.3
31		129.6	141.5	152.6	5.3	2.3	7.4	65.4	19.8	2.5	10.2	34.3	0.3
32		45.2	49.5	48.4	3.1	2.2	4.1	23.0	6.7	0.8	3.9	12.8	0.1
33	100.4	100.9	108.2	115.4	4.1	2.2	6.7	50.5	15.4	2.0	7.5	26.9	0.3
34		110.1	117.1	124.0	4.6	2.2	7.8	54.9	15.2	2.2	8.5	29.3	0.3
35	106.2	118.3	124.5	134.3	4.2	2.5	7.9	59.8	14.5	2.4	8.3	32.6	0.4
36	99.1	116.8	115.5	130.6	4.2	2.8	9.0	58.3	15.4	2.3	8.8	31.8	0.5
37	114.5	127.3	137.8	153.8	4.6	3.5	7.3	67.0	16.0	2.6	9.3	37.5	0.3
38		77.1	81.2	92.4	5.8	6.9	4.4	43.5	12.1	1.6	6.8	24.6	0.4
39	109.2	113.9	127.1	139.1	4.1	4.2	5.6	68.3	17.9	2.2	7.5	29.4	0.3
40		72.3	77.2	83.9	3.3	2.3	5.1	41.3	12.6	1.3	5.3	18.0	0.2
41	91.5	89.8	99.7	104.9	3.1	2.2	6.2	50.7	15.3	1.6	6.5	21.9	0.2
42		156.8	188.3	198.0	2.2	2.6	8.8	93.4	22.1	3.0	11.6	40.3	0.4
43		83.6	95.3	100.7	2.6	2.6	5.9	50.2	15.1	1.5	11.4	15.1	0.2
44		73.1	82.2	88.6	2.4	2.4	4.8	44.2	12.2	1.3	10.5	13.1	0.2
45		40.1	45.3	47.9	3.2	3.0	2.9	26.8	7.9	0.7	7.2	6.3	0.2
46		3.7		-1.7	5.2	86.0	1.0	12.2	24.1	0.0	4.6	65.6	0.4
47	124.8	128.5	154.5	153.2	6.0	3.8	7.0	58.6	17.7	1.9	12.8	38.2	0.3
48	48.2	51.2	44.0	61.3	2.0	3.1	7.8	22.0	18.6	1.5	5.4	15.9	0.1
49		21.7	20.3	21.9	1.6	1.7	3.5	10.2	4.4	0.4	2.2	7.1	0.1
50		171.0	206.7	199.8	5.2	3.8	8.5	94.9	18.0	2.4	13.3	43.4	0.5
51		109.6	118.4	121.5	3.7	2.1	5.4	56.5	12.4	1.5	8.0	26.7	0.3
52	126.0	132.1	160.2	150.3	5.3	2.3	8.9	70.9	16.9	2.2	10.0	33.7	0.3
53	91.7	85.5	104.1	95.3	5.4	1.9	5.4	46.2	11.3	1.4	5.8	22.2	0.2
54		63.5	78.4	69.6	4.8	1.7	3.9	35.5	7.1	0.9	4.0	16.8	0.2
55	100.7	102.0	115.8	120.3	5.8	2.1	6.1	56.7	15.5	1.8	6.9	27.1	0.2
56		117.8	137.5	135.3	5.2	2.2	8.0	65.6	14.6	2.1	8.4	30.6	0.3
57	78.8	93.0	108.3	100.4	4.9	2.3	7.1	50.1	11.3	1.6	6.6	23.7	0.3
58	93.0	91.5	105.4	101.5	4.0	2.0	6.5	49.1	10.7	1.6	6.2	24.1	0.2
59		114.9	129.6	131.8	4.5	2.3	7.6	61.7	14.7	2.2	7.5	30.9	0.3
60	99.0	120.7	144.2	134.9	4.2	2.3	10.0	65.8	13.6	2.3	8.6	32.1	0.4
61	103.6	123.3	145.3	140.3	4.2	2.5	9.1	64.8	16.3	2.4	8.6	33.0	0.5
62		122.3	143.7	141.8	4.5	2.4	8.0	66.5	15.9	2.4	8.1	32.9	0.3
63	28.4	23.0	18.5	22.7	1.9	2.3	3.7	12.3	4.2	0.5	1.9	7.7	0.1
64		58.7	52.8	66.8	6.9	5.2	7.8	39.3	8.8	1.2	4.1	20.7	0.4
65	71.1	67.3	76.9	80.0	4.3	1.8	4.6	40.9	11.5	1.1	4.8	16.8	0.2
66		76.1	94.2	92.6	3.4	1.6	5.7	43.2	15.5	1.5	5.8	19.3	0.1
67	129.5	95.0	118.6	110.7	4.1	1.9	6.6	53.4	16.7	1.8	6.5	23.2	0.2
68	89.1	107.2	122.8	125.1	6.5	2.8	7.9	66.7	15.1	1.7	11.1	23.4	0.3

	Exchangeable cations (corrected) [meq/kg]						Fractional occupancies [-]								
Nr	Na	K	NH_4	Mg	Ca	Sr	N_{Na}	N_K	N_{NH4}	N_{Mg}	N_{Ca}	N_{Sr}	N_{Na}	N_{K+NH4}	$N_{Mg+Ca+Sr}$
1	6.2	10.1	0.7	7.5	12.8	0.2	0.16	0.27	0.02	0.20	0.34	0.00	0.16	0.29	0.55
2	12.1	12.9	0.8	10.1	18.5	0.3	0.22	0.24	0.01	0.18	0.34	0.01	0.22	0.25	0.53
3	11.8	11.6	0.8	9.8	21.0	0.3	0.21	0.21	0.01	0.18	0.38	0.01	0.21	0.22	0.56
4	10.0	11.1	0.8	9.7	16.3	0.3	0.21	0.23	0.02	0.20	0.34	0.01	0.21	0.25	0.55
5	38.6	20.6	1.2	14.2	49.7	0.5	0.31	0.17	0.01	0.11	0.40	0.00	0.31	0.18	0.52
6	7.3	6.2	0.5	14.3	-0.9	0.1									
7	13.6	6.1	0.1	2.3	0.0	0.1									
8	-2.4	1.0	0.1	2.0	1.1	0.2									
9	-1.2	2.1	0.8	2.2	1.7	0.2									
10	1.0	1.8	0.8	2.8	2.8	0.1									
11	80.9	21.8	1.6	16.1	65.7	0.9	0.43	0.12	0.01	0.09	0.35	0.00	0.43	0.12	0.44
12	11.3	6.2	3.0	6.2	10.3	0.1	0.30	0.17	0.08	0.17	0.28	0.00	0.30	0.25	0.45
13	26.8	10.4	0.8	7.3	23.4	0.4	0.39	0.15	0.01	0.11	0.34	0.01	0.39	0.16	0.45
14	55.8	22.1	9.7	13.4	45.2	0.5	0.38	0.15	0.07	0.09	0.31	0.00	0.38	0.22	0.40
15	26.7	9.7	0.8	6.3	18.8	0.3	0.43	0.16	0.01	0.10	0.30	0.00	0.43	0.17	0.41
16	38.9	12.8	1.1	10.0	33.6	0.4	0.40	0.13	0.01	0.10	0.35	0.00	0.40	0.14	0.46
17	29.5	10.2	1.0	7.0	24.6	0.3	0.41	0.14	0.01	0.10	0.34	0.00	0.41	0.15	0.44
18	36.0	10.9	1.0	8.1	30.2	0.7	0.41	0.13	0.01	0.09	0.35	0.01	0.41	0.14	0.45
19	43.3	12.1	1.2	9.6	35.7	0.6	0.42	0.12	0.01	0.09	0.35	0.01	0.42	0.13	0.45
20	53.8	13.8	1.4	14.6	37.7	0.7	0.44	0.11	0.01	0.12	0.31	0.01	0.44	0.12	0.43
21	54.7	15.6	1.6	11.2	47.8	0.7	0.42	0.12	0.01	0.08	0.36	0.01	0.42	0.13	0.45
22	45.0	12.3	1.3	11.4	33.5	0.9	0.43	0.12	0.01	0.11	0.32	0.01	0.43	0.13	0.44
23	31.2	12.2	1.1	9.7	42.1	0.9	0.32	0.13	0.01	0.10	0.43	0.01	0.32	0.14	0.54
24	14.8	7.0	0.6	4.8	10.2	0.5	0.39	0.18	0.02	0.13	0.27	0.01	0.39	0.20	0.41
25	34.7	18.8	1.7	11.8	21.3	0.4	0.39	0.21	0.02	0.13	0.24	0.00	0.39	0.23	0.38
26	48.4	14.2	1.4	8.1	36.0	0.5	0.45	0.13	0.01	0.07	0.33	0.00	0.45	0.14	0.41
27	51.8	19.8	2.2	21.8	53.9	0.7	0.34	0.13	0.01	0.15	0.36	0.00	0.34	0.15	0.51
28	46.3	20.1	2.2	21.1	45.7	0.6	0.34	0.15	0.02	0.16	0.34	0.00	0.34	0.16	0.50
29	17.9	9.0	1.0	10.1	20.6	0.3	0.30	0.15	0.02	0.17	0.35	0.01	0.30	0.17	0.53
30	45.0	15.4	2.0	17.3	49.9	0.7	0.35	0.12	0.02	0.13	0.38	0.01	0.35	0.13	0.52
31	55.5	19.8	2.5	20.3	53.8	0.7	0.36	0.13	0.02	0.13	0.35	0.00	0.36	0.15	0.49
32	15.4	6.7	0.8	7.9	17.4	0.2	0.32	0.14	0.02	0.16	0.36	0.00	0.32	0.15	0.53
33	42.0	15.4	2.0	15.0	40.4	0.5	0.36	0.13	0.02	0.13	0.35	0.00	0.36	0.15	0.48
34	45.9	15.2	2.2	17.1	43.0	0.6	0.37	0.12	0.02	0.14	0.35	0.00	0.37	0.14	0.49
35	50.6	14.5	2.4	16.6	49.4	0.7	0.38	0.11	0.02	0.12	0.37	0.01	0.38	0.13	0.50
36	48.6	15.4	2.3	17.7	45.6	1.1	0.37	0.12	0.02	0.14	0.35	0.01	0.37	0.14	0.49
37	55.5	16.0	2.6	18.7	60.3	0.7	0.36	0.10	0.02	0.12	0.39	0.00	0.36	0.12	0.52
38	23.9	12.1	1.6	13.6	40.5	0.9	0.26	0.13	0.02	0.15	0.44	0.01	0.26	0.15	0.59
39	55.8	17.9	2.2	15.0	47.5	0.6	0.40	0.13	0.02	0.11	0.34	0.00	0.40	0.14	0.45
40	33.4	12.6	1.3	10.5	25.7	0.3	0.40	0.15	0.02	0.13	0.31	0.00	0.40	0.17	0.44
41	43.1	15.3	1.6	13.0	31.4	0.4	0.41	0.15	0.02	0.12	0.30	0.00	0.41	0.16	0.43
42	86.0	22.1	3.0	23.2	63.0	0.7	0.43	0.11	0.02	0.12	0.32	0.00	0.43	0.13	0.44
43	42.5	15.1	1.5	22.8	18.5	0.4	0.42	0.15	0.01	0.23	0.18	0.00	0.42	0.16	0.41
44	37.0	12.2	1.3	21.0	16.7	0.4	0.42	0.14	0.01	0.24	0.19	0.00	0.42	0.15	0.43
45	17.6	7.9	0.7	14.4	6.8	0.4	0.37	0.17	0.01	0.30	0.14	0.01	0.37	0.18	0.45
46					129.1										
					0.0										
47	45.0	17.7	1.9	25.6	62.4	0.6	0.29	0.12	0.01	0.17	0.41	0.00	0.29	0.13	0.58
48	13.9	18.6	1.5	10.7	16.3	0.3	0.23	0.30	0.03	0.17	0.27	0.00	0.23	0.33	0.45
49	5.1	4.4	0.4	4.4	7.2	0.3	0.23	0.20	0.02	0.20	0.33	0.01	0.23	0.22	0.54
50	82.1	18.0	2.4	26.7	69.6	0.9	0.41	0.09	0.01	0.13	0.35	0.00	0.41	0.10	0.49
51	48.5	12.4	1.5	15.9	42.6	0.6	0.40	0.10	0.01	0.13	0.35	0.00	0.40	0.11	0.49
52	60.9	16.9	2.2	20.0	49.7	0.6	0.41	0.11	0.01	0.13	0.33	0.00	0.41	0.13	0.47
53	37.1	11.3	1.4	11.5	33.6	0.4	0.39	0.12	0.01	0.12	0.35	0.00	0.39	0.13	0.48
54	27.3	7.1	0.9	8.0	25.9	0.3	0.39	0.10	0.01	0.12	0.37	0.00	0.39	0.12	0.49
55	46.8	15.5	1.8	13.7	42.0	0.5	0.39	0.13	0.02	0.11	0.35	0.00	0.39	0.14	0.47
56	56.0	14.6	2.1	16.9	45.1	0.6	0.41	0.11	0.02	0.12	0.33	0.00	0.41	0.12	0.46
57	40.5	11.3	1.6	13.2	33.2	0.6	0.40	0.11	0.02	0.13	0.33	0.01	0.40	0.13	0.47
58	41.1	10.7	1.6	12.4	35.2	0.5	0.41	0.11	0.02	0.12	0.35	0.00	0.41	0.12	0.47
59	52.6	14.7	2.2	14.9	46.8	0.6	0.40	0.11	0.02	0.11	0.35	0.00	0.40	0.13	0.47
60	56.9	13.6	2.3	17.1	44.2	0.8	0.42	0.10	0.02	0.13	0.33	0.01	0.42	0.12	0.46
61	55.7	16.3	2.4	17.2	47.8	0.9	0.40	0.12	0.02	0.12	0.34	0.01	0.40	0.13	0.47
62	57.2	15.9	2.4	16.1	49.6	0.6	0.40	0.11	0.02	0.11	0.35	0.00	0.40	0.13	0.47
63	5.9	4.2	0.5	3.9	8.0	0.1	0.26	0.19	0.02	0.17	0.35	0.01	0.26	0.21	0.53
64	22.0	8.8	1.2	8.3	25.8	0.7	0.33	0.13	0.02	0.12	0.39	0.01	0.33	0.15	0.52
65	32.9	11.5	1.1	9.6	24.5	0.4	0.41	0.14	0.01	0.12	0.31	0.01	0.41	0.16	0.43
66	36.7	15.5	1.5	11.5	27.2	0.3	0.40	0.17	0.02	0.12	0.29	0.00	0.40	0.18	0.42
67	45.6	16.7	1.8	13.1	33.2	0.4	0.41	0.15	0.02	0.12	0.30	0.00	0.41	0.17	0.42
68	54.6	15.1	1.7	22.1	31.0	0.5	0.44	0.12	0.01	0.18	0.25	0.00	0.44	0.13	0.43

Tab. A-3: Summary of all the geochemical parameters for the samples from the siting region Zürich Nordost

Samples					Mineralogy								Clay mineralogy					CEC				Total anion & cation exactions										Exchangeable cations (corrected)						Fractional occupancies								
Nr	ID (RWI)	Depth	Group	Formation	Plagioclase	K-feldspat	Quartz	Calcite	Dol/Ank	Siderite	Pyrite	Anhydrite / Celestite	Illite EM	Smectite EM	Kaolinite EM	Chlorite EM	Total clay minerals	CEC-Clay	Ni-CEC	Cs-CEC	∑cations	Cl	SO_4	TIC	Na	K	NH_4	Mg	Ca	Sr	Na	K	NH_4	Mg	Ca	Sr	N_{Na}	N_K	N_{NH4}	N_{Mg}	N_{Ca}	N_{Sr}	N_{Na}	N_{K+NH4}	$N_{Mg+Ca+Sr}$
		[m]			[wt.-%]													[meq/kg]				[mmol/kg]										[meq/kg]						[-]								
1	TRU1-1-722.53/25-PW	722.66	Malm	Wildegg Fm.		2.0	2.7	82.0	1.9		<0.1		7.7	0.7	1.9	0.9	11.1	24.0	24.9	25.9	31.1	3.0	2.0	4.1	15.3	5.5		3.7	8.9	0.1	8.3	5.5	0.0	7.4	9.6	0.3	0.27	0.18		0.24	0.31	0.01	0.27	0.18	0.56
2	TRU1-1-740.15/25-PW	740.28	Dogger	Parkinsoni-Württ.-Sch.	1.3	5.4	21.0	41.3	0.0		0.3		17.9	2.1	8.2	2.4	30.3	62.1	80.4	86.8	101.8	6.0	1.4	6.4	46.2	13.1		7.2	24.4	0.5	37.4	13.1	0.0	14.4	35.8	1.0	0.37	0.13		0.14	0.35	0.01	0.37	0.13	0.50
3	TRU1-1-761.513/25-PW	761.64	Dogger	Parkinsoni-Württ.-Sch.		4.7	15.3	53.2	1.9		0.5		13.9	1.4	6.5	1.9	24.0	46.6	58.9	52.7	73.3	4.3	1.4	6.2	32.3	10.2		5.7	19.1	0.3	25.3	10.2	0.0	11.4	25.8	0.7	0.35	0.14		0.16	0.35	0.01	0.35	0.14	0.52
4	TRU1-1-791.58/25-PW	791.71	Dogger	Wedelsandstein Fm.		5.5	20.0	5.3			0.8		40.0	4.7	15.6	7.5	67.8	139.3	128.5	135.7	178.0	6.7	1.7	9.8	78.4	19.3		12.3	41.9	0.9	68.2	19.3	0.0	24.5	64.3	1.8	0.38	0.11		0.14	0.36	0.01	0.38	0.11	0.51
5	TRU1-1-820.15/25-PW	820.28	Dogger	Opalinus Clay		3.1	17.6	3.9		3.9	2.2		34.6	4.1	22.4	6.8	67.9	123.0	114.1	116.8	150.1	6.8	1.6	12.0	69.4	16.4		11.0	37.4	0.7	59.4	16.4	0.0	22.1	50.7	1.4	0.40	0.11		0.15	0.34	0.01	0.40	0.11	0.49
6	TRU1-1-848.35/25-PW	848.48	Dogger	Opalinus Clay	3.6	5.8	23.1	5.3		3.5	1.2		28.2	3.4	19.2	6.2	56.5	101.5	100.0	104.8	124.0	5.6	1.7	10.2	58.1	13.1		8.9	31.5	0.6	49.2	13.1	0.0	17.9	42.7	1.2	0.40	0.11		0.14	0.34	0.01	0.40	0.11	0.50
7	TRU1-1-876.70/27-PW	876.84	Dogger	Opalinus Clay	3.2	5.7	24.0	7.5		3.7	0.4		26.7	3.3	19.1	5.5	54.5	96.6	98.2	109.1	117.5	5.1	2.0	11.4	56.1	11.9		8.8	31.3	0.6	47.0	11.9	0.0	17.7	39.8	1.2	0.40	0.10		0.15	0.34	0.01	0.40	0.10	0.50
8	TRU1-1-899.40/28-PW	899.54	Dogger	Opalinus Clay	3.5	5.0	22.6	6.7		5.2	0.4		26.7	3.3	20.5	5.0	55.5	97.2	89.4	101.5	106.2	4.4	1.8	11.4	50.3	11.3		8.1	29.0	0.6	42.4	11.3	0.0	16.2	35.2	1.1	0.40	0.11		0.15	0.33	0.01	0.40	0.11	0.49
9	TRU1-1-919.52/25-PW	919.65	Dogger	Opalinus Clay	3.1	4.9	15.9	7.4		3.7	1.1		29.6	3.1	22.7	7.6	63.0	104.1	104.2	116.4	134.0	4.7	2.4	10.4	61.1	14.0		9.4	34.5	0.8	51.6	14.0	0.0	18.7	48.2	1.5	0.38	0.10		0.14	0.36	0.01	0.38	0.10	0.51
10	TRU1-1-938.40/25-PW	938.53	Lias	Staffelegg Fm.	1.8	2.5	9.9	39.4	1.0		3.1		25.8	2.2	4.8	4.1	36.8	80.6	70.7	95.8	106.3	2.5	1.5	5.7	51.0	11.1		6.0	24.1	0.4	45.5	11.1	0.0	12.0	36.8	0.9	0.43	0.10		0.11	0.35	0.01	0.43	0.10	0.47
11	TRU1-1-951.65/25-PW	951.78	Lias	Staffelegg Fm.	3.1	5.1	33.2	6.1	2.0		0.9		26.7	2.9	14.6	4.4	48.5	91.6	85.6	69.5	87.5	6.2	4.9	9.8	43.8	11.3		6.6	26.7	0.6	27.9	11.3	0.0	13.2	33.9	1.3	0.32	0.13		0.15	0.39	0.01	0.32	0.13	0.55
12	MAR1-1-521.29-PW	521.29	Dogger	'Parkinsoni-Württ'	3.0	6.0	22.0	18.6	2.8		0.8		26.5	2.7	12.7	4.2	46.1	88.6	89.7	83.6	94.2	5.1	1.7	6.1	41.3	12.9	1.7	7.9	21.1	0.4	32.9	12.9	1.7	15.8	30.1	0.9	0.35	0.14	0.02	0.17	0.32	0.01	0.35	0.16	0.50
13	MAR1-1-532.18-PW	532.18	Dogger	'Parkinsoni-Württ'	3.0	6.0	16.0	15.1	4.0		1.4		32.8	2.9	13.2	5.0	53.9	105.6	129.6	133.6	142.0	6.7	1.8	8.1	61.6	18.5	2.6	11.8	30.4	0.7	51.2	18.5	2.6	23.7	44.6	1.4	0.36	0.13	0.02	0.17	0.31	0.01	0.36	0.15	0.49
14	MAR1-1-544.94-PW	544.94	Dogger	'Parkinsoni-Württ'	2.0	4.0	17.0	21.6		2.1	1.4		28.2	3.1	14.7	5.2	51.2	97.2	108.1	105.3	113.0	6.3	1.6	6.9	50.2	13.4	1.9	9.4	25.3	0.6	40.8	13.4	1.9	18.8	36.9	1.1	0.36	0.12	0.02	0.17	0.33	0.01	0.36	0.14	0.50
15	MAR1-1-558.62-PW	558.62	Dogger	Wedelsandstein	3.0	6.0	34.0	22.5			1.0		23.2	2.6	4.4	2.8	32.9	77.1	87.2	80.8	87.1	4.5	1.4	4.9	38.5	9.9	1.4	7.4	19.4	0.5	31.0	9.9	1.4	14.9	29.0	0.9	0.36	0.11	0.02	0.17	0.33	0.01	0.36	0.13	0.51
16	MAR1-1-569.87-PW	569.87	Dogger	Wedelsandstein	4.0	6.0	58.0	12.8	0.8		0.1		12.1	1.4	1.6	2.9	17.9	41.1	34.6	35.7	33.6	11.1	2.2	2.0	22.1	6.1	0.3	3.4	8.1	0.8	6.6	6.1	0.3	6.8	12.3	1.5	0.20	0.18	0.01	0.20	0.37	0.05	0.20	0.19	0.61
17	MAR1-1-580.89-PW	580.89	Dogger	Wedelsandstein	3.0	3.0	47.0	16.0			1.0						28.0		84.9	81.6	83.3	5.6	1.6	4.7	38.1	9.6	1.3	7.1	18.8	0.5	29.2	9.6	1.3	14.1	28.1	1.0	0.35	0.11	0.02	0.17	0.34	0.01	0.35	0.13	0.52
18	MAR1-1-588.03-PW	588.03	Dogger	Wedelsandstein	3.0	3.0	32.0	15.0	1.1		0.9						45.0		115.9	119.3	118.3	6.1	2.2	6.9	53.0	13.6	2.2	9.5	26.8	0.7	42.4	13.6	2.2	19.0	39.8	1.3	0.36	0.11	0.02	0.16	0.34	0.01	0.36	0.13	0.51
19	MAR1-1-597.66-PW	597.66	Dogger	Opalinus Clay	2.0	5.0	25.0	20.4	2.1		1.2		23.9	2.4	12.2	4.7	43.3	80.8	95.3	95.1	97.5	4.9	1.7	6.8	43.6	12.1	1.9	8.1	22.4	0.4	35.2	12.1	1.9	16.2	31.2	0.8	0.36	0.12	0.02	0.17	0.32	0.01	0.36	0.14	0.50
20	MAR1-1-605.04-PW	605.04	Dogger	Opalinus Clay	3.0	5.0	24.0	10.3			1.3		28.2	3.1	18.5	5.7	55.4	98.1	113.9	110.8	117.1	5.7	1.7	7.7	52.8	12.6	2.2	9.9	26.6	0.5	43.7	12.6	2.2	19.7	37.8	1.1	0.37	0.11	0.02	0.17	0.32	0.01	0.37	0.13	0.50
21	MAR1-1-618.77-PW	618.77	Dogger	Opalinus Clay	3.0	5.0	25.0	7.8			0.6		28.8	2.7	19.2	6.6	57.3	96.9	97.2	97.6	99.7	5.3	1.4	7.0	44.9	10.9	1.9	8.9	22.7	0.4	36.8	10.9	1.9	17.9	31.3	0.9	0.37	0.11	0.02	0.18	0.31	0.01	0.37	0.13	0.50
22	MAR1-1-630.96-PW	630.96	Dogger	Opalinus Clay	4.0	5.0	22.0	6.3		2.7	1.3		29.4	3.3	20.4	4.5	57.6	102.8	106.6	105.5	108.1	5.1	1.6	7.4	48.1	12.4	2.2	8.6	25.2	0.5	39.8	12.4	2.2	17.2	35.6	0.9	0.37	0.11	0.02	0.16	0.33	0.01	0.37	0.13	0.50
23	MAR1-1-654.25-PW	654.25	Dogger	Opalinus Clay		5.0	26.0	8.1		3.2	0.6		28.2	3.1	18.9	5.7	55.9	99.0	99.2	98.1	95.9	4.5	1.6	6.9	42.1	11.3	2.1	7.6	22.9	0.4	34.4	11.3	2.1	15.2	32.1	0.9	0.36	0.12	0.02	0.16	0.33	0.01	0.36	0.14	0.50
24	MAR1-1-666.13-PW	666.13	Dogger	Opalinus Clay	3.0	5.0	22.0	7.0		3.1	1.1		29.1	3.1	19.2	6.0	57.4	100.6	96.9	103.5	99.2	4.1	1.7	7.7	43.9	11.4	2.2	8.0	23.9	0.4	36.4	11.4	2.2	15.9	32.5	0.8	0.37	0.12	0.02	0.16	0.33	0.01	0.37	0.14	0.50
25	MAR1-1-678.24-PW	678.24	Dogger	Opalinus Clay	0.0	5.0	17.0	3.4		2.3	1.1		34.0	3.5	25.7	6.6	69.8	117.4	123.8	126.8	131.3	5.4	1.9	9.5	58.8	14.2	2.8	10.6	30.8	0.5	49.7	14.2	2.8	21.1	42.5	1.0	0.38	0.11	0.02	0.16	0.32	0.01	0.38	0.13	0.49
26	MAR1-1-689.93-PW	689.93	Dogger	Opalinus Clay	2.0	5.0	19.0	7.1		0.0	0.5		32.1	3.4	23.4	6.3	65.2	111.3	120.0	124.9	123.7	4.7	1.8	9.8	55.5	13.5	2.6	10.3	29.3	0.5	47.2	13.5	2.6	20.5	38.9	0.9	0.38	0.11	0.02	0.17	0.31	0.01	0.38	0.13	0.49
27	MAR1-1-702.63-PW	702.63	Dogger	Opalinus Clay	3.0	5.0	15.0	5.8		2.5	1.2		31.8	3.3	23.9	7.4	66.4	110.7	123.7	126.2	129.8	4.7	2.2	9.0	57.6	13.2	2.6	10.2	31.0	0.5	48.6	13.2	2.6	20.4	44.0	0.9	0.37	0.10	0.02	0.16	0.34	0.01	0.37	0.12	0.50
28	MAR1-1-707.11-PW	707.11	Lias	Staffelegg Fm.	2.0	3.0	7.0	47.6		1.0	0.3		20.8	1.8	11.3	4.6	38.5	67.8	68.2	72.7	74.5	3.6	2.6	5.5	32.3	10.7	1.7	6.2	18.3	0.3	23.6	10.7	1.7	12.5	25.6	0.5	0.32	0.14	0.02	0.17	0.34	0.01	0.32	0.17	0.52
29	MAR1-1-720.33-PW	720.33	Lias	Staffelegg Fm.	3.0	4.0	15.0	13.4		1.1	5.8		31.6	2.8	11.5	5.1	50.9	101.0	106.0	119.0	113.4	3.4	3.0	6.7	54.8	13.1	2.0	7.6	25.2	0.4	45.3	13.1	2.0	15.3	37.0	0.8	0.40	0.12	0.02	0.13	0.33	0.01	0.40	0.13	0.47
30	MAR1-1-732.78-PW	732.78	Lias	Staffelegg Fm.	4.0	6.0	26.0	5.5		2.3	0.3		30.1	3.0	15.8	6.0	54.8	101.0	108.6	114.6	115.4	2.1	1.7	8.1	54.1	13.1	1.9	8.0	25.6	0.3	48.6	13.1	1.9	15.9	35.1	0.7	0.42	0.11	0.02	0.14	0.30	0.01	0.42	0.13	0.45
31	MAR1-1-741.38-PW	741.38	Lias	Staffelegg Fm.	2.0	4.0	23.0				0.8		35.1	4.4	19.9	9.9	69.3	127.4	159.9	173.3	174.3	1.6	1.7	11.3	80.3	17.5	2.6	12.3	38.1	0.5	75.2	17.5	2.6	24.6	53.5	0.9	0.43	0.10	0.01	0.14	0.31	0.01	0.43	0.11	0.45