PHASE 2 INITIAL BOREHOLE DRILLING AND TESTING, IGNACE AREA

WP4C Data Report – Porewater Extraction and Analysis for IG_BH04

APM-REP-01332-0347 **March 2023**

WSP Canada Inc.

NUCLEAR WASTE MANAGEMENT ORGANIZATION
SOCIÉTÉ DE GESTION DES DÉCHETS NUCLÉAIRES

Nuclear Waste Management Organization
22 St. Clair Avenue East, 4th Floor
Toronto, Ontario
M4T 2S3
Canada

Tel: 416-934-9814
Web: www.nwmo.ca

REPORT

PHASE 2 INITIAL BOREHOLE DRILLING AND TESTING, IGNACE AREA

WP4C DATA REPORT – POREWATER EXTRACTION AND ANALYSIS FOR IG_BH04

Submitted to:

Nuclear Waste Management Organization

4th Floor
22 St. Clair Avenue East
Toronto, Ontario, M4T 2S3

Submitted by:

WSP Canada Inc.
3450 Harvester Road, Burlington, Ontario, L7N 3W5

1 (905) 335-2353

NWMO Document: APM-REP-01332-0347

WSP Document Number: SCB1912026-REP-018 R4

March 2023

Distribution List

e-copy - NWMO

e-copy - WSP

e-copy - Hydroisotop

WP4C DATA REPORT – POREWATER EXTRACTION AND ANALYSIS FOR IG_BH04

CLIENT INFORMATION

Project Name: Phase 2 Initial Borehole Drilling and Testing at IG_BH04/05/06, Ignace Area

Project Number: SCB1912026

Client Document Number: APM-REP-01332-0347

Document Name: WP4C DATA REPORT – POREWATER EXTRACTION AND ANALYSIS FOR IG_BH04

Client: Nuclear Waste Management Organization (NWMO)

Address: 22 St. Clair Avenue East, 4th Floor

City: Toronto

Province: Ontario

Postal Code: M4T 2S3

Client Contact:	Laura Kennell-Morrison	Warwick Watt
Telephone:	647-259-3737	647-972-3669
Email:	lkennell@nwmo.ca	wwatt@nwmo.ca

ISSUE/REVISION INDEX

Issue Code	Revision					Revision Details
	No.	By	Revd.	App.	Date	
RR	0				October 14, 2021	Draft for review
RI	1				June 9, 2022	Issued for approval
RI	2				November 30, 2022	Revised comments for RI1. Issued for approval
RI	3				January 26, 2023	Revised comments for RI2. Issued for approval
RI	4				March 28, 2023	Revised comments for RI4. Issued for approval. No changes were made to the appendices R3

Issue Codes: RR = Released for Review and Comments, RI = Released for Information

SIGNATURES

Prepared by:

Dr. Florian Eichinger
Joy Iannotta
Hydroisotop GmbH

21.03.2023
Date:

Reviewed by:

Simon Gautrey
Project Manager

March 28, 2023
Date:

Reviewed & Approved by:

Simon Gautrey
Project Manager

March 28, 2023
Date:

Table of Contents

TABLES

FIGURES

APPENDICES

APPENDIX A
Photo Documentation

APPENDIX B
Analytical Raw Data

APPENDIX C
Error Calculations

1.0 INTRODUCTION

The Initial Borehole Drilling and Testing project in the Ignace Area, Ontario is part of Phase 2 Geoscientific Preliminary Field Investigations of the NWMO's Adaptive Phased Management (APM) Site Selection Phase. This project involves the drilling and testing of borehole IG_BH04 within the northern portion of the Revell batholith.

The project was carried out by a team at Hydroisotop GmbH, subcontracted by WSP on behalf of the NWMO. This report describes the testing methodology and results for Work Package 4c (WP4c): Porewater Extraction and Analysis for IG_BH04.

1.1 Geological Setting

The Potential Repository Areas under investigation is located within the Revell Batholith, a 2.7 billion year old intrusion located within the western part of the Wabigoon Subprovince of the Archean Superior Province. As seen on (Figure 1-1), the batholith is roughly elliptical in shape with the long axis trending northwest, and is approximately 40 km in length, 15 km in width, and covers an area of approximately 455 km^2. Based on geophysical modelling, the batholith has a relatively flat base that extends to depths of nearly 4 km in some regions (SGL, 2020). The batholith is surrounded by supracrustal rocks of the Raleigh Lake (to the north and east) and Bending Lake (to the southwest) greenstone belts.

Four main rock units are identified in the supracrustal rock group: mafic metavolcanic rocks, intermediate to felsic metavolcanic rocks, metasedimentary rocks, and mafic intrusive rocks. Sedimentation within the supracrustal rock assemblage was largely synvolcanic, although sediment deposition in the Bending Lake area may have continued past the volcanic period (Stone, 2009; Stone, 2010a; Stone, 2010b). All supracrustal rocks are affected, to varying degrees, by penetrative brittle-ductile to ductile deformation under greenschist- to amphibolite-facies metamorphic conditions (Blackburn and Hinz, 1996; Stone *et. al*., 1998). In some locations, primary features, such as pillow basalt or bedding in sedimentary rocks are preserved, in other locations, primary relationships are completely masked by penetrative deformation. Uranium-lead (U-Pb) geochronological analysis of the supracrustal rocks produced ages that range between 2734.6 +/-1.1 Ma and 2725 +/-5 Ma (Stone *et. al.*, 2010).

Three main suites of plutonic rock are recognized in the Revell batholith, including, from oldest to youngest: a Biotite Tonalite to Granodiorite suite, a Hornblende Tonalite to Granodiorite suite, and a Biotite Granite to Granodiorite suite. Plutonic rocks of the Biotite Tonalite to Granodiorite suite occur along the southwestern and northeastern margins of the Revell batholith. The principal type of rock within this suite is a white to grey, medium-grained, variably massive to foliated or weakly gneissic, biotite tonalite to granodiorite. One sample of foliated and medium-grained biotite tonalite produced a U-Pb age of 2734.2+/-0.8 Ma (Stone *et. al*., 2010). The Hornblende Tonalite to Granodiorite suite occurs in two irregularly shaped zones surrounding the central core of the Revell batholith. Rocks of the Hornblende Tonalite to Granodiorite suite range compositionally from tonalite through granodiorite to granite and also include significant proportions of quartz diorite and quartz monzodiorite. One sample of coarse-grained grey mesocratic hornblende tonalite produced a U-Pb age of 2732.3+/-0.8 Ma (Stone *et. al*., 2010). Rocks of the Biotite Granite to Granodiorite suite underlie most of the northern, central and southern portions of the Revell batholith. Rocks of this suite are typically coarse-grained, massive to weakly foliated, and white to pink in colour. The Biotite Granite to Granodiorite suite ranges compositionally from granite through granodiorite to tonalite. This suite includes the oval-shaped potassium-feldspar megacrystic granite body in the central portion of the Revell batholith (Figure 1-1). One sample of coarse-grained, pink, massive potassium-feldspar megacrystic biotite granite produced a U-Pb age of 2694.0+/-0.9 Ma (Stone *et. al*., 2010).

Borehole IG_BH04 is located within an investigation area of approximately 19 km^2 in size, situated in the northern portion of the Revell batholith. Bedrock exposure in the area is generally very good due to minimal overburden, few water bodies, and relatively recent logging activities. Ground elevations generally range from 400 to 450 m above sea level. The ground surface broadly slopes towards the northwest as indicated by the flow direction of the main rivers in the area. Local water courses tend to flow to the southwest towards Mennin Lake (Figure 1-2).

The bedrock surrounding IG_BH04 is composed mainly of massive to weakly foliated felsic intrusive rocks that vary in composition between granodiorite and tonalite, and together form a relatively homogeneous intrusive complex. Bedrock identified as tonalite transitions gradationally into granodiorite and no distinct contact relationships between these two rock types are typically observed (SRK and Golder, 2015; Golder and PGW, 2017). Massive to weakly foliated granite is identified at the ground surface to the northwest of the feldspar-megacrystic granite. The granite is observed to intrude into the granodiorite-tonalite bedrock, indicating it is distinct from, and younger than, the intrusive complex (Golder and PGW, 2017).

West-northwest trending mafic dykes interpreted from aeromagnetic data extend across the northern portion of the Revell batholith and into the surrounding greenstone belts. One mafic dyke occurrence, located to the southwest of IG_BH04, is approximately 15-20 m wide. All of these mafic dykes have a similar character and are interpreted to be part of the Wabigoon dyke swarm. One sample from the same Wabigoon swarm produced a U-Pb age of 1887+/-13 Ma (Stone *et. al*., 2010), indicating that these mafic dykes are Proterozoic in age. It is assumed based on surface measurements that these mafic dykes are sub-vertical (Golder and PGW, 2017).

Long, narrow valleys are located along the western and southern limits of the investigation area. These local valleys host creeks and small lakes that drain to the southwest and may represent the surface expression of structural features that extend into the bedrock. A broad valley is located along the eastern limits of the investigation area and hosts a more continuous, un-named water body that flows to the south. The linear and segmented nature of this waterbody's shorelines may also represent the surface expression of structural features that extend into the bedrock.

Regional observations from mapping have indicated that structural features are widely spaced (typically 30 to 500 cm spacing range) and dominantly comprised of sub-vertical joints with two dominant orientations: northeast and northwest trending (Golder and PGW, 2017). Interpreted bedrock lineaments generally follow these same dominant orientations in the northern portion of the Revell batholith (DesRoches *et. al*., 2018). Minor sub-horizontal joints have been observed with minimal alteration, suggesting they are younger and perhaps related to glacial unloading. One mapped regional-scale fault, the Washeibemaga Lake fault, trends east and is located to the west of the Revell batholith. Ductile lineaments, also shown on Figure 1-1, follow the trend of foliation mapped in the surrounding greenstone belts. Additional details of the lithological units and structures found at surface within the investigation area are reported in Golder and PGW (2017).

#

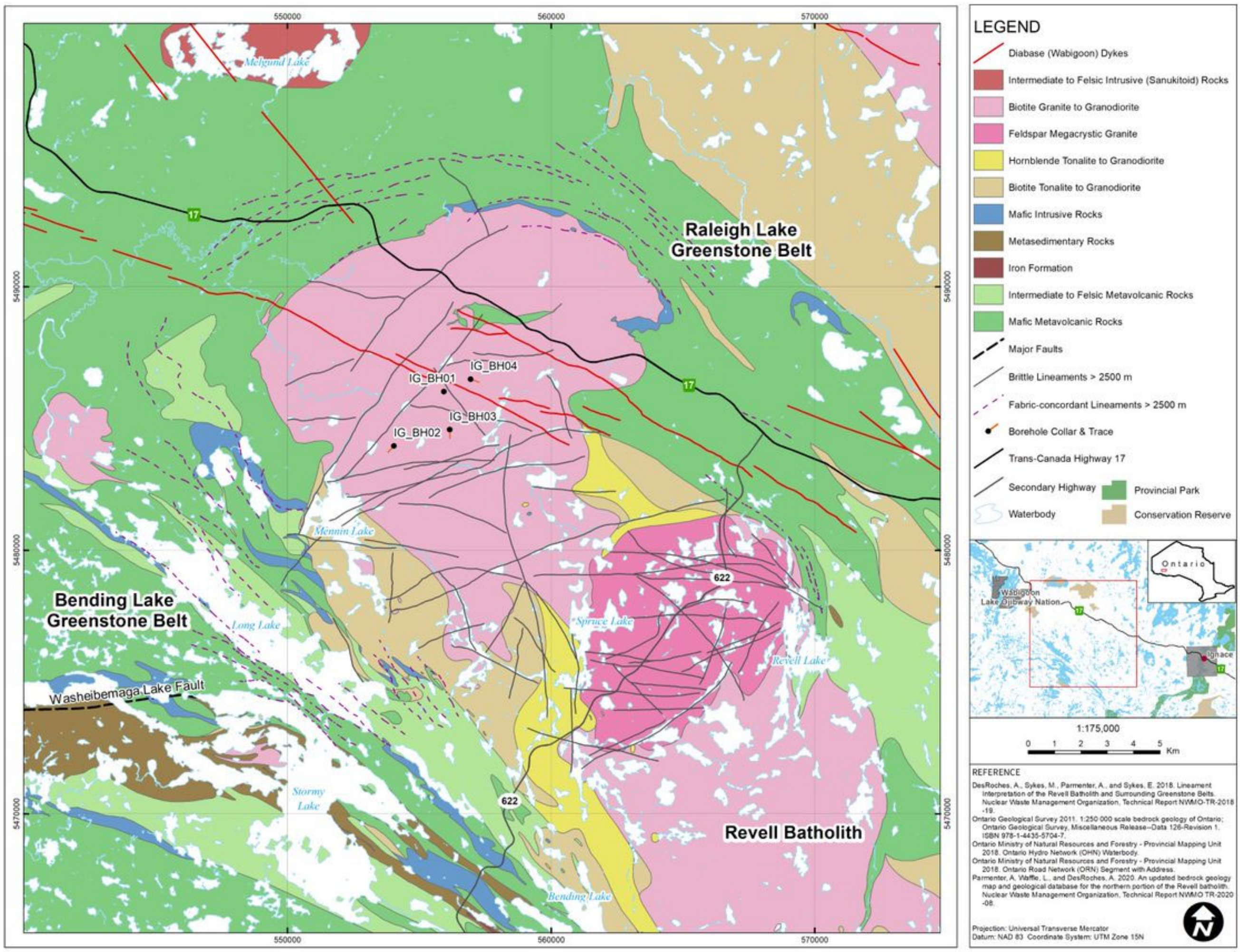


Figure 1-1: Geological Setting of the Northern Portion of the Revell Batholith (Parmenter et al., 2020)

#

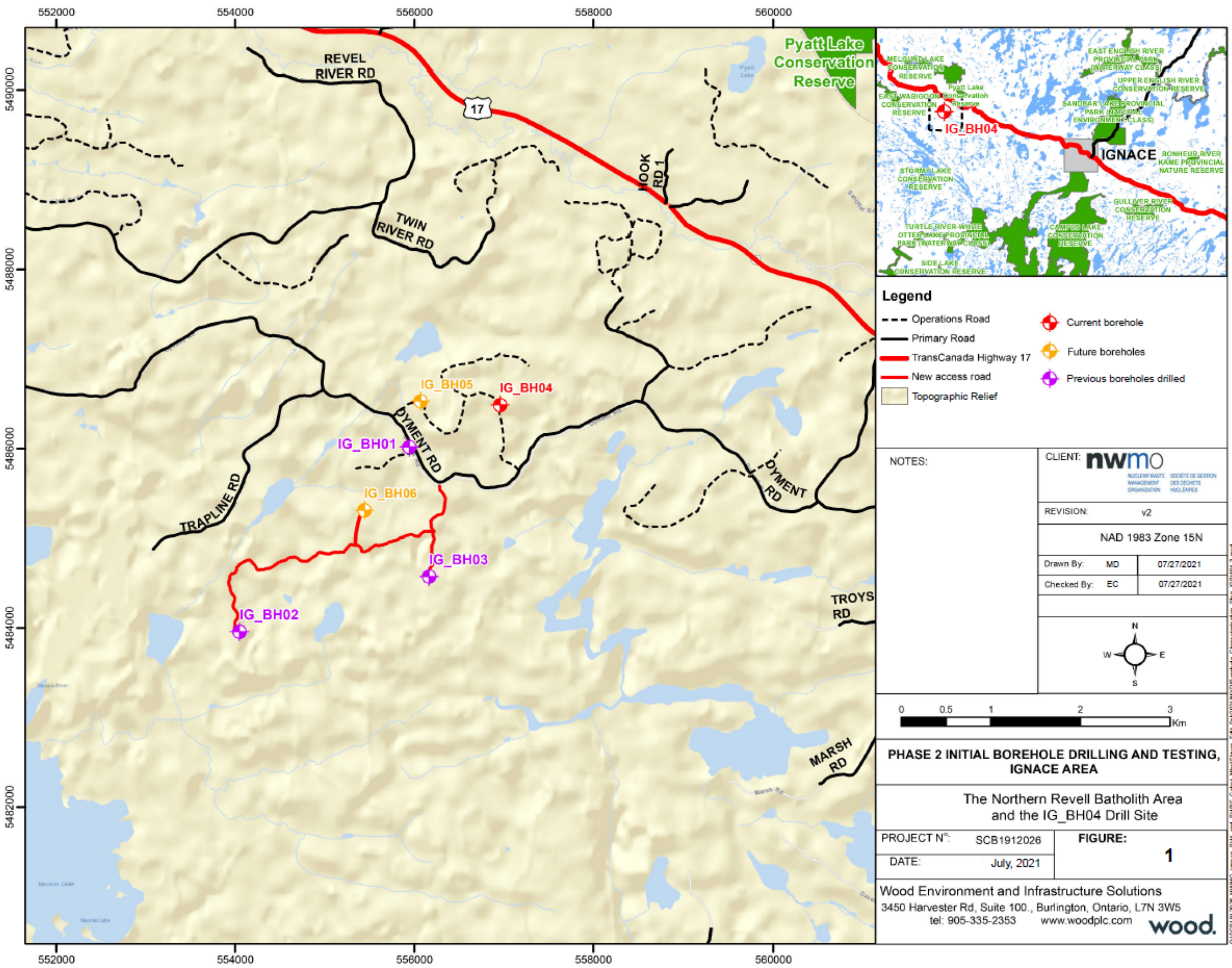


Figure 1-2: Ignace Borehole Site Locations for IG_BH01 to IG_BH06

#

IG_BH04 is an inclined borehole; all depths referred to in the text of this report are in metres below ground surface along the length of the borehole (mbgs (down hole)), or its equivalent metres borehole length (m BHL), rather than true vertical.

1.2 Technical Objectives

The technical objectives of the porewater testing program are to assess the key chemical and transport properties of the crystalline host rock with depth and within the repository horizon (presently assumed to be at depths of > 600 m). The geochemical results will provide information about the palaeohydrogeological evolution of the bedrock system. The porewater chemistry will be evaluated using indirect extraction methods which require the determination of the in-situ water content and connected porosity.

The associated work tasks include:

- Aqueous extraction experiments to determine initial estimates of pore fluid composition and Total Dissolved Solids (TDS);
- Isotope diffusive exchange experiments, for the determination of stable water isotopes ($\delta^{18}O$ and $\delta^{2}H$);
- Out-diffusion experiments, for determination of porewater stable ion concentrations (Cl and Br), as well as the determination of effective diffusion coefficients, D_e, for Cl;
- Determination of elemental elution curves during out-diffusion experiments;
- $\delta^{37}Cl$ analyses; and
- Determination of density, water content and porosity for the various subsamples used in the above-listed analytical suites.

The characterization of the porewater composition and the solute transport processes in the rock matrix contribute important information for the long-term safety assessment of deep geological repositories for radioactive waste. Thus, knowledge of the porewater composition will allow better constraints on the processes affecting the near-field of a repository. In designs where repository construction is restricted to bedrock of low permeability, the first water to interact with the repository barrier materials (e.g., bentonite, Cu-canister) will be the porewater. This interaction could result in changes of the physical and chemical properties of the various barrier materials. Knowledge of the porewater composition and its evolution over recent geological time – particularly during the last thousand to hundreds of thousands of years, in accordance with the expected lifespan of a geologic repository – is considered to be of high importance.

In combination with the knowledge gained about solute transport in the rock matrix, the characterization of porewater also contributes to a better understanding of processes related to the far-field environment around the repository. Thus, it provides valuable information about matrix diffusion as a potential retardation factor for radionuclides, and allows better constraints to be placed on the palaeohydrogeological history of a repository site. Due to the exchange by diffusion between fracture groundwater and matrix porewater, released radionuclides may be temporally immobilized by matrix diffusion, and possible subsequent sorption on mineral surfaces. For radionuclides susceptible to sorption, the accessible surface areas are enhanced by matrix diffusion when compared to the accessible surface area on fracture surfaces alone. Matrix diffusion has the potential to increase solute transport times.

In contrast to fracture groundwater, porewater cannot be sampled by conventional groundwater sampling techniques. The chemical and isotopic composition of porewater has, therefore, to be derived by indirect extraction techniques. In most of these indirect extraction techniques – especially in case of rocks of a porosity below about 2 vol.% – the original porewater concentrations are diluted and need to be back-calculated to in-situ concentrations. This requires a well-defined value for the connected porosity – accessible to different solutes under in-situ conditions. The derivation of connected porosity values, as well as solute concentrations, is prone to various perturbations during drilling, core sampling, storage, and experiments in the laboratory. The obtained data have to be carefully evaluated for potential perturbations induced by drilling activities, rock stress release and sample treatment in the laboratory in order to derive values that are representative of in-situ conditions. This requires detailed characterization of the rock composition, the rock texture, and the local stress field.

Matrix porewater of 31 core samples taken from 162 m to 959 m depth in the borehole IG_BH04, drilled as part of the Phase 2 Initial Borehole Drilling and Testing programme in the Ignace Area for the Nuclear Waste Management Organization (NWMO), was investigated for its chemical and isotopic composition. Additionally, the same set of core samples were characterised for their petrophysical properties, including water content, water-loss porosity, bulk density and chloride pore diffusion coefficients.

2.0 SAMPLING AND SAMPLE PREPARATION

A total of 93 samples from 31 depth intervals were taken from borehole IG_BH04 between December 26, 2019 and March 12, 2020 for the porewater characterization program (Table 2-1) Sampling was conducted by WSP according to the instructions provided by Hydroisotop GmbH (Hydroisotop) via personal training. After recovery from the borehole, the individual core sections (three per depth interval, 31 intervals in total) were photographed and immediately packed in a plastic bag, evacuated and sealed airtight. This procedure was repeated for a second plastic bag and a final Al-coated plastic layer. The samples were stored in a refrigerator on site and then sent to Hydroisotop, Germany, in a cooler.

The samples arrived in the lab between January 10, 2020 and March 26, 2020. All samples were well packed and arrived in the lab with preserved vacuum. At Hydroisotop the samples were stored in the fridge at 4 °C and prepared between January 15, 2020 and March 26, 2020. Two core samples, IG_BH04_PW027 and IG_BH04_PW028, were prepared on April 24, 2020.

One core section from each depth interval was stored and sealed as a retained sample at 4 °C in the fridge. The assigned samples (e.g., one PW and one AQ) were unpacked and immediately wrapped into Parafilm™ and cut by dry-sawing into full-diameter sections. After sawing, the surfaces of the obtained pieces were cleaned with paper towels and again wrapped into Parafilm™. The entire sample preparation was conducted as rapidly as possible (within 10 minutes) after opening the sealed bags, in order to minimize evaporation.

The analytical program conducted on each sample is summarized Table 2-1.

Table 2-1: Overview of the core samples taken from IG_BH04 for porewater investigations

			Depth								
Interval	Sample ID	Hydro Lab Nr.	from	to	ave	Length	Test Type	Date sampled	Time recovered	Date sent	Date arrived
			m	m	m	m			hh:mm		
1	IG_BH04_PW001	337988	162.20	162.70	162.5	0.50	PW	22.12.2019	18:35	03.01.2020	10.01.2020
	IG_BH04_PW002	337989	162.81	163.26	163.0	0.45	PW	22.12.2019	18:37	03.01.2020	10.01.2020
	IG_BH04_PW003	337990	163.58	163.83	163.7	0.25	AQ	22.12.2019	18:40	03.01.2020	10.01.2020
2	IG_BH04_PW004	337991	167.21	167.57	167.4	0.36	PW	23.12.2019	09:24	03.01.2020	10.01.2020
	IG_BH04_PW005	337992	167.57	167.94	167.8	0.37	PW	23.12.2019	09:22	03.01.2020	10.01.2020
	IG_BH04_PW006	337993	167.94	168.21	168.1	0.27	AQ	23.12.2020	09:20	03.01.2020	10.01.2020
3	IG_BH04_PW007	337994	213.00	213.38	213.2	0.38	PW	25.12.2019	16:21	03.01.2020	10.01.2020
	IG_BH04_PW008	337995	213.38	213.79	213.6	0.41	PW	25.12.2020	16:23	03.01.2020	10.01.2020
	IG_BH04_PW009	337996	213.79	214.02	213.9	0.23	AQ	25.12.2019	16:25	03.01.2020	10.01.2020
4	IG_BH04_PW010	337997	236.21	236.65	236.4	0.44	PW	27.12.2019	09:00	03.01.2020	10.01.2020
	IG_BH04_PW011	337998	237.87	238.08	238.0	0.21	AQ	27.12.2019	09:03	03.01.2020	10.01.2020
	IG_BH04_PW012	337999	238.15	238.55	238.4	0.40	PW	27.12.2019	09:06	03.01.2020	10.01.2020
5	IG_BH04_PW013	338000	267.06	267.48	267.3	0.42	PW	28.12.2019	14:20	03.01.2020	10.01.2020
	IG_BH04_PW014	338001	267.48	267.88	267.7	0.40	PW	28.12.2019	14:15	03.01.2020	10.01.2020
	IG_BH04_PW015	338002	267.88	268.11	268.0	0.23	AQ	28.12.2019	14:17	03.01.2020	10.01.2020
6	IG_BH04_PW016	338003	293.21	293.62	293.4	0.41	PW	29.12.2019	23:18	03.01.2020	10.01.2020
	IG_BH04_PW017	338004	293.62	294.03	293.8	0.41	PW	29.12.2019	23:20	03.01.2020	10.01.2020
	IG_BH04_PW018	338005	294.39	294.59	294.5	0.20	AQ	29.12.2019	23:24	03.01.2020	10.01.2020
7	IG_BH04_PW019	338006	317.21	317.59	317.4	0.38	PW	31.12.2019	00:33	03.01.2020	10.01.2020
	IG_BH04_PW020	338007	317.59	318.00	317.8	0.41	PW	31.12.2019	00:35	03.01.2020	10.01.2020
	IG_BH04_PW021	338008	318.00	318.24	318.1	0.24	AQ	31.12.2019	00:39	03.01.2020	10.01.2020
8	IG_BH04_PW022	338009	347.21	347.62	347.4	0.41	PW	01.01.2020	01:03	03.01.2020	10.01.2020
	IG_BH04_PW023	338010	347.62	348.01	347.8	0.39	PW	01.01.2020	01:05	03.01.2020	10.01.2020
	IG_BH04_PW024	338011	348.01	348.34	348.2	0.33	AQ	01.01.2020	01:08	03.01.2020	10.01.2020
9	IG_BH04_PW025	338012	371.52	371.87	371.7	0.35	PW	01.01.2020	13:38	03.01.2020	10.01.2020
	IG_BH04_PW026	338013	371.87	372.04	372.0	0.17	AQ	01.01.2020	13:37	03.01.2020	10.01.2020
	IG_BH04_PW027	338014	372.04	372.40	372.2	0.36	PW	01.01.2020	13:34	03.01.2020	10.01.2020
10	IG_BH04_PW028	339024	397.64	398.03	397.8	0.39	PW	13.01.2020	09:41	24.01.2020	30.01.2020
	IG_BH04_PW029	339025	397.24	397.64	397.4	0.40	PW	13.01.2020	09:42	24.01.2020	30.01.2020
	IG_BH04_PW030	339026	397.04	397.24	397.1	0.20	AQ	13.01.2020	09:44	24.01.2020	30.01.2020

			Depth								
Interval	Sample ID	Hydro Lab Nr.	from	to	ave	Length	Test Type	Date sampled	Time recovered	Date sent	Date arrived
			m	m	m	m			hh:mm		
11	IG_BH04_PW031	339027	423.43	423.80	423.6	0.37	PW	14.01.2020	12:56	24.01.2020	30.01.2020
	IG_BH04_PW032	339028	423.80	424.17	424.0	0.37	PW	14.01.2020	12:57	24.01.2020	30.01.2020
	IG_BH04_PW033	339029	424.17	424.32	424.2	0.15	AQ	14.01.2020	12:58	24.01.2020	30.01.2020
12	IG_BH04_PW034	339030	450.69	451.06	450.9	0.37	PW	16.01.2020	17:06	24.01.2020	30.01.2020
	IG_BH04_PW035	339031	451.06	451.44	451.3	0.38	PW	16.01.2020	17:07	24.01.2020	30.01.2020
	IG_BH04_PW036	339032	451.44	451.62	451.5	0.18	AQ	16.01.2020	17:08	24.01.2020	30.01.2020
13	IG_BH04_PW037	339033	477.91	478.31	478.1	0.40	PW	18.01.2020	00:03	24.01.2020	30.01.2020
	IG_BH04_PW038	339034	478.31	478.71	478.5	0.40	PW	18.01.2020	00:05	24.01.2020	30.01.2020
	IG_BH04_PW039	339035	478.71	478.95	478.8	0.24	AQ	18.01.2020	00:07	24.01.2020	30.01.2020
14	IG_BH04_PW040	339036	504.90	505.28	505.1	0.38	PW	19.01.2020	08:50	24.01.2020	30.01.2020
	IG_BH04_PW041	339037	505.28	505.64	505.5	0.36	PW	19.01.2020	08:51	24.01.2020	30.01.2020
	IG_BH04_PW042	339038	505.64	505.81	505.7	0.17	AQ	19.01.2020	08:52	24.01.2020	30.01.2020
15	IG_BH04_PW043	339039	532.04	532.42	532.2	0.38	PW	20.01.2020	09:27	24.01.2020	30.01.2020
	IG_BH04_PW044	339040	531.66	532.04	531.9	0.38	PW	20.01.2020	09:24	24.01.2020	30.01.2020
	IG_BH04_PW045	339041	532.42	532.61	532.5	0.19	AQ	20.01.2020	09:25	24.01.2020	30.01.2020
16	IG_BH04_PW046	339042	561.08	561.45	561.3	0.37	PW	21.01.2020	09:07	24.01.2020	30.01.2020
	IG_BH04_PW047	339043	561.45	561.81	561.6	0.36	PW	21.01.2020	09:11	24.01.2020	30.01.2020
	IG_BH04_PW048	339044	561.81	561.98	561.9	0.17	AQ	21.01.2020	09:09	24.01.2020	30.01.2020
17	IG_BH04_PW049	340993	586.01	586.40	586.2	0.39	PW	14.02.2020	01:07	18.02.2020	02.03.2020
	IG_BH04_PW050	340994	586.40	586.80	586.6	0.40	PW	14.02.2020	01:09	18.02.2020	02.03.2020
	IG_BH04_PW051	340995	585.79	586.01	585.9	0.22	AQ	14.02.2020	01:12	18.02.2020	02.03.2020
18	IG_BH04_PW052	340996	614.21	614.61	614.4	0.40	PW	17.02.2020	13:25	18.02.2020	02.03.2020
	IG_BH04_PW053	340997	614.65	615.06	614.9	0.41	PW	17.02.2020	13:25	18.02.2020	02.03.2020
	IG_BH04_PW054	340998	615.26	615.51	615.4	0.25	AQ	17.02.2020	13:25	18.02.2020	02.03.2020
19	IG_BH04_PW055	341547	636.62	637.03	636.8	0.41	PW	18.02.2020	03:08	05.03.2020	12.03.2020
	IG_BH04_PW056	341548	637.03	637.43	637.2	0.40	PW	18.02.2020	03:10	05.03.2020	12.03.2020
	IG_BH04_PW057	340999	637.43	637.58	637.5	0.15	AQ	18.02.2020	03:12	18.02.2020	02.03.2020
20	IG_BH04_PW058	341549	665.21	665.61	665.4	0.40	PW	19.02.2020	02:03	05.03.2020	12.03.2020
	IG_BH04_PW059	341550	665.61	666.02	665.8	0.41	PW	19.02.2020	02:06	05.03.2020	12.03.2020
	IG_BH04_PW060	341551	666.02	666.20	666.1	0.18	AQ	19.02.2020	02:09	05.03.2020	12.03.2020

Interval	Sample ID	Hydro Lab Nr.	Depth from	to	ave	Length	Test Type	Date sampled	Time recovered	Date sent	Date arrived
			m	m	m	m			hh:mm		
21	IG_BH04_PW061	341552	692.21	692.60	692.4	0.39	PW	20.02.2020	00:04	05.03.2020	12.03.2020
	IG_BH04_PW062	341553	692.60	692.99	692.8	0.39	PW	20.02.2020	00:07	05.03.2020	12.03.2020
	IG_BH04_PW063	341554	692.99	693.20	693.1	0.21	AQ	20.02.2020	00:10	05.03.2020	12.03.2020
22	IG_BH04_PW064	341555	711.14	711.55	711.3	0.41	PW	21.02.2020	14:32	05.03.2020	12.03.2020
	IG_BH04_PW065	342469	711.55	711.94	711.7	0.39	PW	21.02.2020	14:32	05.03.2020	25.03.2020
	IG_BH04_PW066	342470	711.94	712.28	712.1	0.34	AQ	21.02.2020	14:32	05.03.2020	25.03.2020
23	IG_BH04_PW067	342471	746.14	746.54	746.3	0.40	PW	01.03.2020	05:34	05.03.2020	25.03.2020
	IG_BH04_PW068	342472	746.54	746.94	746.7	0.40	PW	01.03.2020	05:36	05.03.2020	25.03.2020
	IG_BH04_PW069	342473	746.94	747.14	747.0	0.20	AQ	01.03.2020	05:40	05.03.2020	25.03.2020
24	IG_BH04_PW070	342474	771.42	771.82	771.6	0.40	PW	02.03.2020	03:17	05.03.2020	25.03.2020
	IG_BH04_PW071	342475	771.82	772.24	772.0	0.42	PW	02.03.2020	03:20	05.03.2020	25.03.2020
	IG_BH04_PW072	342476	772.24	772.44	772.3	0.20	AQ	02.03.2020	03:25	05.03.2020	25.03.2020
25	IG_BH04_PW073	342477	795.14	795.50	795.3	0.36	PW	03.03.2020	21:21	18.03.2020	25.03.2020
	IG_BH04_PW074	342478	795.50	796.87	796.2	1.37	PW	03.03.2020	21:30	18.03.2020	25.03.2020
	IG_BH04_PW075	342479	795.87	796.03	796.0	0.16	AQ	03.03.2020	21:28	18.03.2020	25.03.2020
26	IG_BH04_PW076	342480	825.14	825.50	825.3	0.36	PW	04.03.2020	23:43	18.03.2020	25.03.2020
	IG_BH04_PW077	342481	825.50	825.86	825.7	0.36	PW	04.03.2020	23:56	18.03.2020	25.03.2020
	IG_BH04_PW078	342482	825.86	826.02	825.9	0.16	AQ	04.03.2020	23:57	18.03.2020	25.03.2020
27	IG_BH04_PW079	342483	849.14	849.49	849.3	0.35	PW	06.03.2020	00:49	18.03.2020	25.03.2020
	IG_BH04_PW080	342498	849.49	849.87	849.7	0.38	PW	06.03.2020	00:51	18.03.2020	26.03.2020
	IG_BH04_PW081	342499	850.01	850.19	850.1	0.18	AQ	06.03.2020	00:54	18.03.2020	26.03.2020
28	IG_BH04_PW082	342500	877.56	877.94	877.8	0.38	PW	07.03.2020	18:39	18.03.2020	26.03.2020
	IG_BH04_PW083	342501	877.94	878.32	878.1	0.38	PW	07.03.2020	18:38	18.03.2020	26.03.2020
	IG_BH04_PW084	342502	878.32	878.52	878.4	0.20	AQ	07.03.2020	18:37	18.03.2020	26.03.2020
29	IG_BH04_PW085	342503	903.76	904.17	904.0	0.41	PW	09.03.2020	13:24	18.03.2020	26.03.2020
	IG_BH04_PW086	342504	904.17	904.56	904.4	0.39	PW	09.03.2020	13:20	18.03.2020	26.03.2020
	IG_BH04_PW087	342505	904.56	904.74	904.7	0.18	AQ	09.03.2020	13:19	18.03.2020	26.03.2020
30	IG_BH04_PW088	342055	930.86	931.34	931.1	0.49	PW	11.03.2020	07:53	18.03.2020	23.03.2020
	IG_BH04_PW089	342056	931.34	931.80	931.6	0.46	PW	11.03.2020	07:55	18.03.2020	23.03.2020
	IG_BH04_PW090	342057	931.90	932.23	932.1	0.33	AQ	11.03.2020	07:57	18.03.2020	23.03.2020
31	IG_BH04_PW091	342058	958.39	958.74	958.6	0.35	PW	12.03.2020	14:04	18.03.2020	23.03.2020
	IG_BH04_PW092	342059	958.74	959.17	959.0	0.43	PW	12.03.2020	14:06	18.03.2020	23.03.2020
	IG_BH04_PW093	342060	959.17	959.41	959.3	0.24	AQ	12.03.2020	14:08	18.03.2020	23.03.2020

Table 2-2: Overview of the analytical porewater program conducted on core samples from IG_BH04 (PW: porewater extraction, AQ: aqueous extraction, RS: reserve sample)

					Experimental and analytical programme													
					Aqueous Extraction			Diffusive isotope exchange experiments			Out-diffusion experiments							Grav. WC
Sample ID	Hydro Lab Nr.	Ave. Depth	Date prepared	Experiment	Exp. Set-Up	Chemical analyses	Grav. WC	Exp. Set-Up	Isotope Analyses	Grav. WC	Exp. Set-Up	Time Series	Analyses ions	Analyses $\delta^{37}Cl$	Grav. WC	Density	Modelling Dp	Extra Pieces
		mbgs																
IG_BH04_PW001	337988	162.5	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW002	337989	163.0	15.01.2020	RS														
IG_BH04_PW003	337990	163.7	15.01.2020	AQ	X	X	X											
IG_BH04_PW004	337991	167.4	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW005	337992	167.8	15.01.2020	RS														
IG_BH04_PW006	337993	168.1	15.01.2020	AQ	X	X	X											
IG_BH04_PW007	337994	213.2	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW008	337995	213.6	15.01.2020	RS														
IG_BH04_PW009	337996	213.9	15.01.2020	AQ	X	X	X											
IG_BH04_PW010	337997	236.4	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW011	337998	238.0	15.01.2020	AQ	X	X	X											
IG_BH04_PW012	337999	238.4	15.01.2020	RS														
IG_BH04_PW013	338000	267.3	15.01.2020	RS														
IG_BH04_PW014	338001	267.7	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW015	338002	268.0	15.01.2020	AQ	X	X	X											
IG_BH04_PW016	338003	293.4	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW017	338004	293.8	15.01.2020	RS														
IG_BH04_PW018	338005	294.5	15.01.2020	AQ	X	X	X											
IG_BH04_PW019	338006	317.4	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW020	338007	317.8	15.01.2020	RS														
IG_BH04_PW021	338008	318.1	15.01.2020	AQ	X	X	X											
IG_BH04_PW022	338009	347.4	15.01.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW023	338010	347.8	15.01.2020	RS														
IG_BH04_PW024	338011	348.2	15.01.2020	AQ	X	X	X											
IG_BH04_PW025	338012	371.7	24.04.2020	RS														
IG_BH04_PW026	338013	372.0	24.04.2020	AQ	X	X	X											
IG_BH04_PW027	338014	372.2	24.04.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW028	339024	397.8	07.02.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW029	339025	397.4	07.02.2020	RS														
IG_BH04_PW030	339026	397.1	08.02.2020	AQ	X	X	X											
IG_BH04_PW031	339027	423.6	07.02.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW032	339028	424.0	07.02.2020	RS														
IG_BH04_PW033	339029	424.2	08.02.2020	AQ	X	X	X											
IG_BH04_PW034	339030	450.9	07.02.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW035	339031	451.3	07.02.2020	RS														
IG_BH04_PW036	339032	451.5	08.02.2020	AQ	X	X	X											
IG_BH04_PW037	339033	478.1	07.02.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW038	339034	478.5	07.02.2020	RS														
IG_BH04_PW039	339035	478.8	08.02.2020	AQ	X	X	X											
IG_BH04_PW040	339036	505.1	07.02.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW041	339037	505.5	07.02.2020	RS														
IG_BH04_PW042	339038	505.7	08.02.2020	AQ	X	X	X											
IG_BH04_PW043	339039	532.2	07.02.2020	RS														
IG_BH04_PW044	339040	531.9	08.02.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW045	339041	532.5	08.02.2020	AQ	X	X	X											

					Experimental and analytical programme													
					Aqueous Extraction			Diffusive isotope exchange experiments			Out-diffusion experiments							Grav. WC
Sample ID	Hydro Lab Nr.	Ave. Depth	Date prepared	Experiment	Exp. Set-Up	Chemical analyses	Grav. WC	Exp. Set-Up	Isotope Analyses	Grav. WC	Exp. Set-Up	Time Series	Analyses ions	Analyses $\delta^{37}Cl$	Grav. WC	Density	Modelling D_P	Extra Pieces
		mbgs																
IG_BH04_PW046	339042	561.3	10.02.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW047	339043	561.6	11.02.2020	RS														
IG_BH04_PW048	339044	561.9	08.02.2020	AQ	X	X	X											
IG_BH04_PW049	340993	586.2	06.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW050	340994	586.6	06.03.2020	RS														
IG_BH04_PW051	340995	585.9	06.03.2020	AQ	X	X	X											
IG_BH04_PW052	340996	614.4	06.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW053	340997	614.9	06.03.2020	RS														
IG_BH04_PW054	340998	615.4	06.03.2020	AQ	X	X	X											
IG_BH04_PW055	341547	636.8	18.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW056	341548	637.2	18.03.2020	RS														
IG_BH04_PW057	340999	637.5	18.03.2020	AQ	X	X	X											
IG_BH04_PW058	341549	665.4	18.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW059	341550	665.8	18.03.2020	RS														
IG_BH04_PW060	341551	666.1	18.03.2020	AQ	X	X	X											
IG_BH04_PW061	341552	692.4	18.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW062	341553	692.8	18.03.2020	RS														
IG_BH04_PW063	341554	693.1	18.03.2020	AQ	X	X	X											
IG_BH04_PW064	341555	711.3	18.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW065	342469	711.7	26.03.2020	RS														
IG_BH04_PW066	342470	712.1	26.03.2020	AQ	X	X	X											
IG_BH04_PW067	342471	746.3	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW068	342472	746.7	26.03.2020	RS														
IG_BH04_PW069	342473	747.0	26.03.2020	AQ	X	X	X											
IG_BH04_PW070	342474	771.6	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW071	342475	772.0	26.03.2020	RS														
IG_BH04_PW072	342476	772.3	26.03.2020	AQ	X	X	X											
IG_BH04_PW073	342477	795.3	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW074	342478	796.2	26.03.2020	RS														
IG_BH04_PW075	342479	796.0	26.03.2020	AQ	X	X	X											
IG_BH04_PW076	342480	825.3	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW077	342481	825.7	26.03.2020	RS														
IG_BH04_PW078	342482	825.9	26.03.2020	AQ	X	X	X											
IG_BH04_PW079	342483	849.3	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW080	342498	849.7	26.03.2020	RS														
IG_BH04_PW081	342499	850.1	26.03.2020	AQ	X	X	X											
IG_BH04_PW082	342500	877.8	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW083	342501	878.1	26.03.2020	RS														
IG_BH04_PW084	342502	878.4	26.03.2020	AQ	X	X	X											
IG_BH04_PW085	342503	904.0	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW086	342504	904.4	26.03.2020	RS														
IG_BH04_PW087	342505	904.7	26.03.2020	AQ	X	X	X											
IG_BH04_PW088	342055	931.1	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW089	342056	931.6	26.03.2020	RS														
IG_BH04_PW090	342057	932.1	26.03.2020	AQ	X	X	X											
IG_BH04_PW091	342058	958.6	26.03.2020	RS														
IG_BH04_PW092	342059	959.0	26.03.2020	PW				X	X	X	X	X	X	X	X	X	X	X
IG_BH04_PW093	342060	959.3	26.03.2020	AQ	X	X	X											

3.0 EXPERIMENTAL SET-UPS AND ANALYTICAL METHODS

Porewater investigations included: 1) the determination of the water content and water-loss porosity on the respective samples, 2) aqueous extraction and out-diffusion experiments to characterise porewater using chemical tracers, 3) isotope diffusive exchange experiments used to determine the porewater $\delta^{18}O$ and $\delta^{2}H$ composition.

Unless otherwise specified, the analytical work has been conducted at Hydroisotop GmbH, Germany.

3.1 Water Content and Water-Loss Porosity

The water content was determined on core material used for aqueous extraction and out-diffusion experiments, as well as on the core pieces used for the isotope diffusive exchange experiments. Water contents also were determined on extra pieces of core available from those used for the out-diffusion experiments.

The quality of sample preservation upon arrival in the laboratory was assessed by the condition of the sample bags and of the core surface (wet vs. dry).

For water content measurements, drill-core pieces were placed in a crystallization dish, weighed and subsequently dried at 105 °C until stable weight conditions. According to the experience and knowledge gained from the investigations of cores from boreholes IG_BH01 to IG_BH03 the first drying step at 45 °C was considered unnecessary. Before taking the initial wet weight of the full diameter core sections, the surface was allowed to dry on the balance until stable weight was achieved for ≈10 sec. During the following drying process, weighing was carried out every 14 days until the sample weight remained constant (±0.002 g) for at least 14 days.

Water contents were determined on core samples used for aqueous extraction experiments (Table 2-2). Therefore, an aliquot of the full disc core (265 – 482 g) was broken by a mortar to an edge length of approximately 1 cm, placed in a crystallization dish, weighed and put in the oven at 105 °C for drying. Additionally, the two cut uneven head pieces with weights between 118 and 358 g were also weighed and put in the oven to determine the water content. Drying times varied between 26 and 89 days for crushed pieces, and 40 to 104 days for full core discs.

Water contents were also determined on core pieces used for out-diffusion experiments, with weights between 1,499 – 1,568 g and drying times between 56 and 131 days. Two extra pieces of the core sample used for out-diffusion and isotope exchange experiments were also taken for the determination of the water content. These sections had weights between 104 and 443 g and drying times between 26 and 69 days.

Gravimetric water contents were further determined on crushed core sections used for the single isotope diffusive exchange experiments after equilibration. The crushed core material (354-480 g) was placed in a crystallizing dish and put in the oven at 105 °C. These samples had weights between 354 g and 480 g and drying times between 27 and 72 days.

The calculation of the water-loss porosity (i.e., the connected porosity) from the gravimetric water content requires a measure of the grain density. In rocks of low porosity, the bulk wet density can be used as a proxy for the grain density. A measure for the bulk wet density of the rocks used for out-diffusion and aqueous extraction experiments was obtained from the volume and saturated mass of the core samples. The volume was calculated from measurements of height and diameter of the core samples using a Vernier Caliper, with an error of ± 0.01 mm.

Core lengths varied between 3.6 and 12.7 cm for aqueous extraction cores, and between 19.6 and 20.1 cm for out-diffusion cores.

From known sample volume and wet mass, the bulk, wet and dry density is obtained by

$$\rho_{bulk,wet} = \frac{m_{rock,wet}}{V_{rock}}, \qquad \rho_{bulk,dry} = \frac{m_{rock,dry}}{V_{rock}} \qquad \text{eq. 1}$$

and the water-loss (connected) porosity, ϕWL, can be calculated according to

$$\emptyset_{WL} = WC_{wet} \times \frac{\rho_{bulk,wet}}{\rho_{water}} \quad \emptyset_{WL} = \frac{m_{pw} \times 100}{r^2 \times h \times \pi \times \rho_{water}} \qquad \text{eq. 2}$$

where WC_{wet} is the water content based on the wet weight of the rock sample and $\rho_{bulk,wet}$ the bulk wet density of the rock. In a first approximation, the density of water, ρ_{water}, is assumed to be 1 g/cm^3. Due to the low water content of the investigated crystalline rocks, the water content and water-loss porosity determined by the wet weight and bulk, wet density of the sample is essentially equal to those values calculated using the dry weight and bulk, dry density.

As shown by Gaussian error propagation (Appendix C), the error of the water content and the water-loss porosity depends predominately on the accuracy of the determination of the mass of porewater measured after unpacking (i.e., on the measured initial wet weight) and the final dry weight of the cores.

3.2 Porewater Extraction Methods

3.2.1 Aqueous Extraction Experiments

Aqueous extraction experiments were conducted prior to out-diffusion and isotope exchange experiments to estimate the salinity of the investigated porewaters.

Saturated full disc core sections were crushed by a mortar and sieved by an analytical sieve to a grain size of < 2 mm, and 75 to 119 g of rock material were put in a PE bottle, where 57 to 76 ml of deionized water were added. Subsequently, the bottle was gently shaken for 24 h. Afterward, the elution was decanted, filtered (0.45 µm) and immediately analysed for alkalinity, pH and specific electrical conductivity (EC) using a Metrohm Titrino 785 and WTW LF 325 system. The main anion and cation concentrations were analysed by ion chromatography (IC) using a Dionex ICS 1500 system. The analytical error of the ion concentration analyses is ± 5 %. Aluminium concentrations were analysed using a ContrAA800 G graphite tube atomic absorbtion spectrometer (AAS) from ThermoFischer with an analytical error of ±10 % and silica concentrations were determined photometrically with an analytical error of ±5 %. DOC concentrations were analysed using a Shimazu TOC-VCSH analyser (analytical error of 3-5 % depending on the concentration range).

The porewater Cl concentration was further calculated according to

$$C_{i,pw} = \frac{C_{i,sol} \times V_{sol} \times 0.001}{m_{pw}} \qquad \text{eq. 3}$$

where $C_{i,pw}$ = porewater elemental concentration, $C_{i,sol}$ = analyzed elemental concentration in the aqueous extraction solution, V_{sol} = Volume of aqueous extraction solution, and m_{pw} = mass of porewater.

3.2.2 Out-diffusion Experiments

Out-diffusion experiments were performed on intact full disc cores by immersion into ultrapure water. The volume of test water varied between 121 and 154 ml, resulting in test water to core mass ratios between 0.08 and 0.10. During the experiments the two water reservoirs, i.e., porewater and test water, were allowed to exchange until equilibrium. Equilibrium with respect to chloride is reached when the Cl concentration has been constant within the analytical error range (= ±5 %) over a minimum of 14 days.

After placing the core sample in the PE-vessel, the vessel was sealed and put in a vibrating water bath (40 rpm) at a constant temperature of 45 °C to accelerate diffusion. The PE-vessels were covered by a vapour-tight lid, which is equipped with two Swagelock™ valves and PEEK™ sampling lines. The core, the experiment container and the test water were weighed before and after the experiment to ensure that no loss of test water occurred during the entire experiment. At specific time intervals of initially a few days, and later a few weeks, 0.5 ml of solution were sampled using a PVC-syringe to determine the chloride concentration as a function of time. The experimental time depended on the equilibration grade in the individual experiments. All out-diffusion experiments were ended between 146 and 188 days.

After equilibrium with respect to chloride was achieved, the vessels were removed from the water bath and cooled to room temperature. Subsequently, the cylinder, the core and the remaining test water were weighed and the supernatant solution was filtered (0.45 µm) and analysed immediately for pH, sp. el. conductivity (EC) and alkalinity (total alkalinity (pH 4.3) and base capacity 8.2), and later for major cations and anions and certain trace elements and isotopes.

The major cations (Na^+, K^+, Ca^{2+}, Mg^{2+}, Sr^{2+}) and anions (F^-, Cl^-, NO_3^-, Br^-, SO_4^{2-}) of the 0.5 ml time series and final test solutions of the out-diffusion experiments were analysed by IC using a Dionex ICS 1500 system or a Thermo Scientific Dionex Aquion and Integrion IC system. The relative analytical error of these analyses is ± 5 % based on multiple measurements of external check standard solutions (1σ). The final test solutions with a volume of app. 100 ml were analysed undiluted and in different dilutions (1:10 and, if necessary, 1:20). The time series samples were analysed timely after sampling. Due to the low volume, the samples could only be measured once in a 1:10 dilution. As such, the detection limit is different for each element in the two different solutions.

The alkalinity titration, pH-value and specific electrical conductivity measurements were performed using Metrohm titration systems and a WTW LF325 probe. TOC and TIC concentrations were analysed on the final solutions using a Shimadzu VCSH analyser with a relative analytical error of ± 5 % based on multiple measurements of external check standard solutions (1σ). Aluminium and lithium concentrations were analysed using a ContrAA800 G graphite tube atomic absorbtion spectrometer (AAS) from ThermoFischer and silica concentrations were determined photometrically. Boron of out-diffusion test solutions was analysed at Analytik Institut Rietzler GmbH, Germany, using an ICP-MS system with a detection limit of 0.0001 mg/l and an analytical uncertainty of 5 %.

The $^{37}Cl/^{35}Cl$ isotope ratio, expressed as $\delta^{37}Cl$ relative to SMOC, was measured by a GC-MS-IRMS system (Thermo Fischer Delta S). Analytical errors were determined by the standard deviation of triplicate analyses of every sample. Strontium isotope signatures were analysed at Iso Analysis UG, Germany, by a Thermo Fischer MC-ICP-MS system with an analytical uncertainty of 0.0005.

Chloride and bromide concentrations of the experiment solution can be converted to porewater concentrations by applying mass balance calculations if equilibrium between test water and porewater is achieved. With knowledge of the mass of porewater in the rock sample, the chloride and bromide concentration of the porewater can be calculated according to

$$C_{pw} = \frac{(m_{pw}+m_{TWi}-\sum^{n} m_s)\times C_{TW\infty}-(m_{TWi}\times C_{TWi})+\sum^{n} m_s\times C_s}{m_{pw}} \quad \text{eq. 4}$$

where C_{pw} = porewater concentration, m_{pw} = mass of porewater, m_{TWi} = initial mass of test water, C_{TWi} = initial Cl concentration of test water, m_s = mass of sub sample used for time series, and C_s = Cl concentration of sub sample used for time series.

The term $\sum m_s * C_s$ (equation 4) describes the amount of Cl removed from the initial experiment solution for Cl time-series samples. A correction for chloride and bromide in the initial experiment solution ($m_{TWi} * C_{TWi}$) is necessary if this solution is not entirely free of chloride and bromide.

The unit for the porewater concentration is given in mg/kg H_2O (and not mg/l) because it is derived on a mass basis rather than a volumetric basis. This is due to the fact that the density of the porewater is not known beforehand, because it depends on the in-situ salinity of the water (which is unknown).

3.3 Isotope Diffusive Exchange Technique

The isotope diffusive exchange technique to determine the water isotope composition, $\delta^{18}O$ and $\delta^{2}H$, of the porewater and the mass of porewater was originally developed by Rogge (1997) and Rübel et al. (2002) for sedimentary rocks and later adapted for crystalline rocks by Waber and Smellie (2005, 2006) and Eichinger et al. (2006). In this method, initially saturated rock material is placed into two vapour-tight containers together with different test waters of known isotope composition. The porewater and test water are then allowed to isotopically equilibrate via the vapour phase without any direct contact between the core material and the test water. The porewater isotope composition and the water content of the rock sample can then be derived by isotope mass balance relationships. It has been shown that the uncertainty of the derived isotope composition largely depends on the ratio of porewater to test water used in the experiments (e.g., Rübel et al. 2002). For crystalline rocks, this ratio was optimised by using larger volumes of rock and smaller volumes of test water in the experiments (e.g., Waber and Smellie 2005, 2006; Eichinger et al. 2006).

For the present samples, 1.8 ml of test water were placed in a Petri dish in the centre of a glass vessel and surrounded by hand crushed core pieces 4-6 cm^3 in size and with a total mass of 354 to 480 g. After an equilibration time of 60 days, the two test waters were removed and analysed by Cavity Ring Down Spectroscopy using a Picarro L 2130-I Analyser. The results for the test waters are reported relative to the VSMOW (Vienna Standard Mean Ocean Water) standard with a precision of ± 0.15 ‰ for $\delta^{18}O$ and ± 1.5 ‰ for $\delta^{2}H$.

Test water and core material were weighed before and after the experiment to assess if test water was lost on the container walls and/or rock material due to evaporation and/or condensation. To minimise condensation, about 0.3 mol of NaCl were dissolved in the test water to lower its water vapour pressure. For every sample, two experiments were performed, one using test water with an isotope composition close to that expected in the porewater ("LAB-sample") and one using test water with an isotope composition far from that expected for the porewater ("ICE-sample").

The test water used for the LAB-sample was normal laboratory tap water ($\delta^{18}O$ = -10.21 to -10.32 ‰ VSMOW; $\delta^{2}H$ = -72.8 to -73.6 ‰ V-SMOW), while that for the ICE-sample was water from an ice core drilled in the Antarctic ($\delta^{18}O$ = -31.29 to 31.82 ‰ V-SMOW; $\delta^{2}H$ = -243.9 to -246.5 ‰ V-SMOW). The equilibration time in the three reservoirs – rock porewater, test water, and the air inside the container as a diaphragm – depends on the volume of the container, the size of the rock pieces and the distance of the rock pieces to the test water (see Rogge 1997). Based on the estimations of the minimum time period required for complete isotopic equilibration (Eichinger et al. 2006) an experimental time of 60 days was chosen.

The isotope diffusive exchange technique can be used to determine porewater $\delta^{18}O$ and $\delta^{2}H$ values and the mass of the porewater present in the connected pore space of the rock sample. These parameters are calculated from the analytical results obtained for the two test water solutions, using mass balance relationships, according to

$$m_{pw} * c_{pw}\Big|_{t=0} + m_{tw} * c_{tw}\Big|_{t=0} = (m_{pw} + m_{tw}) * c_{tw}\Big|_{t=\infty} \qquad \text{eq. 5}$$

where *m* = mass, *c* = isotope ratios expressed in the δ notation, *pw* = porewater, *tw* = test water, *t = 0* represents the isotope concentrations at the beginning of the experiment, and *t* = ∞ represents the isotope concentrations at the end of the experiment.

The water content of the applied samples is calculated by transformation of equation 5 to

$$WC_{IsoEx} = \left[\frac{m_{TW(Std2)} \times m_{Rock(Std1)} \times (C_{TW^0(Std2)} - C_{TW\infty(Std2)}) + m_{TW(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std1)} - C_{TW^0(Std1)})}{m_{Rock(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std2)} - C_{TW\infty(Std1)})}\right] \times 100 \qquad \text{eq. 6}$$

where m_{Rock} = mass of rock, *Std 1* = test solution 1 and *Std 2* = test solution 2.

Equation 6 can be set up for oxygen and hydrogen isotope ratios of the test water, resulting in two independent values for the mass of porewater.

The $\delta^{18}O$- and $\delta^{2}H$- values of the porewater are calculated by transformation of equation 5 to

$$C_{PW} = \frac{C_{TW\infty(Std1)} \times m_{TW(Std2)} \times m_{Rock(Std1)} \times (C_{TW\infty(Std2)} - C_{TW^0(Std2)}) - C_{TW\infty(Std2)} \times m_{TW(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std1)} - C_{TW^0(Std1)})}{m_{TW(Std2)} \times m_{Rock(Std1)} \times (C_{TW\infty(Std2)} - C_{TW^0(Std2)}) - m_{TW(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std1)} - C_{TW^0(Std1)})} \qquad \text{eq. 7}$$

The errors of the calculated $\delta^{18}O$, $\delta^{2}H$ and the mass of porewater are computed for each sample using Gauss' law of error propagation (Appendix C).

4.0 RESULTS OF WATER CONTENT AND WATER-LOSS POROSITY INVESTIGATIONS

Water content, bulk density and water-loss porosity were determined on originally saturated segments of the core samples from borehole IG_BH04. The water content was determined by two independent methods, i.e., gravimetrically by drying rock sections at 105 °C to stable weight conditions, and by using the isotope diffusive exchange technique (see Section 3). The gravimetric water content (WC_{grav}) was determined on different segments of the core samples used for the individual experiments. The initial saturated weight of all these samples was recorded directly after unpacking and preparation of the samples in the laboratory. This ensures that the calculation of the porewater mass is not affected by any possible changes induced during the experiments. Such possible changes were monitored as well by recording the sample weight right after termination of the experiment and before the drying process began. The water loss was calculated using the initial wet weight measured in the lab and the final weight after drying.

The exact determination of the in-situ mass of porewater is of particular importance when using indirect extraction methods because porewater tracer concentrations are calculated by mass balance equations using the mass of porewater (Section 3). Knowledge of the water-loss porosity (calculated from the water content and density) is further required for the derivation of diffusion coefficients (Section 6.2).

4.1 Water Contents

Gravimetric water contents were determined on different segments used for individual experiments (see Section 3).

4.1.1 Gravimetric Water Contents Determined on Aqueous Extraction Core Samples

The gravimetric water contents were determined on different aliquots of the 31 aqueous extraction core samples (AQ) taken between 162 and 959 mbgs (downhole). These values were used for the estimation of porewater Cl and Br concentrations derived from the aqueous extraction experiments (section 6.1).

The gravimetric water contents determined on individual aliquots of the AQ samples vary between 0.10 wt.% and 0.29 wt.%, with weighted values ranging between 0.11 ± 0.01 and 0.23 ± 0.04 wt.% (Table 4-1).

The water contents determined by taking the wet (WC_{wet}) and dry weight (WC_{dry}) are similar within the first two decimal places due to the low water masses in the investigated cores.

The water contents determined on the individual aliquots of the different AQ samples can vary significantly, which is interpreted to be due to mineralogical heterogeneities.

#

Table 4-1: Gravimetric water contents (WC) of aliquots of AQ core samples from IG_BH04 used for aqueous extraction experiments using wet (WCwet) and dry masses (WCdry) of the individual core pieces. The weighted values are calculated by using the individual masses

Sample		Aq.ex. subsample A			Aq.ex. subsample B			Aq.ex. subsample C			WC weighted		
	Depth	mass	WC_{wet}	WC_{dry}	mass	WC_{wet}	WC_{dry}	mass	WC_{wet}	WC_{dry}	WC_{wet}	WC_{dry}	Stdev
	mbgs	g	wt.%	wt.%	g	wt.%	wt.%	g	wt.%	wt.%	wt.%	wt.%	wt.%
IG_BH04_PW003	163.7	130.116	0.21	0.21	187.054	0.20	0.20	398.218	0.16	0.16	0.18	0.18	0.02
IG_BH04_PW006	168.1	161.468	0.17	0.17	130.691	0.18	0.18	337.504	0.16	0.16	0.17	0.17	0.01
IG_BH04_PW009	213.9	173.927	0.22	0.22	152.018	0.21	0.21	365.112	0.18	0.18	0.20	0.19	0.02
IG_BH04_PW011	238.0	178.723	0.19	0.19	191.008	0.19	0.19	391.107	0.16	0.16	0.17	0.17	0.01
IG_BH04_PW015	268.0	190.780	0.16	0.16	208.305	0.17	0.17	381.829	0.15	0.15	0.16	0.16	0.01
IG_BH04_PW018	294.5	171.029	0.19	0.19	167.961	0.20	0.20	330.641	0.17	0.17	0.18	0.18	0.02
IG_BH04_PW021	318.1	167.043	0.21	0.21	172.362	0.19	0.19	297.774	0.19	0.19	0.19	0.19	0.01
IG_BH04_PW024	348.2	256.723	0.11	0.11	273.257	0.12	0.12	387.644	0.10	0.10	0.11	0.11	0.01
IG_BH04_PW026	372.0	183.765	0.14	0.14	133.570	0.15	0.15	284.620	0.13	0.13	0.14	0.14	0.01
IG_BH04_PW030	397.1	206.140	0.17	0.17	178.408	0.17	0.17	482.027	0.16	0.16	0.17	0.17	0.01
IG_BH04_PW033	424.2	192.430	0.18	0.18	174.586	0.19	0.19	371.602	0.15	0.15	0.17	0.17	0.02
IG_BH04_PW036	451.5	130.034	0.17	0.17	131.960	0.16	0.16	330.914	0.14	0.14	0.15	0.15	0.01
IG_BH04_PW039	478.8	155.352	0.13	0.13	171.300	0.16	0.16	360.454	0.14	0.14	0.14	0.14	0.01
IG_BH04_PW042	505.7	358.542	0.17	0.17	156.199	0.19	0.19	277.021	0.16	0.16	0.17	0.17	0.02
IG_BH04_PW045	532.5	119.637	0.18	0.18	204.391	0.17	0.17	310.819	0.14	0.14	0.16	0.16	0.02
IG_BH04_PW048	561.9	152.742	0.17	0.17	133.910	0.19	0.19	290.097	0.15	0.15	0.16	0.16	0.02
IG_BH04_PW051	585.9	118.203	0.29	0.29	155.562	0.21	0.21	360.627	0.22	0.22	0.23	0.23	0.04
IG_BH04_PW054	615.4	235.422	0.17	0.17	207.669	0.18	0.18	358.421	0.16	0.16	0.17	0.17	0.01
IG_BH04_PW057	637.5	179.963	0.17	0.17	257.109	0.15	0.15	310.333	0.14	0.14	0.15	0.15	0.01
IG_BH04_PW060	666.1	161.160	0.13	0.13	179.254	0.13	0.13	310.464	0.12	0.12	0.13	0.13	0.00
IG_BH04_PW063	693.1	224.256	0.11	0.11	188.917	0.11	0.11	379.402	0.10	0.10	0.11	0.11	0.00
IG_BH04_PW066	712.1	296.948	0.15	0.15	223.954	0.15	0.15	338.515	0.14	0.14	0.14	0.14	0.01
IG_BH04_PW069	747.0	230.755	0.18	0.18	173.129	0.13	0.13	306.240	0.12	0.12	0.14	0.14	0.03
IG_BH04_PW072	772.3	199.441	0.12	0.12	184.446	0.12	0.12	323.124	0.11	0.11	0.12	0.12	0.01
IG_BH04_PW075	796.0	198.442	0.24	0.24	141.750	0.21	0.21	271.504	0.19	0.19	0.21	0.21	0.03
IG_BH04_PW078	825.9	116.211	0.20	0.20	167.346	0.22	0.22	286.354	0.20	0.20	0.20	0.20	0.01
IG_BH04_PW081	850.1	143.810	0.18	0.19	162.437	0.19	0.19	331.360	0.17	0.17	0.18	0.18	0.01
IG_BH04_PW084	878.4	210.949	0.24	0.24	231.646	0.20	0.20	265.223	0.17	0.17	0.20	0.20	0.03
IG_BH04_PW087	904.7	176.989	0.13	0.13	182.259	0.17	0.17	323.034	0.12	0.12	0.13	0.13	0.02
IG_BH04_PW090	932.1	265.511	0.16	0.16	178.331	0.14	0.14	347.338	0.12	0.12	0.14	0.14	0.02
IG_BH04_PW093	959.3	221.257	0.19	0.19	229.273	0.20	0.20	320.261	0.19	0.19	0.19	0.19	0.01

Note(s)

41 [mbgs (downhole)]

4.1.2 Gravimetric water contents determined on porewater cores

Gravimetric water contents were determined on different aliquots of the 31 PW samples taken between 162 and 959 mbgs (downhole).

Gravimetric water contents determined on head pieces

During sample preparation, the head pieces with weights between 104 and 443 g were cut, weighed and dried at 105 °C to obtain a first estimate about the water contents of the investigated core samples.

The gravimetric water contents determined on the head pieces of the PW core samples vary between 0.13 wt.% and 0.27 wt.% with weighted WC_{grav} values between 0.14 ± 0.01 wt.% and 0.25± 0.02 wt.% (Table 4-2).

The water contents determined by taking the wet (WC_{wet}) and dry weight (WC_{dry}) are similar within the first two decimal places due to the low water masses in the investigated cores.

The water contents determined on the two head pieces of the different PW samples vary, which is attributed to mineralogical heterogeneities.

Table 4-2: Gravimetric water contents (WC) of aliquots of AQ core samples from IG_BH04 used for aqueous extraction experiments using wet (WCwet) and dry masses (WCdry) of the individual core pieces. The weighted values are calculated by using the individual masses

Sample		Subsample A			Subsample B			WC weighted		
	Depth	mass	WC_{wet}	WC_{dry}	mass	WC_{wet}	WC_{dry}	WC_{wet}	WC_{dry}	Stdev
	mbgs	g	wt.%	wt.%	g	wt.%	wt.%	wt.%	wt.%	wt.%
IG_BH04_PW001	162.5	168.713	0.23	0.23	443.495	0.17	0.17	0.18	0.19	0.05
IG_BH04_PW004	167.4	111.799	0.17	0.17	229.610	0.17	0.17	0.17	0.17	0.01
IG_BH04_PW007	213.2	230.246	0.20	0.20	220.839	0.18	0.18	0.19	0.19	0.02
IG_BH04_PW010	236.4	243.542	0.20	0.20	277.887	0.21	0.21	0.20	0.20	0.01
IG_BH04_PW014	267.7	238.333	0.19	0.19	191.003	0.15	0.15	0.17	0.17	0.02
IG_BH04_PW016	293.4	258.065	0.27	0.27	192.855	0.18	0.18	0.23	0.23	0.07
IG_BH04_PW019	317.4	208.736	0.23	0.23	172.595	0.20	0.20	0.22	0.22	0.02
IG_BH04_PW022	347.4	252.485	0.15	0.15	221.034	0.17	0.17	0.16	0.16	0.01
IG_BH04_PW027	372.2	212.193	0.16	0.16	161.354	0.16	0.16	0.16	0.16	0.01
IG_BH04_PW028	397.8	223.134	0.16	0.16	107.715	0.18	0.18	0.16	0.16	0.02
IG_BH04_PW031	423.6	203.775	0.18	0.18	194.217	0.21	0.21	0.19	0.19	0.02
IG_BH04_PW034	450.9	172.390	0.19	0.19	190.891	0.17	0.17	0.18	0.18	0.02
IG_BH04_PW037	478.1	189.469	0.18	0.18	133.384	0.14	0.14	0.16	0.16	0.02
IG_BH04_PW040	505.1	205.842	0.17	0.17	182.463	0.17	0.17	0.17	0.17	0.01
IG_BH04_PW044	531.9	192.270	0.22	0.22	174.217	0.21	0.21	0.21	0.21	0.01
IG_BH04_PW046	561.3	142.324	0.15	0.15	229.676	0.18	0.18	0.17	0.17	0.02
IG_BH04_PW049	586.2	201.429	0.20	0.20	183.186	0.19	0.19	0.20	0.20	0.01
IG_BH04_PW052	614.4	288.580	0.16	0.16	175.975	0.17	0.17	0.16	0.17	0.01
IG_BH04_PW055	636.8	232.680	0.16	0.16	128.611	0.18	0.18	0.17	0.17	0.01
IG_BH04_PW058	665.4	164.144	0.13	0.13	245.474	0.15	0.15	0.14	0.14	0.01
IG_BH04_PW061	692.4	175.059	0.13	0.13	227.645	0.16	0.16	0.14	0.14	0.02
IG_BH04_PW064	711.3	227.558	0.14	0.14	174.514	0.13	0.13	0.14	0.14	0.01
IG_BH04_PW067	746.3	260.701	0.14	0.14	260.701	0.14	0.14	0.14	0.14	0.01
IG_BH04_PW070	771.6	178.264	0.13	0.13	208.017	0.15	0.15	0.15	0.15	0.01
IG_BH04_PW073	795.3	208.643	0.14	0.14	172.987	0.20	0.20	0.21	0.21	0.01
IG_BH04_PW076	825.3	168.397	0.22	0.22	112.627	0.19	0.19	0.20	0.20	0.01

Sample		Subsample A			Subsample B			WC weighted		
	Depth	mass	WC_{wet}	WC_{dry}	mass	WC_{wet}	WC_{dry}	WC_{wet}	WC_{dry}	Stdev
	mbgs	g	wt.%	wt.%	g	wt.%	wt.%	wt.%	wt.%	wt.%
IG_BH04_PW079	849.3	170.257	0.20	0.20	104.073	0.18	0.18	0.17	0.17	0.01
IG_BH04_PW082	877.8	162.269	0.17	0.17	184.852	0.26	0.26	0.25	0.25	0.02
IG_BH04_PW085	904.0	162.878	0.24	0.24	276.682	0.16	0.16	0.17	0.17	0.01
IG_BH04_PW088	931.1	149.218	0.18	0.18	213.059	0.18	0.18	0.18	0.18	0.01
IG_BH04_PW092	959.0	129.712	0.19	0.19	257.860	0.15	0.15	0.17	0.17	0.02

Note(s)
41 [mbgs (downhole)]

Gravimetric water contents determined on out-diffusion cores

Gravimetric water contents determined on the large sized 1,500 g to 1,569 g heavy core pieces were determined by the weights taken before and after their long-term immersion in deionised water during the out-diffusion experiments. For 19 samples, the weights of cores were higher, beyond the assumed error of 0.05 g (uncertainty in the determination of the weight with dry surface) after the experiment than before the experiment (Table 4-3, Figure 4-3). The weight gain and hence intake of water during the experiments, which is between 0.057 and 0.580 g can be caused by:

- The filling of pore space created post drilling by stress release;
- The filling of pore space that was desaturated during the time period between core recovery (during drilling) and packaging; or
- Uncertainty of the determination of the initial wet weight during drying of the surface water.

Major evaporation effects in the period between the recovery out of the borehole and sample packing can, in principle, be excluded because most of the samples arrived with moist surfaces in the lab.

Six samples showed lower (>0.05 g) weights after the experiments than before (0.111 – 0.207 g, negative Δ-values in Table 4-3). The differences are presumed to be due to the fact that determination of the initial weight is done after drying the surfaces of the cores.

The gravimetric water contents determined on the out-diffusion cores vary between 0.13 ± 0.04 wt.% and 0.21 ± 0.02 wt.%, as calculated using the wet weight (dry surface) of the core before the experiment (b.e.), and between 0.14 ± 0.02 wt.% and 0.23 ± 0.03 wt.%, as calculated using the wet weight (dry surface) of the core after the experiment (a.e.) (Table 4-3). The weight differences of the core samples determined before (b.e.) and after the experiments (a.e.) result in water content variations of 0.01-0.03 wt.% (Table 4-3, Figure 4-1). These differences are within the error ranges determined by Gaussian error propagation (Table 4-3, Figure 4-1). The weight differences before and after the experiments, and the corresponding differences in porewater masses expressed as water content, are considered for the calculation of the porewater Cl and Br concentrations.

The water contents determined by taking the wet (WC_{wet}) and dry weight (WC_{dry}) are similar within the first two decimal places due to the low water masses in the investigated cores (Table 4-3).

Table 4-3: Gravimetric water contents of out-diffusion core samples from IG_BH04 calculated by the mass of cores determined before (b.e.) and after (a.e.) experiments using wet (WC_{wet}) and dry masses (WC_{dry}) of the individual core pieces; the error of the water content is determined by Gaussian error propagation (Appendix C)

Sample		Mass Core			Mass Porewater		WCgrav.wet		WCgrav.dry		Error WCgrav
	Depth	wet b.e. (dry surface)	wet a.e. (dry surface)	Δmcore (a.e.-b.e.)	mPW b.e.	mPW a.e.	WCcore b.e.	WCcore a.e.	WCcore b.e.	WCcore a.e.	
	mbgs	g	g	g	g	g	g	wt.%	wt.%	wt.%	wt.%
IG_BH04_PW001	162.5	1552.060	1552.240	0.180	2.646	2.826	0.17	0.18	0.17	0.18	0.01
IG_BH04_PW004	167.4	1561.953	1562.115	0.162	2.625	2.787	0.17	0.18	0.17	0.18	0.01
IG_BH04_PW007	213.2	1520.000	1520.330	0.330	2.618	2.948	0.17	0.19	0.17	0.19	0.02
IG_BH04_PW010	236.4	1568.973	1568.985	0.012	3.079	3.091	0.20	0.20	0.20	0.20	0.01
IG_BH04_PW014	267.7	1553.765	1554.140	0.375	2.347	2.722	0.15	0.18	0.15	0.18	0.03
IG_BH04_PW016	293.4	1556.602	1556.610	0.008	2.724	2.732	0.17	0.18	0.18	0.18	0.01
IG_BH04_PW019	317.4	1561.248	1561.305	0.057	2.842	2.899	0.18	0.19	0.18	0.19	0.01
IG_BH04_PW022	347.4	1533.661	1533.690	0.029	2.440	2.469	0.16	0.16	0.16	0.16	0.01
IG_BH04_PW027	372.2	1547.028	1547.012	-0.016	2.553	2.537	0.17	0.16	0.17	0.16	0.01
IG_BH04_PW028	397.8	1531.613	1531.502	-0.111	2.428	2.317	0.16	0.15	0.16	0.15	0.01
IG_BH04_PW031	423.6	1536.805	1536.683	-0.122	2.637	2.515	0.17	0.16	0.17	0.16	0.01
IG_BH04_PW034	450.9	1523.905	1523.670	-0.235	2.299	2.064	0.15	0.14	/0.15	0.14	0.02
IG_BH04_PW037	478.1	1519.162	1519.202	0.040	2.114	2.154	0.14	0.14	0.14	0.14	0.01
IG_BH04_PW040	505.1	1519.367	1519.160	-0.207	2.482	2.275	0.16	0.15	0.16	0.15	0.02
IG_BH04_PW044	531.9	1503.544	1503.266	0.247	2.429	2.676	0.16	0.18	0.16	0.18	0.02
IG_BH04_PW046	561.3	1504.206	1504.050	-0.156	2.337	2.181	0.16	0.15	0.16	0.15	0.01
IG_BH04_PW049	586.2	1555.679	1555.780	0.101	3.308	3.409	0.21	0.22	0.21	0.22	0.01
IG_BH04_PW052	614.4	1518.334	1518.478	0.144	2.910	3.054	0.19	0.20	0.19	0.20	0.01
IG_BH04_PW055	636.8	1537.568	1537.644	0.076	2.402	2.478	0.16	0.16	0.16	0.16	0.01
IG_BH04_PW058	665.4	1546.004	1546.403	0.399	2.657	3.056	0.17	0.20	0.17	0.20	0.03
IG_BH04_PW061	692.4	1531.519	1531.970	0.451	2.109	2.560	0.14	0.17	0.14	0.17	0.03
IG_BH04_PW064	711.3	1564.920	1565.140	0.220	2.314	2.534	0.15	0.16	0.15	0.16	0.02
IG_BH04_PW067	746.3	1549.030	1549.610	0.580	1.953	2.533	0.13	0.16	0.13	0.16	0.04
IG_BH04_PW070	771.6	1550.371	1550.870	0.499	2.359	2.858	0.15	0.18	0.15	0.18	0.04
IG_BH04_PW073	795.3	1518.800	1518.970	0.170	3.137	3.307	0.21	0.22	0.21	0.22	0.01
IG_BH04_PW076	825.3	1521.900	1522.310	0.410	3.117	3.527	0.20	0.23	0.21	0.23	0.03
IG_BH04_PW079	849.3	1560.300	1560.730	0.430	2.970	3.400	0.19	0.22	0.19	0.22	0.03
IG_BH04_PW082	877.8	1499.654	1499.455	-0.199	3.201	3.002	0.21	0.20	0.21	0.20	0.02
IG_BH04_PW085	904.0	1540.600	1540.550	-0.050	2.512	2.462	0.16	0.16	0.16	0.16	0.01
IG_BH04_PW088	931.1	1521.035	1521.200	0.165	2.838	3.003	0.19	0.20	0.19	0.20	0.01
IG_BH04_PW092	959.0	1531.237	1531.441	0.204	2.312	2.516	0.15	0.16	0.15	0.16	0.02

Note(s)

41 [mbgs (downhole)]

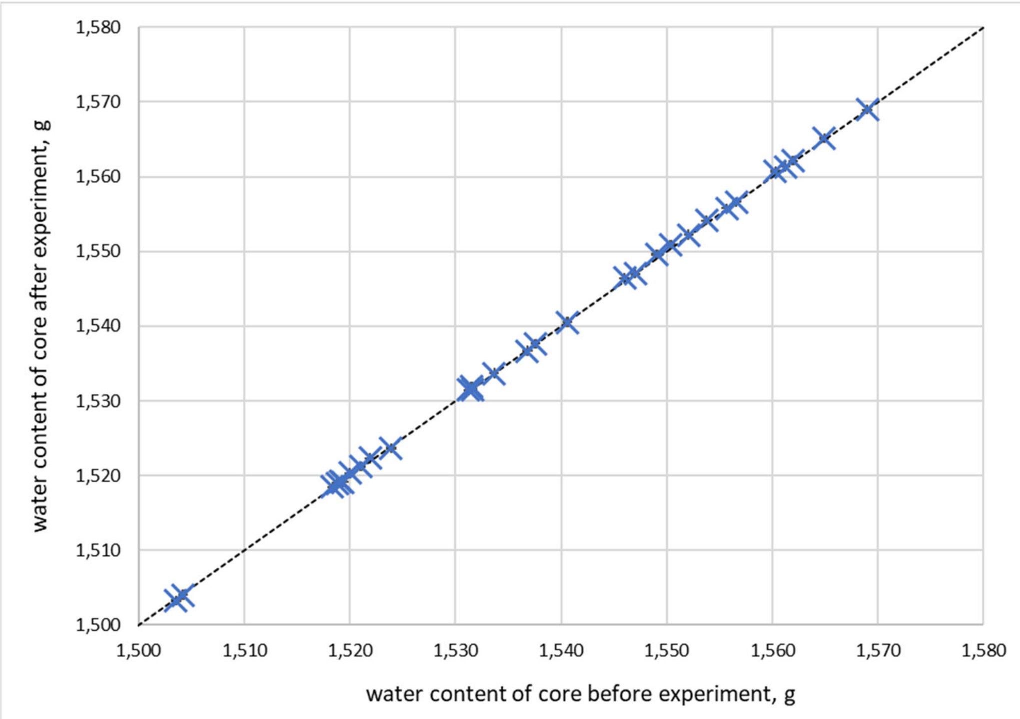


Figure 4 1: Mass of core samples from IG_BH04 before and after the out-diffusion experiments; the uncertainty of the core mass is ± 0.05 g

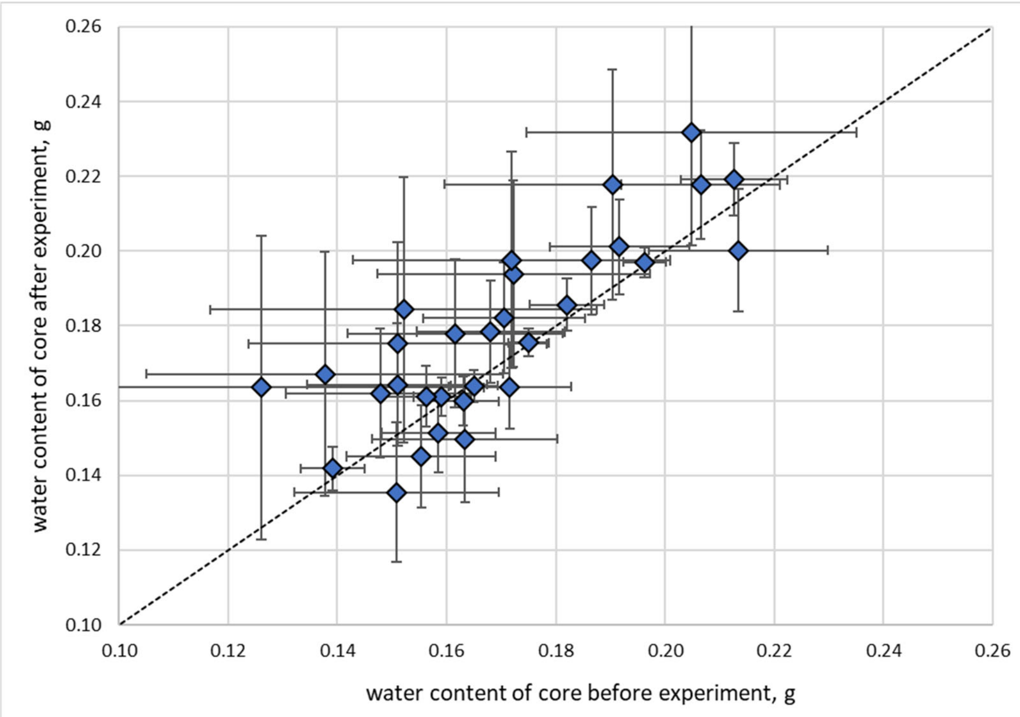


Figure 4-1: Water content calculated from the wet mass (dry surface) before and after the out-diffusion experiments of core sections from IG_BH04; the error of the water content is determined by Gaussian error propagation (Appendix III)

Water contents determined by isotope diffusive exchange

Gravimetric water contents were determined on crushed core pieces used for the isotope diffusive exchange experiments. The masses of the used rock material were measured before and after the experiments. During the experiments the rocks remain saturated. A weight change of the rocks above the analytical uncertainty of ± 0.05 g at constant total weight was observed in 22 experiments (Table 4-4). Therefore, the gravimetric water contents were corrected for the weight loss or gain.

The gravimetric water contents determined on rock pieces used for isotope diffusive exchange experiments ($WC_{IsoEx,grav,corr.}$) vary between 0.09 wt.% and 0.23 wt.% with weighted $WCI_{soEx,grav}$ values ranging from 0.09 ± 0.01 wt.% to 0.23 ± 0.01 wt.% (Table 4-4).

The water contents determined by the isotope diffusive exchange technique ($WC_{IsoEx,average}$) for core samples from borehole IG_BH04 vary between 0.11 ± 0.01 wt.% and 0.27 ± 0.01 wt.% (Table 4-5).

During the isotope diffusive exchange experiment water uptake of 0.004 to 0.1 g was observed for 39 individual experiments. For 23 individual experiments the rock mass was 0.001 to 0.05 g lower after the experiment.

Hence, the gravimetric water content of crushed rock samples used for isotope diffusive exchange experiments were corrected by calculating the mass difference ($\Delta m_{(rock,wet)} = m_{(rock,wet)}$ after experiment – $m_{(rock,wet)}$ before experiment) of the crushed rock sample in the container. The porewater mass was then corrected by this mass difference and the gravimetric water contents were calculated using the corrected porewater mass values.

The water contents determined by the isotope diffusive exchange technique are slightly higher compared to gravimetric values determined on the same core pieces ((Table 4-4 and Table 4-5, Figure 4-2). For the samples IG_BH04_PW004, PW027, PW028, PW031, PW044, PW044 and PW073 the water contents determined by isotope diffusive exchange are >0.05 wt% higher than those determined gravimetrically (Table 4-4). Based on the experimental quality check, it was decided to classify these values as reliable.

It is known from many sites, that generally the water contents determined by the isotope diffusive exchange (WCIsoEx) technique are slightly higher than those determined gravimetrically ($WC_{IsoEx, grav}$) (e.g. Eichinger et al., 2010, 2018, Eichinger, 2021). This can be observed in argillaceous and crystalline rocks and is explained by the isotopic exchange of the test water with interlayer and bound water, which is generally more pronounced in argillaceous rocks and altered crystalline rocks (e.g. Pearson et al., 2003; Gimmi et al., 2022).

For the further use of the values, it is recommended to take the weighted gravimetric water contents (Table 4-6).

Table 4-4: Gravimetric water contents determined on core samples from IG_BH04 used for isotope diffusive exchange experiments ($WC_{IsoEx, grav}$); Water contents are corrected for weight changes during experiments (b.e. = before experiment, a.e. = after experiment); the gravimetric water contents determined on the rock pieces used in the experiments with LAB – and ICE water are weighted taking their weights into account; the error of the water content is determined by Gaussian error propagation (Appendix C)

Sample		LAB				ICE				
	Depth	mass	Δm_{rock} (a.e.-b.e.)	$WC_{IsoEx, grav}$	$WC_{IsoEx, grav, corr.}$	mass	Δm_{rock} (a.e.-b.e.)	$WC_{IsoEx, grav}$	$WC_{IsoEx, grav, corr}$	$WC_{IsoEx, grav}$ weighted
	mbgs	G	g	wt.%	wt.%	g	wt.%	wt.%	wt.%	wt.%
IG_BH04_PW001	162.5	480.421	-0.039	0.14	0.15	447.775	-0.003	0,14	0.14	0.15
IG_BH04_PW004	167.4	354.568	0.010	0.16	0.15	356.172	-0.001	0.16	0.16	0.16
IG_BH04_PW007	213.2	355.325	0.004	0.15	0.15	353.962	0.018	0.15	0.14	0.15
IG_BH04_PW010	236.4	433.805	-0.014	0.16	0.17	443.399	-0.019	0.16	0.17	0.17
IG_BH04_PW014	267.7	458.337	0.067	0.14	0.12	451.422	0.006	0.14	0.14	0.13
IG_BH04_PW016	293.4	463.643	0.051	0.16	0.15	427.197	0.047	0.16	0.15	0.15
IG_BH04_PW019	317.4	419.477	0.049	0.23	0.22	418.919	0.041	0.25	0.24	0.23
IG_BH04_PW022	347.4	432.376	0.041	0.14	0.13	446.050	0.054	0.14	0.13	0.13
IG_BH04_PW027	372.2	370.247	0.091	0.13	0.10	369.738	0.071	0.13	0.11	0.11
IG_BH04_PW028	397.8	442.266	-0.073	0.12	0.14	444.937	-0.063	0.12	0.13	0.13
IG_BH04_PW031	423.6	404.912	-0.067	0.12	0.14	402.226	-0.065	0.13	0.15	0.14
IG_BH04_PW034	450.9	407.364	-0.092	0.11	0.13	407.631	-0.096	0.11	0.13	0.13
IG_BH04_PW037	478.1	457.166	0.013	0.13	0.13	454.878	-0.051	0.14	0.16	0.14
IG_BH04_PW040	505.1	385.414	-0.074	0.11	0.13	382.827	-0.111	0.11	0.14	0.14
IG_BH04_PW044	531.9	381.933	-0.113	0.11	0.14	380.475	-0.101	0.12	0.15	0.14
IG_BH04_PW046	561.3	405.708	-0.083	0.11	0.13	407.853	-0.057	0.11	0.13	0.13
IG_BH04_PW049	586.2	356.872	-0.002	0.17	0.17	360.591	0.012	0.17	0.17	0.17
IG_BH04_PW052	614.4	422.374	-0.126	0.11	0.14	420.453	-0.100	0.12	0.14	0.14
IG_BH04_PW055	636.8	462.890	0.087	0.15	0.13	463.396	0.081	0.15	0.13	0.13
IG_BH04_PW058	665.4	407.533	0.046	0.12	0.11	406.741	0.063	0.12	0.11	0.11
IG_BH04_PW061	692.4	427.295	0.087	0.14	0.12	428.019	0.093	0.15	0.13	0.13
IG_BH04_PW064	711.3	459.403	0.055	0.11	0.10	454.553	0.046	0.11	0.10	0.10
IG_BH04_PW067	746.3	461.837	0.096	0.12	0.10	458.478	0.095	0.11	0.09	0.09
IG_BH04_PW070	771.6	409.132	0.092	0.14	0.12	411.179	0.092	0.13	0.11	0.11
IG_BH04_PW073	795.3	330.811	0.048	0.19	0.18	332.431	0.064	0.18	0.16	0.17
IG_BH04_PW076	825.3	380.171	0.026	0.16	0.16	380.923	0.045	0.16	0.15	0.15
IG_BH04_PW079	849.3	310.307	0.059	0.16	0.15	309.940	0.068	0.17	0.15	0.15
IG_BH04_PW082	877.8	427.214	-0.018	0.15	0.15	426.714	-0.042	0.14	0.15	0.15
IG_BH04_PW085	904.0	499.719	0.053	0.13	0.12	498.045	0.061	0.12	0.11	0.11

Sample		LAB				ICE				
	Depth	mass	Δm_{rock} (a.e.-b.e.)	$WC_{IsoEx, grav}$	$WC_{IsoEx, grav, corr.}$	mass	Δm_{rock} (a.e.-b.e.)	$WC_{IsoEx, grav}$	$WC_{IsoEx, grav, corr}$	$WC_{IsoEx, grav}$ weighted
	mbgs	G	g	wt.%	wt.%	g	wt.%	wt.%	wt.%	wt.%
IG_BH04_PW088	931.1	482.253	0.123	0.15	0.12	482.362	0.084	0.16	0.14	0.13
IG_BH04_PW092	959.0	479.874	0.083	0.13	0.11	481.792	0.071	0.13	0.11	0.02

Note(s)
41 [mbgs (downhole)]

Table 4-5: Water contents of core samples from IG_BH04 calculated by isotope diffusive exchange method (eq. 7); the error of the water content is determined by Gaussian error propagation (Appendix C)

Sample	WC_{IsoEx} ($\delta^{18}O$)	WC_{IsoEx} ($\delta^{2}H$)	WC_{IsoEx} average
	wt.%	wt.%	wt.%
IG_BH04_PW001	0.16±0.01	0.17±0.01	0.16±0.01
IG_BH04_PW004	0.21±0.01	0.22±0.02	0.22±0.01
IG_BH04_PW007	0.15±0.01	0.17±0.01	0.16±0.01
IG_BH04_PW010	0.19±0.01	0.19±0.01	0.19±0.01
IG_BH04_PW014	0.15±0.01	0.15±0.01	0.15±0.01
IG_BH04_PW016	0.17±0.01	0.17±0.01	0.17±0.01
IG_BH04_PW019	0.27±0.01	0.27±0.02	0.27±0.01
IG_BH04_PW022	0.15±0.01	0.15±0.01	0.15±0.01
IG_BH04_PW027	0.20±0.01	0.18±0.01	0.19±0.01
IG_BH04_PW028	0.17±0.01	0.17±0.01	0.17±0.01
IG_BH04_PW031	0.19±0.01	0.19±0.01	0.19±0.01
IG_BH04_PW034	0.14±0.01	0.14±0.01	0.14±0.01
IG_BH04_PW037	0.17±0.01	0.16±0.01	0.16±0.01
IG_BH04_PW040	0.18±0.01	0.17±0.01	0.17±0.01
IG_BH04_PW044	0.19±0.02	0.20±0.01	0.19±0.01
IG_BH04_PW046	0.19±0.01	0.19±0.01	0.19±0.01
IG_BH04_PW049	0.19±0.01	0.20±0.01	0.19±0.01
IG_BH04_PW052	0.15±0.01	0.15±0.01	0.15±0.01
IG_BH04_PW055	0.17±0.01	0.17±0.01	0.17±0.01
IG_BH04_PW058	0.12±0.02	0.12±0.01	0.12±0.01
IG_BH04_PW061	0.14±0.01	0.13±0.01	0.13±0.01
IG_BH04_PW064	0.13±0.01	0.12±0.01	0.13±0.01
IG_BH04_PW067	0.11±0.01	0.11±0.01	0.11±0.01
IG_BH04_PW070	0.13±0.01	0.12±0.01	0.12±0.01
IG_BH04_PW073	0.26±0.02	0.26±0.02	0.26±0.01
IG_BH04_PW076	0.17±0.01	0.17±0.01	0.17±0.01
IG_BH04_PW079	0.17±0.01	0.17±0.02	0.17±0.02
IG_BH04_PW082	0.17±0.01	0.17±0.01	0.17±0.01
IG_BH04_PW085	0.14±0.01	0.13±0.01	0.14±0.01
IG_BH04_PW088	0.18±0.01	0.17±0.01	0.17±0.01
IG_BH04_PW092	0.14±0.01	0.13±0.01	0.14±0.01

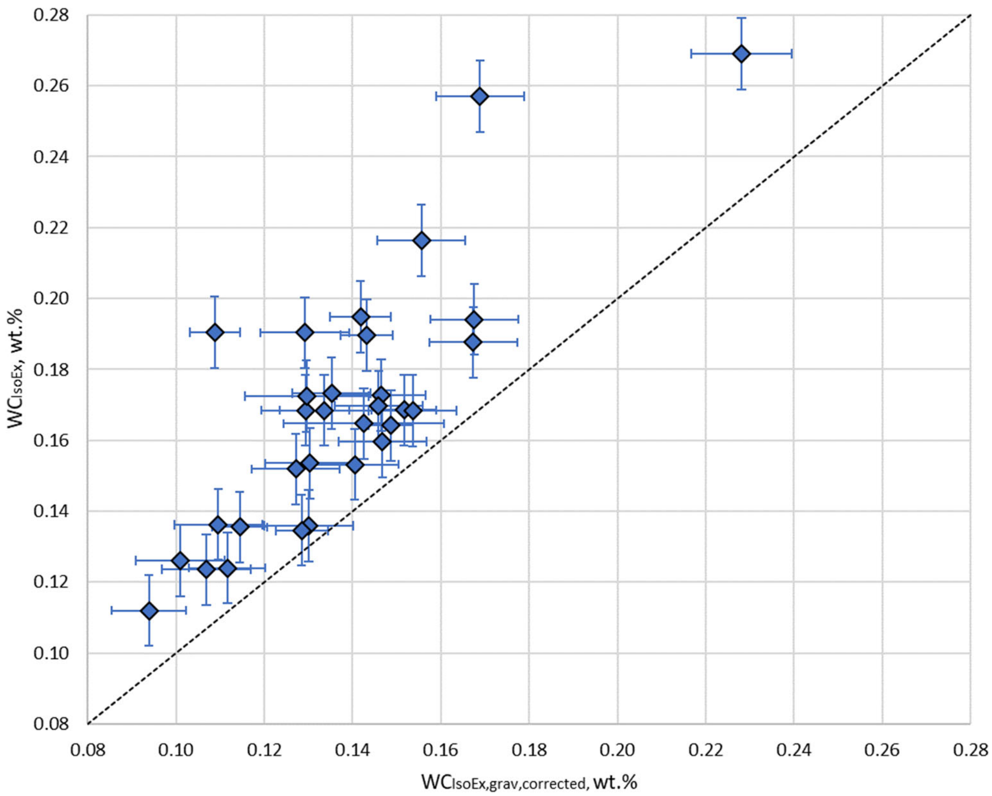


Figure 4-2: Comparison of water contents determined by isotope diffusive exchange (WC_{IsoEx}) and gravimetrically ($WC_{IsoEx,\ grav,\ corr.}$ by wet weight, corrected for weight change during experiments) on the same core pieces; the error of the water content is determined by Gaussian error propagation (Appendix III)

Summary and depth profiles of water content results

The gravimetric water contents determined on different portions of the core pieces for the AQ and the PW investigations are weighted using the masses of the individual rock pieces (see Table 4-6). The weighted water contents represent the entire cores, with masses between 570 g and 867 g for AQ cores and between 2,447 g and 3,093 g for PW cores. As shown in the previous paragraphs, the water contents of the individual aliquots can vary significantly, and is inferred to be caused by mineralogical heterogeneities. This indicates that water content values cannot be extrapolated.

The weighted gravimetric water contents of the AQ- and PW-core samples taken between 162.5 mbgs and 959.3 mbgs vary between 0.11±0.01 wt.% and 0.23 ±0.04 wt.% (Table 4-6, Figure 4-4).

Table 4-6: Weighted gravimetric water contents of aqueous extraction and porewater core samples taken from borehole IG_BH04 and their corresponding total masses; the uncertainties of the water content values are the weighted standard deviations of the individual aliquots showing the density of water contents in one entire sample

Sample	Depth	$m_{rock\ tot}$	WC_{grav} weighted (wet)	WC_{grav} weighted (dry)
	mbgs*	g	wt.%	wt.%
Aqueous Extraction cores (AQ)				
IG_BH04_PW003	163.7	715.4	0.18±0.02	0.18±0.02
IG_BH04_PW006	168.1	629.7	0.17±0.01	0.17±0.01
IG_BH04_PW009	213.9	691.1	0.20±0.02	0.20±0.02
IG_BH04_PW011	238.0	760.8	0.17±0.01	0.17±0.01
IG_BH04_PW015	268.0	780.9	0.16±0.01	0.16±0.01
IG_BH04_PW018	294.5	669.6	0.18±0.02	0.18±0.02
IG_BH04_PW021	318.1	637.2	0.19±0.01	0.19±0.01
IG_BH04_PW024	348.2	917.6	0.11±0.01	0.11±0.01
IG_BH04_PW026	372.0	602.0	0.14±0.01	0.14±0.01
IG_BH04_PW030	397.1	866.6	0.17±0.01	0.17±0.01
IG_BH04_PW033	424.2	738.6	0.17±0.02	0.17±0.02
IG_BH04_PW036	451.5	592.9	0.15±0.01	0.15±0.01
IG_BH04_PW039	478.8	687.1	0.14±0.01	0.14±0.01
IG_BH04_PW042	505.7	791.8	0.17±0.02	0.17±0.02
IG_BH04_PW045	532.5	634.8	0.16±0.02	0.16±0.02
IG_BH04_PW048	561.9	576.7	0.16±0.02	0.16±0.02
IG_BH04_PW051	585.9	634.4	0.23±0.04	0.23±0.04
IG_BH04_PW054	615.4	801.5	0.17±0.01	0.17±0.01
IG_BH04_PW057	637.5	747.4	0.15±0.01	0.15±0.01
IG_BH04_PW060	666.1	650.9	0.13±0.01	0.13±0.01
IG_BH04_PW063	693.1	792.6	0.11±0.01	0.11±0.01
IG_BH04_PW066	712.1	859.4	0.14±0.01	0.14±0.01
IG_BH04_PW069	747.0	710.1	0.14±0.03	0.14±0.03
IG_BH04_PW072	772.3	707.0	0.12±0.01	0.12±0.01
IG_BH04_PW075	796.0	611.7	0.21±0.03	0.21±0.03

Sample	Depth	$m_{rock\ tot}$	WC_{grav} weighted (wet)	WC_{grav} weighted (dry)
	mbgs*	g	wt.%	wt.%
Porewater cores (PW)				
IG_BH04_PW001	162.5	3092.5	0.17±0.02	0.17±0.02
IG_BH04_PW004	167.4	2614.1	0.17±0.01	0.17±0.01
IG_BH04_PW007	213.2	2680.4	0.17±0.02	0.17±0.02
IG_BH04_PW010	236.4	2967.6	0.19±0.02	0.19±0.02
IG_BH04_PW014	267.7	2892.9	0.15±0.02	0.15±0.02
IG_BH04_PW016	293.4	2898.4	0.17±0.04	0.18±0.04
IG_BH04_PW019	317.4	2781.0	0.20±0.02	0.20±0.02
IG_BH04_PW022	347.4	2885.6	0.15±0.02	0.15±0.02
IG_BH04_PW027	372.2	2660.6	0.15±0.03	0.15±0.03
IG_BH04_PW028	397.8	2749.7	0.15±0.02	0.15±0.02
IG_BH04_PW031	423.6	2741.9	0.17±0.02	0.17±0.03
IG_BH04_PW034	450.9	2702.2	0.15±0.03	0.15±0.03
IG_BH04_PW037	478.1	2754.1	0.14±0.01	0.14±0.01
IG_BH04_PW040	505.1	2675.9	0.16±0.02	0.16±0.02
IG_BH04_PW044	531.9	2632.4	0.16±0.04	0.16±0.04
IG_BH04_PW046	561.3	2689.8	0.15±0.02	0.15±0.02
IG_BH04_PW049	586.2	2657.8	0.20±0.02	0.20±0.02
IG_BH04_PW052	614.4	2825.7	0.17±0.03	0.17±0.03
IG_BH04_PW055	636.8	2825.1	0.15±0.02	0.15±0.02
IG_BH04_PW058	665.4	2769.9	0.15±0.03	0.15±0.03
IG_BH04_PW061	692.4	2789.5	0.14±0.01	0.14±0.01
IG_BH04_PW064	711.3	2880.9	0.13±0.02	0.13±0.02
IG_BH04_PW067	746.3	2908.3	0.12±0.02	0.12±0.02
IG_BH04_PW070	771.6	2787.3	0.14±0.02	0.14±0.02
IG_BH04_PW073	795.3	2523.4	0.20±0.02	0.20±0.02

Sample	Depth	$m_{rock\ tot}$	WC_{grav} weighted (wet)	WC_{grav} weighted (dry)
	mbgs*	g	wt.%	wt.%
IG_BH04_PW078	825.9	569.9	0.20±0.01	0.20±0.01
IG_BH04_PW081	850.1	637.6	0.18±0.01	0.18±0.01
IG_BH04_PW084	878.4	707.8	0.20±0.03	0.20±0.03
IG_BH04_PW087	904.7	682.3	0.13±0.02	0.13±0.02
IG_BH04_PW090	932.1	791.2	0.14±0.02	0.14±0.02
IG_BH04_PW093	959.3	770.8	0.19±0.01	0.19±0.01

Sample	Depth	$m_{rock\ tot}$	WC_{grav} weighted (wet)	WC_{grav} weighted (dry)
	mbgs*	g	wt.%	wt.%
IG_BH04_PW076	825.3	2565.9	0.19±0.03	0.19±0.03
IG_BH04_PW079	849.3	2446.9	0.18±0.02	0.18±0.02
IG_BH04_PW082	877.8	2701.3	0.20±0.05	0.20±0.05
IG_BH04_PW085	904.0	2964.3	0.15±0.03	0.15±0.03
IG_BH04_PW088	931.1	2828.4	0.17±0.03	0.17±0.03
IG_BH04_PW092	959.0	3006.7	0.14±0.03	0.14±0.03

Note(s)
[mbgs (downhole)]

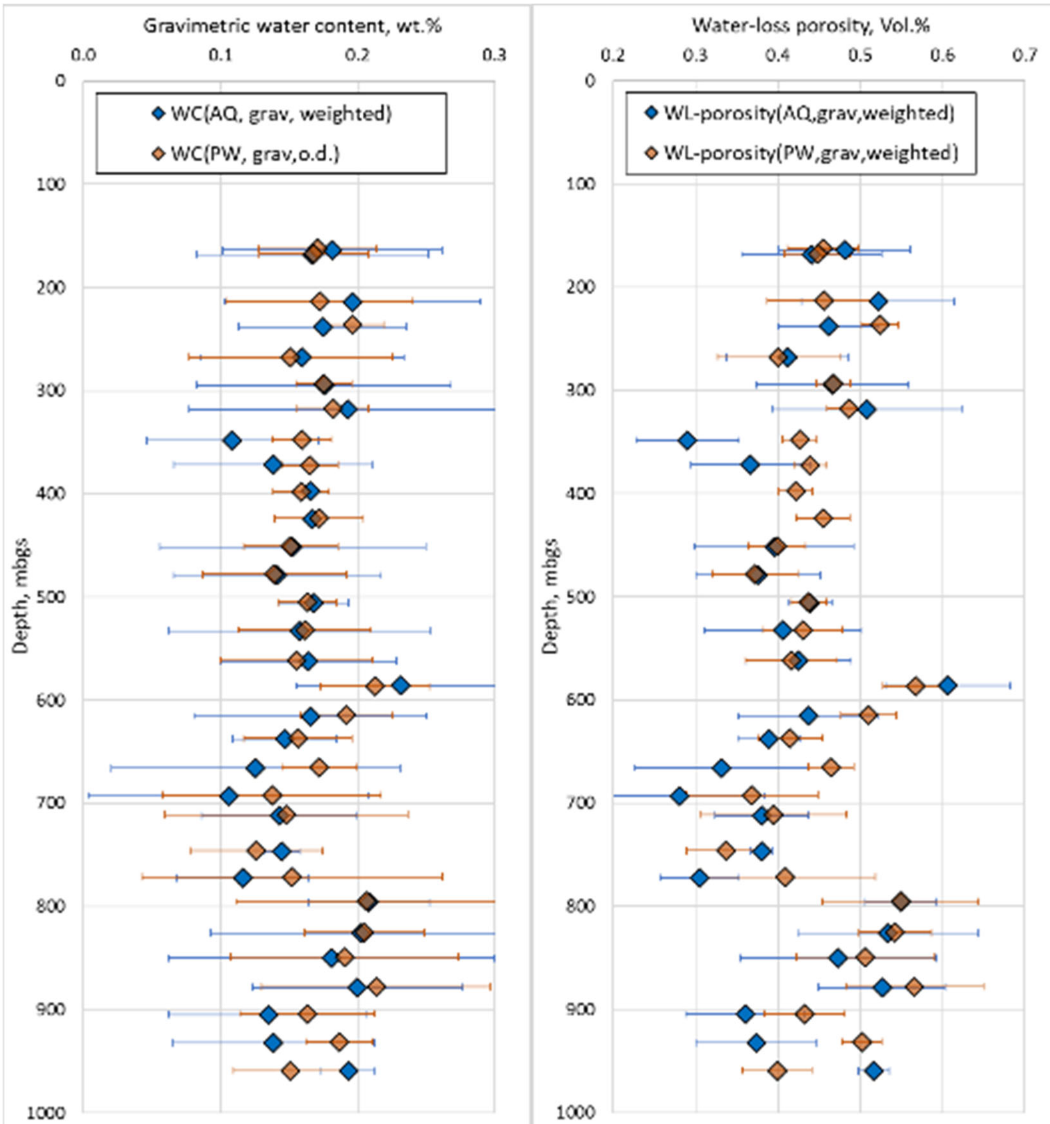


Figure 4 4: Water content and water-loss porosity of core samples from IG_BH04

5.0 CHEMICAL COMPOSITION OF EXPERIMENT SOLUTIONS OF AQUEOUS EXTRACTION AND OUT-DIFFUSION EXPERIMENTS

Out-diffusion and aqueous extraction experiments were performed on 31 core samples taken from borehole IG_BH04.

5.1 Chemical Composition of Aqueous Extraction Solutions

The purpose of aqueous extraction experiments is to obtain an initial estimate of the porewater salinity, which is necessary for the adjustment of the ion concentration in the test waters for the indirect porewater extraction methods.

Crushing and grinding of the rock material additionally liberates fluid trapped in mineral fluid inclusions. During leaching, all salts will become dissolved in addition to the limited dissolution of the original mineral assemblage. The mineralization of a leach solution is therefore the sum of: (i) the constituents originally dissolved in the porewater, (ii) the constituents present in fluid inclusions, and (iii) water-rock interactions during the leaching process. Aqueous leach solutions represent a complex composition in rocks with abundant fluid inclusions and/or rapidly reacting mineral phases.

The aqueous extraction solutions produced by the immersion of crushed cores from borehole IG_BH04 in deionized water (procedure in Section 3.3.1) have pH values between 9.1 and 9.9, and a mineralization between 54 and 108 mg/l (specific electrical conductivity = 90 – 171 µS/cm, Table 5-1). The dissolved constituents consist predominately of Na^+, K^+, Ca^{2+}, HCO_3^-, Cl^-, SO_4^{2-} and Si in different concentrations and proportions (Table 5-1, Figure 5-1). Minor concentrations of Mg^{2+} (not all samples), F^- and Br^- could be detected. Concentrations of Sr were very low (0.01-0.11 mg/l) or below detection limit (Table 5-1). Silica and aluminium could be detected in concentrations between 4.2 and 8.7 mg/l (Si) and between 0.47 and 4.8 mg/l (Al).

The DOC (dissolved organic carbon) was detected in concentrations between 1.8 and 10.9 mg/l.

Table 5-1: Analytical results of the aqueous extraction solutions of crushed core samples from borehole IG_BH04; Test solution types are classified after Jäckli et al. 1971

Sample		IG_BH04_PW003	IG_BH04_PW006	IG_BH04_PW009	IG_BH04_PW011	IG_BH04_PW015	IG_BH04_PW018	IG_BH04_PW021	IG_BH04_PW024	IG_BH04_PW026	IG_BH04_PW030	IG_BH04_PW033
Interval	mbgs	163.7	168.1	213.9	238.0	268.0	294.5	318.1	348.2	372.0	397.1	424.2
MISCELLANEOUS PROPERTIES												
pH (lab)	-log(H+)	9.7	9.7	9.9	9.9	9.8	9.9	9.9	9.8	9.1	9.4	9.2
Electr. Conductivity	µS/cm	102	122	145	144	97	119	121	127	123	107	90
Sample Temperature	°C	20	20	20	20	20	20	20	20	20	20	20
Alkalinity (pH 4,3) Lab.	mmol/l	0.72	0.98	1.02	1.00	0.82	1.06	1.04	1.04	0.69	0.46	0.42
Alkalinity (pH 8,2) Lab.	mmol/l	< 0.5	0.76	0.94	0.84	0.54	0.54	0.54	0.62	< 0.5	< 0.5	< 0.5
DOC	mg/l	2.0	2.6	2.8	2.7	2.1	2.0	1.9	1.8	3.6	3.2	2.1
DISSOLVED CONSTITUENTS												
CATIONS												
Sodium (Na+)	mg/l	18	26	27	29	19	26	25	21	17	13	12
Potassium (K+)	mg/l	5.0	3.7	7.5	5.5	4.2	2.9	3.2	8.9	7.5	6.8	5.1
Magnesium (Mg+2)	mg/l	< 0,2	0.25	0.27	0.25	< 0,2	0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2
Calcium (Ca+2)	mg/l	2.3	2.3	1.8	1.9	1.9	1.6	1.7	2.7	3.2	1.6	2.0
Strontium (Sr+2)	mg/l	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	0.04	< 0.1	< 0.1
Silicon (Si+4)	mg/l	6.9	7.9	8.7	8.3	7.7	8.1	8.5	6.9	6.7	7.7	6.2
Aluminium (Al+3)	mg/l	1.36	1.52	2.00	2.20	1.50	1.60	1.20	1.40	1.40	1.10	1.00
ANIONS												
Fluoride (F-)	mg/l	0.26	0.45	0.41	0.48	0.37	0.40	0.33	0.26	0.12	0.29	0.23
Chloride (Cl-)	mg/l	8.7	12	16	15	7.1	7.1	7.7	6.8	11.8	8.5	8.6
Bromide (Br-)	mg/l	1.00	0.72	0.34	3.5	0.85	0.42	0.21	0.10	0.31	0.73	0.15
Sulfate (SO4-2)	mg/l	0.6	1.1	1.1	1.3	0.73	0.88	0.63	0.84	1.6	0.85	0.61
Nitrate (NO3-)	mg/l	0.2	< 0.2	< 0.2	0.2	< 0.2	< 0.2	< 0.2	< 0.2	<0.2	0.3	< 0.2
Total Alkalinity as HCO3	mg/l	43.9	59.8	62.2	61.0	50.0	64.7	63.5	63.5	41.9	28.3	25.4
PARAMETERS CALCULATED FROM ANALYTICAL DATA												
Sum of Analysed Constituents	mg/l	80	106	117	118	84	104	102	104	83	60	54
Water type		Na-(K)-(Ca)-HCO3-Cl	Na-HCO3-Cl	Na-(K)-HCO3-Cl	Na-HCO3-Cl	Na-(K)-HCO3-(Cl)	Na-HCO3-(Cl)	Na-HCO3-(Cl)	Na-(K)-(Ca)-HCO3-(Cl)	Na-(K)-(Ca)-HCO3-Cl	Na-K-HCO3-Cl	Na-(K)-(Ca)-HCO3-Cl

Sample		IG_BH04_PW036	IG_BH04_PW039	IG_BH04_PW042	IG_BH04_PW045	IG_BH04_PW048	IG_BH04_PW051	IG_BH04_PW054	IG_BH04_PW057	IG_BH04_PW060	IG_BH04_PW063
Interval	mbgs	451.5	478.8	505.7	532.5	561.9	585.9	615.4	637.5	666.1	693.1
MISCELLANEOUS PROPERTIES											
pH (lab)	-log(H+)	9.4	9.3	9.4	9.2	9.2	9.2	9.1	9.4	9.3	9.3
Electr. Conductivity	µS/cm	111	112	104	131	117	138	118	110	111	118
Sample Temperature	°C	20	20	20	20	20	20	20	20	20	20
Alkalinity (pH 4,3) Lab.	mmol/l	0.55	0.5	0.45	0.53	0.43	0.30	0.39	0.37	0.31	0.30
Alkalinity (pH 8,2) Lab.	mmol/l	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
DOC	mg/l	2.0	1.8	2.1	2.0	2.2	2.7	3.6	3.9	3.7	3.2
DISSOLVED CONSTITUENTS											
CATIONS											
Sodium (Na+)	mg/l	14	13	12	16	15	15	12	12	9.6	11
Potassium (K+)	mg/l	8.4	6.0	8.3	11	9.2	7.1	9.5	9.1	15	14
Magnesium (Mg+2)	mg/l	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	0.22	< 0.2	0.29	0.20
Calcium (Ca+2)	mg/l	1.9	2.7	1.6	2.6	2.8	5.6	3.9	3.5	1.7	1.9
Strontium (Sr+2)	mg/l	< 0.1	< 0.1	< 0.1	< 0.1	< 0.1	0.11	0.06	0.07	0.03	0.03
Silicon (Si+4)	mg/l	7.5	7.8	7.5	7.6	6.5	8.1	6.3	8.0	6.4	5.6
Aluminium (Al+3)	mg/l	1.7	0.54	1.8	1.6	0.76	0.47	1.8	4.8	4.4	4.2
ANIONS											
Fluoride (F-)	mg/l	0.21	0.16	0.11	0.19	0.23	0.22	0.17	0.28	0.22	0.20
Chloride (Cl-)	mg/l	11	11	9.1	18	17	10	9.7	5.2	11	14
Bromide (Br-)	mg/l	0.71	0.85	0.23	2.6	0.87	0.93	1.3	0.26	0.4	2.0
Sulfate (SO4-2)	mg/l	0.58	< 0.5	< 0.5	0.53	1.2	19	8.9	7.7	3.2	2.3
Nitrate (NO3-)	mg/l	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2
Total Alkalinity as HCO3	mg/l	33.4	30.3	27.6	32.3	26.4	18.0	23.5	22.5	19.2	18.3
PARAMETERS CALCULATED FROM ANALYTICAL DATA											
Sum of Analysed Constituents	mg/l	70	64	59	83	73	76	70	61	60	64
Water type		Na-K-(Ca)-HCO3-Cl	Na-(K)-(Ca)-HCO3-Cl	Na-K-HCO3-Cl	Na-K-(Ca)-HCO3-Cl	Na-K-(Ca)-HCO3-Cl	Na-Ca-(K)-SO4-HCO3-Cl	Na-K-(Ca)-HCO3-Cl-SO4	Na-K-(Ca)-HCO3-SO4-Cl	Na-K-HCO3-Cl-SO4	Na-K-(Ca)-Cl-HCO3

Sample		IG_BH04_PW066	IG_BH04_PW069	IG_BH04_PW072	IG_BH04_PW075	IG_BH04_PW078	IG_BH04_PW081	IG_BH04_PW084	IG_BH04_PW087	IG_BH04_PW090	IG_BH04_PW093
Interval	mbgs	712.1	747.0	772.3	796.0	825.9	850.1	878.4	904.7	932.1	959.3
MISCELLANEOUS PROPERTIES											
pH (lab)	-log(H+)	9.2	9.1	9.3	9.2	9.2	9.2	9.1	9.5	9.3	9.3
Electr. Conductivity	µS/cm	138	171	117	125	140	170	165	125	168	124
Sample Temperature	ºC	20	20	20	20	20	20	20	20	20	20
Alkalinity (pH 4,3) Lab.	mmol/l	0.60	0.60	0.83	0.48	0.56	0.31	0.31	0.36	0.82	0.35
Alkalinity (pH 8,2) Lab.	mmol/l	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5	< 0.5
DOC	mg/l	7.1	11	8.0	8.1	11	1.9	1.8	2.3	9.8	4.2
DISSOLVED CONSTITUENTS											
CATIONS											
Sodium (Na+)	mg/l	14	19	12	11	12	14	13	12	18	14
Potassium (K+)	mg/l	14	15	12	12	15	18	16	14	20	9.5
Magnesium (Mg+2)	mg/l	0.29	0.42	0.25	0.27	0.45	0.4	0.46	< 0.2	< 0.2	0.26
Calcium (Ca+2)	mg/l	3.8	3.1	4.9	4.2	5.3	3.6	5.0	1.3	1.7	2.7
Strontium (Sr+2)	mg/l	0.03	0.03	0.03	0.03	0.03	0.03	0.04	0.01	0.04	0.03
Silicon (Si+4)	mg/l	5.4	4.2	6.0	7.4	6.4	5.7	4.9	6.5	5.4	4.5
Aluminium (Al+3)	mg/l	2.1	2.5	2.6	2.5	1.4	1.0	0.87	1.7	2.1	1.4
ANIONS											
Fluoride (F-)	mg/l	0.20	0.40	0.31	0.25	0.34	0.40	0.32	0.22	0.44	0.30
Chloride (Cl-)	mg/l	17	26	8.0	18	21	32	30	19	16	18
Bromide (Br-)	mg/l	1.7	2.5	0.37	1.4	0.92	1.3	3.4	0.80	0.42	0.55
Sulfate (SO4-2)	mg/l	1.8	2.1	1.5	1.1	1.4	1.3	1.5	1.4	2.0	4.5
Nitrate (NO3-)	mg/l	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2
Total Alkalinity as HCO3	mg/l	36.8	36.8	50.5	29.2	33.9	19.0	19.2	21.7	49.7	21.5
PARAMETERS CALCULATED FROM ANALYTICAL DATA											
Sum of Analysed Constituents	mg/l	90	105	90	77	90	90	89	70	108	71
Water type		Na-K-(Ca)-HCO3-Cl	Na-K-(Ca)-Cl-HCO3	Na-K-(Ca)-HCO3-Cl	Na-K-Ca-Cl-HCO3	Na-K-Ca-Cl-HCO3	Na-K-(Ca)-Cl-HCO3	Na-K-(Ca)-Cl-HCO3	Na-K-Cl-HCO3	Na-K-HCO3-Cl	Na-K-(Ca)-Cl-HCO3

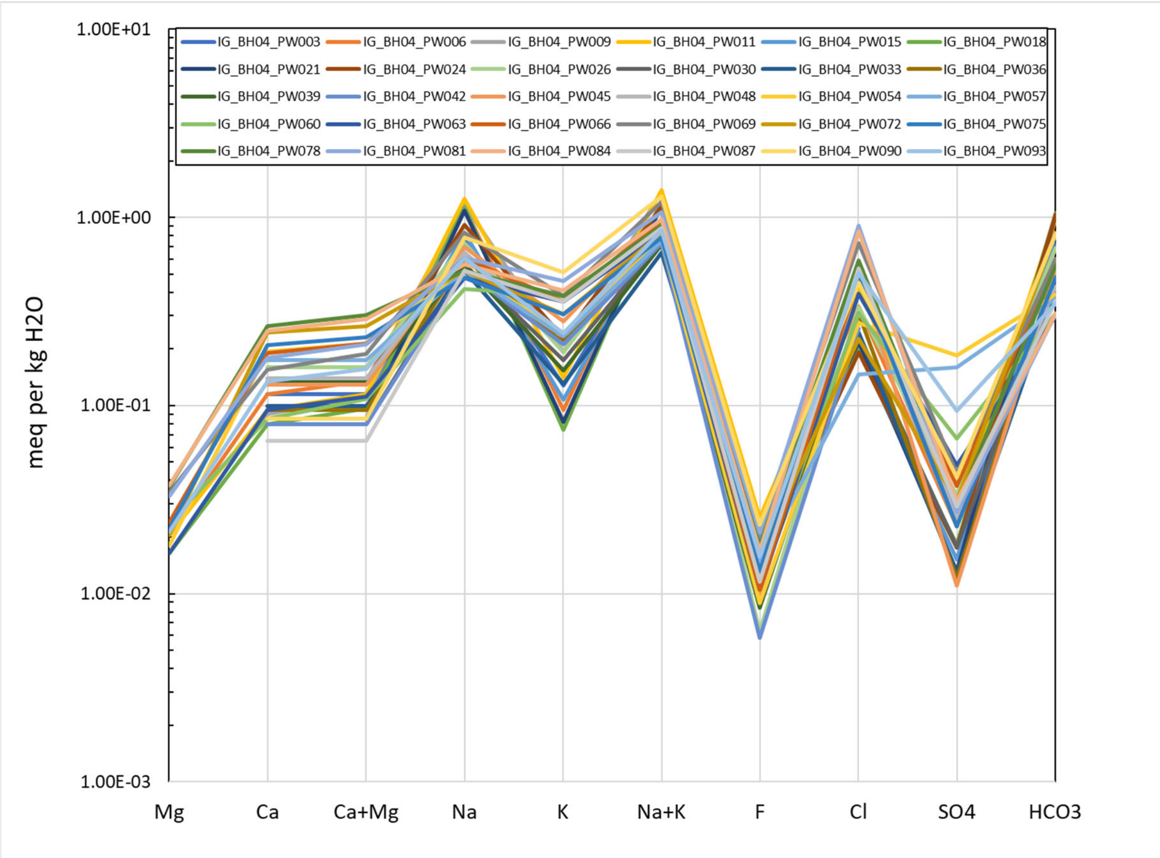


Figure 5 1: Schoeller diagram of experiment solutions from aqueous extraction experiments conducted with core samples from borehole IG_BH04

5.2 Chemical Composition of Out-diffusion Experiment Solutions

Out-diffusion experiments were performed on 31 core samples from borehole IG_BH04 to derive the porewater chloride and bromide concentrations, porewater □^{37}Cl isotopic ratios, and chemical composition of the test solutions - which are the basis for the hydrogeochemical modelling of porewater chemical compositions. The core sections varied in diameter between 60.2 mm and 61.3 mm, with lengths between 195 mm and 204 mm. The corresponding volume of the sections varied between 561 cm^3 and 589 cm^3 and the saturated mass was between 1,500 g and 1,569 g. In the out-diffusion experiments, the mass ratio of experiment solution to rock samples was between 0.077 and 0.103 (Table 5-2).

During the out-diffusion experiments, a continuous exchange between porewater and test water takes place until equilibrium conditions with respect to conservative, non-reactive compounds are achieved. The experiments use intact large-sized core pieces and so, there is no release and/or influence of fluids from within fluid inclusions. The exchange appears to occur mainly by diffusion (Section 6). For chemically conservative elements, such as chloride and bromide, for which the porewater is the only source, the porewater concentration can be calculated using the gravimetrically determined porewater mass of the rock sample. For reactive elements and compounds, such as Ca^{2+}, Mg^{2+}, Na^{+}, K^{+}, Sr^{2+}, Si, Al, SO_4^{2-} and HCO_3^{-}, the contribution of mineral dissolution reactions during the experiment has to be taken into account. Those reactions are evaluated by the determination of the concentrations of the non-conservative elements taken in time-series (Section 6.1).

In parallel to the out-diffusion experiments conducted for core samples from IG_BH04, a blank set-up containing only test water, which was sampled at the same frequency as the normal experiments and finished after 141 days, was conducted. After the experimental period, the “Blank” water, with a pH of 5.8 and a specific electrical conductivity (EC) of 3 µS/cm, contained 3.1 mg/L dissolved constituents, mainly composed of Ca^{2+}, Na^{+} and HCO_3^- (Table 5-2, Figure 5-2). The “Blank” test solution has a DOC concentration of 1.7 mg/L and a TIC concentration of 0.51 mg/L. The comparison of the TIC concentration analysed directly (0.51 mg/L) and that calculated from the acid capacity determined by titration (0.48 mg/L) shows that the determination of the HCO_3^- concentration by titration is not influenced by organic acids and is reliable. Lithium, magnesium, strontium, aluminium, boron, fluoride, bromide and nitrate are below detection limit.

The pH of the experiment solutions varies between 7.3 and 8.0 with a total mineralization between 111 mg/L and 353 mg/L (EC = 191 – 704 µS/cm, Table 5-2). It should be noted that the total mineralization obtained for the experiment solutions depends on the water content of the sample and the water/rock ratio used in the experiment and does not directly reflect differences in porewater salinity.

The experimental solutions contain Na^{+} (17.8 – 69.6 mg/L), Ca^{2+} (5.6 – 88.8 mg/L), K^{+} (2.2 – 8.4 mg/L), HCO_3^- (25.1 – 232 mg/L), Cl^- (5.2 – 177 mg/L) and SO_4^{2-} (3.1 – 14.2 mg/L) in varying proportions and concentrations (Table 5-2, Figure 5-2).

Based on the out-diffusion test solutions, samples are characterized by Na^{+} and HCO_3^{-} dominated water between 162.5 mbgs and 586.2 mbgs, and transition to a Ca^{2+} and Cl^- dominated water below, as observed clearly in samples from 771.6 mbgs and 904.0 mbgs. The two last samples from 931.1 and 959.0 mbgs tend to a Na^{+} and Cl^- dominated water (Table 5-2, Figure 5-2).

Silicon (expressed as Si) is present in concentrations between 3.2 and 11 mg/L. Lithium, magnesium, strontium, aluminium, boron, fluoride, bromide and nitrate are below detection limit or present in low or trace concentrations (Table 5-2).

The concentrations of dissolved organic carbon (DOC) vary between 3.5 and 17.6 mg/L (Table 5-2).

The DIC/TIC concentrations (DIC = TIC, because analyses are performed on filtered samples) determined by TIC analyser vary between 4.9 and 45.7 mg/L. The comparison of the TIC concentrations determined by direct analyses with those determined by acid titration (AC4.3) shows that the total alkalinity is mainly determined by HCO_3^-.

The strontium $^{87}Sr/^{86}Sr$ isotope ratios of the out-diffusion test solutions vary between 0.722494 and 0.758015, with Sr^{2+} concentrations varying between 0.05 and 1.82 mg/L (Table 5-2).

Table 5-2: Analytical results of the test solutions of out-diffusion experiments using core samples from borehole IG_BH04; Test solution types are classified after Jäckli et al. 1971

Sample		IG_BH03_Blank	IG_BH04_PW001	IG_BH04_PW004	IG_BH04_PW007	IG_BH04_PW010	IG_BH04_PW014	IG_BH04_PW016	IG_BH04_PW019	IG_BH04_PW022	IG_BH04_PW027
Hydroisotop Nr.		338402	345810	345811	345812	345813	345814	345815	345816	345817	351159
Interval	mbgs		162.5	167.4	213.2	236.4	267.7	293.4	317.4	347.4	372.2
Ratio Exp.Water : Rock	g/g		0.084	0.077	0.084	0.078	0.084	0.085	0.079	0.081	0.080
Ratio TW:PW	g/g		49.3	46.1	48.5	39.9	55.3	48.5	43.4	51.1	48.3
MISCELLANEOUS PROPERTIES											
pH (lab)	-log(H+)	5.8	7.5	7.3	7.3	7.4	7.5	7.4	7.6	7.5	7.5
Spec. electr. conductivity	µS/cm	3	245	198	376	276	285	222	405	221	241
Acid Capacity (4.3)	mmol	0.04	1.54	1.33	1.95	1.86	2.1	1.72	3.81	1.99	1.50
Base Capacity (8.2)	mmol	0.152	0.11	0.13	0.18	0.16	0.15	0.13	0.18	0.12	0.09
Sample Temperature	ºC	18.8	24.1	23.5	23.9	23.7	23.4	23.2	23.5	23.6	25.6
DOC	mg/l	1.70	13.2	15.1	13.0	12.8	11.4	13.3	17.6	12.3	7.40
TIC	mg/l	0.5	18.5	16.0	23.4	22.3	25.2	20.6	45.7	23.8	18.0
DISSOLVED CONSTITUENTS											
CATIONS											
Sodium (Na+)	mg/l	0.12	35.3	34.5	60.0	50.9	48.0	43.1	69.6	40.3	35.0
Potassium (K+)	mg/l	< 0.1	4.60	4.00	4.40	3.70	3.60	2.20	5.40	3.70	4.00
Lithium (Li+)	mg/L	< 0.01	0.022	0.012	0.016	0.010	0.025	< 0.01	0.053	< 0.01	0.014
Calcium (Ca+2)	mg/l	0.49	14.0	6.70	14.9	11.6	11.4	5.60	21.9	9.50	12.9
Magnesium (Mg+2)	mg/l	< 0.2	0.32	0.25	< 0.2	< 0.2	0.34	< 0.2	0.27	< 0.2	< 0.2
Strontium (Sr+2)	mg/l	<0.01	0.17	0.11	0.11	0.09	0.13	0.05	0.19	0.07	0.20
Aluminium (Al+3)	mg/l	< 0.01	0.036	0.035	0.019	0.051	0.018	0.118	0.022	0.049	0.032
Silicon (Si+4)	mg/l	< 0.1	7.10	3.20	3.95	3.40	10.7	4.30	9.2	4.0	8.2
Boron (B)	mg/l	< 0.01	0.19	0.21	0.11	0.10	0.20	0.14	0.15	0.14	0.10
ANIONS											
Fluoride (F-)	mg/l	< 0.1	1.40	0.31	0.66	0.53	0.51	0.42	0.34	0.25	0.40
Chloride (Cl-)	mg/l	0.02	17.4	9.70	44.4	18.7	17.8	10.9	12.1	6.50	16.7
Bromide (Br-)	mg/l	< 0.1	2.40	1.40	1.20	3.10	4.10	1.60	0.22	0.12	0.66
Nitrate (NO3-)	mg/l	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2
Sulphate (SO4-2)	mg/l	< 0.2	5.80	6.80	10.1	9.20	7.00	6.30	6.10	4.50	10.6
Total Alkalinity	meq/l	0.04	1.54	1.33	1.95	1.86	2.10	1.72	3.81	1.99	1.50
Total Alkalinity as HCO3	mg/l	2.4	94.15	81.33	118.9	113.5	128.0	104.7	232.4	121.1	91.52
PARAMETERS CALCULATED FROM ANALYTICAL DATA											
Sum of Analysed Constituents	mg/l	3	176	145	255	211	221	175	349	186	172
Difference/Total		-15.51%	2.66%	4.76%	0.10%	4.39%	-0.80%	0.33%	-0.16%	1.01%	1.14%
WATER TYPE		Na-Ca-HCO3	Na-(Ca)-HCO3-Cl	Na-HCO3-(Cl)	Na-(Ca)-HCO3-Cl	Na-(Ca)-HCO3-Cl	Na-(Ca)-HCO3-(Cl)	Na-HCO3-(Cl)	Na-(Ca)-HCO3	Na-(Ca)-HCO3	Na-(Ca)-HCO3-Cl
ION-ION RATIOS											
Br*1000/Cl weight		/	137.9	144.3	27.0	165.8	230.3	146.8	18.2	18.5	39.5
Br*1000/Cl molal	mol/mol	/	61.2	64.0	12.0	73.6	102.2	65.1	8.1	8.2	17.5
Na/Cl molal	mol/mol	3.129	5.485	2.084	4.198	4.159	6.098	8.870	9.561	3.232	4.282
K/Na molal	mol/mol	/	0.077	0.068	0.043	0.043	0.044	0.030	0.046	0.054	0.067
SO4/Cl molal	mol/mol	/	0.123	0.259	0.084	0.182	0.145	0.213	0.186	0.256	0.234
Na/(Cl+SO4)	mol/mol	9.253	2.786	4.357	1.923	3.553	3.631	5.026	7.479	7.615	2.619
ISOTOPE RATIOS											
d37Cl	pm SMOC	Cl too low	0.55	0.49	1.21	0.59	1.06	0.64	0.39	0.75	0.38
error d37Cl	pm SMOC		0.27	0.15	0.15	0.18	0.20	0.17	0.15	0.21	0.18
87Sr/86Sr		Sr too low	0.732677	0.726491	0.729765	0.732912	0.729133	0.728684	0.72415	0.726197	0.726583
error 87Sr/86Sr			0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005

Sample		IG_BH03_Blank	IG_BH04_PW001	IG_BH04_PW028	IG_BH04_PW031	IG_BH04_PW034	IG_BH04_PW037	IG_BH04_PW040	IG_BH04_PW044	IG_BH04_PW046	IG_BH04_PW049	IG_BH04_PW052	IG_BH04_PW055	IG_BH04_PW058
Hydroisotop Nr.		338402	345810	349117	349118	349119	349120	349121	349328	349329	349520	349521	351146	351147
Interval	mbgs		162.5	397.8	423.6	450.9	478.1	505.1	531.9	561.3	586.2	614.4	636.8	665.4
Ratio Exp.Water : Rock	g/g		0.084	0.092	0.085	0.089	0.095	0.095	0.103	0.093	0.080	0.087	0.082	0.084
Ratio TW:PW	g/g		49.3	56.9	47.3	55.4	68.1	50.7	57.1	57.0	37.6	42.1	52.2	48.1
MISCELLANEOUS PROPERTIES														
pH (lab)	-log(H+)	5.8	7.5	7.8	7.7	7.7	7.6	7.6	7.5	7.5	7.4	7.3	8.0	7.9
Spec. electr. conductivity	µS/cm	3	245	202	195	191	169	289	234	240	251	197	214	397
Acid Capacity (4.3)	mmol	0.04	1.54	1.28	1.44	1.10	1.10	1.21	0.91	0.85	1.24	0.41	1.39	1.17
Base Capacity (8.2)	mmol	0.152	0.11	0.04	0.056	0.041	0.054	0.067	0.055	0.057	0.108	0.042	0.016	0.025
Sample Temperature	ºC	18.8	24.1	26.3	28.5	29.2	26.1	26.8	27.2	26.1	26.2	26.7	25.3	25.4
DOC	mg/l	1.70	13.2	14.8	15.1	9.90	9.40	14.2	8.30	8.90	5.00	3.80	6.20	5.10
TIC	mg/l	0.5	18.5	15.4	17.3	13.2	13.2	14.6	11.0	10.2	14.9	4.90	16.7	14.0
DISSOLVED CONSTITUENTS														
CATIONS														
Sodium (Na+)	mg/l	0.12	35.3	28.6	23.4	20.9	17.8	23.0	19.0	24.0	23.9	18.1	24.4	27.5
Potassium (K+)	mg/l	< 0.1	4.60	3.90	4.80	3.80	3.20	5.20	4.70	4.00	5.30	3.90	3.90	5.10
Lithium (Li+)	mg/L	< 0.01	0.022	0.035	0.021	0.014	< 0.01	0.024	0.020	0.035	0.025	0.012	0.047	0.029
Calcium (Ca+2)	mg/l	0.49	14.0	10.8	13.3	14.4	14.8	26.8	19.6	17.7	20.6	15.9	17.4	40.0
Magnesium (Mg+2)	mg/l	< 0.2	0.32	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	0.25	< 0.2	< 0.2	0.25
Strontium (Sr+2)	mg/l	<0.01	0.17	0.15	0.17	0.15	0.16	0.24	0.25	0.23	0.31	0.27	0.33	0.68
Aluminium (Al+3)	mg/l	< 0.01	0.036	0.128	0.120	0.222	0.177	0.108	0.126	0.154	0.114	0.131	0.039	0.051
Silicon (Si+4)	mg/l	< 0.1	7.10	8.9	11	9.2	9.50	10.7	9.6	8.5	7.0	3.8	8.8	7.4
Boron (B)	mg/l	< 0.01	0.19	0.10	0.11	0.07	0.03	0.02	< 0.02	0.07	0.20	0.10	0.13	0.071
ANIONS														
Fluoride (F-)	mg/l	< 0.1	1.40	0.63	0.62	0.20	0.13	< 0.1	< 0.1	< 0.1	2.4	< 0.1	0.40	0.40
Chloride (Cl-)	mg/l	0.02	17.4	10.3	5.20	14.4	10.8	33.2	29.0	32.0	22.7	32.0	15.1	66.1
Bromide (Br-)	mg/l	< 0.1	2.40	0.46	0.08	0.86	0.38	0.95	3.70	1.40	1.30	5.50	0.28	2.50
Nitrate (NO3-)	mg/l	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	< 0.2	0.29	0.28	0.23
Sulphate (SO4-2)	mg/l	< 0.2	5.80	5.10	3.70	5.50	3.80	6.90	3.60	4.40	6.40	7.10	3.00	8.50
Total Alkalinity	meq/l	0.04	1.54	1.28	1.44	1.10	1.10	1.21	0.91	0.85	1.24	0.41	1.39	1.17
Total Alkalinity as HCO3	mg/l	2.4	94.15	78.10	87.86	67.06	67.24	74.01	55.71	51.68	75.84	25.08	84.99	71.33
PARAMETERS CALCULATED FROM ANALYTICAL DATA														
Sum of Analysed Constituents	mg/l	3	176	140	144	127	118	172	136	135	159	111	157	223
Difference/Total		-15.51%	2.66%	4.95%	3.15%	2.58%	3.25%	3.58%	2.06%	4.51%	1.62%	4.70%	3.31%	1.39%
WATER TYPE		Na-Ca-HCO3	Na-(Ca)-HCO3-Cl	Na-(Ca)-HCO3-(Cl)	Na-Ca-HCO3	Na-Ca-HCO3-Cl	Na-Ca-HCO3-Cl	Na-Ca-HCO3-Cl	Na-Ca-HCO3-Cl	Na-Ca-HCO3-Cl	Na-Ca-HCO3-Cl	Na-Ca-Cl-HCO3	Na-Ca-HCO3-Cl	Na-Ca-Cl-HCO3
ION-ION RATIOS														
Br*1000/Cl weight		/	137.9	44.7	15.4	59.7	35.2	28.6	127.6	43.8	57.3	171.9	18.5	37.8
Br*1000/Cl molal	mol/mol	/	61.2	19.8	6.8	26.5	15.6	12.7	56.6	19.4	25.4	76.3	8.2	16.8
Na/Cl molal	mol/mol	3.129	5.485	6.940	2.238	2.542	1.068	1.010	1.157	1.624	0.872	2.492	0.642	0.713
K/Na molal	mol/mol	/	0.077	0.080	0.121	0.107	0.106	0.133	0.145	0.098	0.130	0.127	0.094	0.109
SO4/Cl molal	mol/mol	/	0.123	0.183	0.263	0.141	0.130	0.077	0.046	0.051	0.104	0.082	0.073	0.047
Na/(Cl+SO4)	mol/mol	9.253	2.786	3.620	5.496	1.962	2.250	0.992	0.966	1.101	1.471	0.806	2.322	0.613
ISOTOPE RATIOS														
d37Cl	pm SMOC	Cl too low	0.55	0.50	0.47	0.66	0.46	0.86	0.64	0.87	0.22	0.40	0.12	0.32
error d37Cl	pm SMOC		0.27	0.31	0.34	0.15	0.18	0.18	0.23	0.15	0.16	0.35	0.15	0.26
87Sr/86Sr		Sr too low	0.732677	0.727698	0.726040	0.726111	0.725324	0.727537	0.728847	0.727063	0.728203	0.758015	0.721527	0.725668
error 87Sr/86Sr			0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005

Sample		IG_BH03_Blank	IG_BH04_PW001	IG_BH04_PW061	IG_BH04_PW064	IG_BH04_PW067	IG_BH04_PW070	IG_BH04_PW073	IG_BH04_PW076	IG_BH04_PW079	IG_BH04_PW082	IG_BH04_PW085	IG_BH04_PW088	IG_BH04_PW092
Hydroisotop Nr.		338402	345810	351148	351149	351150	351151	351152	351153	351154	351155	351156	351157	351158
Interval	mbgs		162.5	692.4	711.3	746.3	771.6	795.3	825.3	849.3	877.8	904.0	931.1	959.0
Ratio Exp.Water : Rock	g/g		0.084	0.090	0.087	0.081	0.079	0.091	0.088	0.085	0.088	0.087	0.088	0.084
Ratio TW:PW	g/g		49.3	65.4	57.6	63.6	51.1	43.7	41.6	43.6	39.9	52.0	45.9	54.8
MISCELLANEOUS PROPERTIES														
pH (lab)	-log(H+)	5.8	7.5	7.5	7.6	7.5	7.6	7.6	7.7	7.6	7.8	7.6	7.9	7.7
Spec. electr. conductivity	µS/cm	3	245	311	358	461	510	439	562	704	633	499	514	477
Acid Capacity (4.3)	mmol	0.04	1.54	1.03	0.66	1.13	0.92	0.56	0.59	0.58	0.84	0.70	0.99	0.69
Base Capacity (8.2)	mmol	0.152	0.11	0.064	0.032	0.076	0.049	0.03	0.029	0.032	0.031	0.036	0.027	0.032
Sample Temperature	ºC	18.8	24.1	25.5	25.6	25.3	25.4	25.8	25.6	25.8	25.7	25.6	25.5	25.8
DOC	mg/l	1.70	13.2	5.10	4.80	7.70	3.50	4.70	4.00	5.10	6.20	6.40	8.00	4.20
TIC	mg/l	0.5	18.5	12.4	7.9	13.6	11.1	6.70	7.00	7.00	10.1	8.30	11.8	8.20
DISSOLVED CONSTITUENTS														
CATIONS														
Sodium (Na+)	mg/l	0.12	35.3	23.3	25.9	29.2	25.3	21.7	25.0	27.4	26.8	27.8	42.8	33.5
Potassium (K+)	mg/l	< 0.1	4.60	3.80	5.30	5.80	4.60	4.60	6.20	6.80	6.80	8.40	4.10	7.80
Lithium (Li+)	mg/L	< 0.01	0.022	0.016	0.018	0.014	0.024	0.032	0.051	0.060	0.045	0.025	0.028	0.031
Calcium (Ca+2)	mg/l	0.49	14.0	30.5	32.8	48.1	58.8	50.4	66.1	88.8	77.3	52.9	46.3	40.0
Magnesium (Mg+2)	mg/l	< 0.2	0.32	0.25	< 0.2	0.33	0.29	< 0.2	0.38	0.28	0.38	0.60	0.51	0.62
Strontium (Sr+2)	mg/l	<0.01	0.17	0.51	0.68	0.82	1.09	0.92	1.46	1.82	1.69	0.89	0.51	0.79
Aluminium (Al+3)	mg/l	< 0.01	0.036	0.024	0.031	0.029	0.039	0.049	0.041	0.033	0.045	0.021	0.037	0.028
Silicon (Si+4)	mg/l	< 0.1	7.10	8.4	7.8	8.3	8.9	7.7	7.1	7.3	7.0	8.2	7.1	7.3
Boron (B)	mg/l	< 0.01	0.19	0.038	0.027	0.033	0.061	0.04	0.057	0.033	0.035	0.094	0.190	0.220
ANIONS														
Fluoride (F-)	mg/l	< 0.1	1.40	< 0.1	< 0.1	0.54	1.9	2.2	1.9	1.4	1.8	0.62	1.9	1.7
Chloride (Cl-)	mg/l	0.02	17.4	50.4	72.3	84.2	107	99.1	138	177	147	115	108	92.0
Bromide (Br-)	mg/l	< 0.1	2.40	2.80	4.30	4.50	5.30	4.40	3.70	6.10	10.7	5.20	2.40	2.10
Nitrate (NO3-)	mg/l	< 0.2	< 0.2	0.47	< 0.2	< 0.2	0.50	< 0.2	0.70	0.36	< 0.2	< 0.2	< 0.2	< 0.2
Sulphate (SO4-2)	mg/l	< 0.2	5.80	5.20	4.70	6.80	5.50	4.90	9.20	8.20	10.0	7.60	10.5	14.2
Total Alkalinity	meq/l	0.04	1.54	1.03	0.66	1.13	0.92	0.56	0.59	0.58	0.84	0.70	0.99	0.69
Total Alkalinity as HCO3	mg/l	2.4	94.15	62.78	40.33	69.13	56.32	34.17	35.82	35.33	51.25	42.47	60.22	41.86
PARAMETERS CALCULATED FROM ANALYTICAL DATA														
Sum of Analysed Constituents	mg/l	3	176	180	186	249	267	222	288	353	334	261	277	235
Difference/Total		-15.51%	2.66%	1.35%	1.08%	1.71%	-0.35%	-0.43%	-2.33%	-0.26%	-1.46%	-0.75%	-0.59%	0.39%
WATER TYPE		Na-Ca-HCO3	Na-(Ca)-HCO3-Cl	Na-Ca-Cl-HCO3	Na-Ca-Cl-HCO3	Na-Ca-Cl-HCO3	Ca-Na-Cl-HCO3	Ca-Na-Cl-(HCO3)	Ca-Na-Cl-(HCO3)	Ca-Na-Cl	Ca-Na-Cl-(HCO3)	Ca-Na-Cl-(HCO3)	Na-Ca-Cl-HCO3	Na-Ca-Cl-(HCO3)
ION-ION RATIOS														
Br*1000/Cl weight		/	137.9	55.6	59.5	53.4	49.5	44.4	26.8	34.5	72.8	45.2	22.2	22.8
Br*1000/Cl molal	mol/mol	/	61.2	24.7	26.4	23.7	22.0	19.7	11.9	15.3	32.3	20.1	9.9	10.1
Na/Cl molal	mol/mol	3.129	5.485	0.552	0.535	0.365	0.338	0.279	0.239	0.281	0.373	0.611	0.562	0.562
K/Na molal	mol/mol	/	0.077	0.096	0.120	0.117	0.107	0.125	0.146	0.146	0.149	0.178	0.056	0.137
SO4/Cl molal	mol/mol	/	0.123	0.038	0.024	0.030	0.019	0.018	0.025	0.017	0.025	0.024	0.036	0.057
Na/(Cl+SO4)	mol/mol	9.253	2.786	0.687	0.539	0.519	0.358	0.332	0.273	0.235	0.274	0.364	0.590	0.531
ISOTOPE RATIOS														
d37Cl	pm SMOC	Cl too low	0.55	0.68	0.48	0.33	0.35	0.34	0.72	0.34	0.03	0.18	0.35	-0.12
error d37Cl	pm SMOC		0.27	0.20	0.14	0.35	0.15	0.27	0.30	0.24	0.15	0.15	0.18	0.15
87Sr/86Sr		Sr too low	0.732677	0.722494	0.724474	0.726201	0.733826	0.732951	0.735922	0.733718	0.742868	0.727157	0.722521	0.723765
error 87Sr/86Sr			0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005	0.00005

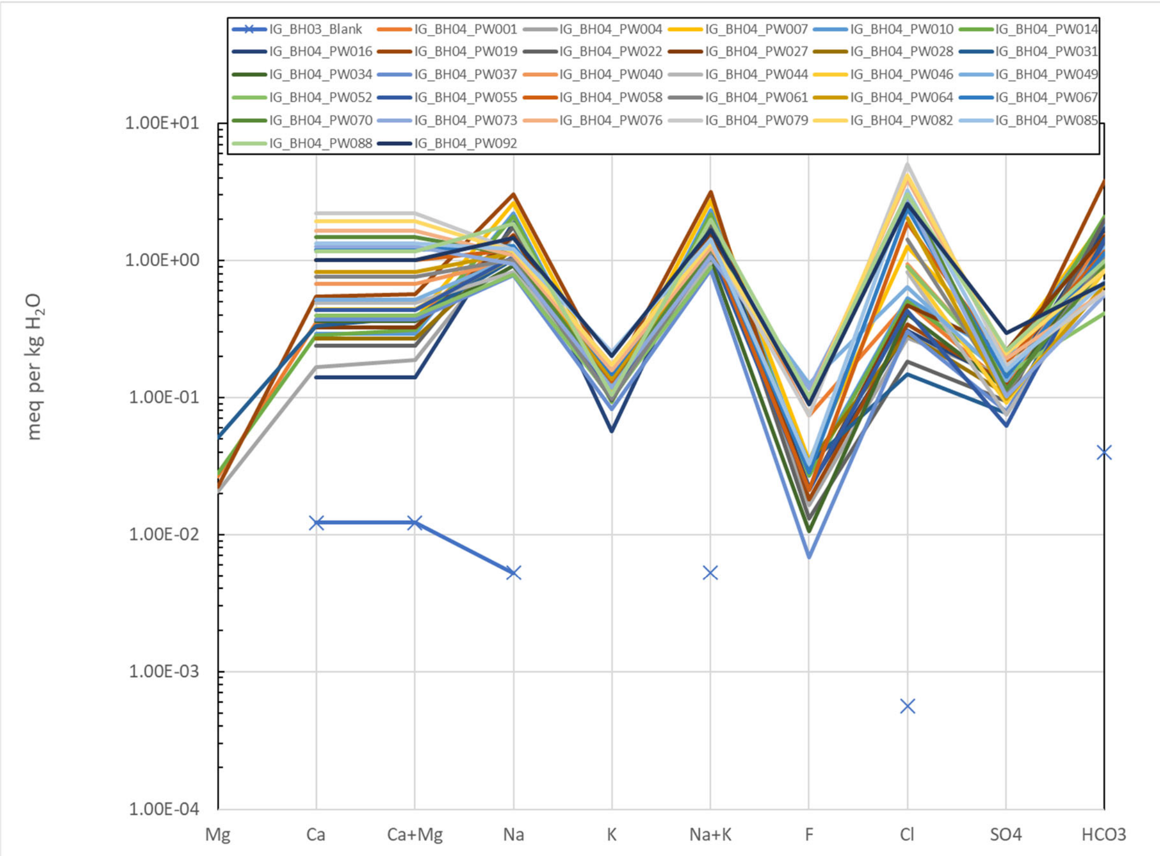


Figure 5 2: Schoeller diagram of experiment solutions from out-diffusion experiments conducted with core samples from borehole IG_BH04

6.0 ELEMENTAL TIME SERIES AND PORE DIFFUSION COEFFICIENT OF CHLORIDE

6.1 Elemental Elution Curves

Non-destructive out-diffusion experiments are performed based on the concept of chemical exchange between porewater residing in the rock matrix and a test solution of known composition surrounding the rock sample. The experimental setup is maintained until well-defined conditions between the two solution reservoirs are attained. Because of the closed system character of out-diffusion experiments, the target conditions to be achieved between the two solution reservoirs are equilibrium for any solutes for which the porewater is the only source, and which are only subjected to transport processes.

For the present study, improved analytical techniques allowed continuous monitoring of all major solute concentrations in the eluate solutions during out-diffusion. This allows definition of mineral reactions and – at a later stage – possible determination of solute-specific transport (e.g., ion-specific accessible porosity) in the matrix of crystalline rocks.

Porewater chloride and bromide concentrations are calculated based on the final concentrations in the out-diffusion test solutions and the water content of the individual core samples (Section 3). The approach to equilibrium was monitored by periodically taking sub-samples and analysing them for their Cl and Br concentrations. The criterion for attainment of equilibrium conditions is defined by a difference of less than 5 % in Cl and Br concentrations between the last sub-sample and the final test solution at the end of the experiment. This corresponds to the analytical uncertainty of the Cl and Br measurements. Sub-samples were collected as a function of time during all conducted out-diffusion experiments.

Out-diffusion experiments were run for 146 to 188 days. Equilibrium with respect to Cl and Br was attained for all samples with respect to the above-mentioned criteria after 48 – 90 days and 29 – 90 days, respectively (Figure 6-1). For core samples IG_BH04_PW022 and IG_BH04_PW031 the Br concentration of the sub-samples are below the detection limit of 0.1 mg/l. However, in the final test solutions of these samples very low Br concentrations of 0.12 and 0.08 mg/l were detected resulting in a sharp-like shape of the Br elution curves. Due to the much higher sample volume (about 110 to 140 ml) of the final test solutions compared to the sub-samples (0.5 ml) the measurements could be performed with lower dilutions, hence very low Br concentrations could be detected.

The calculated Br*1000/Cl mass ratios (further expressed as Br/Cl ratio) of the individual out-diffusion experiments either increase within the first days or weeks of elution and are subsequently constant or are constant over the entire period of elution (Figure 6-1). This indicates that there is no significant influence of diffusional fractionation between bromide and chloride. For core samples IG_BH04_PW022 and IG_BH04_PW031 the Br concentration of the sub-samples are below the detection limit of 0.1 mg/l and therefore no time series elution curve for Br*1000/Cl is available.

Sodium appears to elute similar to chloride and bromide in the first app. 30 to 50 days of the experiments. In a different way from the conservative elements, Cl^- and Br^-, Na^- shows a slight increasing trend in the later course of the experiments (see Figure 6-1). In several experiments, sodium was in equilibrium after app. 120 days (Figure 6-1). These trends indicate that the main proportion of sodium in the test solutions originates from porewater, which exchanged by diffusion with the test water, and a low proportion originates from water-rock interactions of Na-bearing plagioclases within the experiments.

Potassium, in contrast, shows a trend similar to Cl^- and Br^- and reaching equilibrium in all samples after just a few weeks. The consistent trend of K-elution indicates that there is no influence of interactions of K-bearing alkali feldspar observable from the K-elution curves. The main proportion of K appears to originate from the diffusive accessible porewater.

The concentrations of Ca^{2+} are also constant in most test solutions after an experimental period of 60 to 120 days (Figure 6-1). Exceptions to this trend occur in eight samples (IG_BH04_PW001, PW019, PW040, PW046, PW055, PW058, PW067 and PW082) which show a slight increasing trend for the duration of the experiments. The general elution behaviour of Ca^{2+} in most of the experiments indicates that there is no main influence of Ca-dissolution reactions of Ca-bearing plagioclase and/or its alteration products on the Ca^{2+}-contents of the test solutions.

The sulphate concentrations show for almost all samples a continuous increase during the entire elution period (Figure 6-1), which is caused by the oxidation and elution of sulphide minerals (present in the core samples as accessories (chapter 4.3)).

The Magnesium concentrations of samples from IG_BH04 are very low with values between 0.2 and 0.6 mg/l or below the detection limit of 0.2 mg/l. For samples with Magnesium concentration below the detection limit no time series elution curve is shown in Figure 6-1.

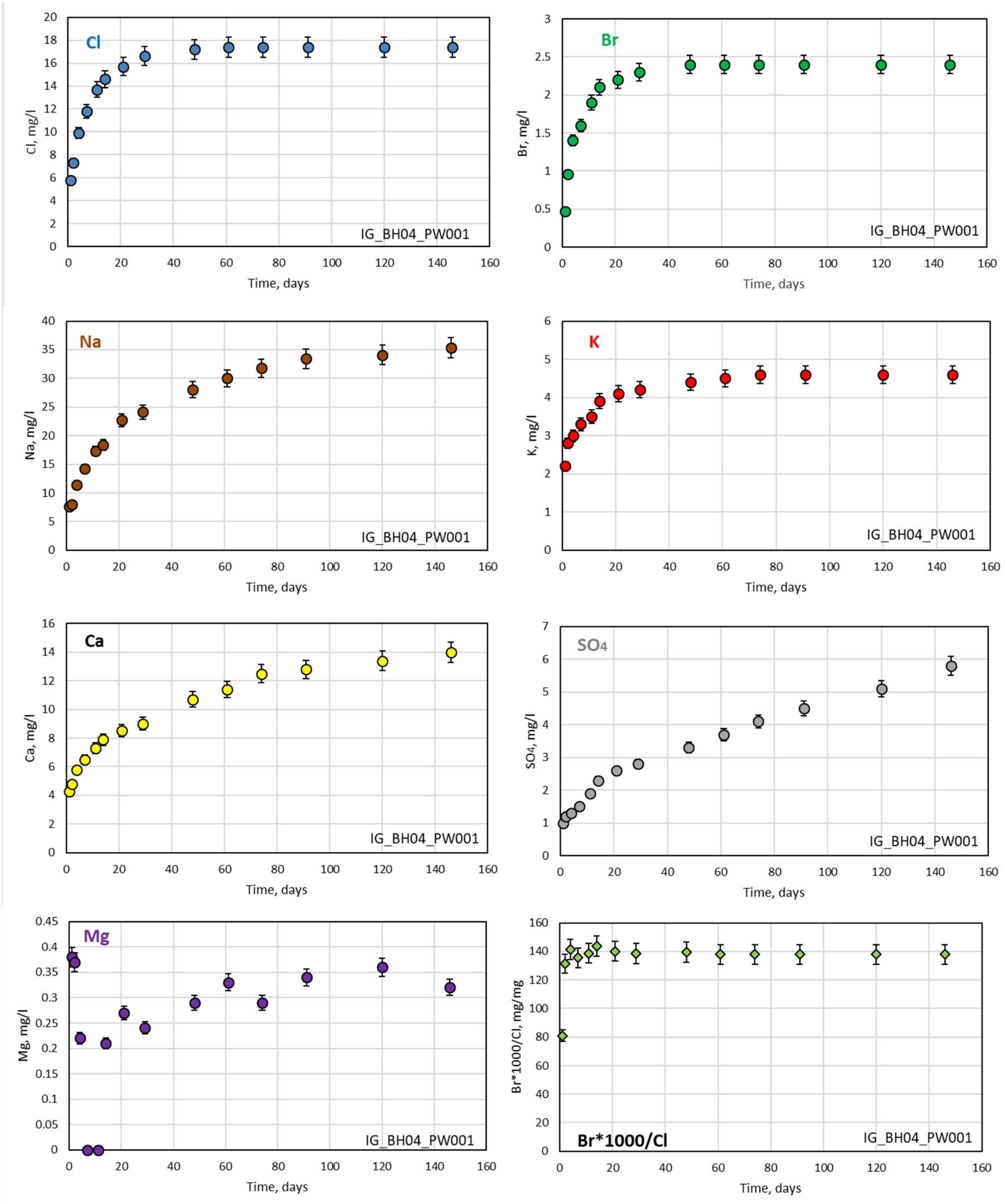


Figure 6-1: Elution curves of different main anions and cations set-up by the periodic sampling of test solutions of out-diffusion experiments applying core samples from IG_BH04; the errors are the analytical uncertainty of ± 5 %. The analyses of the last samples are conducted on the large volume fully equilibrated test solutions. Hence, the detection limits are higher for these samples, which can be predominately observed on some of the bromide elution curves.

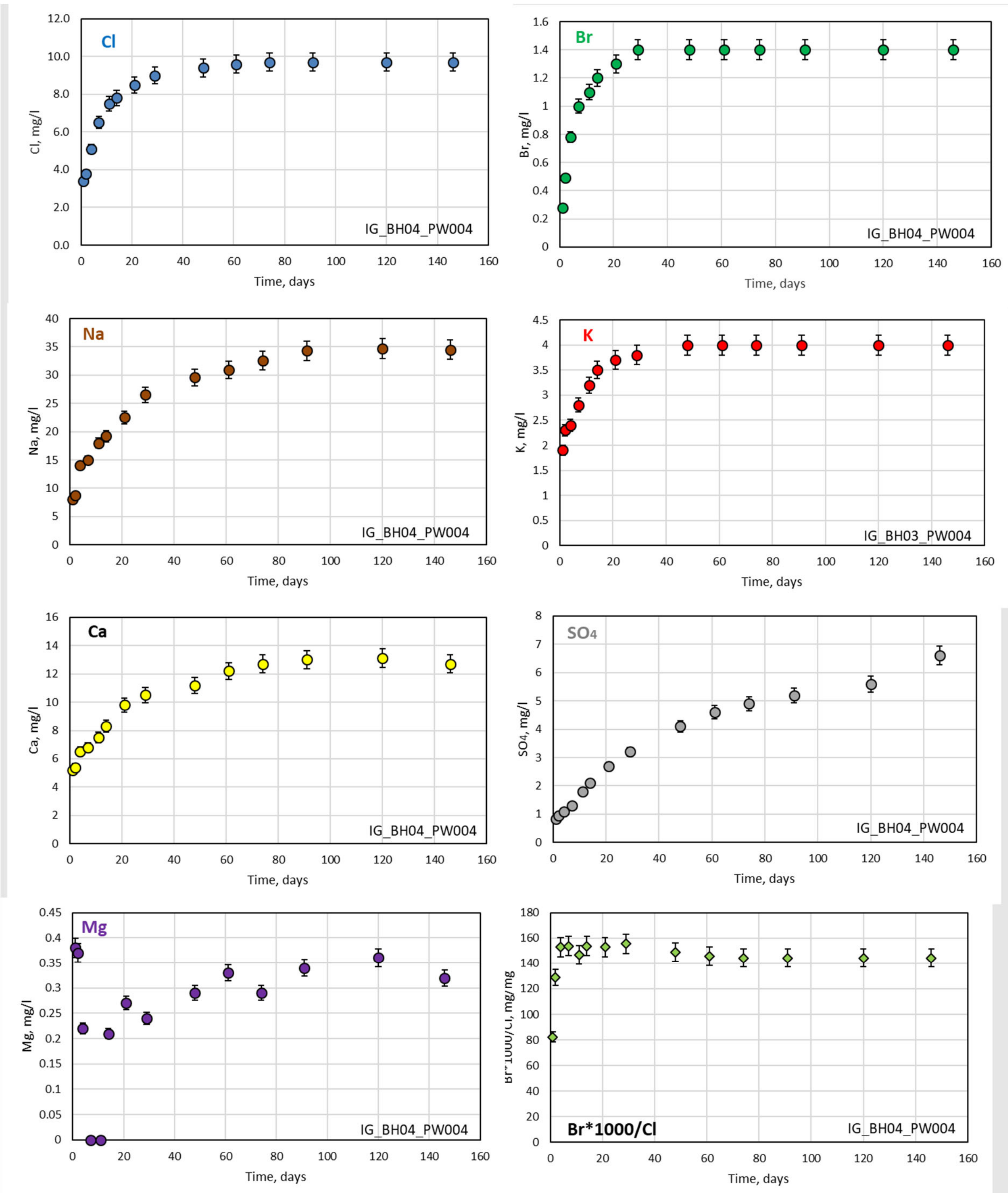


Figure 6-1 continued

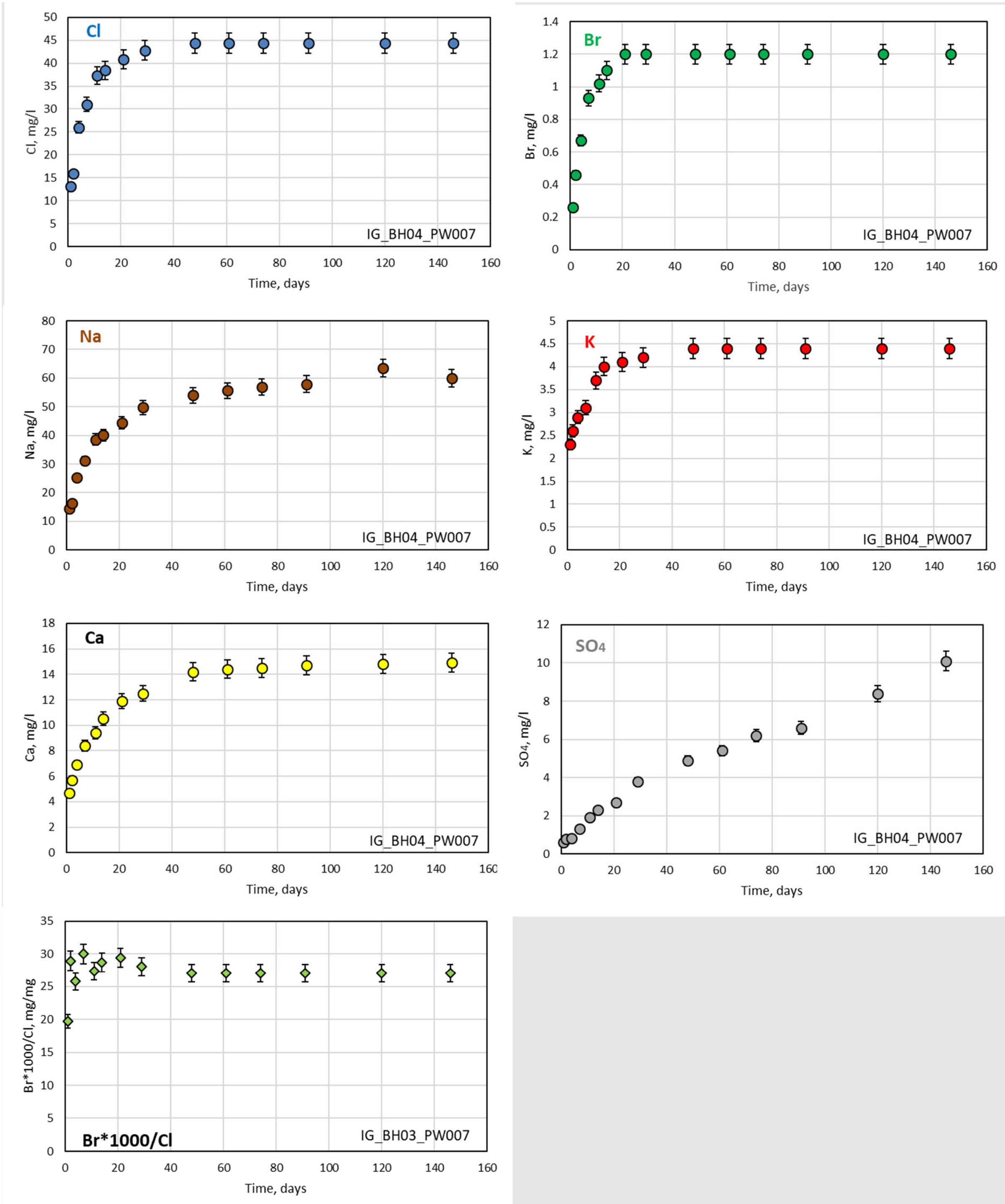


Figure 6-1 continued

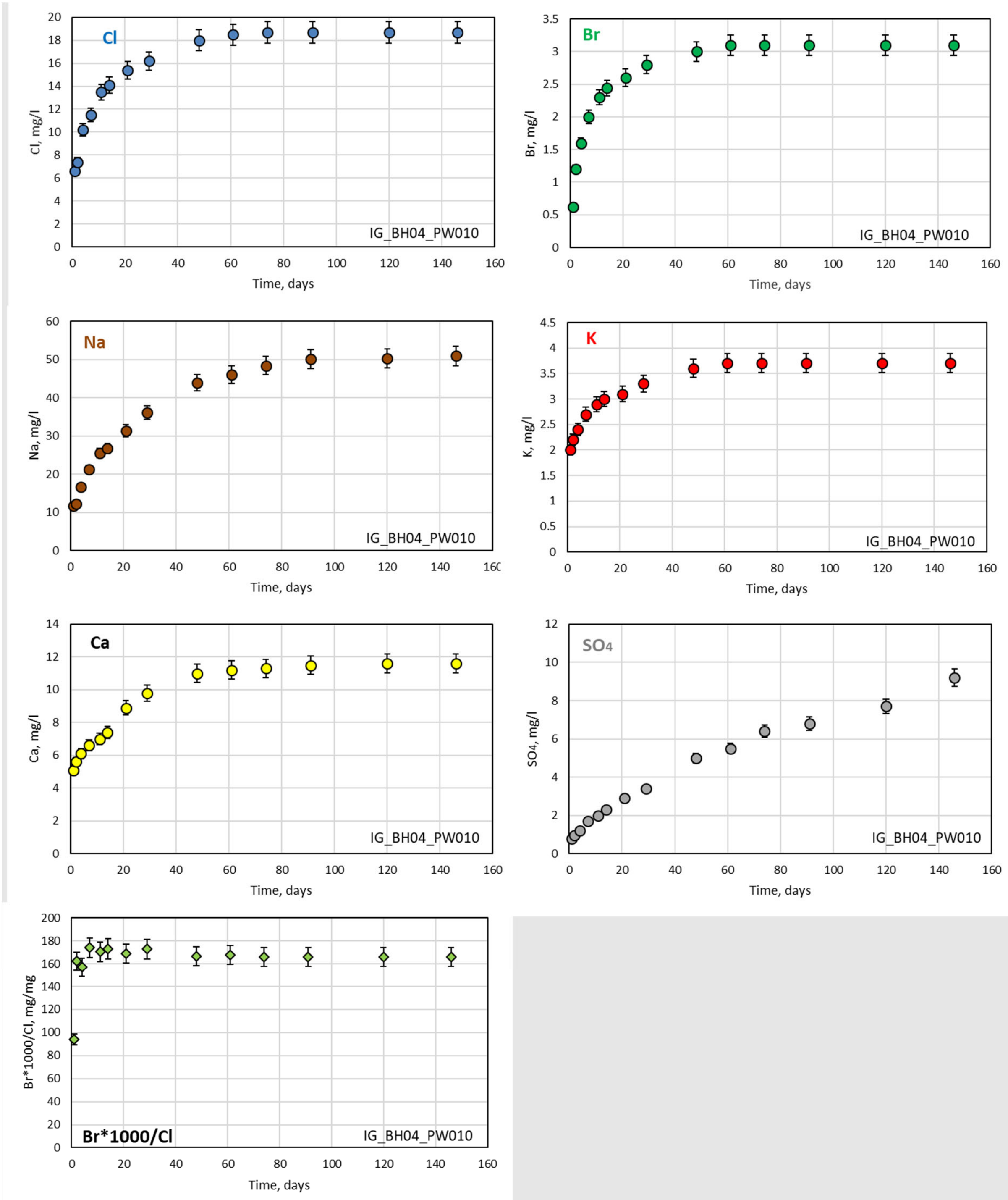


Figure 6-1 continued

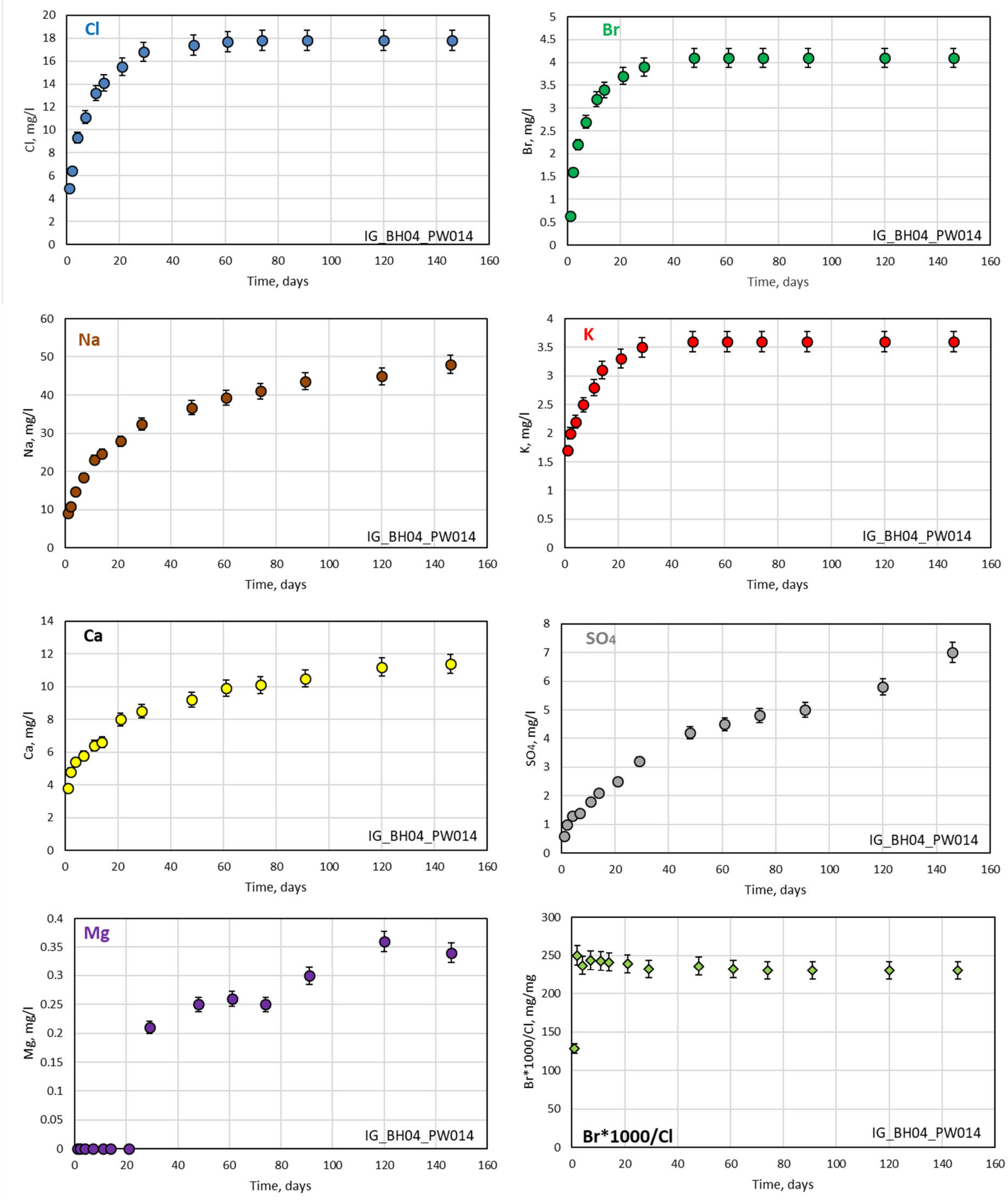


Figure 6-1 continued

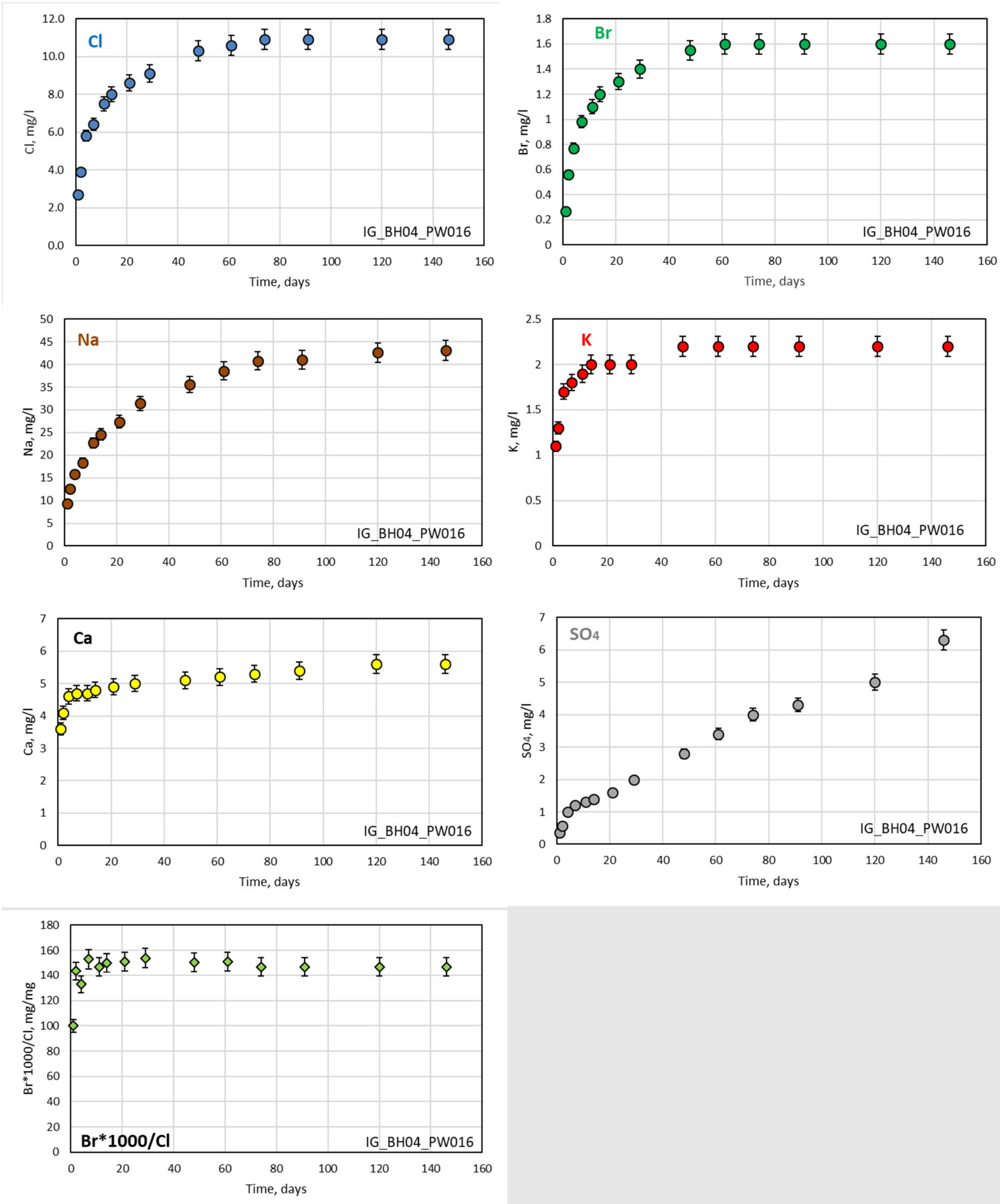


Figure 6-1 continued

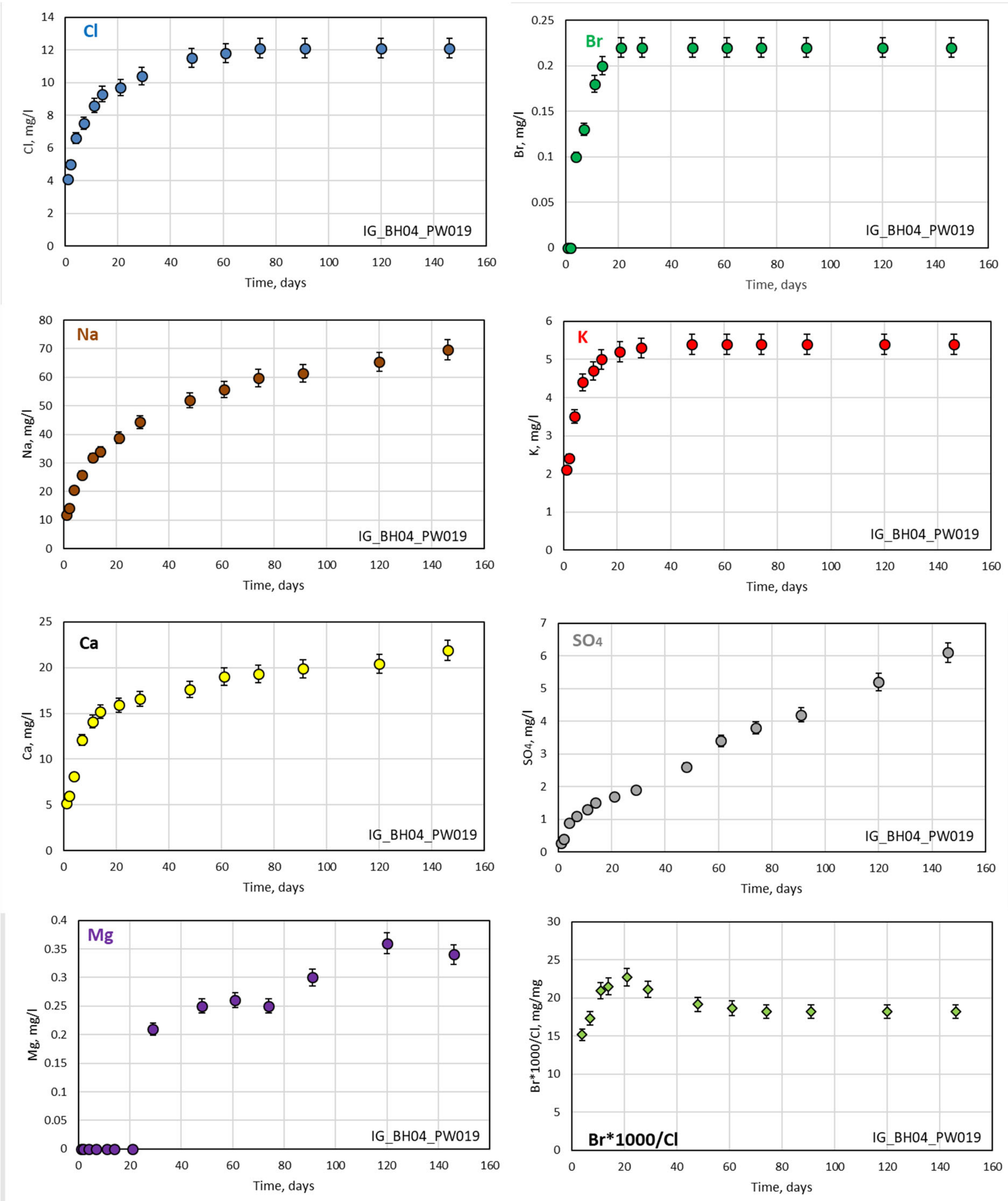


Figure 6-1 continued

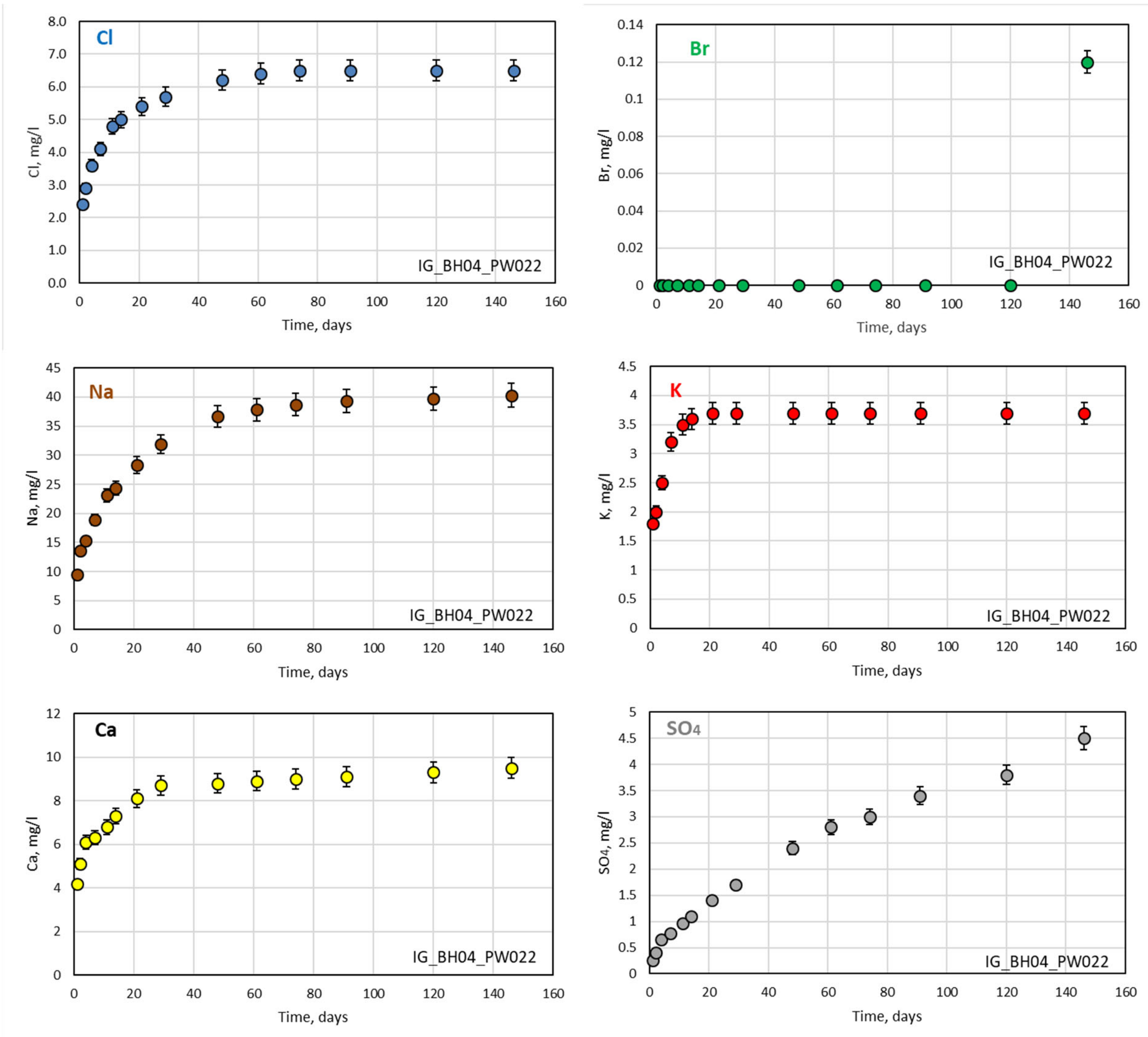


Figure 6-1 continued

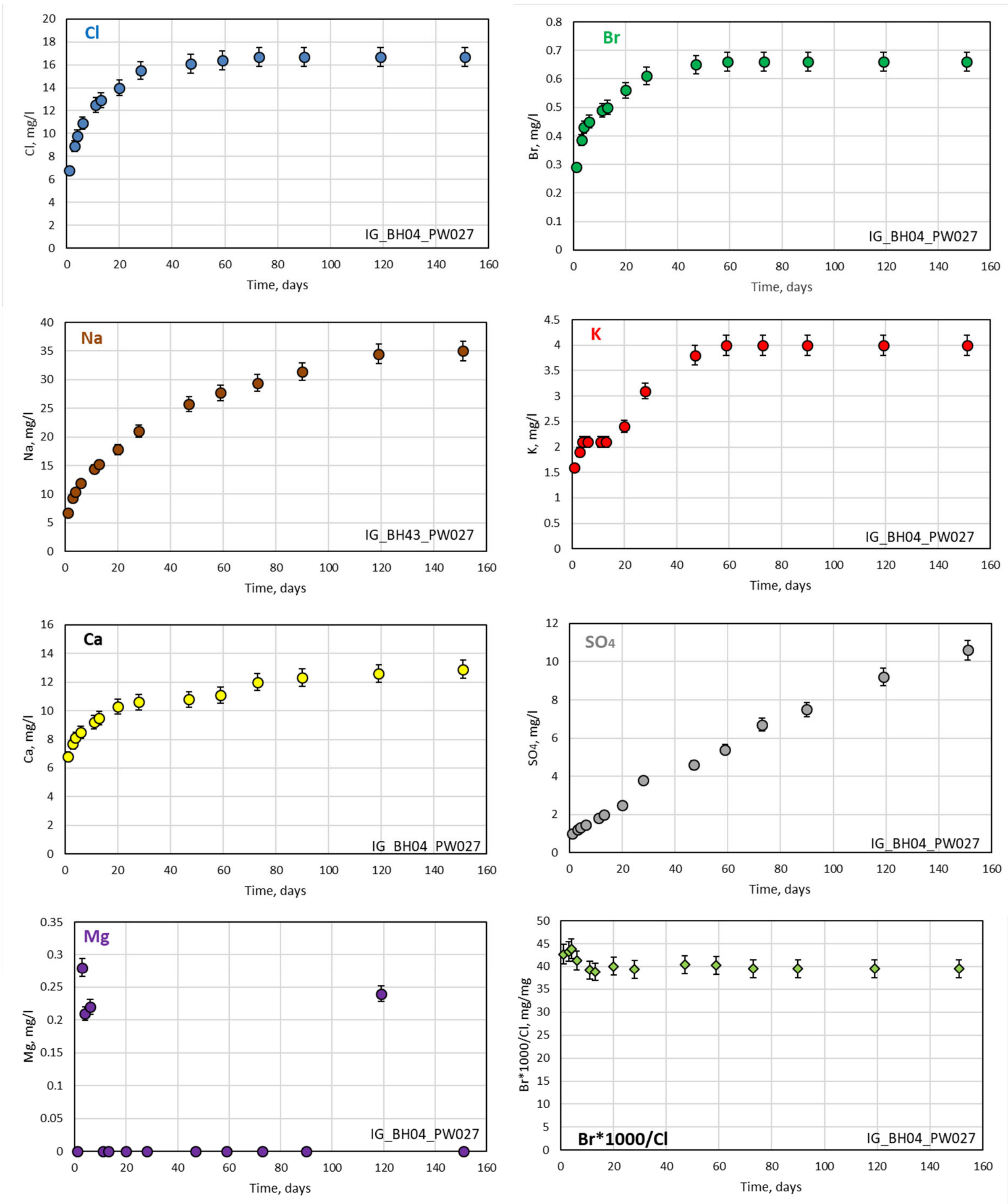


Figure 6-1 continued

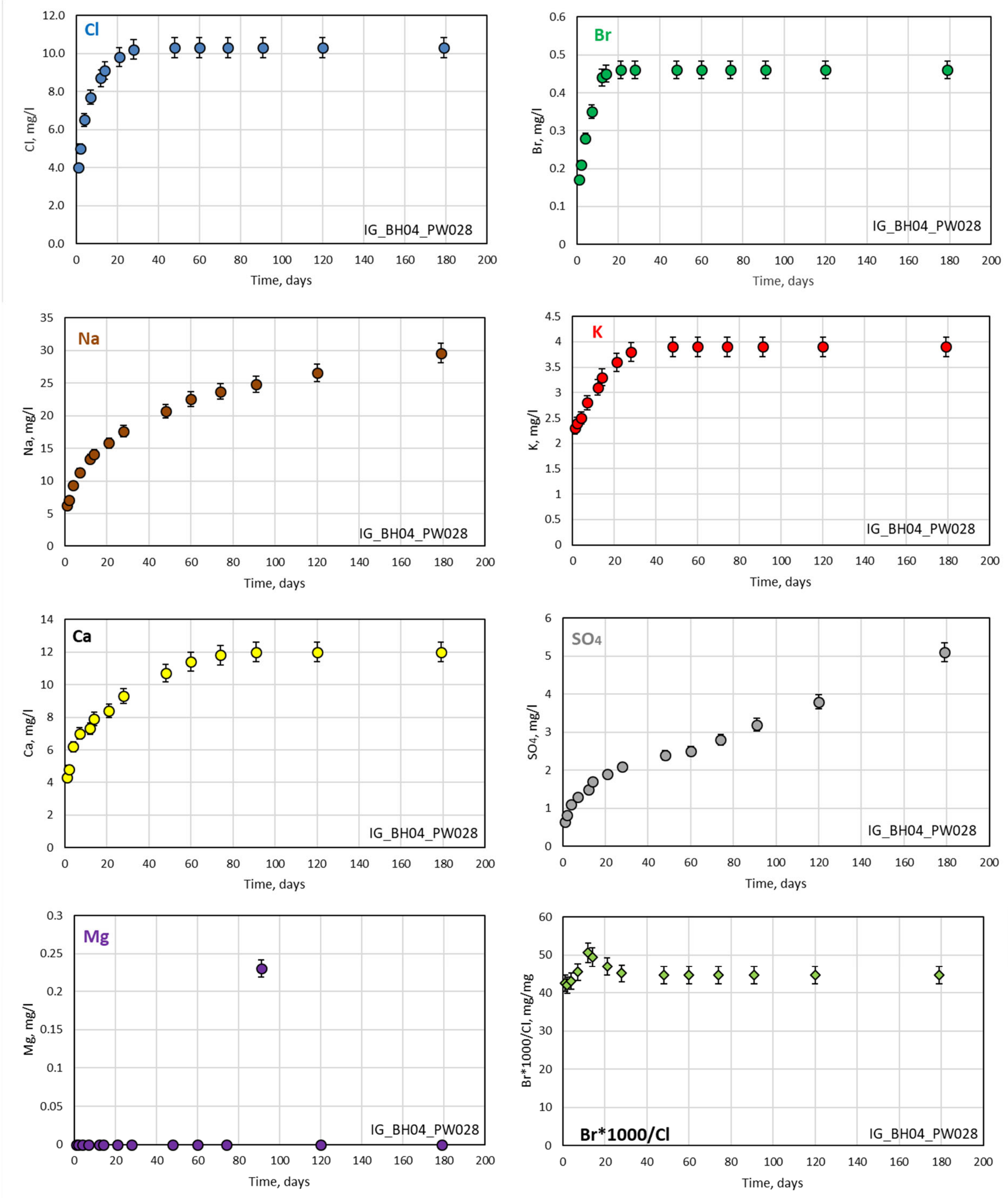


Figure 6-1 continued

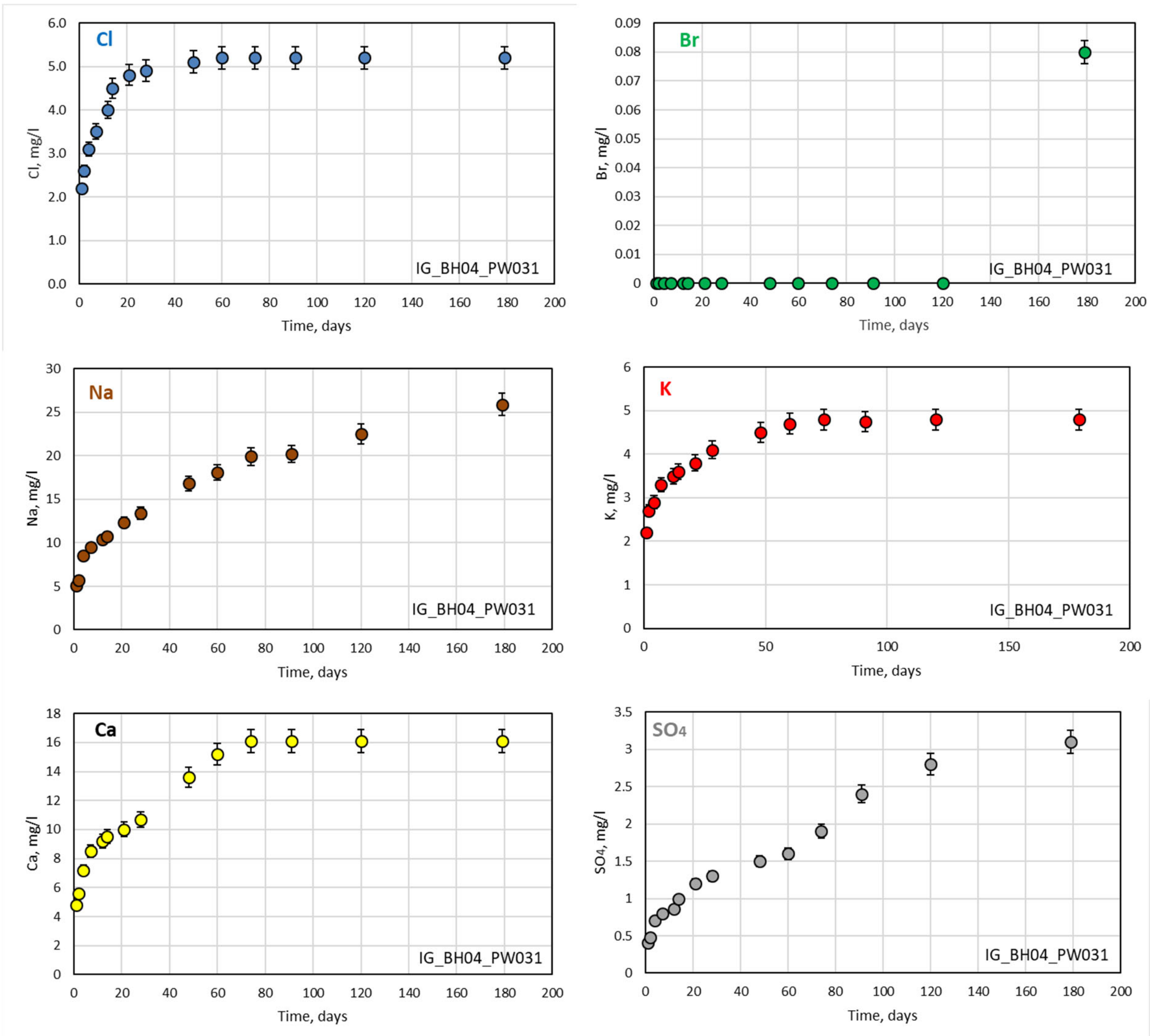


Figure 6-1 continued

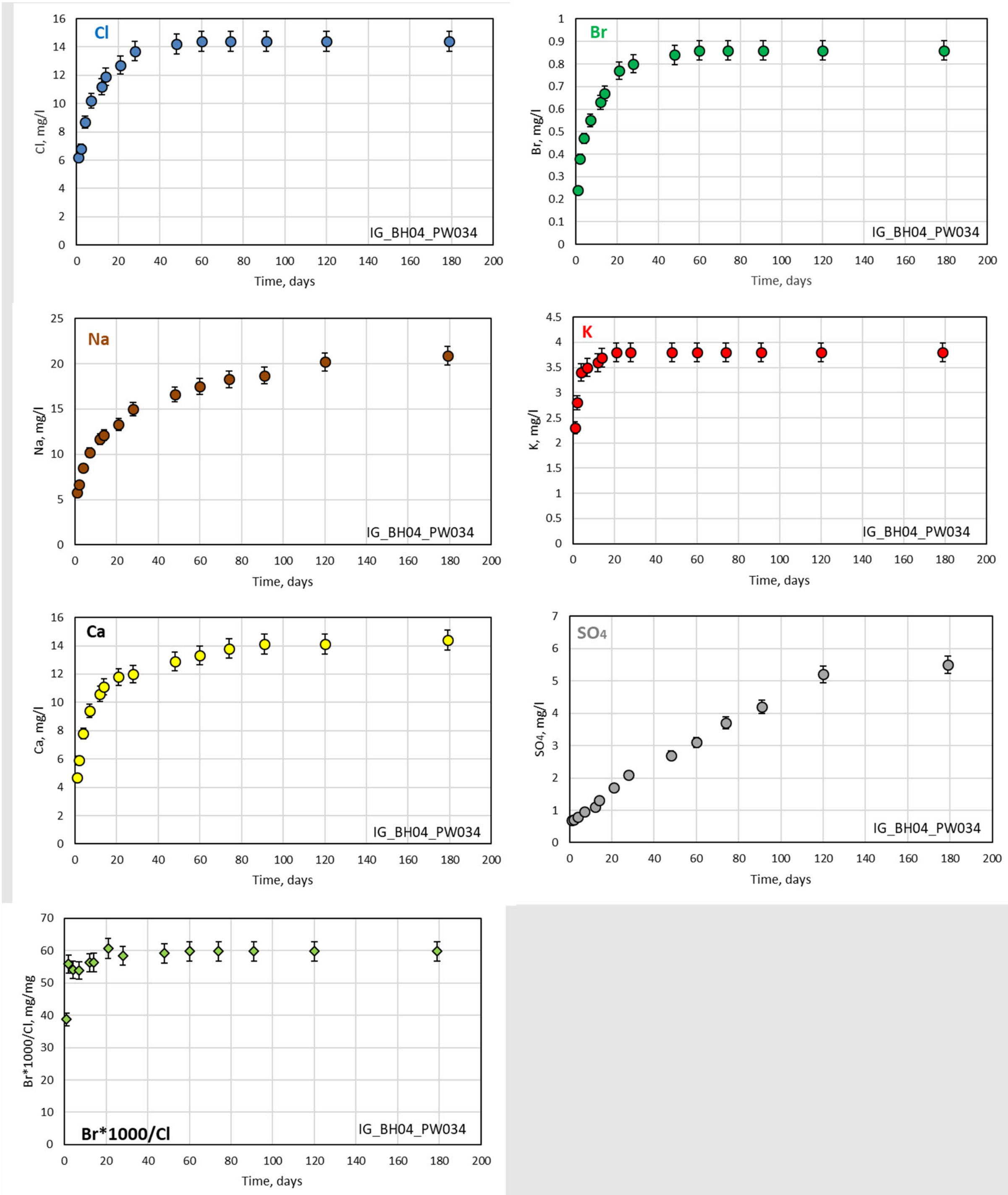


Figure 6-1 continued

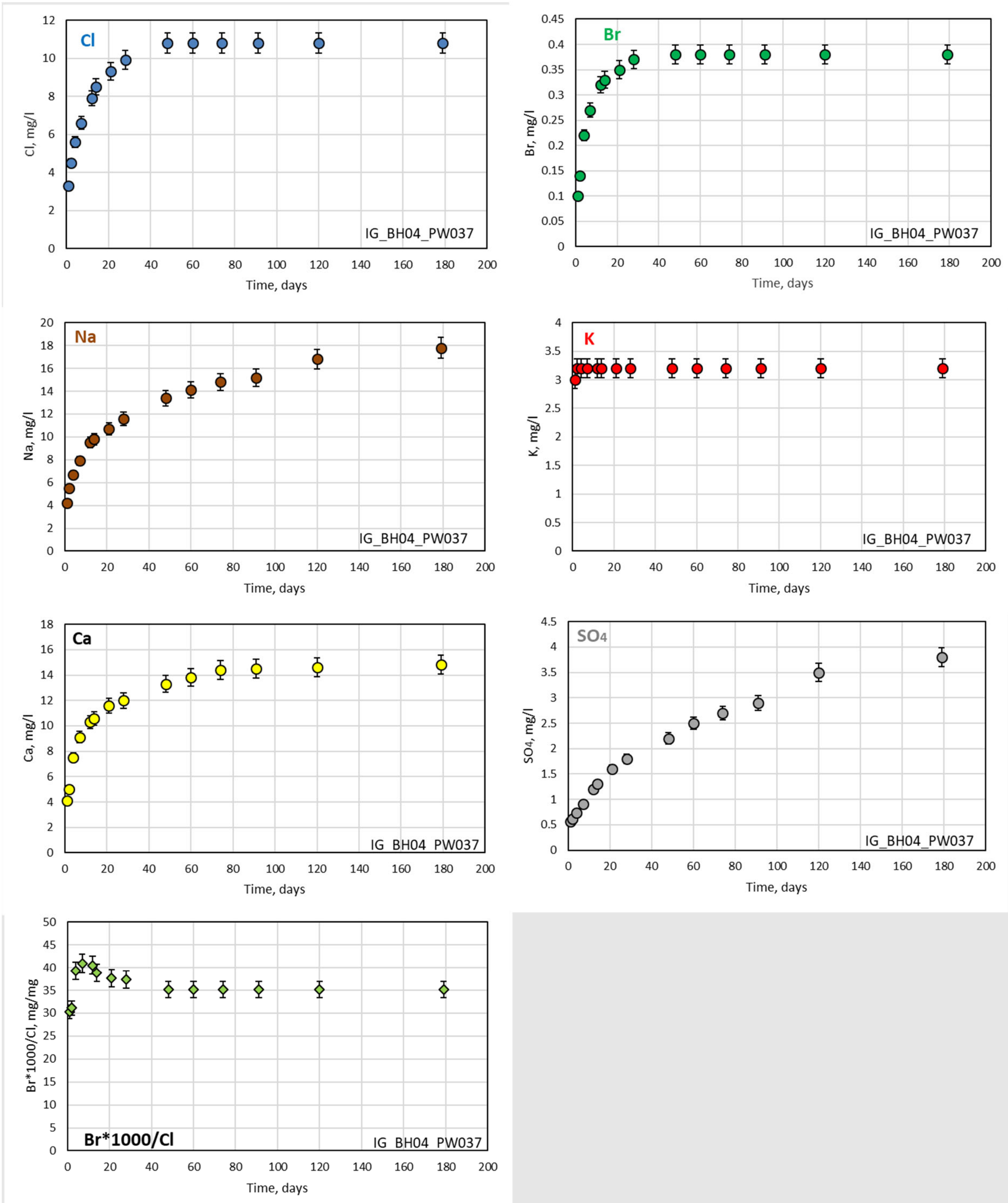


Figure 6-1 continued

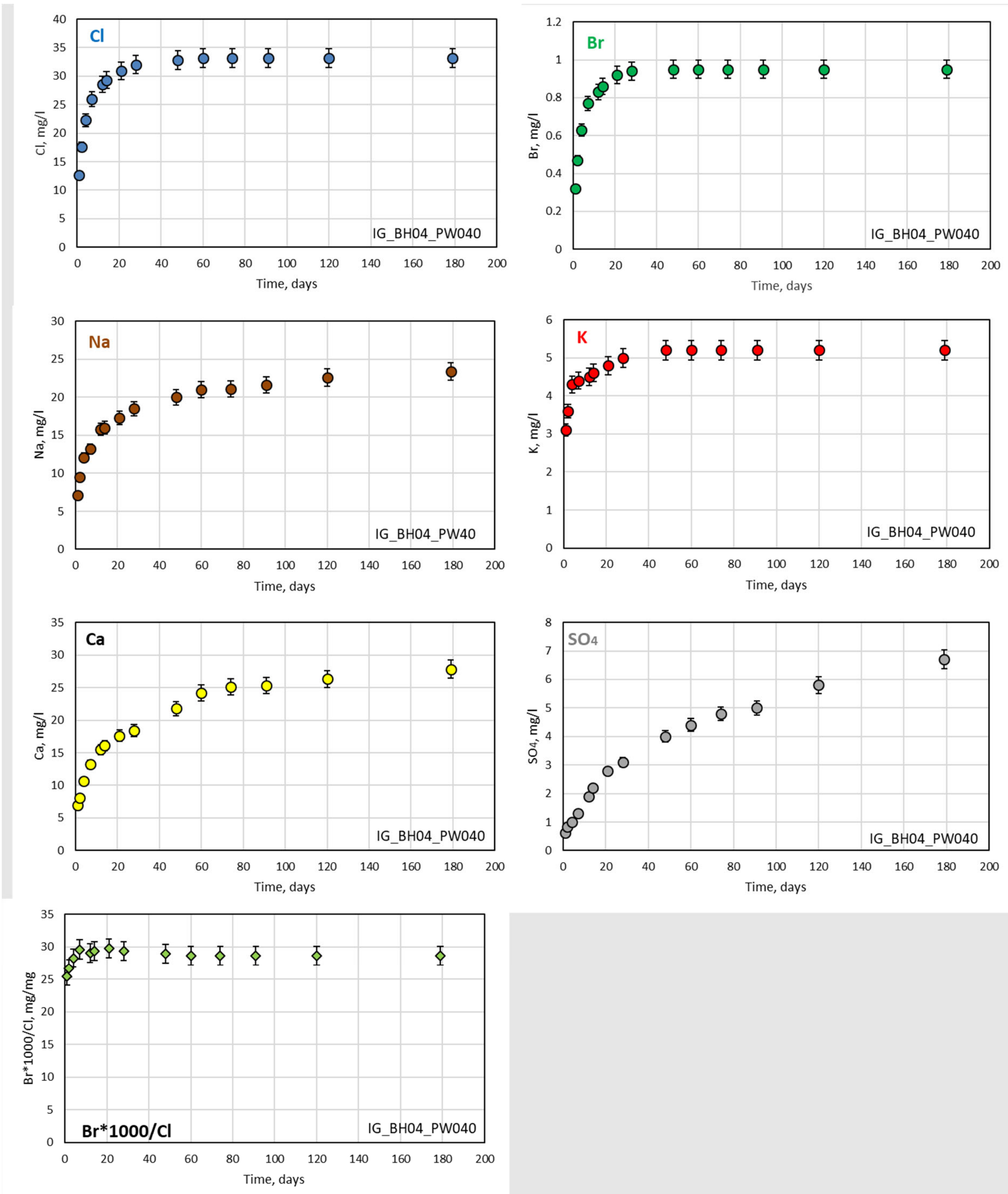


Figure 6-1 continued

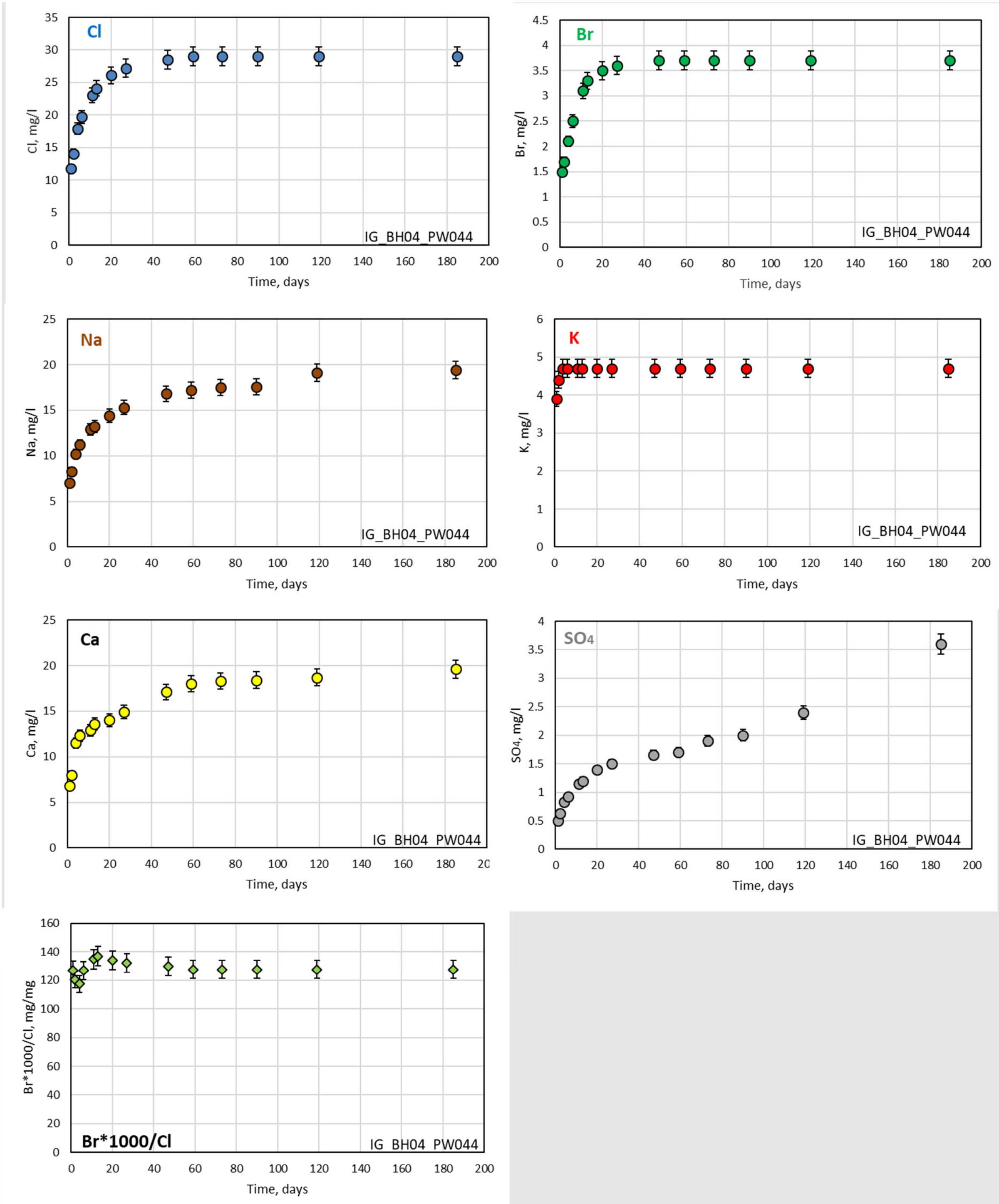


Figure 6-1 continued

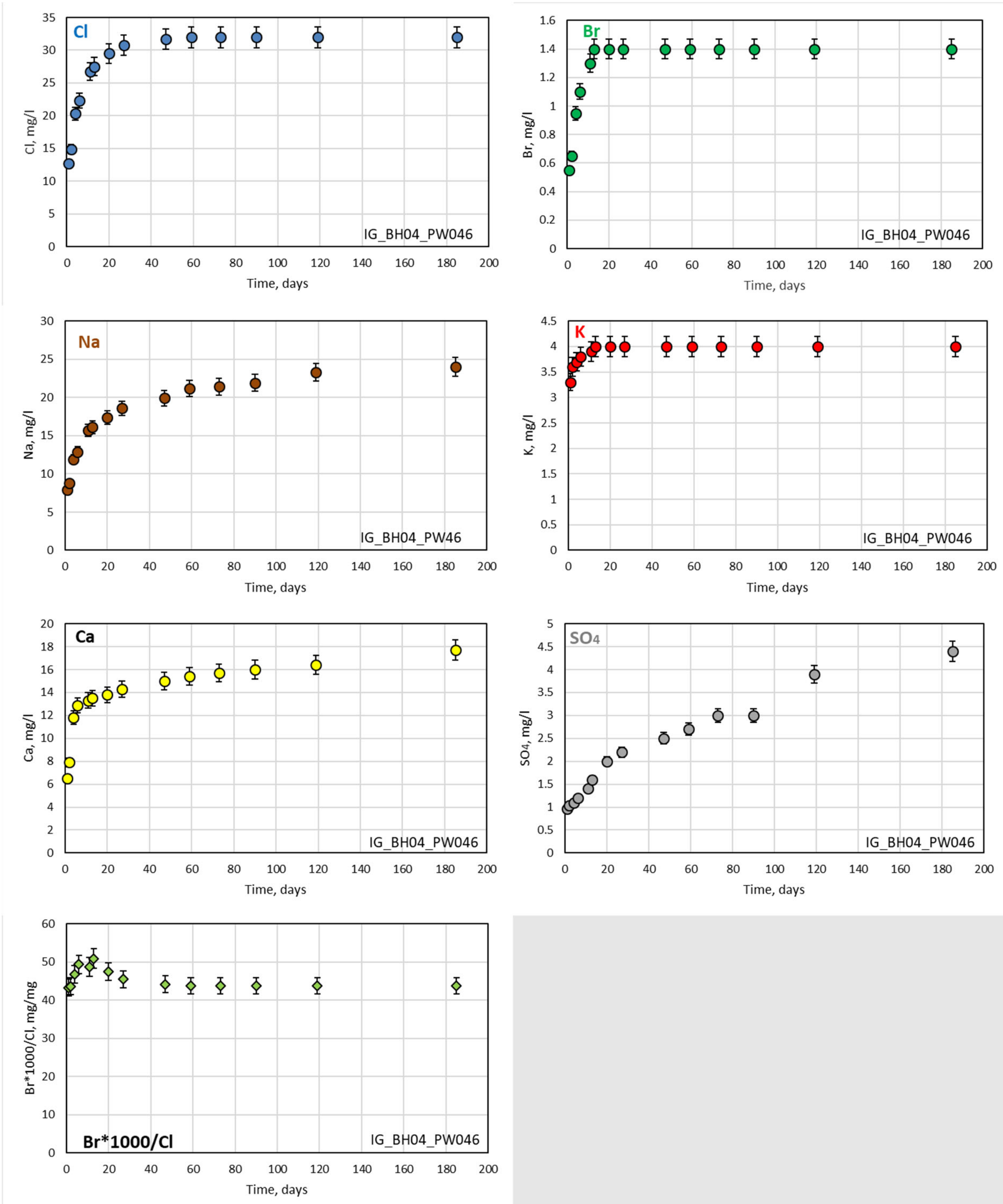


Figure 6-1 continued

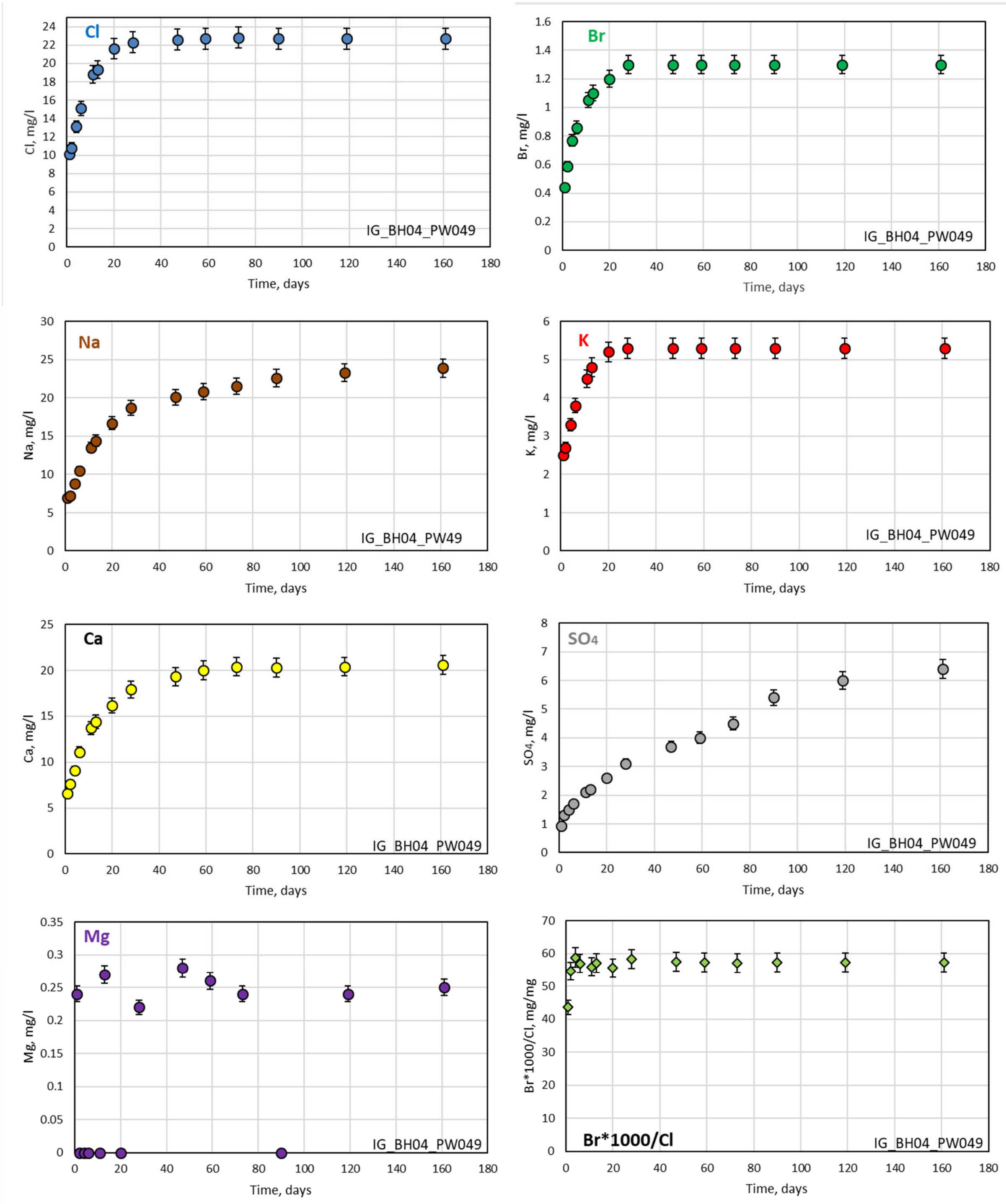


Figure 6-1 continued

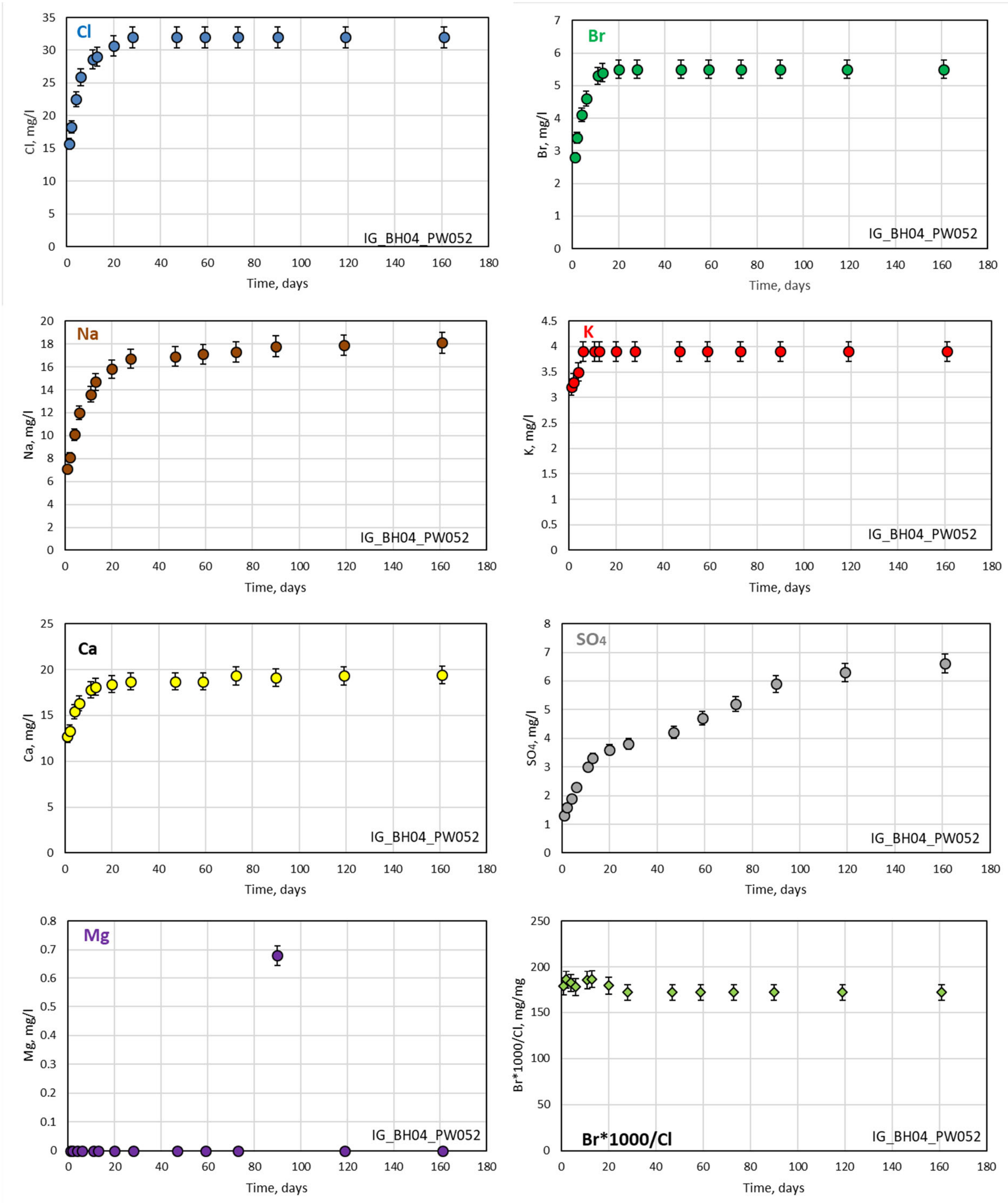


Figure 6-1 continued

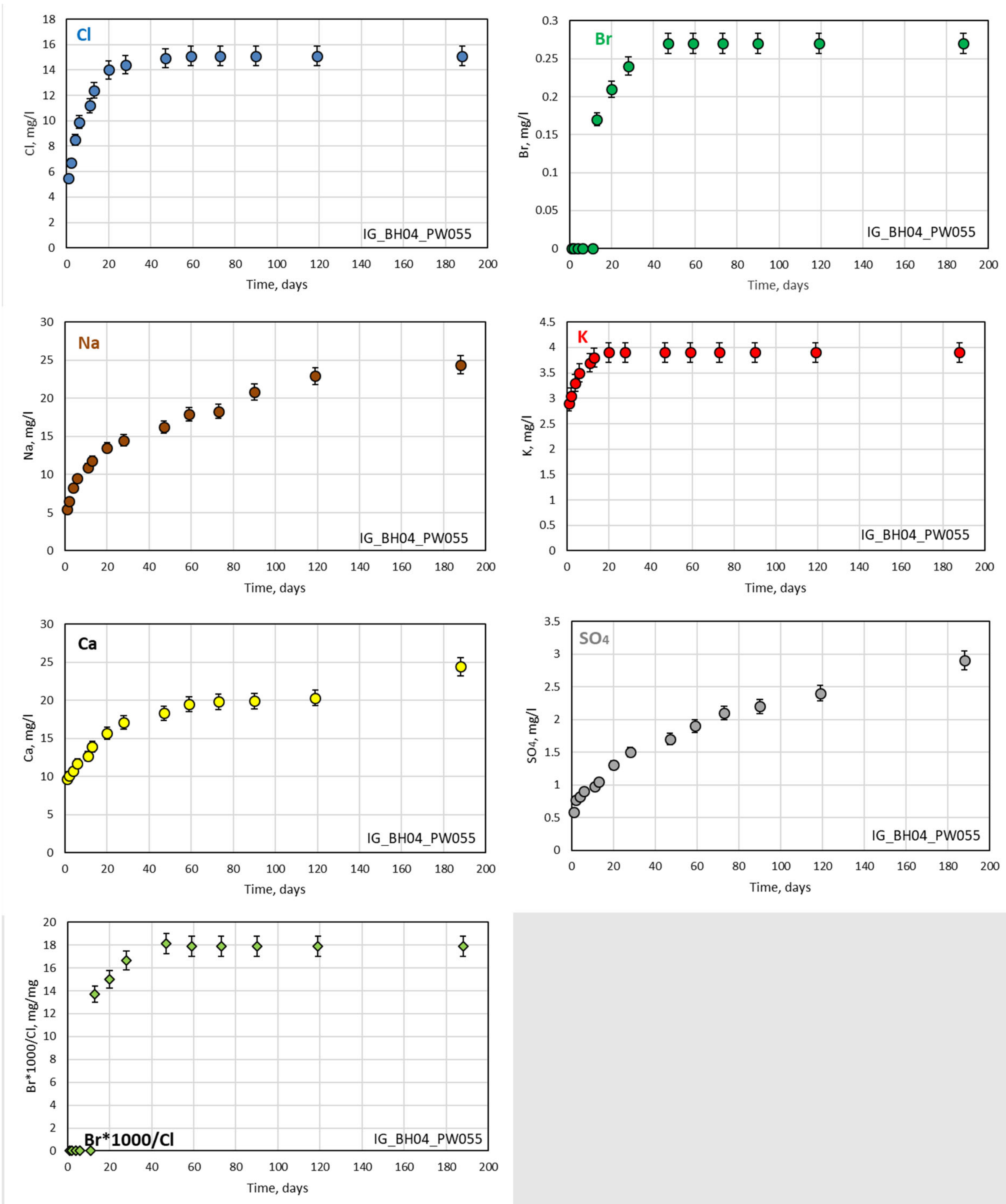


Figure 6-1 continued

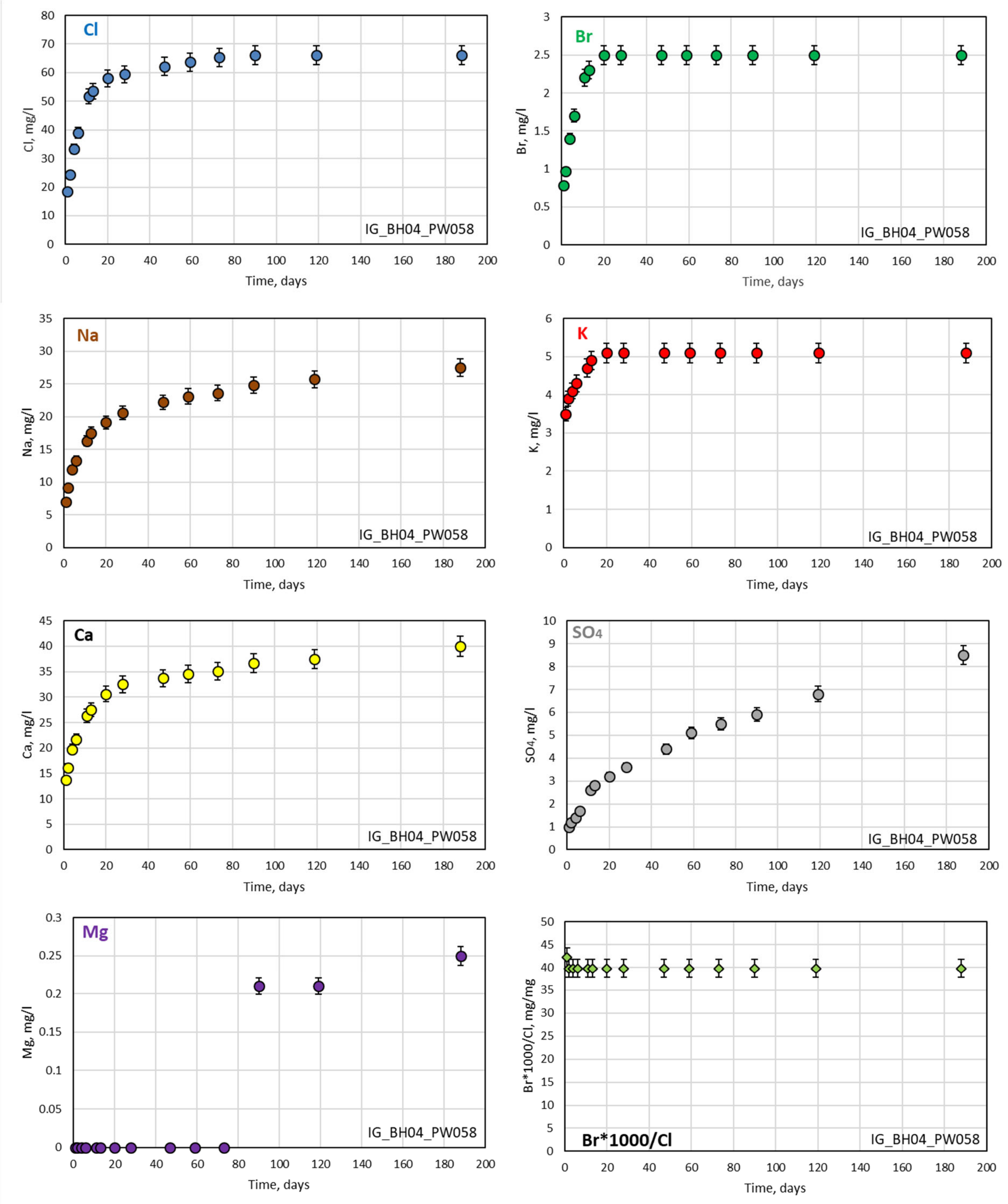


Figure 6-1 continued

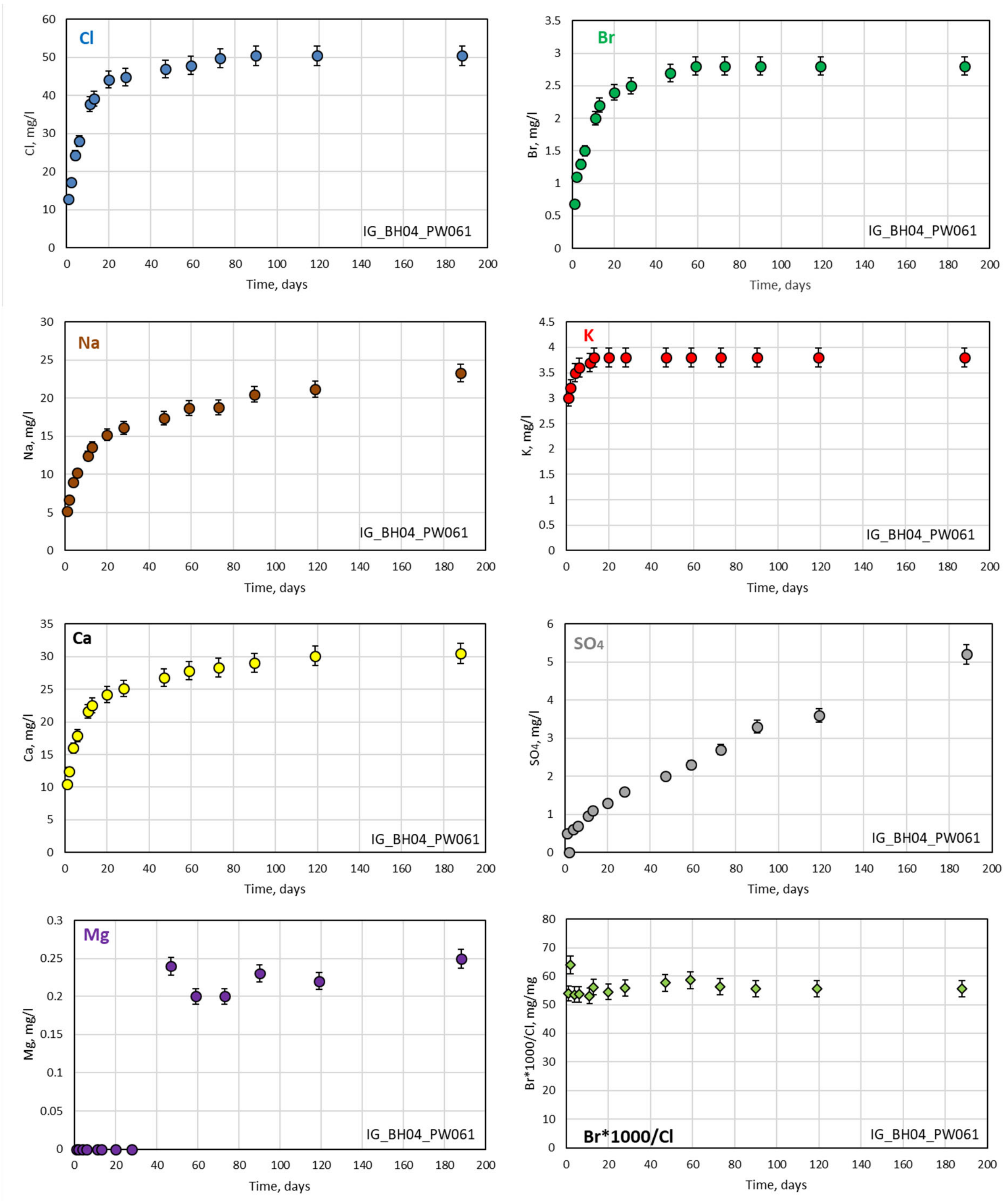


Figure 6-1 continued

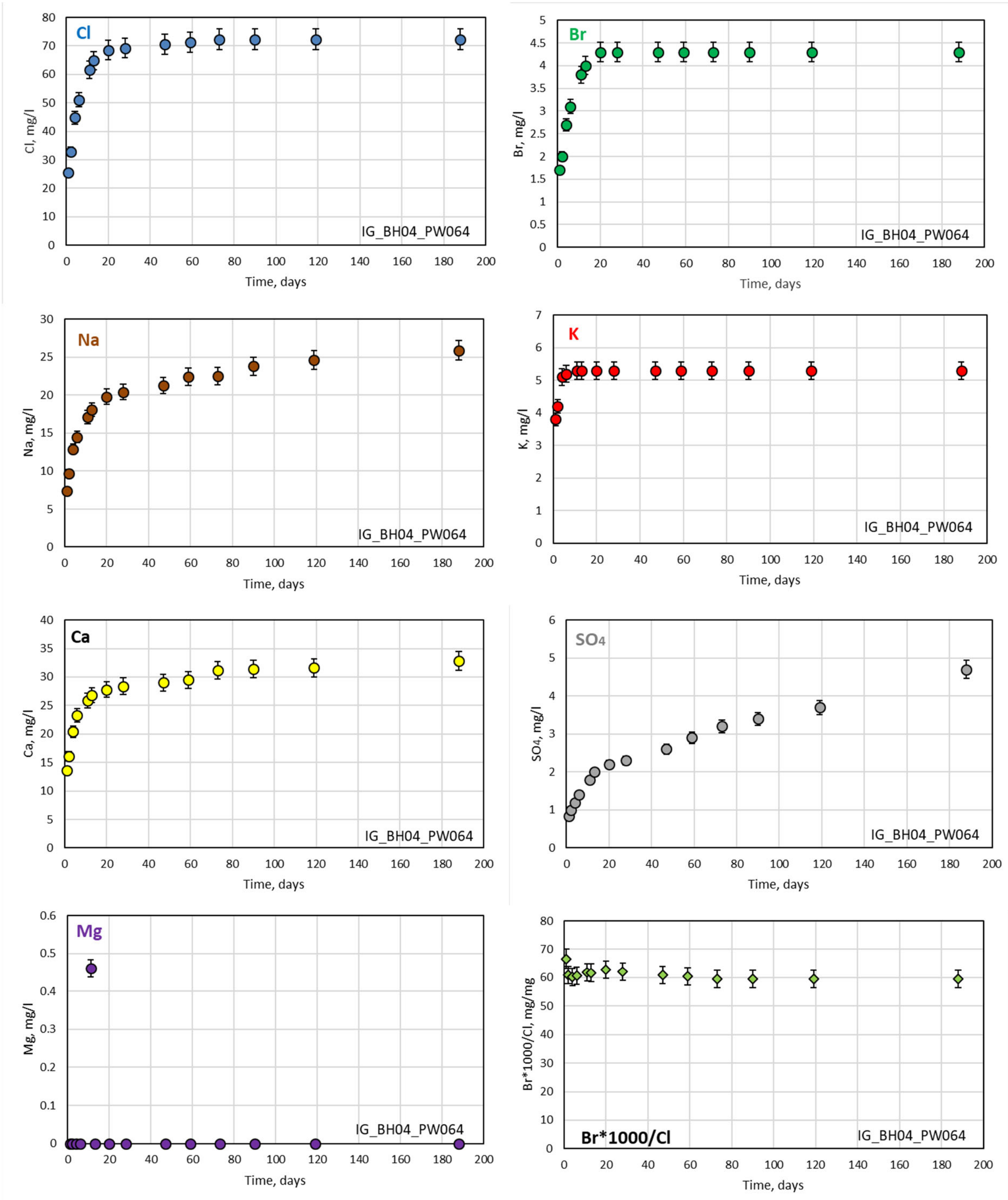


Figure 6-1 continued

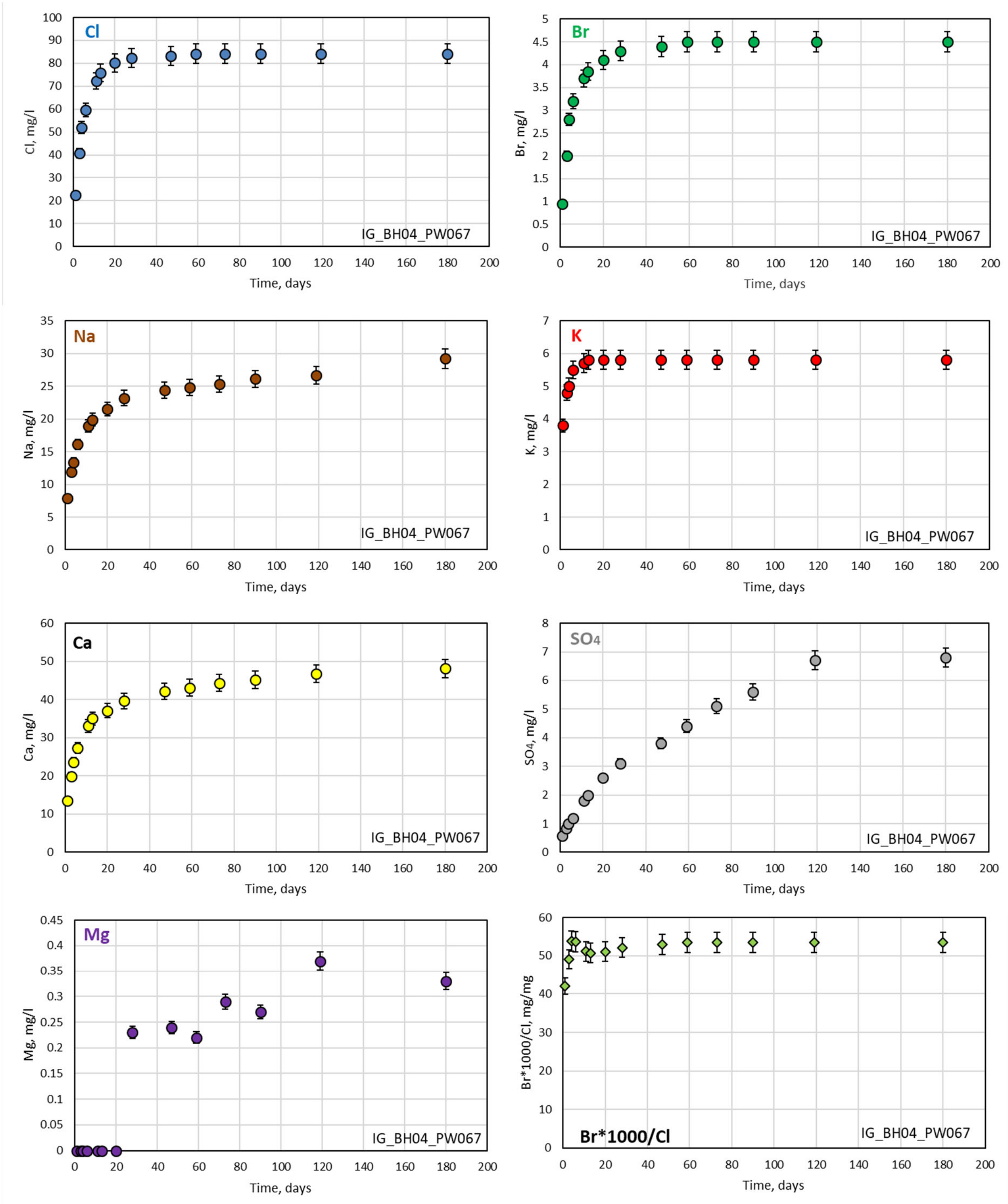


Figure 6-1 continued

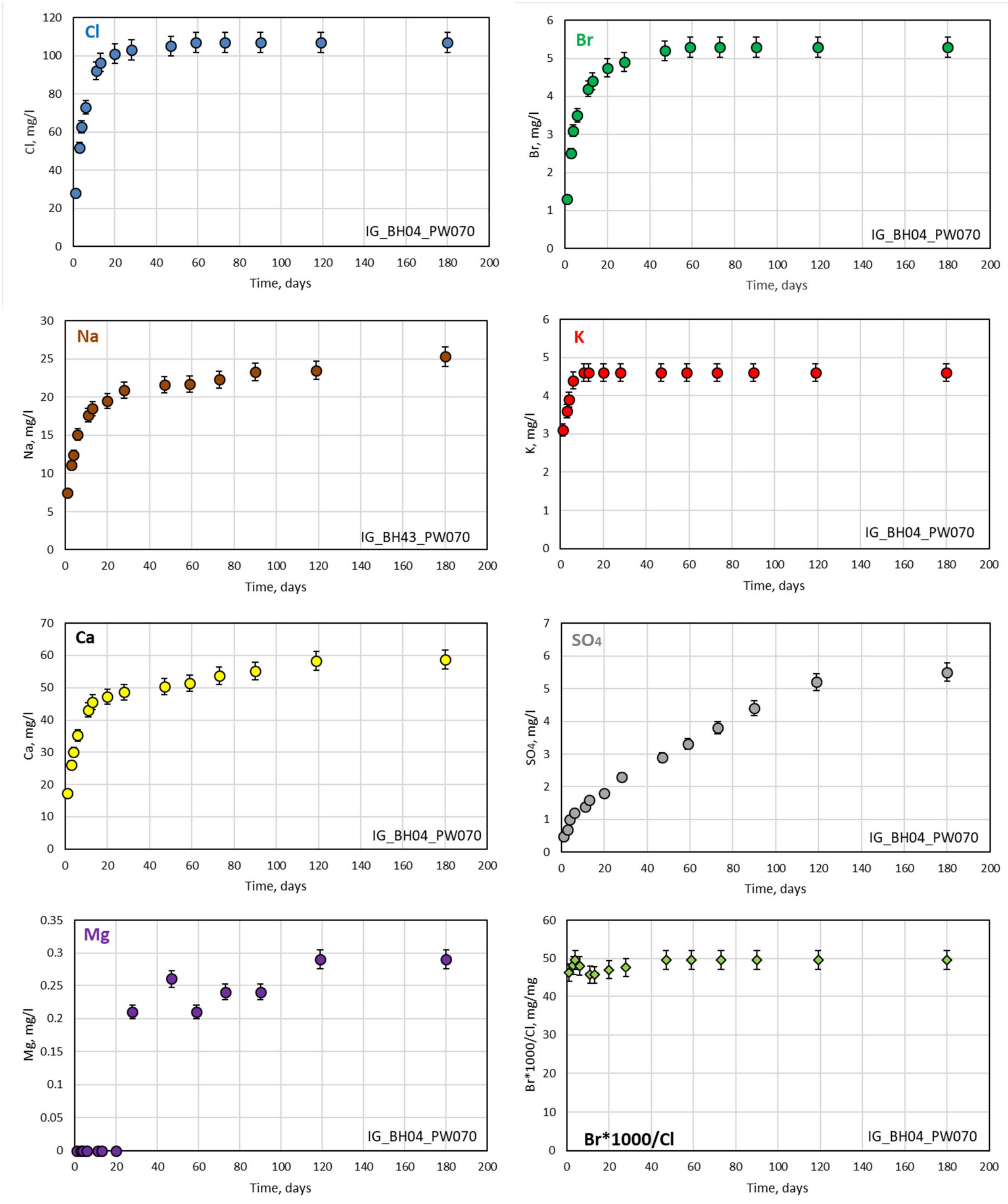


Figure 6-1 continued

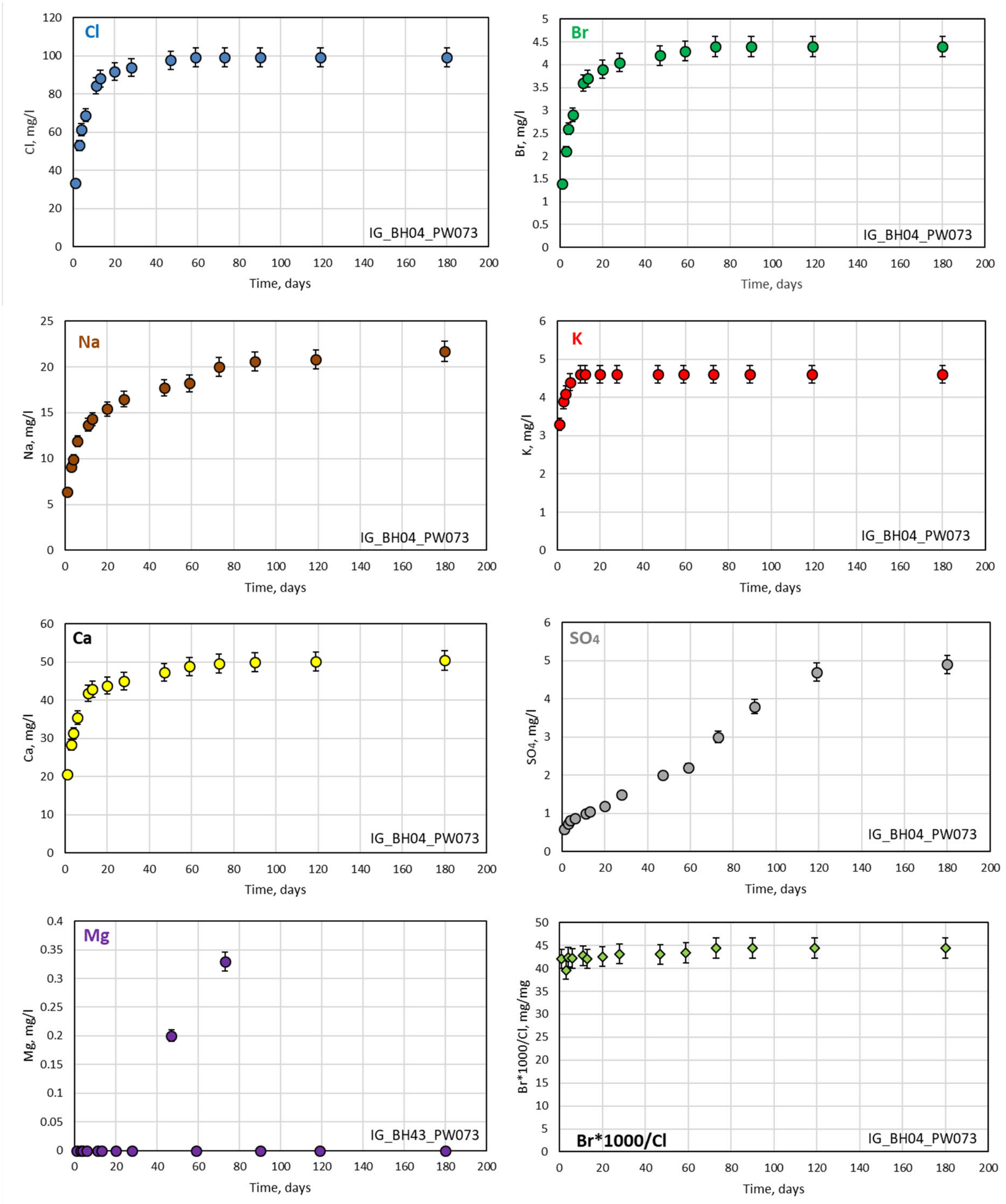


Figure 6-1 continued

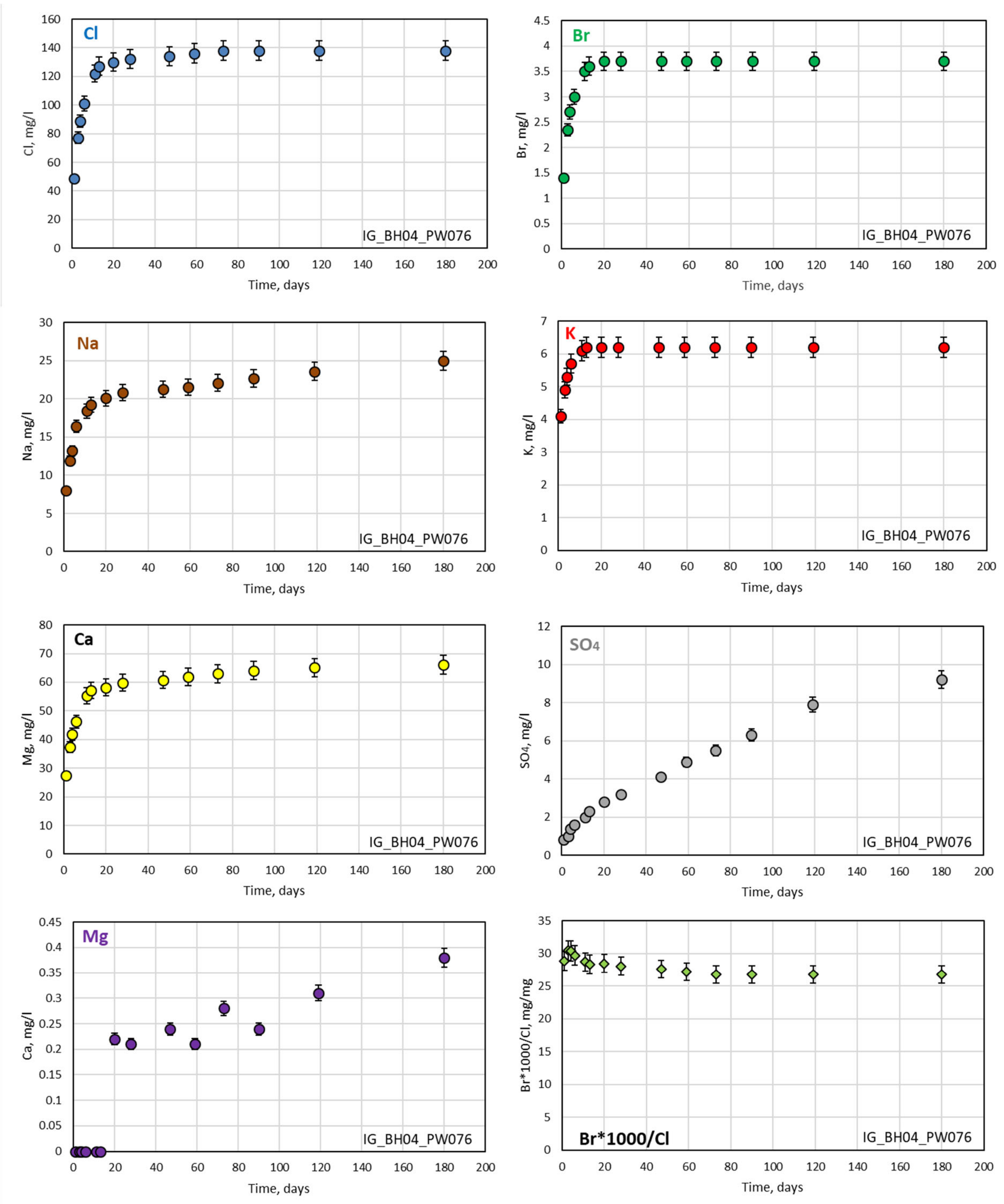


Figure 6-1 continued

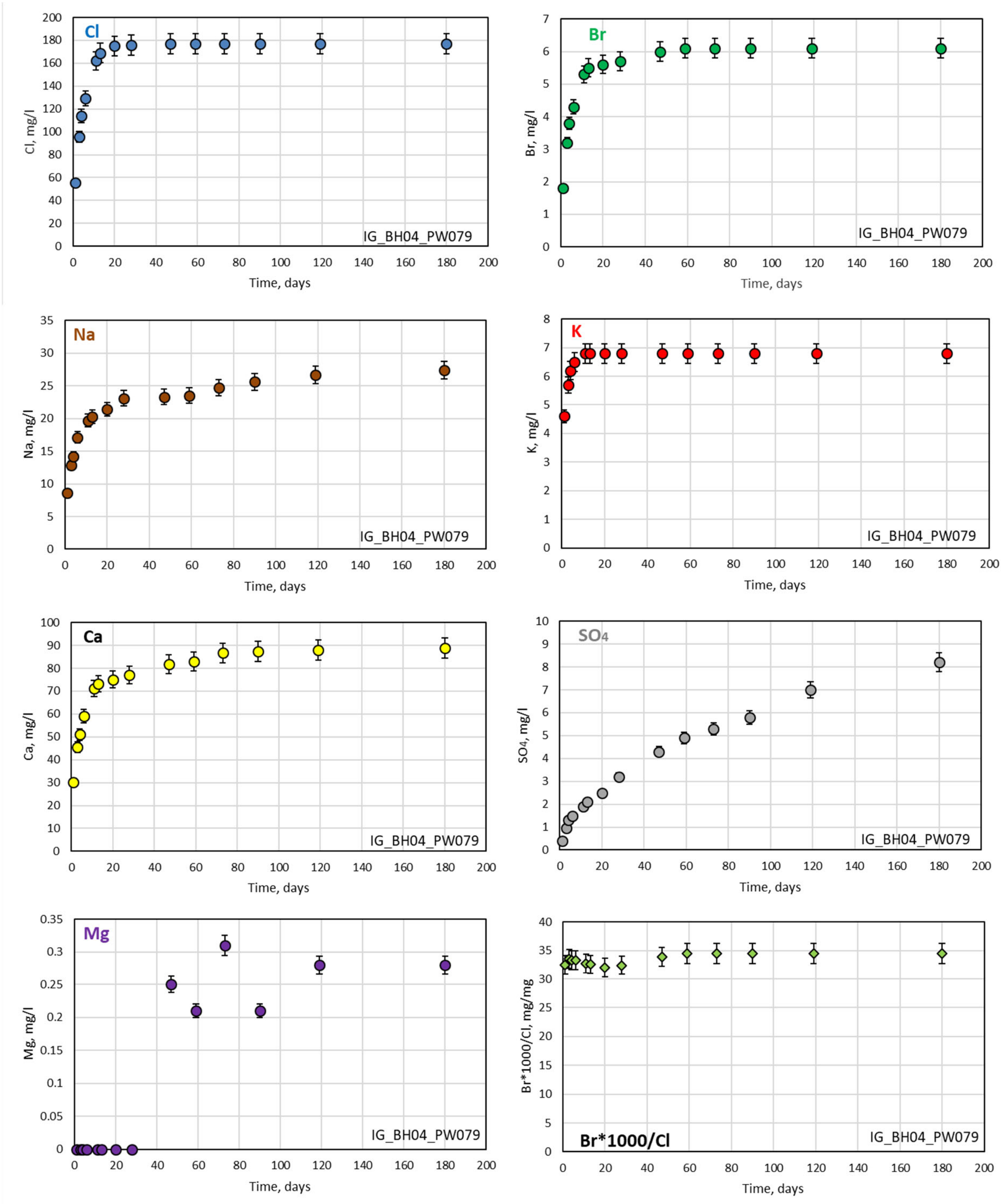


Figure 6-1 continued

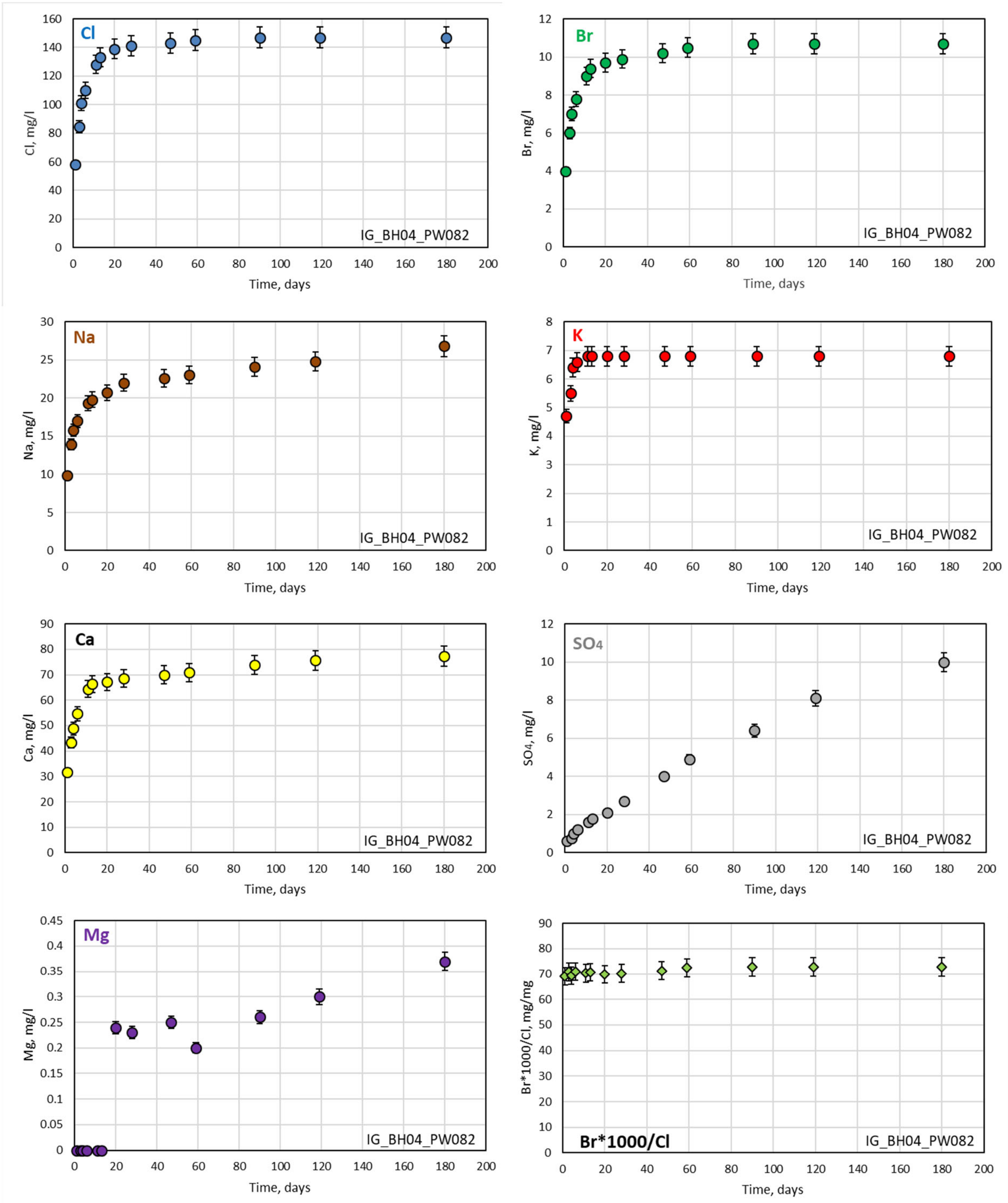


Figure 6-1 continued

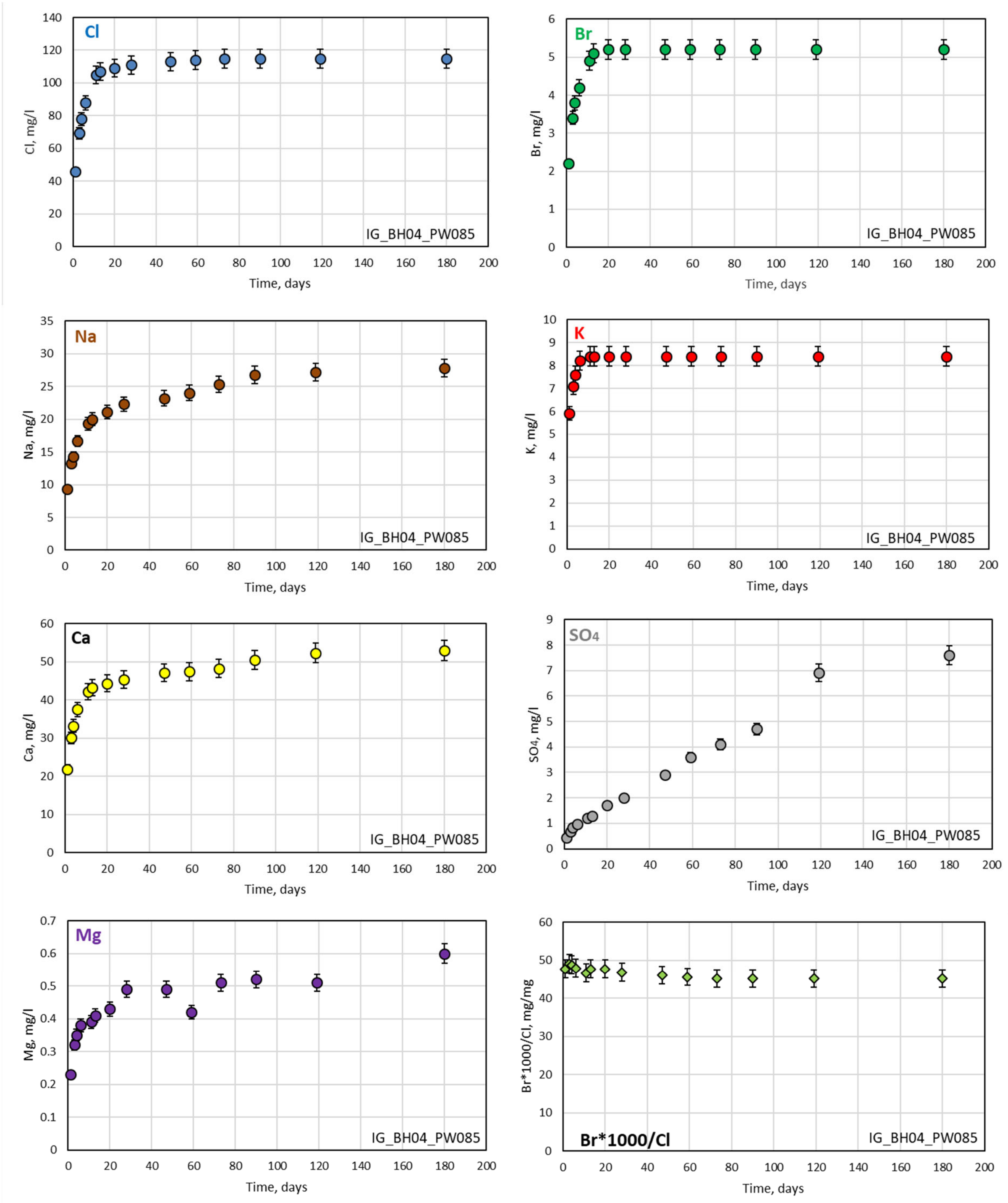


Figure 6-1 continued

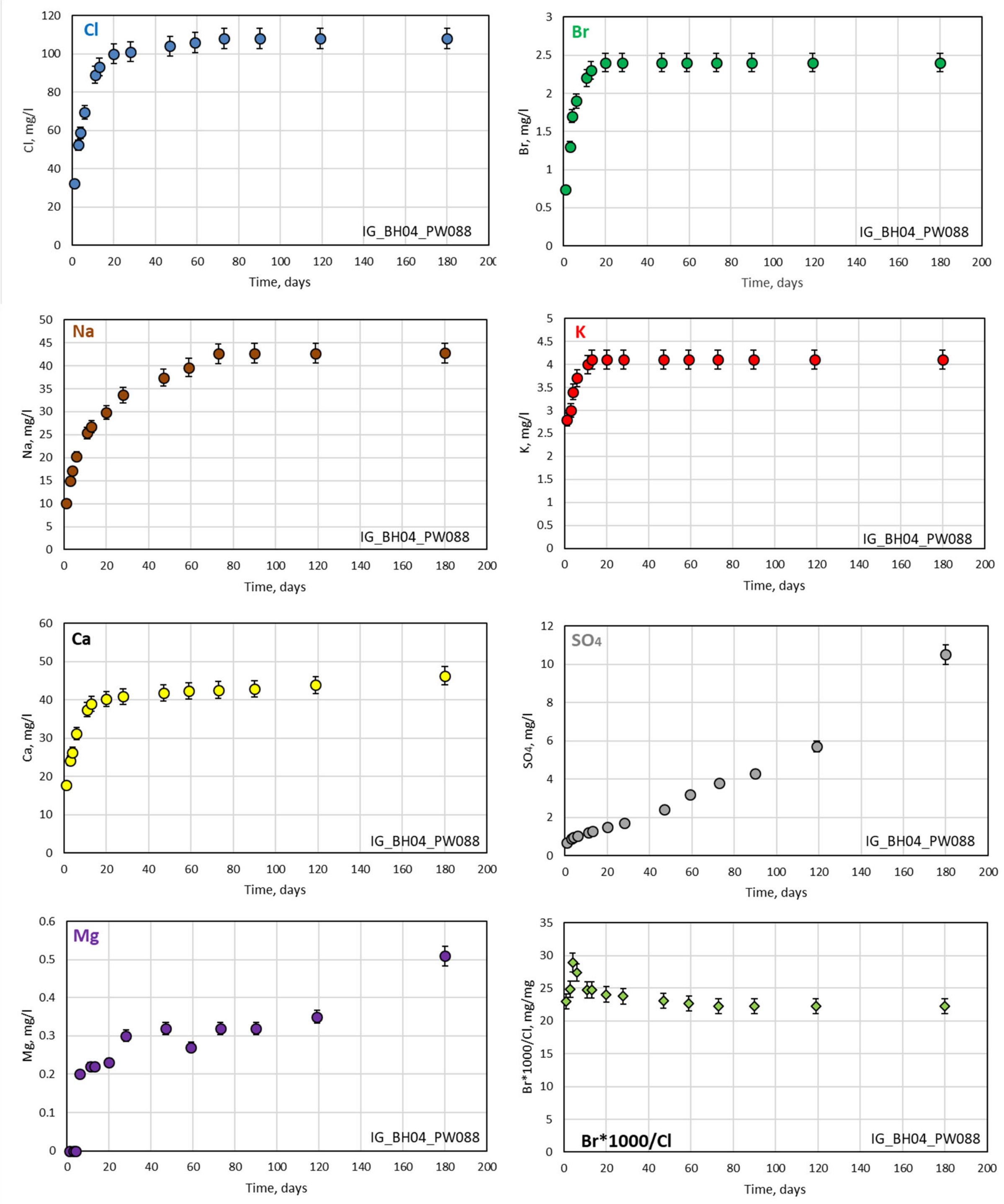


Figure 6-1 continued

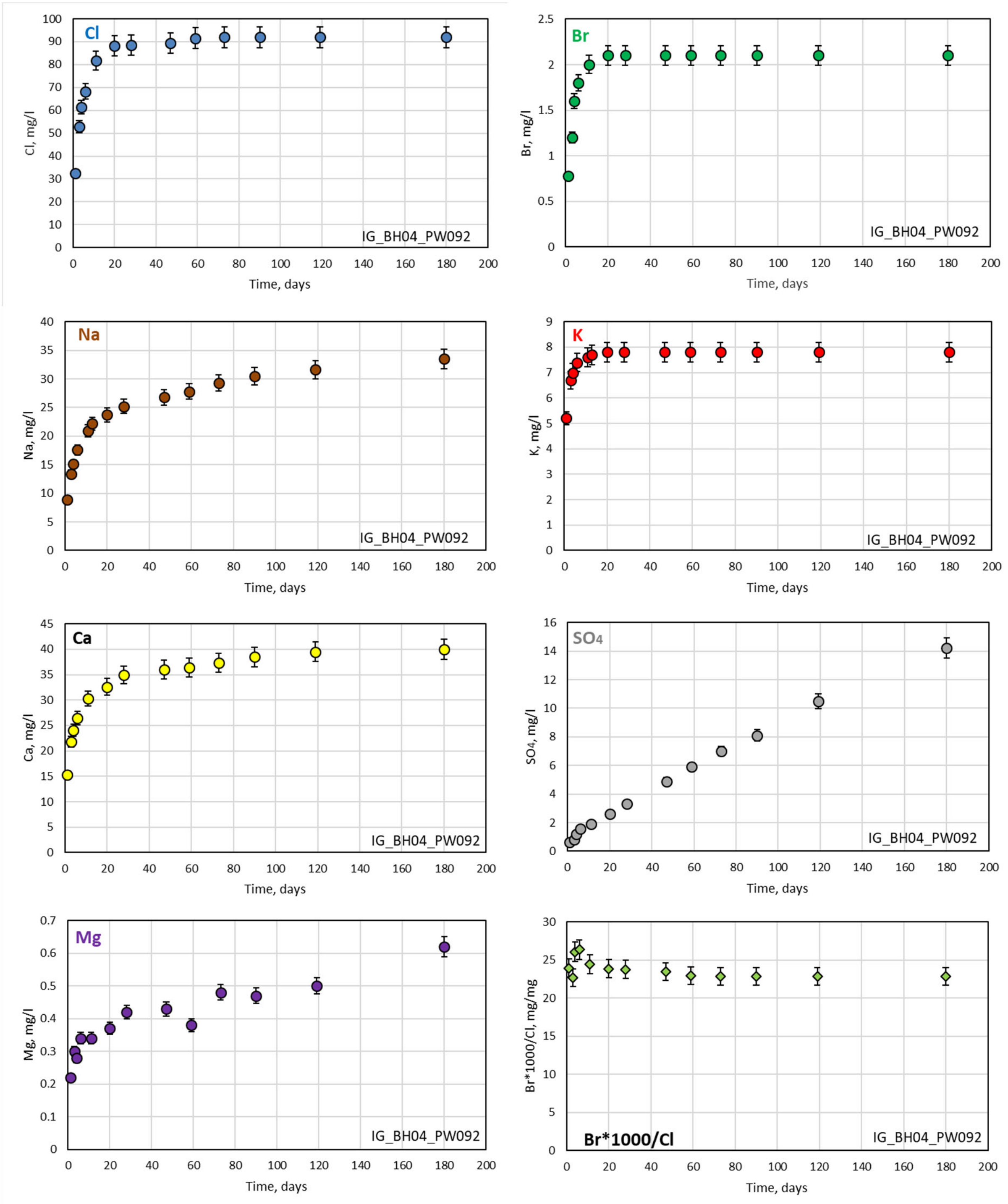


Figure 6-1 continued

6.2 Modelling of Pore Diffusion Coefficients

Chloride pore diffusion coefficients were derived by modelling the chloride breakthrough curves obtained from the out-diffusion experiments of all 31 samples from borehole IG_BH04. The chloride breakthrough curves are deduced from the Cl contents in the small-sized sub-samples that were collected periodically during the out-diffusion experiments (Section 3.3.2, 6.1). The pore diffusion coefficient is obtained by fitting the observed data with an analytical solution for one-dimensional radial diffusion out of the cylinder into a well-mixed solution reservoir (Crank 1975). The applied model (T. Gimmi, RWI, University of Bern) is restricted to homogeneous hydraulic properties (porosity, diffusion coefficient) across the core cylinder, and cannot consider heterogeneous properties due to rock anisotropy or induced effects, such as a drilling disturbed zone and/or stress release (Meier et al., 2015).

The pore diffusion coefficient, D_p, of a solute in a geological media mainly depends on the shape and size of water conducting pores (constrictivity) and on the pathways given by the connected pore network (tortuosity, e.g., Ohlsson and Neretnieks 1995). It can be defined as

$$D_p = D_w \frac{\delta_D}{\tau^2} \qquad \text{eq. 8}$$

where D_P = pore-diffusion coefficient in m^2/s, D_W = diffusion coefficient in pure water in m^2/s, δ_D = constrictivity, τ = tortuosity, and the term δ_D/τ^2 is called the geometry factor.

In a first assumption the pore diffusion coefficient of a given species, D_P, can be converted to the effective diffusion coefficient of this species, D_e, according to

$$D_e = D_p \Phi_{WC} \qquad \text{eq. 9}$$

where D_e is the effective diffusion coefficient in m^2/s and Φ_{WC} the species-accessible porosity.

The shape of the Cl elution curves obtained for all core samples from borehole IG_BH04 suggests a heterogeneous transport system from the rim to the centre of the core (Figure 6-2). The initial slopes are steeper (in the transient state) during the first five to ten days of out-diffusion than the more moderate slopes observed later in the experiments.

The quality of the D_P fits is controlled by the difference ($\Delta_{meas-mod}$) of the measured and modelled Cl concentration at equal time and shown graphically by logarithmic plots (Figure 6-2). To determine the lowest $\Delta_{meas-mod}$ values, a stepwise adjustment (±0.5*10^{-10}m$^{2/}$s) of the single points was conducted and the $\Delta_{meas-mod}$ values were calculated for every measured point. The determination of the best fits per sampling point indicates a gradual decrease of the modelled pore diffusion coefficients as diffusion progresses deeper into the cores.

The modelled D_P values, which were determined at 45 °C, are additionally converted to 10 °C and 25°C by the Stoke-Einstein equation (Lide 1994).

For the investigated core samples, the influence of the disturbed zone results in a pore diffusion coefficient that is a factor 1.5 to 4.0 higher than that of the inner core (Table 6-1, Figure 6-2).

The average pore diffusion coefficients (DP) of the 31 crystalline core samples vary between 0.7 and 1.6*10 10 m^2/s (10 °C), resulting in effective diffusion coefficients (De) between 0.3 and 0.8*10 12 m2/s (10 °C) (Table 6 1, Figure 6-1).

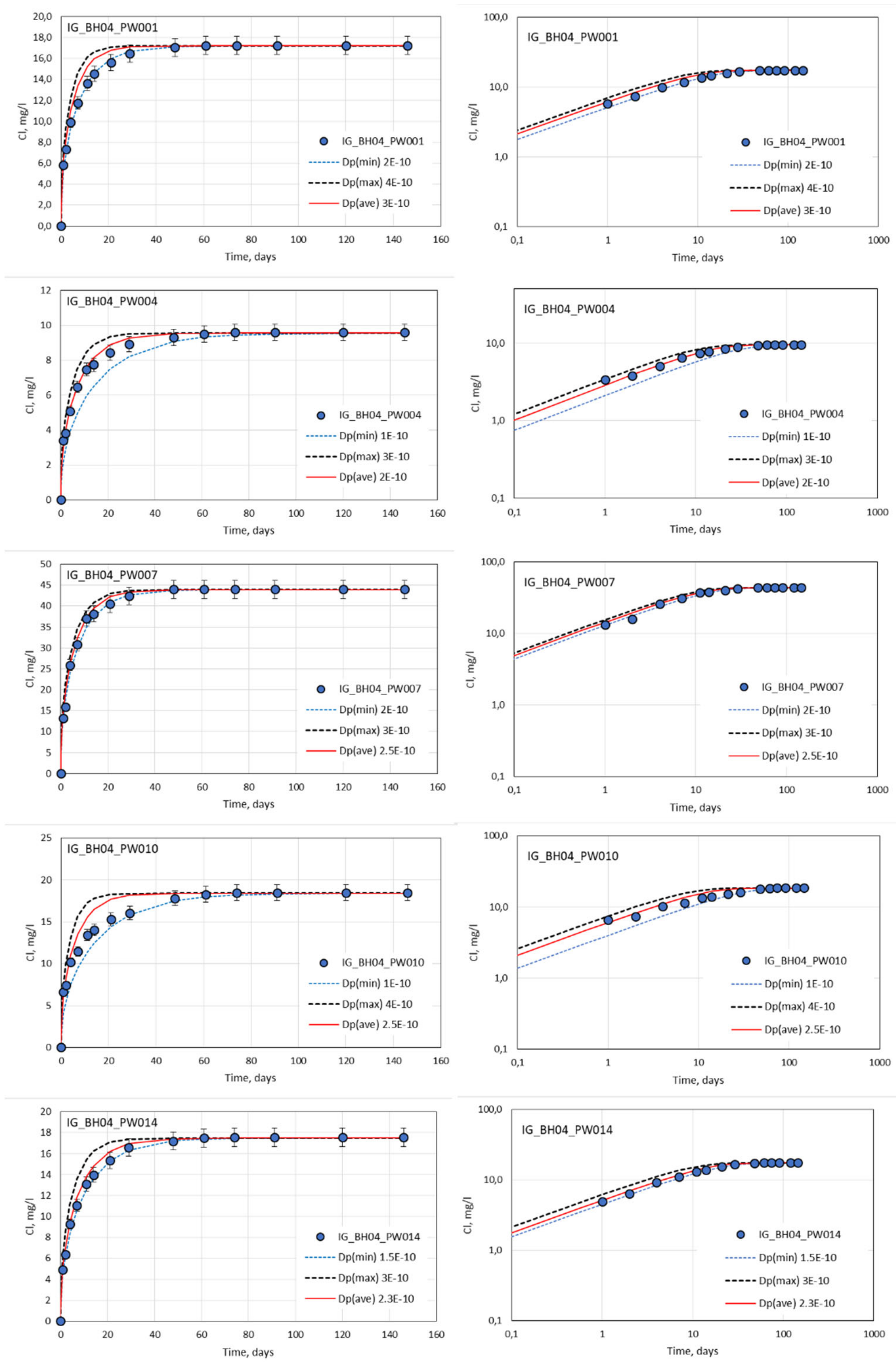


Figure 6-2: Maximum (Dp(max)) and minimum (Dp(min)) pore diffusion coefficients (45 °C) determined ba a best fit of Cl elution curves in linear and logarithmic time and concentration scale; the solid lines mark the average diffusion coefficients (45 °C, Dp (ave))

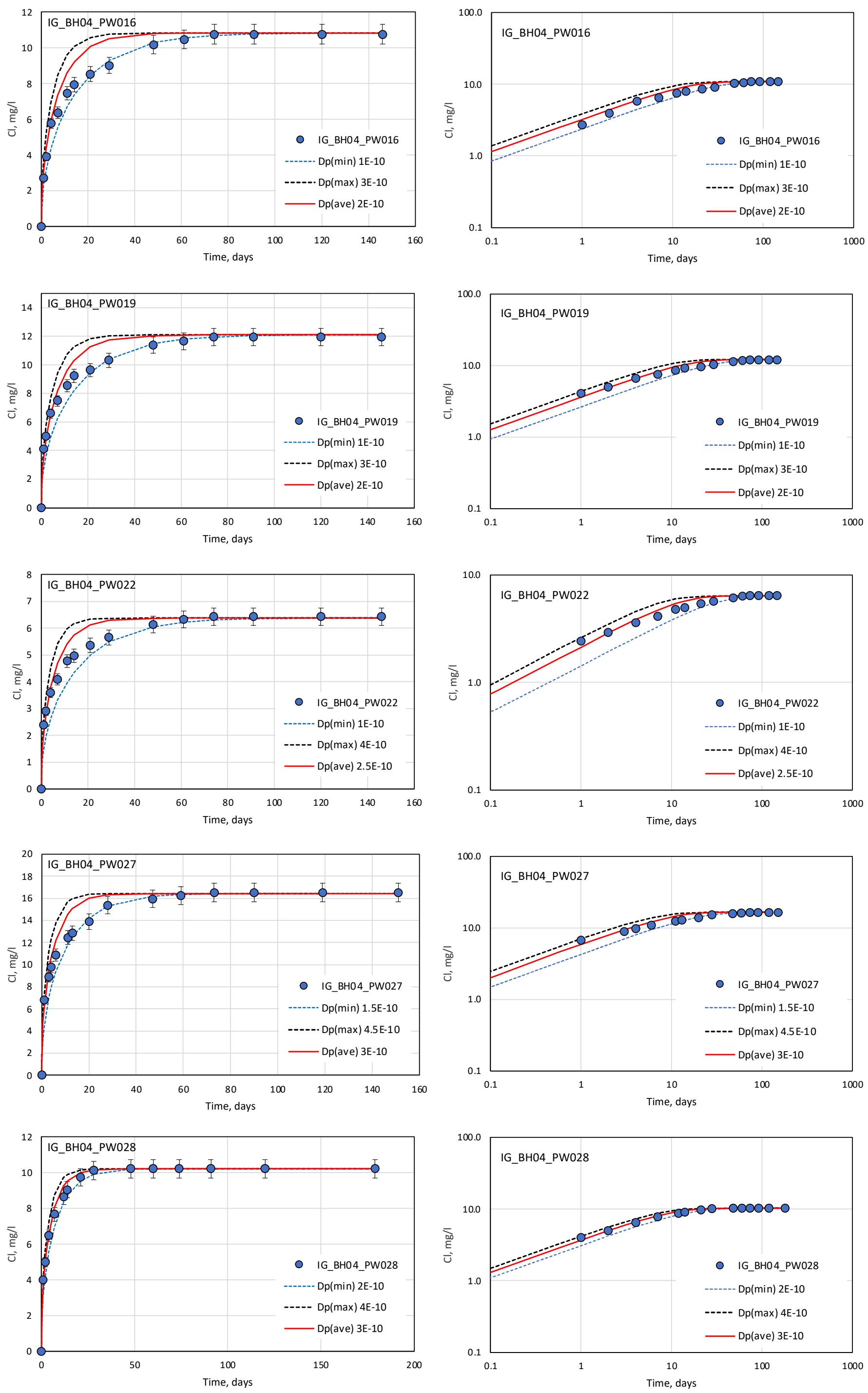


Figure 6-2 continued

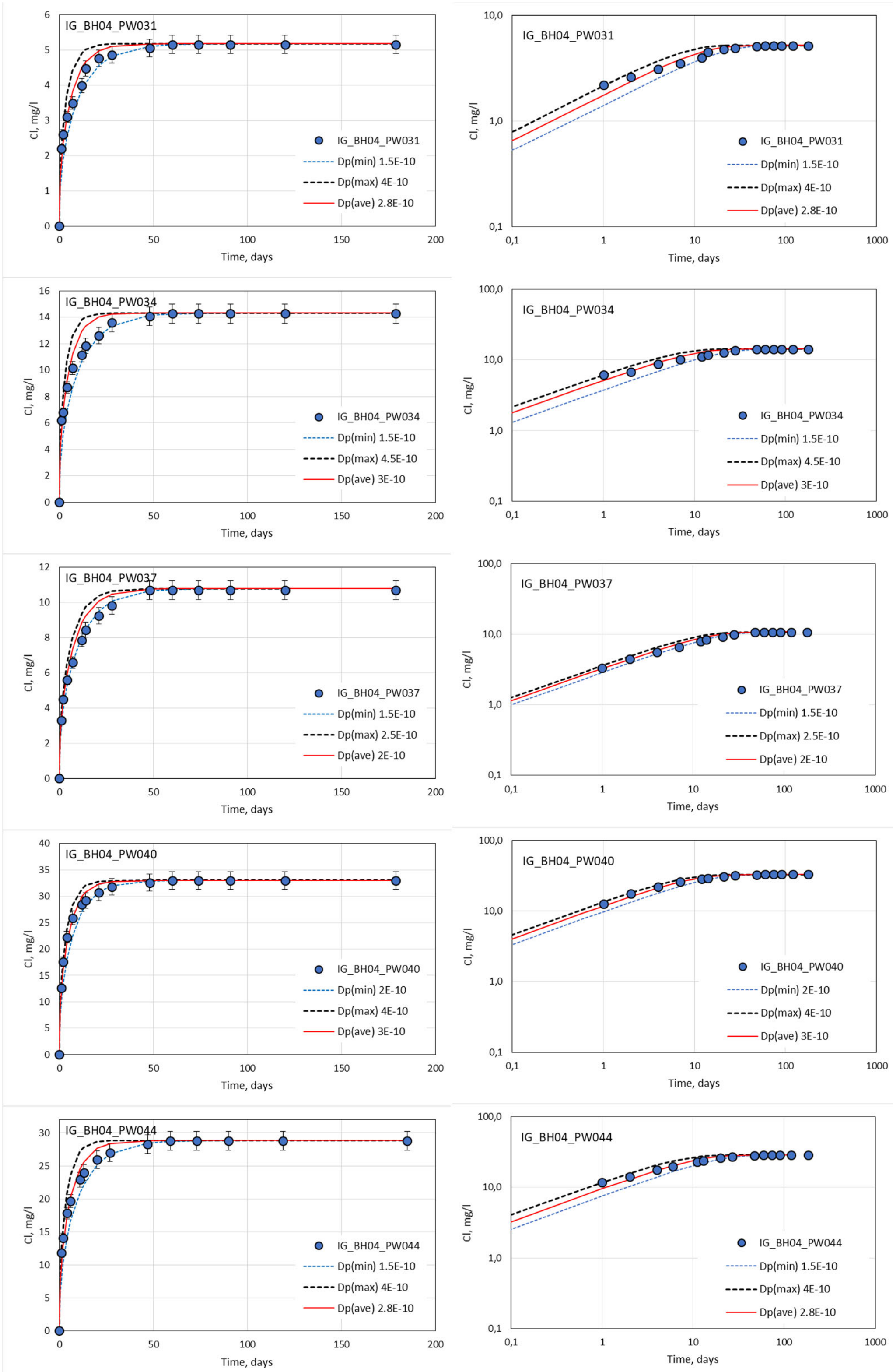


Figure 6-2 continued

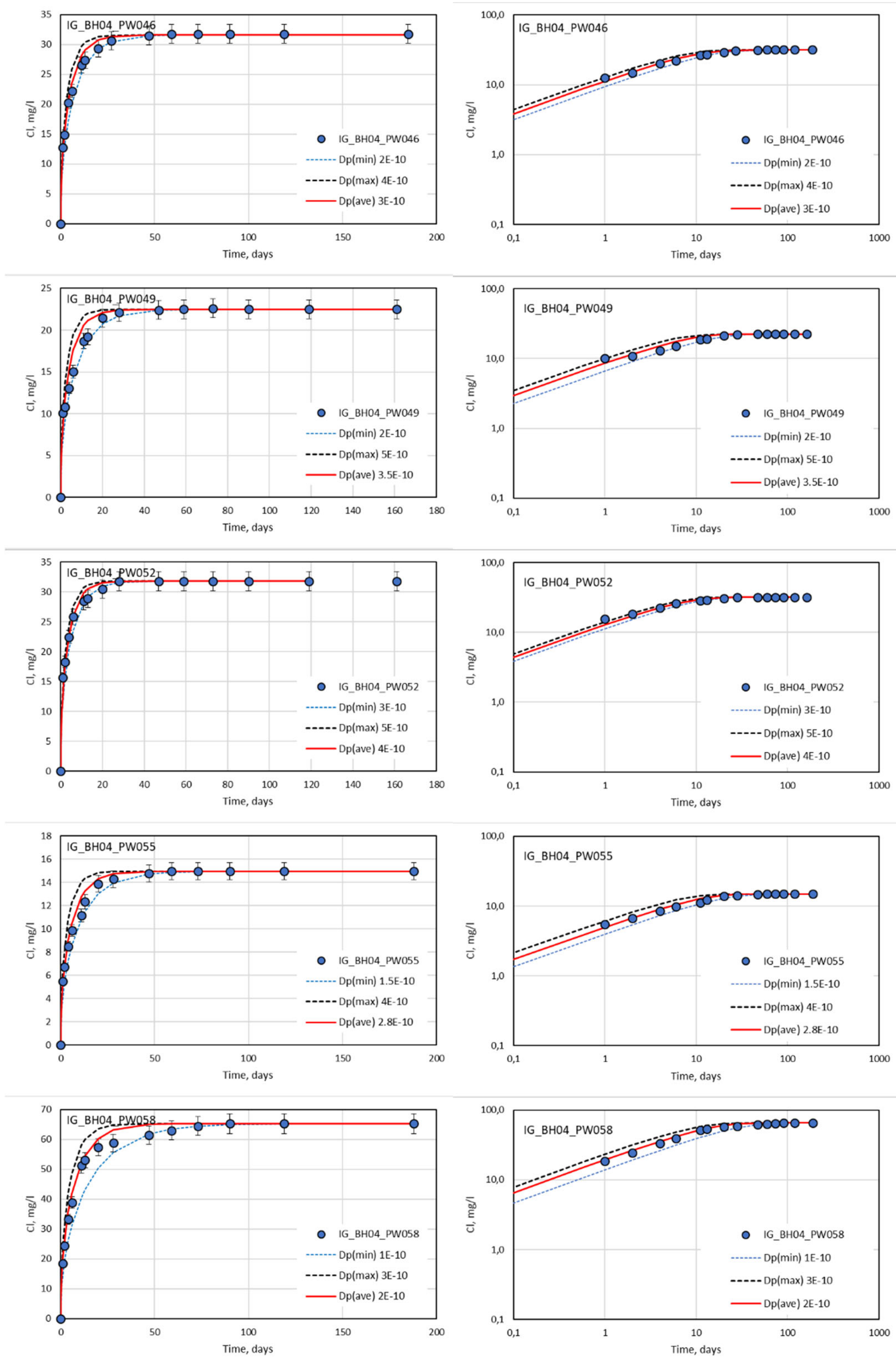


Figure 6-2 continued

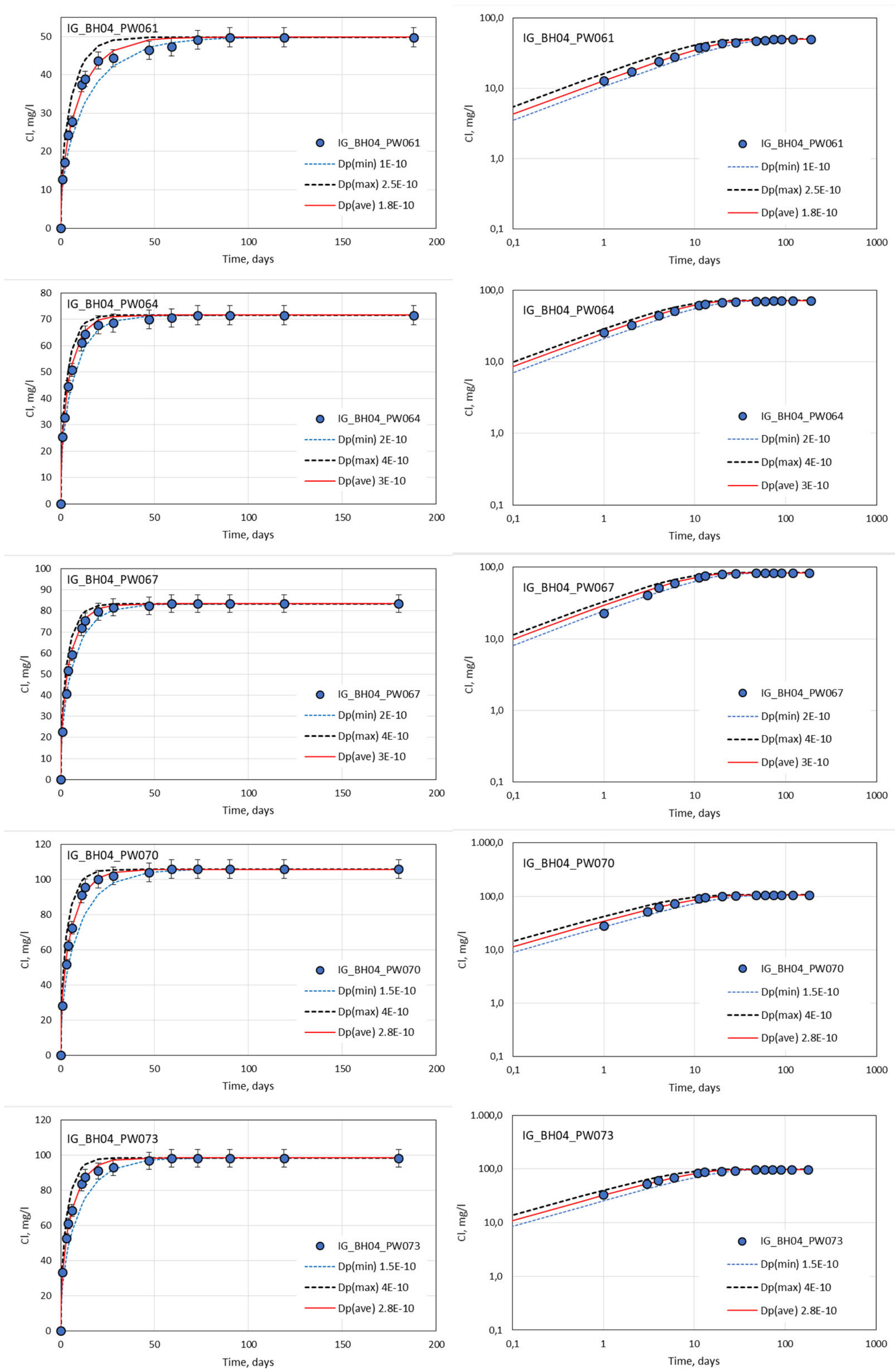


Figure 6-2 continued

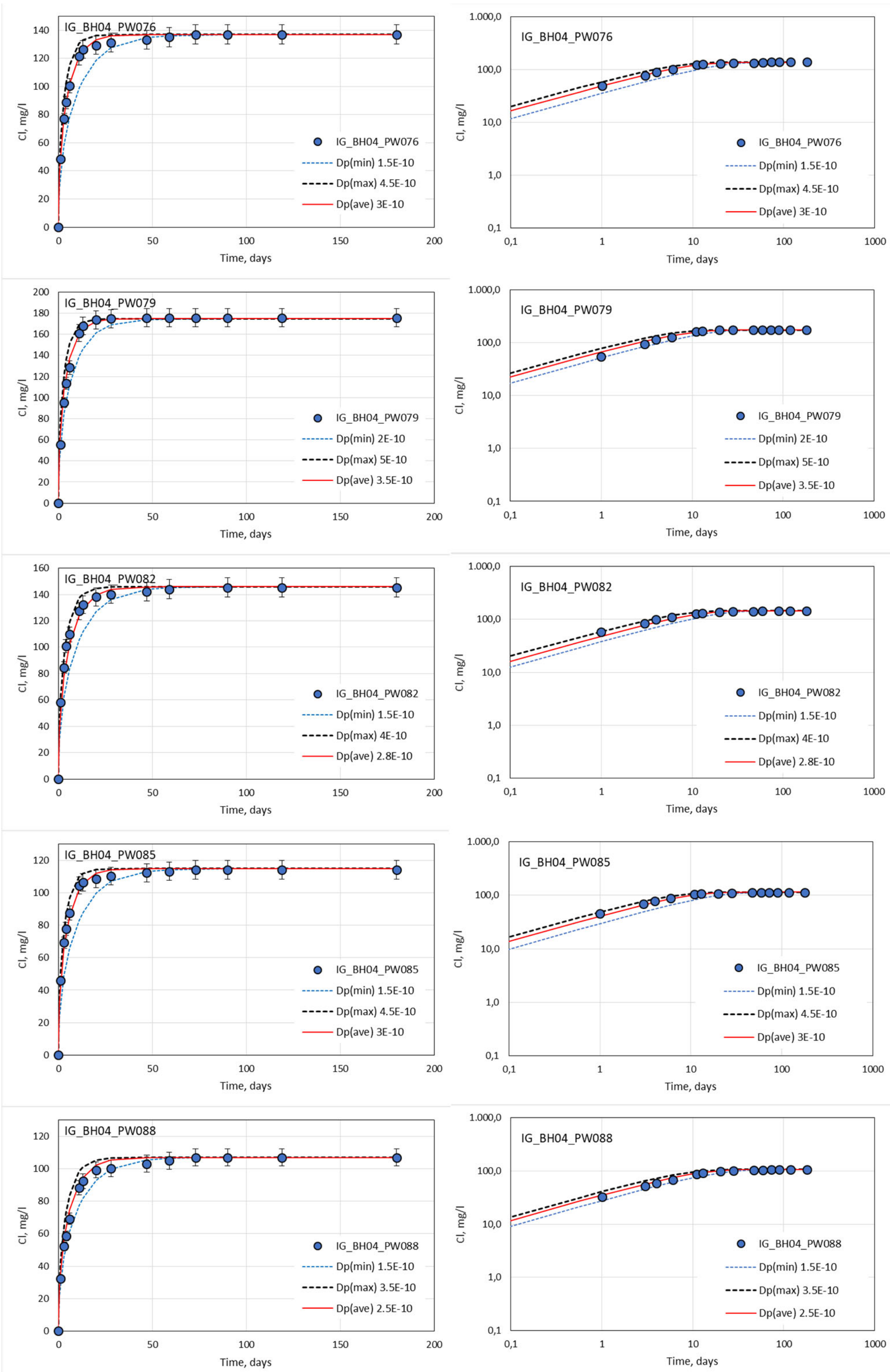
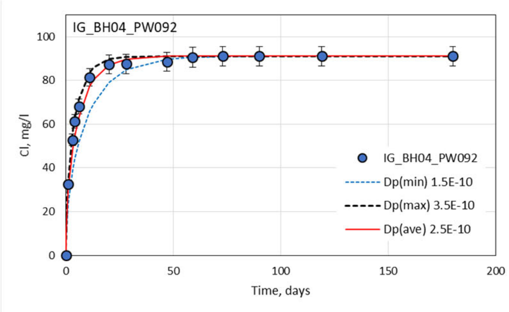


Figure 6-2 continued



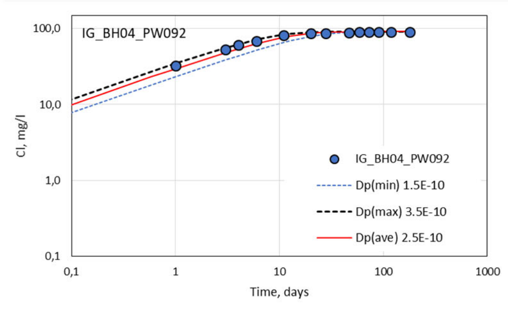


Figure 6-2 continued

Table 6-1: Minimum (min), maximum (max) and average (ave) pore and effective diffusion coefficients determined by 1-dimensional modelling of Cl elution curves of out-diffusion experiments on core samples from IG_BH04 at 45 °C and calculated by the Stoke-Einstein-equation for 10 °C and 25 °C

Sample	Depth	WL-Porosity	$D(P)*10^{-10}$ (45 °C)			$D(P)*10^{-10}$ (10 °C)			$D(e)*10^{-12}$ (10 °C)			$D(P)*10^{-10}$ (25 °C)			$D(e)*10^{-12}$ (25 °C)		
			max	min	ave	max	min	ave	max	min	ave	max	min	ave	max	min	ave
	mbgs	Vol.%	m^2/s			m^2/s			m^2/s			m^2/s			m^2/s		
IG_BH04_PW001	162.5	0.45	2.0	4.0	3.0	0.8	1.6	1.2	0.4	0.7	0.5	1.3	2.5	1.9	0.6	1.1	0.8
IG_BH04_PW004	167.4	0.44	1.0	3.0	2.0	0.4	1.2	0.8	0.2	0.5	0.4	0.6	1.9	1.3	0.3	0.8	0.6
IG_BH04_PW007	213.2	0.46	2.0	3.0	2.5	0.8	1.2	1.0	0.4	0.6	0.5	1.3	1.9	1.6	0.6	0.9	0.7
IG_BH04_PW010	236.4	0.52	1.0	4.0	2.5	0.4	1.6	1.0	0.2	0.8	0.5	0.6	2.5	1.6	0.3	1.3	0.8
IG_BH04_PW014	267.7	0.40	1.5	3.0	2.3	0.6	1.2	0.9	0.2	0.5	0.4	0.9	1.9	1.4	0.4	0.7	0.6
IG_BH04_PW016	293.4	0.47	1.0	3.0	2.0	0.4	1.2	0.8	0.2	0.6	0.4	0.6	1.9	1.3	0.3	0.9	0.6
IG_BH04_PW019	317.4	0.54	1.0	3.0	2.0	0.4	1.2	0.8	0.2	0.7	0.4	0.6	1.9	1.3	0.3	1.0	0.7
IG_BH04_PW022	347.4	0.40	1.0	4.0	2.5	0.4	1.6	1.0	0.2	0.7	0.4	0.6	2.5	1.6	0.3	1.0	0.6
IG_BH04_PW027	372.2	0.41	1.5	4.5	3.0	0.6	1.8	1.2	0.2	0.7	0.5	0.9	2.8	1.9	0.4	1.1	0.8
IG_BH04_PW028	397.8	0.41	2.0	4.0	3.0	0.8	1.6	1.2	0.3	0.7	0.5	1.3	2.5	1.9	0.5	1.0	0.8
IG_BH04_PW031	423.6	0.45	1.5	4.0	2.8	0.6	1.6	1.1	0.3	0.7	0.5	0.9	2.5	1.7	0.4	1.1	0.8
IG_BH04_PW034	450.9	0.41	1.5	4.5	3.0	0.6	1.8	1.2	0.2	0.7	0.5	0.9	2.8	1.9	0.4	1.2	0.8
IG_BH04_PW037	478.1	0.38	1.5	2.5	2.0	0.6	1.0	0.8	0.2	0.4	0.3	0.9	1.6	1.3	0.4	0.6	0.5
IG_BH04_PW040	505.1	0.46	2.0	4.0	3.0	0.8	1.6	1.2	0.4	0.7	0.6	1.3	2.5	1.9	0.6	1.1	0.9
IG_BH04_PW044	531.9	0.46	1.5	4.0	2.8	0.6	1.6	1.1	0.3	0.8	0.5	0.9	2.5	1.7	0.4	1.2	0.8
IG_BH04_PW046	561.3	0.41	2.0	4.0	3.0	0.8	1.6	1.2	0.3	0.7	0.5	1.3	2.5	1.9	0.5	1.0	0.8
IG_BH04_PW049	586.2	0.53	2.0	5.0	3.5	0.8	2.0	1.4	0.4	1.1	0.8	1.3	3.1	2.2	0.7	1.7	1.2
IG_BH04_PW052	614.4	0.48	3.0	5.0	4.0	1.2	2.0	1.6	0.6	1.0	0.8	1.9	3.1	2.5	0.9	1.5	1.2
IG_BH04_PW055	636.8	0.40	1.5	4.0	2.8	0.6	1.6	1.1	0.2	0.6	0.4	0.9	2.5	1.7	0.4	1.0	0.7
IG_BH04_PW058	665.4	0.40	1.0	3.0	2.0	0.4	1.2	0.8	0.2	0.5	0.3	0.6	1.9	1.3	0.3	0.8	0.5
IG_BH04_PW061	692.4	0.36	1.0	2.5	1.8	0.4	1.0	0.7	0.1	0.4	0.3	0.6	1.6	1.1	0.2	0.6	0.4
IG_BH04_PW064	711.3	0.35	2.0	4.0	3.0	0.8	1.6	1.2	0.3	0.6	0.4	1.3	2.5	1.9	0.4	0.9	0.7
IG_BH04_PW067	746.3	0.32	2.0	4.0	3.0	0.8	1.6	1.2	0.3	0.5	0.4	1.3	2.5	1.9	0.4	0.8	0.6
IG_BH04_PW070	771.6	0.38	1.5	4.0	2.8	0.6	1.6	1.1	0.2	0.6	0.4	0.9	2.5	1.7	0.4	0.9	0.6
IG_BH04_PW073	795.3	0.53	1.5	4.0	2.8	0.6	1.6	1.1	0.3	0.9	0.6	0.9	2.5	1.7	0.5	1.3	0.9
IG_BH04_PW076	825.3	0.51	1.5	4.5	3.0	0.6	1.8	1.2	0.3	0.9	0.6	0.9	2.8	1.9	0.5	1.4	1.0
IG_BH04_PW079	849.3	0.48	2.0	5.0	3.5	0.8	2.0	1.4	0.4	1.0	0.7	1.3	3.1	2.2	0.6	1.5	1.0
IG_BH04_PW082	877.8	0.54	1.5	4.0	2.8	0.6	1.6	1.1	0.3	0.9	0.6	0.9	2.5	1.7	0.5	1.3	0.9
IG_BH04_PW085	904.0	0.40	1.5	4.5	3.0	0.6	1.8	1.2	0.2	0.7	0.5	0.9	2.8	1.9	0.4	1.1	0.7
IG_BH04_PW088	931.1	0.46	1.5	3.5	2.5	0.6	1.4	1.0	0.3	0.6	0.5	0.9	2.2	1.6	0.4	1.0	0.7
IG_BH04_PW092	959.0	0.38	1.5	3.5	2.5	0.6	1.4	1.0	0.2	0.5	0.4	0.9	2.2	1.6	0.4	0.8	0.6

7.0 CHLORIDE, BROMIDE AND CHLORIDE ISOTOPES IN POREWATER OF CORE SAMPLES FROM BOREHOLE IG_BH04

Chloride and bromide concentrations of porewater were determined by aqueous extraction experiments (Section 3.3.1) and out-diffusion experiments (Section 3.3.2). Aqueous extraction experiments were conducted prior to the other longer-term experiments to obtain preliminary information about porewater salinities.

7.1 Porewater Chloride Concentrations Estimated by Aqueous Extraction Experiments

Aqueous extraction experiments were conducted on 31 core samples from each of the sampled depth intervals. Approximate estimates of porewater Cl concentrations were calculated according to equation 3 (Section 3.3.1). During crushing of the rock samples, saline fluids from fluid inclusions in quartz and feldspar are released, which contribute to the Cl and Br inventory of the samples. This means that the chloride concentrations determined by aqueous extraction overestimate the actual porewater Cl concentrations.

Estimated porewater Cl concentrations for core samples from borehole IG_BH04 determined by aqueous extractions vary between 2.0 and 9.5 g/kg H_2O (Table 7-1, Figure 7-1).

Based on the Cl concentration range of porewater in core samples taken from borehole IG_BH04 (2.0 – 9.5 g/kg H_2O = 0.06 - 0.28 mol), the salinity of the isotope diffusive exchange experiment solutions was defined at 0.3 mol NaCl (see Section 8.0).

#

Table 7-1: Porewater Cl and Br concentrations and Br*1000/Cl mass ratios estimated using aqueous extraction experiments; the errors of porewater Cl and Br concentrations and Br*1000/Cl mass ratios are calculated by Gaussian error propagation (Appendix C)

Sample	Depth	Estimated ClPW (aq.ex.)	Estimated BrPW (aq.ex.)	Estimated Br*1000/Cl (aq.ex.)
	mbgs*	mg/kg H_2O	mg/kg H_2O	mg/mg
IG_BH04_PW003	163.7	3610	415	115
IG_BH04_PW006	168.1	3760	226	60
IG_BH04_PW009	213.9	4688	100	21
IG_BH04_PW011	238.0	4579	1068	233
IG_BH04_PW015	268.0	3186	381	120
IG_BH04_PW018	294.5	2851	169	59
IG_BH04_PW021	318.1	2727	74	27
IG_BH04_PW024	348.2	2862	42	15
IG_BH04_PW030	397.1	2563	220	86
IG_BH04_PW033	424.2	3330	58	17
IG_BH04_PW036	451.5	2960	191	65
IG_BH04_PW039	478.8	3761	291	77
IG_BH04_PW042	505.7	2772	70	25
IG_BH04_PW045	532.5	4598	664	144
IG_BH04_PW048	561.9	5704	292	51
IG_BH04_PW051	585.9	3052	284	93
IG_BH04_PW054	615.4	3545	475	134
IG_BH04_PW057	637.5	1978	99	50
IG_BH04_PW060	666.1	4418	161	36
IG_BH04_PW063	693.1	6428	918	143
IG_BH04_PW066	712.1	6077	608	100

Sample	Depth	Estimated ClPW (aq.ex.)	Estimated BrPW (aq.ex.)	Estimated Br*1000/Cl (aq.ex.)
	mbgs*	mg/kg H_2O	mg/kg H_2O	mg/mg
IG_BH04_PW069	747.0	7297	702	96
IG_BH04_PW072	772.3	3908	181	46
IG_BH04_PW075	796.0	7513	584	78
IG_BH04_PW078	825.9	6477	284	44
IG_BH04_PW081	850.1	9383	381	41
IG_BH04_PW084	878.4	9479	1074	113
IG_BH04_PW087	904.7	7929	334	42
IG_BH04_PW090	932.1	4847	127	26
IG_BH04_PW093	959.3	7660	234	31

Note(s)
41 [mbgs (downhole)]

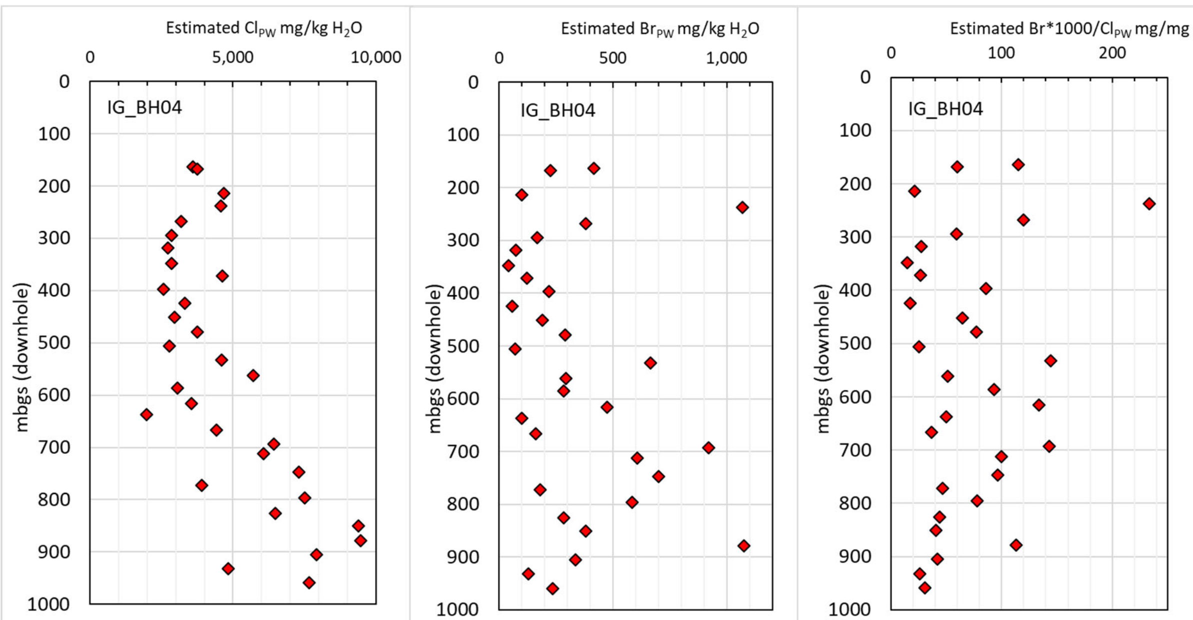


Figure 7-1: Borehole IG_BH04: Estimated porewater Cl and Br concentrations and Br*1000/Cl mass ratios verus depth by aqueous extraction experiments

#

7.2 Porewater Chloride Concentrations Estimated by Out-diffusion Experiments

The conservative behaviour of chloride and bromide, the absence of Cl- and Br-bearing minerals in the rock, and the non-destructive character of the out-diffusion method, make the porewater the only source for dissolved Cl and Br in the experimental solutions. This allows calculation of the Cl and Br concentration in the porewaters by mass balance according to equation 4 (Section 3.3.2), given that equilibrium in the out-diffusion experiments is achieved. As shown by their chloride and bromide elution curves, this latter condition is fulfilled for all samples (Section 6.1).

The mass ratio of the two conservative elements, Cl and Br, can serve as a tracer of the origin of Cl and Br in porewater and fracture groundwater. The $\delta^{37}Cl$ ratio measured for the experiment solutions directly corresponds to the porewater Cl isotope signature. This is because the attained equilibrium in the out-diffusion experiment with respect to total Cl is also expected to result in equilibrium with respect to the Cl isotopes (Gimmi and Waber 2004).

Chloride concentrations of porewater taken between 162.2 mbgs and 959.0 mbgs from borehole IG_BH04 vary between 245 and 6,070 mg/kg H_2O (Table 7-2, Figure 7-2). Porewater bromide concentrations of the same respective samples from borehole IG_BH04 vary between 3.8 and 442 mg/kg H_2O (Table 7-2, Figure 7-2). The Br*1000/Cl mass ratios (=Br/Cl ratio) of porewater from borehole IG_BH04 vary between 15 and 230 (Table 7-2, Figure 7-2). In the bromide versus chloride diagram, porewaters extracted from borehole IG_BH04 cores plot significantly above the seawater dilution line (Br*1000/Cl mass ratio of seawater = 3.4, Figure 7-3).

Porewater δ^{37}Cl isotope signatures vary between -0.12±0.15 and 1.21±0.15 ‰ SMOC along the depth profile between 162.5 and 959.0 mbgs (downhole) (Table 7-2, Figure 7-2). Porewater stable chlorine isotope signatures do not show a trend that correlates with porewater Cl concentrations (see Figures 7-23 and 7-4).

#

Table 7-2: Porewater Cl and Br concentrations, Br*1000/Cl mass ratios and δ^{37}Cl isotope signatures. Cl concentrations are determined by out-diffusion experiments; the errors of porewater Cl and Br concentrations and Br*1000/Cl mass ratios are calculated by Gaussian error propagation (Appendix C); the errors of δ^{37}Cl values are the standard deviation of triplicate analyses

Sample	Depth	ClPW	BrPW	Br*1000/Cl	δ^{37}Cl
	mbgs*	mg/kg H_2O	mg/kg H_2O	mg/mg	‰ SMOC
IG_BH04_PW001	162.5	862±66	119±9	138±15	0.55±0.27
IG_BH04_PW004	167.4	447±37	64.5±5.4	144±17	0.49±0.15
IG_BH04_PW007	213.2	2173±253	58.7±6.8	27±4	1.21±0.15
IG_BH04_PW010	236.4	752±46	125±7.6	166±14	0.59±0.18
IG_BH04_PW014	267.7	985±125	227±29	230±41	1.06±0.20
IG_BH04_PW016	293.4	528±32	77.5±4.7	147±12	0.64±0.17
IG_BH04_PW019	317.4	527±29	9.6±0.5	18±1	0.39±0.15
IG_BH04_PW022	347.4	330±23	6.1±0.4	18±2	0.75±0.21
IG_BH04_PW027	372.2	810±50	32.0±2.0	40±3	0.38±0.18
IG_BH04_PW028	397.8	595±46	26.6±2.0	45±5	0.50±0.31
IG_BH04_PW031	423.6	255±19	3.9±0.3	15±2	0.47±0.34
IG_BH04_PW034	450.9	854±118	51.0±7.1	60±12	0.66±0.15
IG_BH04_PW037	478.1	737±40	25.9±1.4	35±3	0.46±0.18
IG_BH04_PW040	505.1	1946±220	55.7±6.3	29±5	0.86±0.18
IG_BH04_PW044	531.9	1853±177	236±23	128±17	0.64±0.23
IG_BH04_PW046	561.3	1929±181	84.4±7.9	44±6	0.87±0.15
IG_BH04_PW049	586.2	864±62	49.5±3.5	57±6	0.22±0.16
IG_BH04_PW052	614.4	1464±119	252±21	172±20	0.40±0.35
IG_BH04_PW055	636.8	796±47	14.8±0.9	19±2	0.12±0.15
IG_BH04_PW058	665.4	3240±394	123±15	38±7	0.32±0.26
IG_BH04_PW061	692.4	3305±499	184±28	56±12	0.68±0.20
IG_BH04_PW064	711.3	4262±393	254±23	59±8	0.48±0.14
IG_BH04_PW067	746.3	5417±975	290±52	53±14	0.33±0.35
IG_BH04_PW070	771.6	5571±832	276±41	50±10	0.35±0.15
IG_BH04_PW073	795.3	4448±310	198±14	44±4	0.34±0.27
IG_BH04_PW076	825.3	6004±671	161±18	27±4	0.72±0.30
IG_BH04_PW079	849.3	7993±947	276±33	34±6	0.34±0.24
IG_BH04_PW082	877.8	6230±560	454±41	73±9	0.03±0.15
IG_BH04_PW085	904.0	5985±349	271±16	45±4	0.18±0.15

Sample	Depth mbgs*	ClPW mg/kg H_2O	BrPW mg/kg H_2O	Br*1000/Cl mg/mg	$\delta^{37}Cl$ ‰ SMOC
IG_BH04_PW088	931.1	5049±362	112±8	22±2	0.35±0.18
IG_BH04_PW092	959.0	5390±476	123±11	23±3	-0.12±0.15

Note(s)
[mbgs (downhole)]

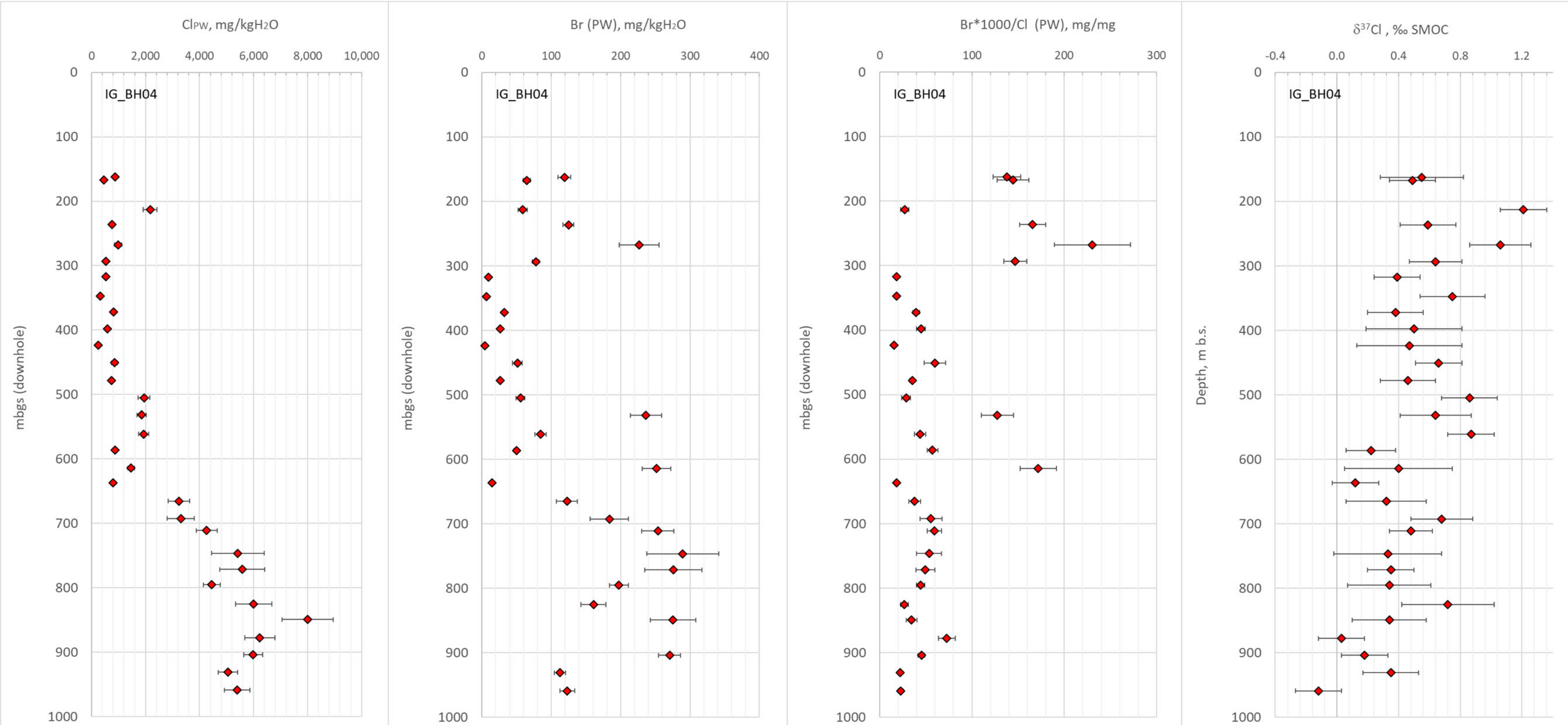


Figure 7-2: Porewater chloride, bromide, Br*1000/Cl mass ratios and δ37Cl isotope signatures extracted from cores from borehole IG_BH04 as function of depth

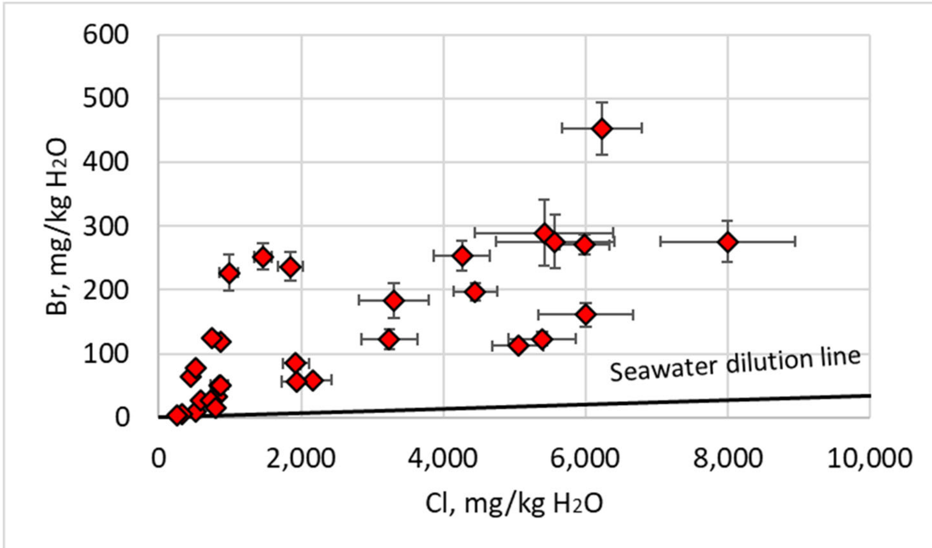


Figure 7-3: Porewater Cl versus Br concentrations determined by out-diffusion experiments on core samples from IG_BH04

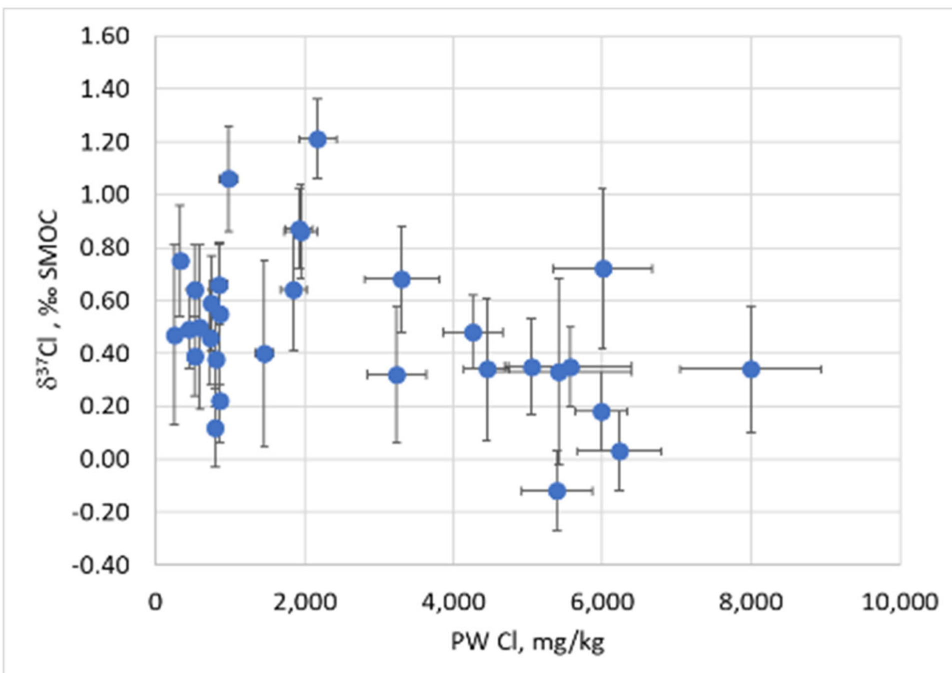


Figure 7-4: Porewater δ37Cl isotope signatures versus porewater Cl concentrations

8.0 δ^{18}O AND δ^{2}H OF POREWATER OF CORE SAMPLES FROM IG_BH04

Isotope diffusive exchange experiments were carried out on 31 core samples (62 individual experiments) from borehole IG_BH04. The δ^{18}O and δ^{2}H values of porewater are calculated according to equation 7 (Section 3.3.3), expressed relative to the standard VSMOW, and are listed in Table 8-1 and graphically shown in Figure 8-1 and Figure 8-2. The calculated porewater isotope signatures, which are based on the isotope analyses of the test waters, are carefully evaluated for potential artefacts (mainly due to evaporation of test water during the experiments, test water storage and handling). Evaporation of porewater during storage and handling was minimized by careful handling of the core samples (Section 3.3.3). These processes might result in discrepancies between the gravimetric water content and that calculated from isotope mass balance and 2) errors in the resulting (calculated) porewater isotopic signatures. Such differences were not observed in this study (Section 4.1.2). Some samples showed a higher (>0.5 wt.%) water content determined by isotope diffusive exchange than determined gravimetrically (cf. chapter 4.1.2). According to the quality check of the raw data we decided to qualify those data as reliable, also if the water contents differ for >0.5 wt%. Evaporation within the experiment was monitored by keeping track of all individual weights before and after the experiments. None of the experiments suffered evaporation > 2 % of the total water mass in the experiments (= mass of porewater determined gravimetrically + mass of test water) during the time of equilibration.

The maximum Cl concentration determined by aqueous extraction prior to the set-up of the isotope diffusive exchange experiments is 9.5 g/kg H_2O, which relates to 0.28 mol $NaCl_{eq}$. Out-diffusion experiments showed an actual maximum Cl concentration of 7.8 g/kg H_2O, which relates to 0.22 mol $NaCl_{eq}$. Based on the aqueous extraction results, it was decided to adjust the salinity of the test solutions to 0.3 mol NaCl to prevent mass transfer from the test water reservoir to the rocks.

Stable oxygen and hydrogen isotope signatures of porewater extracted from core samples from borehole IG_BH04 vary between -14.34 and -7.03 ‰ V-SMOW for δ^{18}O and -112.1 and -55.7 ‰ V-SMOW for δ^{2}H (Table 8-1, Figure 8-1).

Porewaters from borehole IG_BH04 of core samples taken between 162.5 mbgs and 959.0 mbgs (downhole) plot on or slightly to the right of (i.e., below) the global meteoric water line (GMWL) on the δ^{18}O-δ^{2}H diagram (Figure 8-2).

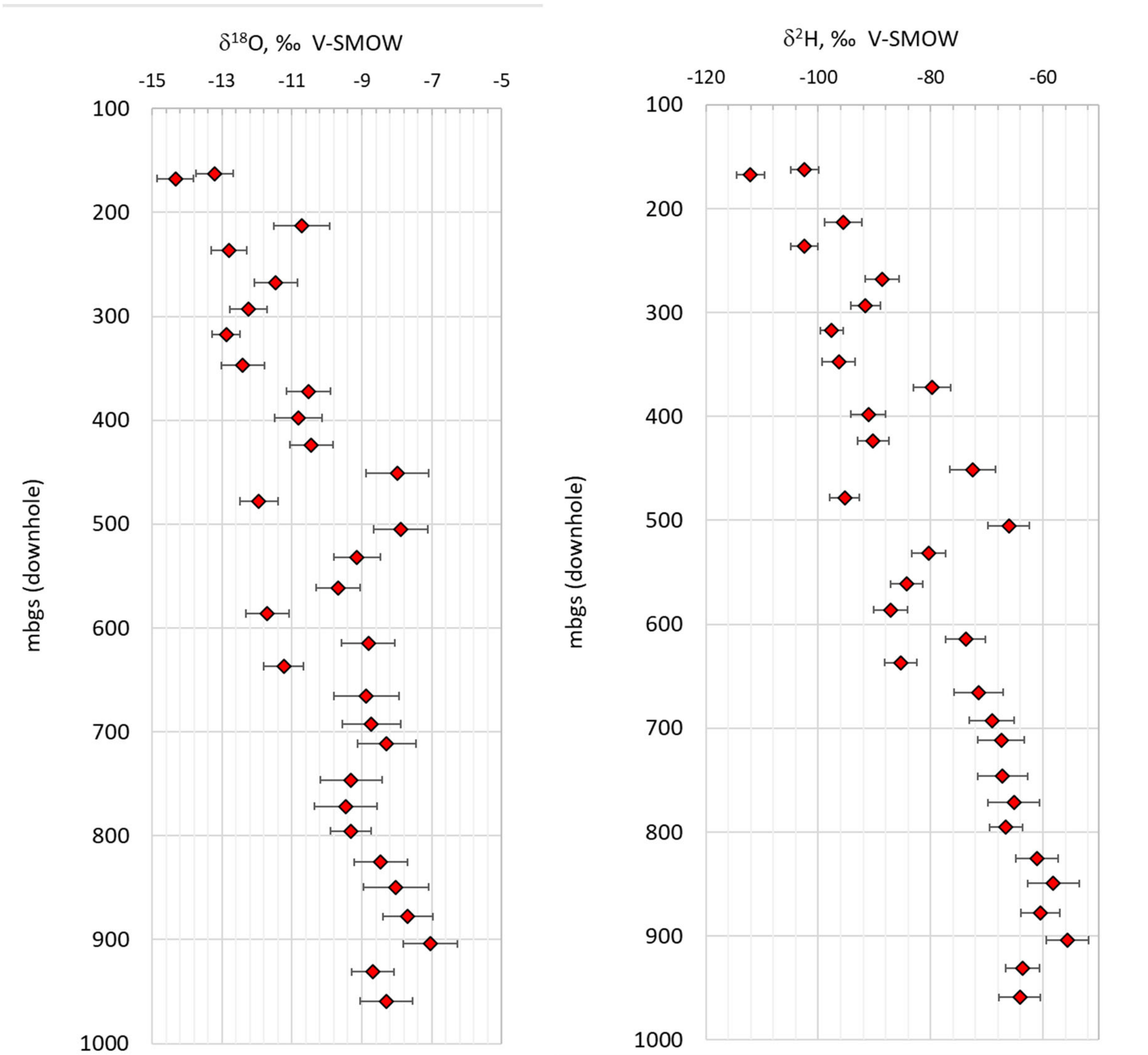


Figure 8-1: $\delta^{18}O$ and $\delta^{2}H$ porewater signatures as function of depth along borehole IG_BH04; the errors are calculated by Gaussian error propagation (Appendix C)

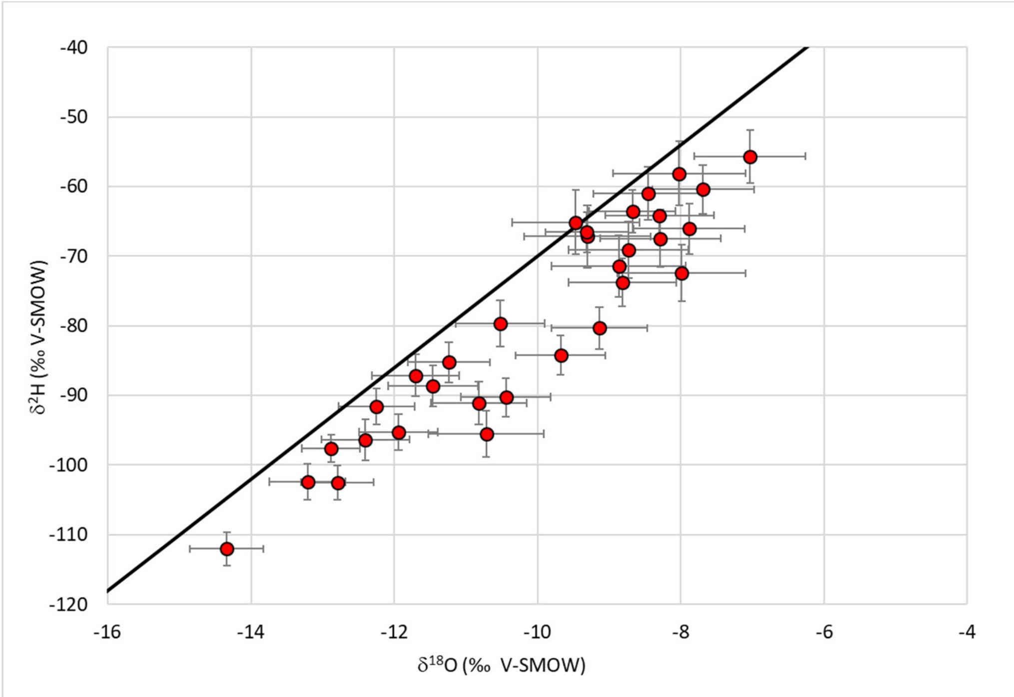


Figure 8-2: $\delta^{18}O$ versus $\delta^{2}H$ values of porewater; the black line marks the global meteoric water line; the errors of the stable isotope ratios are calculated by Gausssian error propagation (Appendix C)

Table 8-1: $\delta^{18}O$ and $\delta^{2}H$ values of porewater of core samples from IG_BH04; the errors are calculated by Gaussian error propagation (Appendix C)

Sample	Depth	$\delta^{18}O$	Error $\delta^{18}O$	$\delta^{2}H$	Error $\delta^{2}H$
	mbgs	‰ V-SMOW	‰ V-SMOW	‰ V-SMOW	‰ V-SMOW
IG_BH04_PW001	162.5	-13.21	0.53	-102.4	2.5
IG_BH04_PW004	167.4	-14.34	0.51	-112.1	2.4
IG_BH04_PW007	213.2	-10.72	0.81	-95.5	3.3
IG_BH04_PW010	236.4	-12.79	0.51	-102.5	2.4
IG_BH04_PW014	267.7	-11.46	0.63	-88.6	3.0
IG_BH04_PW016	293.4	-12.25	0.53	-91.6	2.6
IG_BH04_PW019	317.4	-12.88	0.40	-97.6	2.0
IG_BH04_PW022	347.4	-12.40	0.61	-96.3	2.9
IG_BH04_PW027	372.2	-10.52	0.62	-79.7	3.3
IG_BH04_PW028	397.8	-10.82	0.67	-91.1	3.1
IG_BH04_PW031	423.6	-10.44	0.62	-90.2	2.8
IG_BH04_PW034	450.9	-7.99	0.90	-72.5	4.0
IG_BH04_PW037	478.1	-11.94	0.55	-95.3	2.6
IG_BH04_PW040	505.1	-7.88	0.77	-66.1	3.7
IG_BH04_PW044	531.9	-9.14	0.67	-80.3	3.0
IG_BH04_PW046	561.3	-9.68	0.63	-84.2	2.8
IG_BH04_PW049	586.2	-11.70	0.61	-87.2	3.0
IG_BH04_PW052	614.4	-8.82	0.75	-73.8	3.5
IG_BH04_PW055	636.8	-11.24	0.57	-85.3	2.9
IG_BH04_PW058	665.4	-8.87	0.93	-71.4	4.4
IG_BH04_PW061	692.4	-8.73	0.84	-69.1	4.0
IG_BH04_PW064	711.3	-8.29	0.84	-67.5	4.1
IG_BH04_PW067	746.3	-9.30	0.88	-67.2	4.5
IG_BH04_PW070	771.6	-9.47	0.89	-65.1	4.6
IG_BH04_PW073	795.3	-9.31	0.58	-66.6	2.9
IG_BH04_PW076	825.3	-8.46	0.76	-61.0	3.8
IG_BH04_PW079	849.3	-8.02	0.92	-58.1	4.6
IG_BH04_PW082	877.8	-7.69	0.71	-60.4	3.5
IG_BH04_PW085	904.0	-7.03	0.78	-55.7	3.8
IG_BH04_PW088	931.1	-8.68	0.60	-63.6	3.0
IG_BH04_PW092	959.0	-8.30	0.76	-64.1	3.7

Note(s)

41 [mbgs (downhole)]

9.0 SUMMARY

Porewater investigations applying different indirect methods were completed on 31 crystalline core samples taken between 162.5 and 959.4 mbgs from borehole IG_BH04 drilled in the Revell batholith at Ignace, Ontario.

Potential major sampling-, preservation-, preparation-, experimental- and analytical artefacts, were considered and assessed during the investigation and were observed to be minimal.

The gravimetrically determined water contents (weighted for the entire core sample) vary along the depth profile between 0.11 and 0.23 wt.%, corresponding to water-loss porosities between 0.28 and 0.61 Vol.%. The water contents determined by the isotope diffusive exchange technique are slightly higher compared to gravimetric values determined on the same core pieces. The bulk, wet density values are between 2.58 and 2.70 g/cm^3.

Pore diffusion coefficients were determined by 1-dimensional diffusion modelling based on the fitting of Cl-elution curves, established by taking periodic sub-samples from the out-diffusion experiments. Elution curves could not be fitted by a single pore diffusion coefficient. All cores showed a faster diffusion in the outer rim of the cores (potentially the drilling disturbed zone) and a slower diffusion in the inner cores. The average pore diffusion coefficients (10 °C) vary between 0.7*10^{-10} and 1.6*10^{-10} m^2/s, corresponding to effective diffusion coefficients between 0.3*10^{-12} and 0.8*10^{-12} m^2/s.

Out-diffusion experiments ran for 144 to 188 days. The analyses of time series samples showed that all experiments were in equilibrium with respect to Cl before they were terminated. Test water chemistries are dominated by sodium, calcium, potassium, bicarbonate and chloride in varying proportions and concentrations.

Porewater Cl and Br concentrations were calculated using out-diffusion concentrations and the gravimetrically determined mass of porewater. They vary between 245 and 6,070 mg/kg H_2O for Cl, and 3.8 and 442 mg/kg H_2O for Br, resulting in Br*1000/Cl mass ratios between 15 and 230. Chlorine isotope signatures of porewater vary along the profile between -0.02 and 1.21 ‰ SMOC and show no correlation to porewater Cl concentrations.

Porewater stable water isotope signatures were determined by isotope diffusive exchange experiments. Along the depth profile encountered by borehole IG_BH04, porewater $\delta^{18}O$ signatures range from -14.34 to -7.03 ‰ VSMOW, and δ^2H signatures from -112.1 to -55.7 ‰ VSMOW.

10.0 REFERENCES

Crank, J., 1975. The Mathematics of Diffusion; Oxford Science Publications; Oxford.

Eichinger, F.L., Waber, H.N., Smellie, J.A.T., 2006. Characterisation of Matrix Porewater at the Olkiluoto Investigation Site, Finland. Posiva Working Report 2006-103, Posiva OY, Olkiluoto Finland.

Eichinger, F. Hämmerli, J., Waber, H.N., Smellie, J.A.T., 2010. Characterisation of Matrix Pore Water and Fluid Inclusions in Olkiluoto Bedrock from Drilling OL-KR47. Posiva Working Report 20010-58, Posiva OY, Olkiluoto Finland.

Eichinger, F., Rufer, D., Waber, H.N., 2018. Matrix Porewater and Gases in Porewater in Olkiluoto Bedrock from Drilling OL-KR56. Posiva Working Report 2018-07, Posiva OY, Olkiluoto Finland.

Eichinger, F., 2021. Matrix Porewater in Olkiluoto Bedrock from Drilling OL-KR58. Posiva Working Report 2021-03, Posiva OY, Olkiluoto Finland.

Gimmi, T. and Waber, H.N., 2004. Modelling of Tracer Profiles in Pore Water of Argillaceous Rocks in the Benken Borehole: Stable Water Isotopes, Chloride, and Chlorine Isotopes; Nagra Tech. Rep. 2004-05, Nagra, Wettingen, Switzerland.

Gimmi, T., Aschwanden, L., Camesi, L., Gaucher, E., Jenni, A., et al., 2022. TBO Bözberg-2-1: Data Report Dossier VIII – Rock Properties, Porewater Characterisation and Natural Tracer Profiles. NAB 21-22, NAGRA, Wettingen, Switzerland.

Jäckli, H., 1970. Kriterien zur Klassifikation von Grundwasservorkommen. Ecologae geol. Helv., 63 (2), 389-434.

Lide, D.R., 1994. CRC Handbook of chemistry and physics. 75th ed., CRC Press, Boca Raton, USA.

Meier, D.B., Waber, H.N., Gimmi, T., Eichinger, F., Diamond, L.W., 2015. Reconstruction of in-situ porosity and porewater compositions of low-permeability crystalline rocks: Magnitude of artefacts induced by drilling and sample recovery. Journal of Contaminant Hydrology, 183, 55-71.

Ohlsson, Y. and Neretnieks, I., 1995. Literature survey of matrix diffusion theory and of experiments and data including natural analogues; SKB Tech. Rep. 95-12, Svensk Kärnbränslehantering AB, Stockholm, Sweden.

Pearson et al., 2003. Mont Terri Project – Geochemistry of Water in the Opalinus Clay Formation at the Mont Terri Rock Laboratory. Federal Office of Water and Geology, Geology Series No. 5, Bern, Switzerland.

Rogge, T., 1997. Eine molekular-diffusive Methode zur Bestimmung des Porenwassergehaltes und der Zusammensetzung von stabilen Isotopen im Porenwasser von Gestein; unveröffentlichte Diplomarbeit; Heidelberg.

Rübel, A.P., Sonntag, Ch., Lippmann, J., Pearson, F.J. and Gautschi, A., 2002. Solute transport in formations of very low permeability: Profiles of stable isotope and dissolved noble gas contents of pore water in the Opalinus Clay. Mont Terri, Switzerland; Geochim. Cosmochim. Acta, 66, 1311-1321.

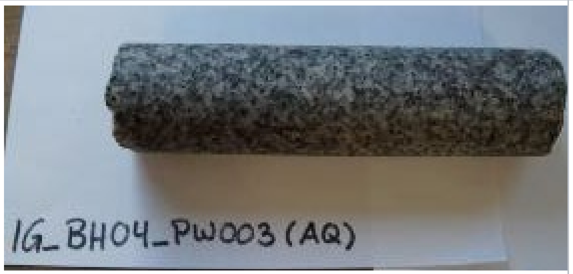
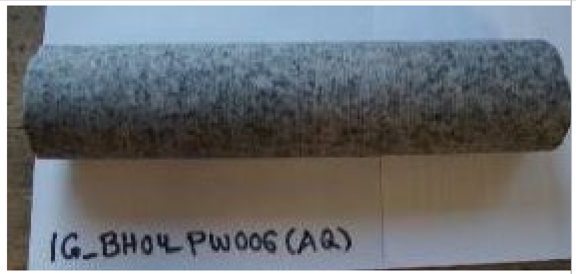
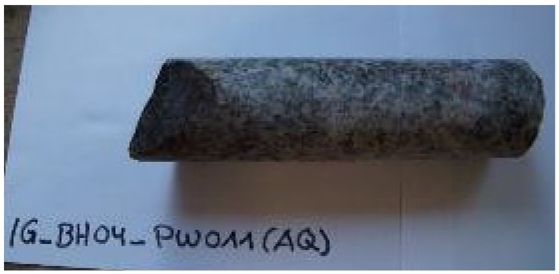
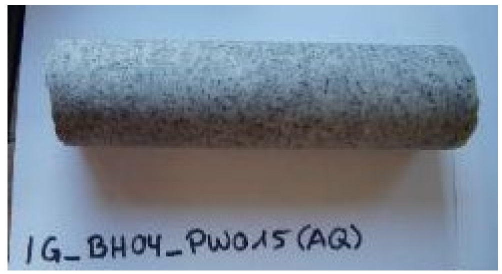
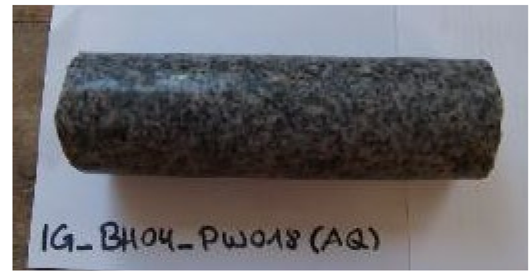
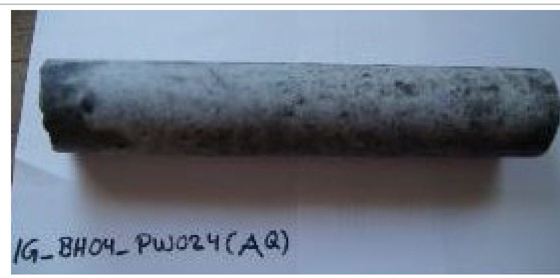
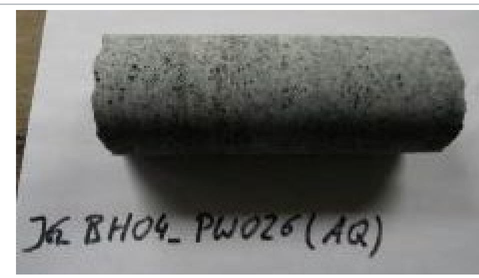
Waber, H.N. and Smellie, J.A.T., 2005. SKB Site Investigations Forsmark – Borehole KFM06: Characterisation of porewater. Part I: Diffusion experiments; SKB P-Rep. P-05-196, Svensk Kärnbränslehantering AB, Stockholm, Sweden.

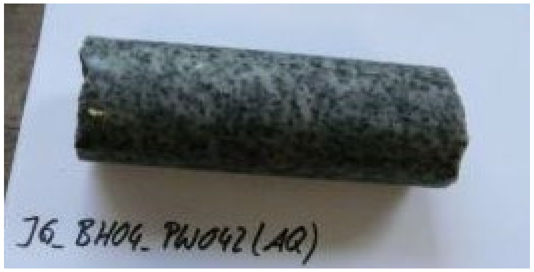
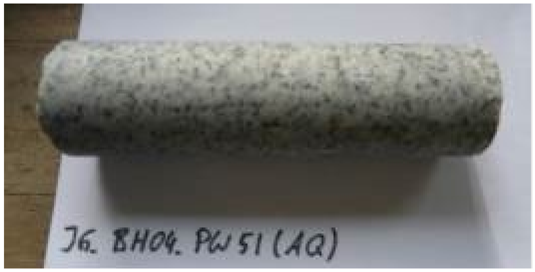
Waber, H.N. and Smellie, J.A.T., 2006. Oskarshamn site investigations. Borehole KLX03: Characterisation of porewater. Part 2: Rock properties and diffusion experiments; SKB P-Report P-06-77. Svensk Kärnbränslehantering AB, Stockholm, Sweden.

APPENDIX A

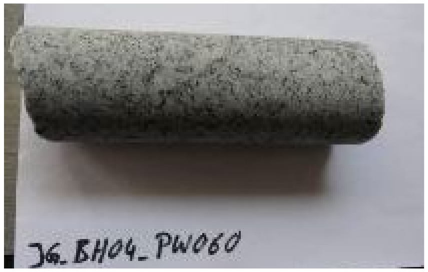
Photo Documentation

Appendix Table 10-1: Core samples used for aqueous extraction experiments

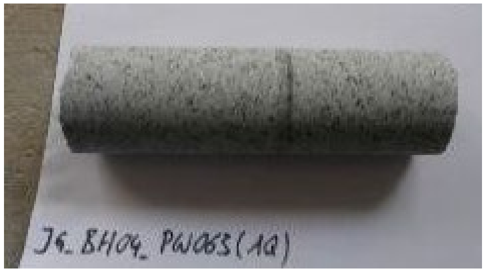
 IG_BH04_PW003: 163.58-163.83 m	 IG_BH04_PW006: 167.94-168.21 m	 IG_BH04_PW009: 213.79-214.02 m
 IG_BH03_AQ004: 504.12-504.27 m	 IG_BH04_PW015: 267.88-268.11 m	 IG_BH04_PW018: 294.39-294.59 m
 IG_BH04_PW021: 318.00-318.24 m	 IG_BH04_PW024: 348.01-348.34 m	 IG_BH04_PW026: 371.87-372.04 m

 IG_BH04_PW030: 397.04-397.24 m	 IG_BH04_PW033: 424.17-424.32 m	 IG_BH04_PW036: 451.44-451.62 m
 IG_BH04_PW039: 478.71-478.95 m	 IG_BH04_PW042: 505.64-505.81 m	 IG_BH04_PW045: 532.42-532.61 m
 IG_BH04_PW048: 561.81-561.98 m	 IG_BH04_PW051: 585.79-5856.01 m	 IG_BH04_PW054: 615.26-615.51 m

IG_BH04_PW057: 637.43-637.58 m



IG_BH04_PW060: 666.02-666.20 m



IG_BH04_PW063: 692.99-693.20 m

IG_BH04_PW066: 711.94-712.28 m

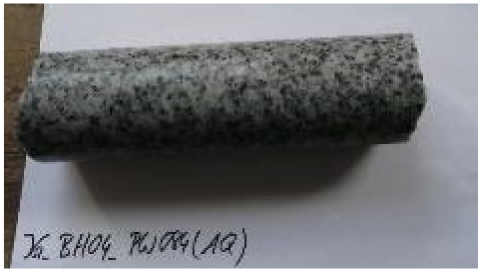
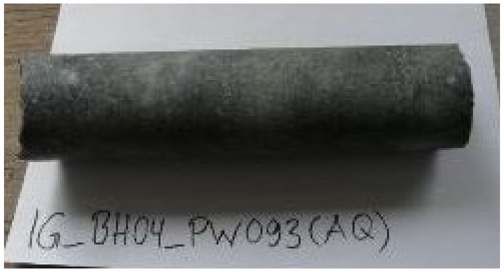
IG_BH04_PW069: 746.94-747.14 m

IG_BH04_PW072: 772.24-772.44 m

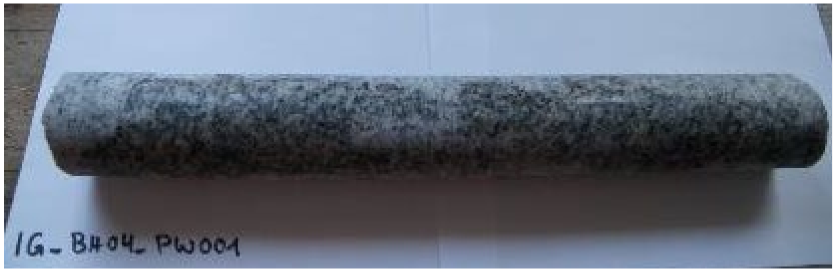
IG_BH04_PW075: 795.87-796.03 m

IG_BH04_PW078: 825.86-826.02 m

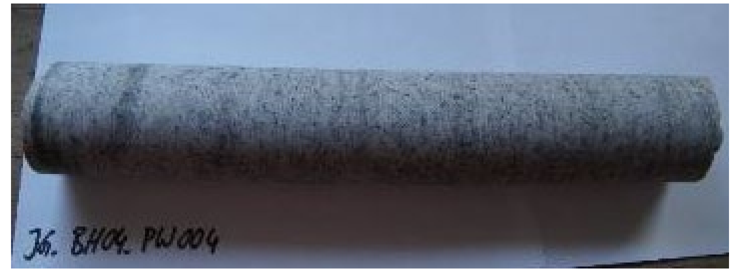
IG_BH04_PW081: 850.01-850.19 m

 IG_BH04_PW084: 878.32-878.52 m	 IG_BH04_PW087: 904.56-904.74 m	 IG_BH04_PW090: 931.90-932.23 m
 IG_BH04_PW093: 959.17-959.41 m		

Appendix Table 10-2: Core samples used for out-diffusion and isotope diffusive exchange experiments



IG_BH04_PW001: 162.20-162.70 m



IG_BH04_PW004: 167.21-167.57 m

IG_BH04_PW007: 213.00-213.38 m

IG_BH04_PW010: 236.21-236.65 m

IG_BH04_PW014: 267.48-267.88 m

IG_BH04_PW016: 293.21-293.62 m

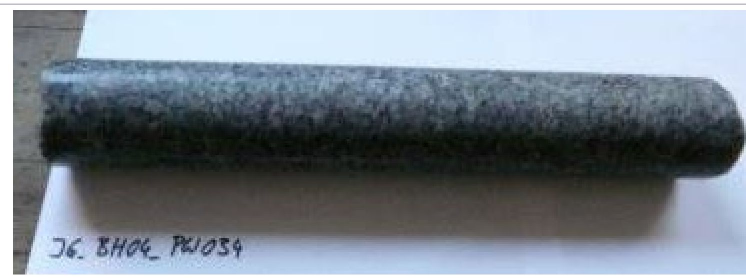
IG_BH04_PW019: 317.21-317.59 m

IG_BH04_PW022: 347.21.347.62 m

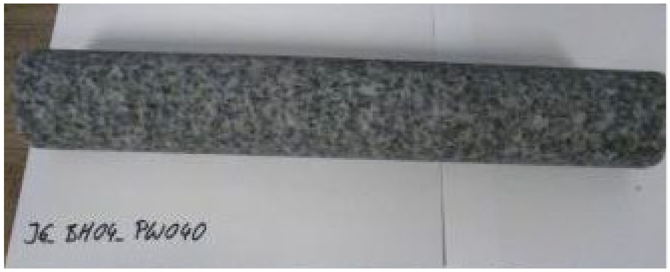
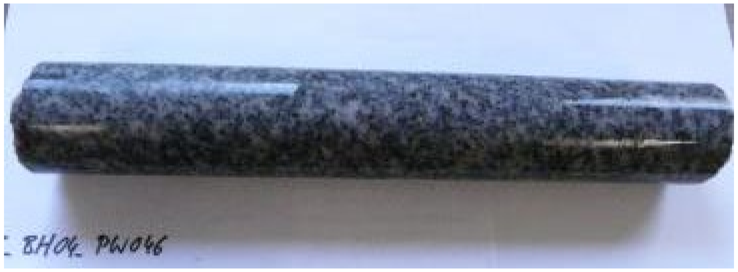
IG_BH04_PW027: 372.04-372.40 m

IG_BH04_PW028: 397.64-398.03 m

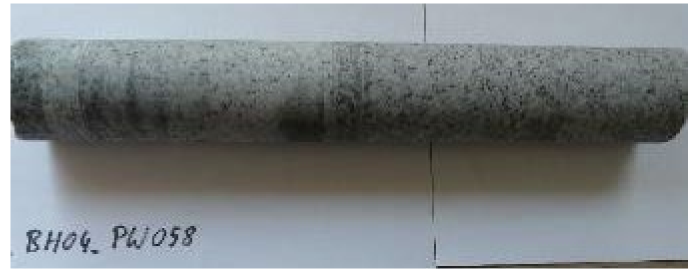
IG_BH04_PW031: 423.43-423.80 m



IG_BH04_PW034: 450.69-451.06 m

 IG_BH04_PW037: 477.91-478.31 m	 IG_BH04_PW040: 504.90-505.28 m
 IG_BH04_PW044: 531.66-532.04 m	 IG_BH04_PW046: 561.08-561.45 m
 IG_BH04_PW049: 568.01-568.40 m	 IG_BH04_PW052: 614.21-614.61 m

IG_BH04_PW055: 1636.62-637.03 m



IG_BH04_PW058: 665.21-665.61 m

IG_BH04_PW061: 692.21-692.60 m

IG_BH04_PW064: 711.14-711.55 m

IG_BH04_PW067: 746.14-746.54 m

IG_BH04_PW070: 771.42-771.82 m

IG_BH04_PW067: 795.14-795.50 m

IG_BH04_PW067: 825.14-825.50 m

IG_BH04_PW079: 849.14-849.49 m

IG_BH04_PW082: 977.56-977.94 m

IG_BH04_PW085: 903.76-904.17 m

IG_BH04_PW088: 930.86-931.34 m

IG_BH04_PW092: 958.74-959.17 m

APPENDIX B

Analytical Raw Data

CALCULATION OF WATER CONTENT VALUES: RAW DATA

Appendix Table 10-3: Determination of gravimetric water content; sample weights, drying times and calculated water contents of core pieces used for aqueous extraction experiments

Sample	Date prepared	m (cryst.dish)	m (cryst+ rock)	16.03.2020	31.03.2020	13.04.2020					Sample	m (rock, wet)	m (rock, dry)
Drying times	days			61	76	89						g	g
PW003 (AQ)	15.01.2020	88,733	486,951	486,315	486,304	486,305					PW003 (AQ)	398,218	397,571
PW006 (AQ)	15.01.2020	91,306	428,810	428,269	428,271						PW006 (AQ)	337,504	336,963
PW009 (AQ)	15.01.2020	88,733	453,845	453,185	453,187						PW009 (AQ)	365,112	364,452
PW011 (AQ)	15.01.2020	87,323	478,430	477,790	477,790						PW011 (AQ)	391,107	390,467
PW015 (AQ)	15.01.2020	91,260	473,089	472,513	472,511						PW015 (AQ)	381,829	381,251
PW018 (AQ)	15.01.2020	87,788	418,429	417,870	417,870						PW018 (AQ)	330,641	330,082
PW021 (AQ)	15.01.2020	87,284	385,058	384,506	384,503	384,505					PW021 (AQ)	297,774	297,219
PW024 (AQ)	15.01.2020	90,804	478,448	478,054	478,053						PW024 (AQ)	387,644	387,249
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**08.05.2020**	**20.05.2020**								
Drying times	**days**			14	26								
PW026 (AQ)	24.04.2020	88,618	373,238	372,862	372,860						PW026 (AQ)	284,620	284,242
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**17.03.2020**	**31.03.2020**	**14.04.2020**							
Drying times	**days**			38	52	66							
PW030 (AQ)	08.02.2020	84,668	566,695	565,939	565,929	565,928					PW030 (AQ)	482,027	481,260
PW033 (AQ)	08.02.2020	86,535	458,137	457,585	457,577	457,579					PW033 (AQ)	371,602	371,042
PW036 (AQ)	08.02.2020	87,165	418,079	417,613	417,603	417,605					PW036 (AQ)	330,914	330,438
PW039 (AQ)	08.02.2020	86,413	446,867	446,387	446,378	446,380					PW039 (AQ)	360,454	359,965
PW042 (AQ)	08.02.2020	83,841	360,862	360,431	360,433						PW042 (AQ)	277,021	276,590
PW045 (AQ)	08.02.2020	84,543	395,362	394,926	394,929						PW045 (AQ)	310,819	310,383
PW048 (AQ)	08.02.2020	88,662	378,759	378,334	378,333						PW048 (AQ)	290,097	289,671
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**20.03.2020**	**03.04.2020**	**16.04.2020**							
Drying times	**days**			14	28	41							
PW051 (AQ)	06.03.2020	88,325	448,952	448,169	448,152	448,154					PW051 (AQ)	360,627	359,827
PW054 (AQ)	06.03.2020	92,195	450,616	450,071	450,06	450,061					PW054 (AQ)	358,421	357,865
PW057 (AQ)	06.03.2020	90,942	401,275	400,855	400,851	400,853					PW057 (AQ)	310,333	309,909
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**01.04.2020**	**15.04.2020**	**29.04.2020**	**13.05.2020**	**27.05.2020**	**10.06.2020**				
Drying times	**days**			14	28	42	56	70	84				
PW060 (AQ)	18.03.2020	89,833	400,297	399,929	399,927	399,934	399,923	399,916	399,92		PW060 (AQ)	310,464	310,083
PW063 (AQ)	18.03.2020	97,341	476,743	476,355	476,353	476,359	476,357				PW063 (AQ)	379,402	379,012
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**07.04.2020**	**21.04.2020**	**07.05.2020**	**20.05.2020**	**03.06.2020**	**17.06.2020**				
Drying times	**days**			12	26	42	55	69	83				
PW066 (AQ)	26.03.2020	92,806	431,321	430,863	438,870	438,855	438,853				PW066 (AQ)	338,515	338,057
PW069 (AQ)	26.03.2020	88,079	394,319	393,954	393,962	393,946	393,948				PW069 (AQ)	306,240	305,867
PW072 (AQ)	26.03.2020	86,346	409,470	409,113	409,117	409,108	409,108				PW072 (AQ)	323,124	322,762
PW075 (AQ)	26.03.2020	88,640	360,144	359,640	359,647	359,644	359,635	359,647	359,654		PW075 (AQ)	271,504	270,995
PW078 (AQ)	26.03.2020	86,232	372,586	372,032	372,046	372,020	372,033	372,035			PW078 (AQ)	286,354	285,788
PW081 (AQ)	26.03.2020	87,193	418,553	417,996	417,997	417,976	417,993	417,996	418,002		PW081 (AQ)	331,360	330,783
PW084 (AQ)	26.03.2020	89,126	354,349	353,905	353,901	353,895	353,903	353,91	353,92		PW084 (AQ)	265,223	264,769
PW087 (AQ)	26.03.2020	92,881	415,915	415,523	415,534	415,531	415,521	415,539	415,544		PW087 (AQ)	323,034	322,640
PW090 (AQ)	26.03.2020	89,010	436,348	435,940	435,954	435,937	435,943	435,945			PW090 (AQ)	347,338	346,927
PW093 (AQ)	26.03.2020	85,364	405,625	405,025	405,031	405,028	405,02	405,027	405,038		PW093 (AQ)	320,261	319,656

Appendix Table 10-3: continued

			m(dry surf)	**16.03.2020**	**31.03.2020**	**14.04.2020**	**28.04.2020**					**Sample**	**m (rock, wet)**	**m (rock, dry)**
Drying times	**days**			61	76	90	104						**g**	**g**
PW003 (AQ) A	15.01.2020		130,116	129,856	129,849	129,847						PW003 (AQ) A	130,116	129,847
PW003 (AQ) B	15.01.2020		187,054	186,678	186,674	186,672						PW003 (AQ) B	187,054	186,672
PW006 (AQ) A	15.01.2020		161,468	161,200	161,192	161,193						PW006 (AQ) A	161,468	161,192
PW006 (AQ) B	15.01.2020		130,691	130,464	130,459	130,457						PW006 (AQ) B	130,691	130,457
PW009 (AQ) A	15.01.2020		173,927	173,569	173,559	173,553	173,552					PW009 (AQ) A	173,927	173,552
PW009 (AQ) B	15.01.2020		152,018	151,712	151,703	151,697	151,696					PW009 (AQ) B	152,018	151,696
PW011 (AQ) A	15.01.2020		178,723	178,400	178,391	178,389						PW011 (AQ) A	178,723	178,389
PW011 (AQ) B	15.01.2020		191,008	190,671	190,661	190,653	190,653					PW011 (AQ) B	191,008	190,653
PW011 (AQ Frnc)	15.01.2020		312,851	312,027	312,017	312,017								
PW015 (AQ) A	15.01.2020		190,780	190,486	190,482	190,475	190,476					PW015 (AQ) A	190,780	190,475
PW015 (AQ) B	15.01.2020		208,305	207,954	207,946	207,945						PW015 (AQ) B	208,305	207,945
PW018 (AQ) A	15.01.2020		171,029	170,721	170,716	170,710	170,711					PW018 (AQ) A	171,029	170,710
PW018 (AQ) B	15.01.2020		167,961	167,637	167,631	167,618	167,618					PW018 (AQ) B	167,961	167,618
PW021 (AQ) A	15.01.2020		167,043	166,715	166,704	166,700	166,698					PW021 (AQ) A	167,043	166,698
PW021 (AQ) B	15.01.2020		172,362	172,047	172,037	172,034	172,035					PW021 (AQ) B	172,362	172,034
PW024 (AQ) A	15.01.2020		256,723	256,458	256,447	256,439	256,440					PW024 (AQ) A	256,723	256,439
PW024 (AQ) B	15.01.2020		273,257	272,956	272,948	272,942	372,941					PW024 (AQ) B	273,257	272,942
			m(dry surf)	**08.05.2020**	**20.05.2020**	**03.06.2020**								
Drying times	**days**			14	26	40								
PW026 (AQ) A	24.04.2020		183,765	183,509	183,509	183,506						PW026 (AQ) A	183,765	183,506
PW026 (AQ) B	24.04.2020		133,570	133,380	133,380	133,376						PW026 (AQ) B	133,570	133,376
			m(dry surf)	**18.02.2020**	**03.03.2020**	**17.03.2020**	**31.03.2020**	**14.04.2020**	**28.04.2020**	**12.05.2020**				
Drying times	**days**			10	24	38	52	66	80	94				
PW030 (AQ) A	08.02.2020		206,140	205,806	205,803	205,793	205,786	205,782	205,783			PW030 (AQ) A	206,140	205,782
PW030 (AQ) B	08.02.2020		178,408	178,124	178,124	178,115	178,108	178,103	178,098	178,100		PW030 (AQ) B	178,408	178,098
PW033 (AQ) A	08.02.2020		192,430	192,117	192,109	192,097	192,092	192,086	192,085			PW033 (AQ) A	192,430	192,085
PW033 (AQ) B	08.02.2020		174,586	174,289	174,281	174,271	174,264	174,258	174,259			PW033 (AQ) B	174,586	174,258
PW036 (AQ) A	08.02.2020		130,034	129,846	129,842	129,836	129,829	129,817	129,818			PW036 (AQ) A	130,034	129,817
PW036 (AQ) B	08.02.2020		131,960	131,779	131,772	131,766	131,755	131,751	131,749			PW036 (AQ) B	131,960	131,749
PW039 (AQ) A	08.02.2020		155,352	155,160	155,156	155,151	155,145	155,144				PW039 (AQ) A	155,352	155,144
PW039 (AQ) B	08.02.2020		171,300	171,046	171,042	171,036	171,031	171,026	171,026			PW039 (AQ) B	171,300	171,026
PW042 (AQ) A	08.02.2020		358,542	357,972	357,964	357,953	357,950	357,945	357,946			PW042 (AQ) A	358,542	357,945
PW042 (AQ) B	08.02.2020		156,199	155,927	155,915	155,906	155,901	155,899				PW042 (AQ) B	156,199	155,899
PW045 (AQ) A	08.02.2020		119,637	119,449	119,441	119,435	119,426	119,424				PW045 (AQ) A	119,637	119,424
PW045 (AQ) B	08.02.2020		204,391	204,073	204,068	204,054	204,042	204,040				PW045 (AQ) B	204,391	204,040
PW048 (AQ) A	08.02.2020		152,742	152,502	152,492	152,485	152,479	152,477				PW048 (AQ) A	152,742	152,477
PW048 (AQ) B	08.02.2020		133,910	133,686	133,676	133,670	133,660	133,656	133,656			PW048 (AQ) B	133,910	133,656
			m(dry surf)	**20.03.2020**	**03.04.2020**	**16.04.2020**	**30.04.2020**							
Drying times	**days**			14	28	41	55							
PW051 (AQ) A	06.03.2020		118,203	117,965	117,957	117,862	117,863					PW051 (AQ) A	118,203	117,862
PW051 (AQ) B	06.03.2020		155,562	155,246	155,237	155,236						PW051 (AQ) B	155,562	155,236
PW054 (AQ) A	06.03.2020		235,422	235,032	235,022	235,021						PW054 (AQ) A	235,422	235,021
PW054 (AQ) B	06.03.2020		207,669	207,316	207,303	207,301						PW054 (AQ) B	207,669	207,301
PW057 (AQ) A	06.03.2020		179,963	179,682	179,670	179,665	179,665					PW057 (AQ) A	179,963	179,665
PW057 (AQ) B	06.03.2020		257,109	256,750	256,734	256,736						PW057 (AQ) B	257,109	256,734
			m(dry surf)	**01.04.2020**	**16.04.2020**	**29.04.2020**								
Drying times	**days**			14	29	42								
PW060 (AQ) A	18.03.2020		161,160	160,965	160,958	160,959						PW060 (AQ) A	161,160	160,958
PW060 (AQ) B	18.03.2020		179,254	179,033	179,020	179,021						PW060 (AQ) B	179,254	179,020
PW063 (AQ) A	18.03.2020		224,256	224,018	224,009	224,011						PW063 (AQ) A	224,256	224,009
PW063 (AQ) B	18.03.2020		188,917	188,719	188,715	188,716						PW063 (AQ) B	188,917	188,715
			m(dry surf)	**07.04.2020**	**22.04.2020**	**07.05.2020**	**20.05.2020**							
Drying times	**days**			12	27	42	55							
PW066 (AQ) A	26.03.2020		296,948	296,528	296,511	296,510						PW066 (AQ) A	296,948	296,510
PW066 (AQ) B	26.03.2020		223,954	223,639	223,624	223,623						PW066 (AQ) B	223,954	223,623
PW069 (AQ) A	26.03.2020		230,755	230,344	230,337	230,335						PW069 (AQ) A	230,755	230,335
PW069 (AQ) B	26.03.2020		173,129	172,902	172,898	172,896						PW069 (AQ) B	173,129	172,896
PW072 (AQ) A	26.03.2020		199,441	199,208	199,205	199,205						PW072 (AQ) A	199,441	199,205
PW072 (AQ) B	26.03.2020		184,446	184,225	184,221	184,221						PW072 (AQ) B	184,446	184,221
PW075 (AQ) A	26.03.2020		198,442	197,985	197,975	197,971	197,971					PW075 (AQ) A	198,442	197,971
PW075 (AQ) B	26.03.2020		141,750	141,465	141,457	141,456						PW075 (AQ) B	141,750	141,456
PW078 (AQ) A	26.03.2020		116,211	115,993	115,985	115,984						PW078 (AQ) A	116,211	115,984
PW078 (AQ) B	26.03.2020		167,346	167,001	166,988	166,985	166,984					PW078 (AQ) B	167,346	166,984
PW081 (AQ) A	26.03.2020		143,810	143,554	143,546	143,544						PW081 (AQ) A	143,810	143,544
PW081 (AQ) B	26.03.2020		162,437	162,141	162,129	162,128						PW081 (AQ) B	162,437	162,128
PW084 (AQ) A	26.03.2020		210,949	210,461	210,447	210,446						PW084 (AQ) A	210,949	210,446
PW084 (AQ) B	26.03.2020		231,646	231,202	231,190	231,189						PW084 (AQ) B	231,646	231,189
PW087 (AQ) A	26.03.2020		176,989	176,775	176,767	176,766						PW087 (AQ) A	176,989	176,766
PW087 (AQ) B	26.03.2020		182,259	181,973	181,962	181,959	181,957					PW087 (AQ) B	182,259	181,957
PW090 (AQ) A	26.03.2020		265,511	265,081	265,078	265,076						PW090 (AQ) A	265,511	265,076
PW090 (AQ) B	26.03.2020		178,331	178,087	178,084	178,082						PW090 (AQ) B	178,331	178,082
PW093 (AQ) A	26.03.2020		221,257	220,848	220,843	220,840	220,840					PW093 (AQ) A	221,257	220,840
PW093 (AQ) B	26.03.2020		229,273	228,812	228,808	228,807						PW093 (AQ) B	229,273	228,807

Appendix Table 10-4: Determination of gravimetric water content; sample weights, drying times and calculated water contents of rim core pieces of samples used for out-diffusion and isotope diffusive exchange experiments

	Set-up date	m(dry surf)	16.03.2020	31.03.2020	15.04.2020			m wet	m dry
Drying time (days)			14	29	44			g	g
PW001 A	02.03.2020	168,713	168,435	168,429	168,320			168,713	168,32
PW001 B	02.03.2020	443,495	442,771	442,761	442,756			443,495	442,756
PW004 A	02.03.2020	111,799	111,609	111,607				111,799	111,607
PW004 B	02.03.2020	229,610	229,232	229,224	229,213			229,610	229,213
PW007 A	02.03.2020	230,246	229,812	229,803	229,785			230,246	229,785
PW007 B	02.03.2020	220,839	220,474	220,463	220,449			220,839	220,449
PW010 A	02.03.2020	243,542	243,076	243,070	243,058			243,542	243,058
PW010 B	02.03.2020	277,887	277,324	277,316	277,305			277,887	277,305
PW014 A	02.03.2020	238,333	237,966	237,955	237,890			238,333	237,89
PW014 B	02.03.2020	191,003	190,726	190,720	190,709			191,003	190,709
PW016 A	02.03.2020	258,065	257,368	257,627	257,619			258,065	257,368
PW016 B	02.03.2020	192,855	192,532	192,522	192,514			192,855	192,514
PW019 A	02.03.2020	208,736	208,270	208,261	208,256			208,736	208,256
PW019 B	02.03.2020	172,595	172,266	172,255	172,251			172,595	172,251
PW022 A	02.03.2020	252,485	252,135	252,119	252,108			252,485	252,108
PW022 B	02.03.2020	221,034	220,689	220,675	220,667			221,034	220,667
	Set-up date	**m(dry surf)**	**08.05.2020**	**20.05.2020**					
Drying time (days)			14	26					
PW027 A	24.04.2020	212,193	211,860	211,860				212,193	211,86
PW027 B	24.04.2020	161,354	161,101	161,099				161,354	161,099
	Set-up date	**m(dry surf)**	**18.02.2020**	**03.03.2020**	**17.03.2020**	**31.03.2020**	**15.04.2020**		
Drying time (days)			11	25	39	53	68		
PW028 A	07.02.2020	223,134	222,808	222,800	222,793	222,789	222,783	223,134	222,783
PW028 B	07.02.2020	107,715	107,547	107,541	107,535	107,531	107,522	107,715	107,522
PW031 A	07.02.2020	203,775	203,449	203,434	203,421	203,417	203,410	203,775	203,41
PW031 B	07.02.2020	194,217	193,865	193,850	193,837	193,824	193,814	194,217	193,814
PW034 A	07.02.2020	172,390	172,096	172,085	172,074	172,068	172,057	172,390	172,057
PW034 B	07.02.2020	190,891	190,603	190,591	190,583	190,578	190,568	190,891	190,568
PW037 A	07.02.2020	189,469	189,175	189,147	189,137	189,137		189,469	189,137
PW037 B	07.02.2020	133,384	133,221	133,217	133,201	133,198	133,191	133,384	133,191
PW040 A	07.02.2020	205,842	205,514	205,509	205,501	205,497	205,488	205,842	205,488
PW040 B	07.02.2020	182,463	182,183	182,169	182,159	182,156	182,148	182,463	182,148
PW044 A	08.02.2020	192,270	191,899	191,884	191,870	191,860	191,851	192,270	191,851
PW044 B	08.02.2020	174,217	173,919	173,915	173,904	173,900	173,857	174,217	173,857
PW046 A	08.02.2020	142,324	142,122	142,115	142,111	142,109		142,324	142,109
PW046 B	08.02.2020	229,676	229,325	229,319	229,311	229,281	229,271	229,676	229,271

Appendix Table 10-4: continued

	Set-up date	m(dry surf)	20.03.2020	03.04.2020	16.04.2020	30.04.2020			m wet	m dry
Drying time (days)			14	28	41	55			g	g
PW049 A	06.03.2020	201,429	201,037	201,029	201,027				201,429	201,027
PW049 B	06.03.2020	183,186	182,848	182,838	182,836				183,186	182,836
PW052 A	06.03.2020	288,580	288,127	288,115	288,110	288,112			288,580	288,11
PW052 B	06.03.2020	175,975	175,683	175,677	175,671	175,673			175,975	175,671
	Set-up date	**m(dry surf)**	**01.04.2020**	**15.04.2020**	**29.04.2020**	**12.05.2020**				
Drying time (days)			14	28	42	55				
PW055 A	18.03.2020	232,680	232,304	232,297	232,298				232,680	232,297
PW055 B	18.03.2020	128,611	128,393	128,379	128,376	128,374			128,611	128,374
PW058 A	18.03.2020	164,144	163,932	163,928	163,925	163,923			164,144	163,923
PW058 B	18.03.2020	245,474	245,118	245,107	245,109				245,474	245,107
PW061 A	18.03.2020	175,059	174,843	174,836	174,836				175,059	174,836
PW061 B	18.03.2020	227,645	227,299	227,291	227,292				227,645	227,291
PW064 A	18.03.2020	227,558	227,244	227,238	227,240				227,558	227,238
PW064 B	18.03.2020	174,514	174,290	174,281	174,283				174,514	174,281
	Set-up date	**m(dry surf)**	**08.04.2020**	**22.04.2020**	**07.05.2020**	**20.05.2020**	**03.06.2020**			
Drying time (days)			13	27	42	55	69			
PW067 A	26.03.2020	260,701	260,354	260,348	260,345	260,342	260,342		260,701	260,342
PW067 B	26.03.2020	178,264	178,033	178,030	178,027	178,024	178,024		178,264	178,024
PW070 A	26.03.2020	208,017	207,713	207,707	207,705				208,017	207,705
PW070 B	26.03.2020	208,643	208,353	208,349	208,347				208,643	208,347
PW073 A	26.03.2020	172,987	172,643	172,635	172,635				172,987	172,635
PW073 B	26.03.2020	168,397	168,029	168,027	168,022	168,021			168,397	168,021
PW076 A	26.03.2020	112,627	112,420	112,417	112,414	112,412			112,627	112,412
PW076 B	26.03.2020	170,257	169,923	169,916	169,914				170,257	169,914
PW079 A	26.03.2020	104,073	103,901	103,891	103,889				104,073	103,889
PW079 B	26.03.2020	162,269	162,001	161,997	161,995				162,269	161,995
PW082 A	26.03.2020	184,852	184,388	184,381	184,378	184,372	184,371		184,852	184,371
PW082 B	26.03.2020	162,878	162,505	162,494	162,492				162,878	162,492
PW085 A	26.03.2020	276,682	276,246	276,233	276,231				276,682	276,231
PW085 B	26.03.2020	149,218	148,970	148,964	148,961	148,958	148,956		149,218	148,956
PW088 A	26.03.2020	213,059	212,680	212,677	212,675				213,059	212,675
PW088 B	26.03.2020	129,712	129,467	129,464	129,464				129,712	129,464
PW092 A	26.03.2020	257,860	257,481	257,477	257,474	257,471	257,471		257,860	257,471
PW092 B	26.03.2020	255,948	255,485	255,481	255,478	255,476			255,948	255,476

Appendix Table 10-5: Determination of gravimetric water content; sample weights, drying times and calculated water contents of core pieces used for isotope-diffusive exchange experiments

Sample	Date start drying	Drying times (days)	m (cryst.dish)	m (cryst+ rock)	01.04.2020	14.04.2020	27.04.2020	12.05.2020	27.05.2020		mass dry	m rock wet	m rock dry
PW001 LAB	18.03.2020	27	86,252	566,673	565,981	565,983					565,981	480,421	479,729
PW001 ICE	18.03.2020	27	88,299	536,074	535,428	535,430					535,428	447,775	447,129
PW004 LAB	18.03.2020	27	90,021	444,589	444,034	444,035					444,034	354,568	354,013
PW004 ICE	18.03.2020	27	87,593	443,765	443,205	443,207					443,205	356,172	355,612
PW007 LAB	18.03.2020	27	86,230	441,555	441,020	441,022					441,020	355,325	354,790
PW007 ICE	18.03.2020	27	90,447	444,409	443,881	443,885					443,881	353,962	353,434
PW010 LAB	18.03.2020	70	88,295	522,100	521,391	521,385	521,397	521,388	521,386		521,385	433,805	433,090
PW010 ICE	18.03.2020	27	89,510	532,909	532,190	532,189					532,189	443,399	442,679
PW014 LAB	18.03.2020	27	89,350	547,687	547,057	547,055					547,055	458,337	457,705
PW014 ICE	18.03.2020	27	88,438	539,860	539,233	539,234					539,233	451,422	450,795
PW016 LAB	18.03.2020	27	86,927	550,570	549,842	549,845					549,842	463,643	462,915
PW016 ICE	18.03.2020	27	87,597	514,794	514,119	514,121					514,119	427,197	426,522
PW019 LAB	18.03.2020	70	90,904	510,381	509,412	509,409	509,427	509,419	509,420		509,409	419,477	418,505
PW019 ICE	18.03.2020	27	91,511	510,430	509,400	509,403					509,400	418,919	417,889
PW022 LAB	18.03.2020	55	88,390	520,766	520,178	520,170	520,178	520,170			520,170	432,376	431,780
PW022 ICE	18.03.2020	27	90,684	536,734	536,118	536,121					536,118	446,05	445,434
Sample	**Date start drying**	**Drying times (days)**	**m (cryst.dish)**	**m (cryst+ rock)**	**14.07.2020**	**28.07.2020**							
PW027 LAB	30.06.2020	28	87,228	457,475	456,996	459,994					456,996	370,247	369,768
PW027 ICE	30.06.2020	28	90,452	460,190	459,702	459,702					459,702	369,738	369,250
Sample	**Date start drying**	**Drying times (days)**	**m (cryst.dish)**	**m (cryst+ rock)**	**29.04.2020**	**13.05.2020**	**27.05.2020**	**10.06.2020**					
PW028 LAB	15.04.2020	28	89,356	531,622	531,097	531,097					531,097	442,266	441,741
PW028 ICE	15.04.2020	56	83,840	528,777	528,264	528,253	528,260	528,262			528,253	444,937	444,413
PW031 LAB	15.04.2020	42	90,805	495,717	495,224	495,221	495,223				495,221	404,912	404,416
PW031 ICE	15.04.2020	56	87,788	490,014	489,499	489,486	489,492	489,495			489,486	402,226	401,698
PW034 LAB	15.04.2020	42	91,261	498,625	498,197	498,192	498,192				498,192	407,364	406,931
PW034 ICE	15.04.2020	56	88,818	496,449	496,020	496,014	496,010	496,014			496,010	407,631	407,192
PW037 LAB	15.04.2020	42	88,663	545,829	545,233	545,226	545,223				545,223	457,166	456,560
PW037 ICE	15.04.2020	42	89,546	544,424	543,774	543,768	543,769				543,768	454,878	454,222
PW040 LAB	15.04.2020	42	90,679	476,093	475,678	475,670	475,672				475,670	385,414	384,991
PW040 ICE	15.04.2020	28	87,804	470,631	470,200	470,201					470,200	382,827	382,396
PW044 LAB	15.04.2020	42	91,195	473,128	472,724	472,720	472,718				472,718	381,933	381,523
PW044 ICE	15.04.2020	56	87,498	467,973	467,532	467,516	467,523	467,528			467,516	380,475	380,018
PW046 LAB	15.04.2020	56	91,786	497,494	497,050	497,046	497,051	497,058			497,046	405,708	405,260
PW046 ICE	15.04.2020	42	89,567	497,420	496,964	496,957	496,959				496,957	407,853	407,390

Appendix Table 10-5: continued

Sample	Date start drying	Drying times (days)	m (cryst.dish)	m (cryst+ rock)	28.05.2020	10.06.2020	24.06.2020			mass dry	m rock wet	m rock dry
PW049 LAB	07.05.2020	48	81,570	438,442	437,860	437,848	437,85			437,848	356,872	356,278
PW049 ICE	07.05.2020	34	86,422	447,013	446,395	446,397				446,395	360,591	359,973
PW052 LAB	07.05.2020	34	89,012	511,386	510,916	510,917				510,916	422,374	421,904
PW052 ICE	07.05.2020	34	92,197	512,650	512,162	512,163				512,162	420,453	419,965
Sample	Date start drying	ying times (da	m (cryst.dish)	m (cryst+ rock)	02.06.2020	16.06.2020	01.07.2020	15.07.2020	29.07.2020			
PW055 LAB	18.05.2020	44	87,823	550,713	550,030	550,048	550,05			550,030	462,89	462,207
PW055 ICE	18.05.2020	58	90,887	554,283	553,600	553,627	553,624	553,623		553,600	463,396	462,713
PW058 LAB	18.05.2020	72	84,302	491,835	491,347	491,367	491,36	491,355	491,354	491,347	407,533	407,045
PW058 ICE	18.05.2020	44	85,987	492,728	492,237	492,245	492,243			492,237	406,741	406,250
PW061 LAB	18.05.2020	44	86,108	513,403	512,792	512,787	512,785			512,785	427,295	426,677
PW061 ICE	18.05.2020	58	93,415	521,434	520,775	520,783	520,775	520,773		520,773	428,019	427,358
PW064 LAB	18.05.2020	44	91,127	550,530	550,019	550,025	550,024			550,019	459,403	458,892
PW064 ICE	18.05.2020	44	88,338	542,891	542,378	542,389	542,387			542,378	454,553	454,040
Sample	Date start drying	Drying times (days)	m (cryst.dish)	m (cryst+ rock)	10.06.2020	24.06.2020	14.07.2020	28.07.2020				
PW067 LAB	29.05.2020	26	88,793	550,630	550,073	550,075				550,073	461,837	461,280
PW067 ICE	29.05.2020	26	85,239	543,717	543,219	543,221				543,219	458,478	457,980
PW070 LAB	29.05.2020	46	88,914	498,046	497,477	497,474	497,472			497,472	409,132	408,558
PW070 ICE	29.05.2020	26	88,053	499,232	498,708	498,706				498,706	411,179	410,653
PW073 LAB	29.05.2020	46	90,745	421,556	420,935	420,928	420,926			420,926	330,811	330,181
PW073 ICE	29.05.2020	60	93,925	426,356	425,766	425,762	425,754	425,755		425,754	332,431	331,829
PW076 LAB	29.05.2020	60	88,468	468,639	468,029	468,026	468,017	468,017		468,017	380,171	379,549
PW076 ICE	29.05.2020	60	86,249	467,172	466,576	466,571	466,569	466,569		466,569	380,923	380,320
PW079 LAB	29.05.2020	60	89,364	399,671	399,169	399,165	399,16	399,159		399,159	310,307	309,795
PW079 ICE	29.05.2020	60	87,295	397,235	396,727	396,721	396,715	396,716		396,715	309,94	309,420
PW082 LAB	29.05.2020	26	91,407	518,621	517,987	517,986				517,986	427,214	426,579
PW082 ICE	29.05.2020	60	87,600	514,314	513,713	513,703	513,697	513,697		513,697	426,714	426,097
PW085 LAB	29.05.2020	60	90,420	590,139	589,493	589,5	589,492	589,495		589,492	499,719	499,072
PW085 ICE	29.05.2020	26	86,961	585,006	584,398	584,397				584,397	498,045	497,436
PW088 LAB	29.05.2020	26	84,663	566,916	566,216	566,216				566,216	482,253	481,553
PW088 ICE	29.05.2020	26	86,550	568,912	568,155	568,155				568,155	482,362	481,605
PW092 LAB	29.05.2020	60	86,266	566,140	565,536	565,548	565,537	565,535		565,535	479,874	479,269
PW092 ICE	29.05.2020	26	91,547	573,339	572,736	572,738				572,736	481,792	481,189

Appendix Table 10-6: Determination of gravimetric water content; sample weights, drying times and calculated water contents of core pieces used for out-diffusion experiments

			before experiment (b.e.)		after experiment (a.e.)											
Sample	**Date start drying**	**Drying times (days)**	**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**23.06.2020**	**08.07.2020**	**21.07.2020**	**04.08.2020**	**18.08.2020**	**01.09.2020**	**16.09.2020**	**29.09.2020**	**07.10.2020**	
			g	g	g	g	g	g	g	g	g	g	g	g	g	
Drying time (days)																
PW001	09.06.2020	120	1552,100	1552,060	1552,482	1552,240	1549,470	1549,467	1549,458	1549,453	1549,469	1549,433	1549,452	1549,414	1549,420	
PW004	09.06.2020	56	1561,972	1561,953	1562,281	1562,115	1559,364	15589,348	1559,330	1559,328						
PW007	09.06.2020	120	1520,128	1520,000	1520,561	1520,330	1517,444	1517,441	1517,432	1517,424	1517,439	1517,411	1517,422	1517,382	1517,386	
PW010	09.06.2020	120	1569,103	1568,973	1569,186	1568,985	1565,976	1565,968	1565,955	1565,948	1565,962	1565,924	1565,940	1565,894	1565,896	
PW014	09.06.2020	120	1553,836	1553,765	1554,344	1554,140	1551,472	1551,469	1551,460	1551,456	1551,478	1551,440	1551,463	1551,418	1551,420	
PW016	09.06.2020	120	1556,613	1556,602	1556,776	1556,610	1553,966	1553,952	1553,938	1553,927	1553,951	1553,908	1553,932	1553,878	1553,880	
PW019	09.06.2020	56	1561,256	1561,248	1561,485	1561,305	1558,484	1558,436	1558,408	1558,406						
PW022	09.06.2020	120	1533,689	1533,661	1533,862	1533,690	1531,353	1531,297	1531,272	1531,262	1531,581	1531,241	1531,261	1531,221	1531,222	
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**06.10.2020**	**20.10.2020**	**03.11.2020**	**17.11.2020**	**04.12.2020**	**18.12.2020**	**01.01.2021**			
			g	g	g	g	g	g	g	g	g	g	g			
Drying time (days)																
PW027	22.09.2020	101	1547,140	1547,028	1547,172	1547,012	1544,649	1544,603	1544,526	1544,489	1544,524	1544,475	1544,524			
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**18.08.2020**	**01.09.2020**	**16.09.2020**	**29.09.2020**	**07.10.2020**	**21.10.2020**	**03.11.2020**	**10.11.2020**	**25.11.2020**	**11.12.2020**
			g	g	g	g	g	g	g	g	g	g	g	g	g	g
Drying time (days)																
PW028	04.08.2020	64	1531,650	1531,613	1531,762	1531,502	1529,271	1529,223	1529,23	1529,187	1529,185					
PW031	04.08.2020	129	1536,922	1536,805	1536,910	1536,683	1534,356	1534,295	1534,298	1534,25	1534,243	1534,216	1534,204	1534,198	1534,170	1534,168
PW034	04.08.2020	64	1524,063	1523,905	1524,132	1523,670	1521,686	1521,643	1521,653	1521,608	1521,606					
PW037	04.08.2020	98	1519,176	1519,162	1519,515	1519,202	1517,175	1517,13	1517,136	1517,091	1517,086	1517,058	1517,048	1517,048		
PW040	04.08.2020	64	1519,733	1519,367	1520,041	1519,160	1516,964	1516,921	1516,933	1516,885	1516,887					
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**25.08.2020**	**08.09.2020**	**23.09.2020**	**06.10.2020**	**20.10.2020**	**03.11.2020**				
			g	g	g	g	g	g	g	g	g	g				
Drying time (days)																
PW044	11.08.2020	84	1503,821	1503,544	1503,791	1503,266	1501,204	1501,167	1501,167	1501,142	1501,115	1501,115				
PW046	11.08.2020	84	1504,325	1504,206	1504,541	1504,050	1501,920	1501,984	1501,907	1501,891	1501,871	1501,869				
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**28.08.2020**	**16.09.2020**	**28.09.2020**	**15.10.2020**	**29.10.2020**	**12.11.2020**	**25.11.2020**	**11.12.2020**	**23.12.2020**	
			g	g	g	g	g	g	g	g	g	g	g	g	g	
Drying time (days)																
PW049	14.08.2020	119	1555,679	1555,679	1556,148	1555,780	1552,569	1552,578	1552,545	1552,413	1552,371	1552,495	1552,417	1552,415		
PW052	14.08.2020	131	1518,550	1518,334	1519,001	1518,478	1515,649	1515,641	1515,625	1515,5	1515,483	1515,553	1515,541	1515,424	1515,425	
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**06.10.2020**	**20.10.2020**	**03.11.2020**	**17.11.2020**	**04.12.2020**	**18.12.2020**	**01.01.2021**			
			g	g	g	g	g	g	g	g	g	g	g			
Drying time (days)																
PW055	22.09.2020	101	1537,588	1537,568	1537,786	1537,644	1535,369	1535,281	1535,260	1535,220	1535,185	1535,166	1535,175			
PW058	22.09.2020	101	1546,038	1546,004	1546,620	1546,403	1543,47	1543,436	1543,422	1543,389	1543,366	1543,347	1543,362			
PW061	22.09.2020	87	1531,521	1531,519	1532,210	1531,970	1529,535	1529,491	1529,458	1529,434	1529,410	1529,412				
PW064	22.09.2020	73	1564,960	1564,920	1565,362	1565,140	1562,706	1562,676	1562,666	1562,606	1562,608					
PW067	22.09.2020	87	1549,043	1549,030	1549,885	1549,610	1547,174	1547,145	1547,139	1547,105	1547,077	1547,080				
PW070	22.09.2020	73	1550,393	1550,371	1551,134	1550,870	1548,129	1548,099	1548,069	1548,012	1548,014					
PW073	22.09.2020	101	1518,842	1518,800	1519,220	1518,970	1515,798	1515,755	1515,745	1515,683	1515,673	1515,663	1515,684			
PW076	22.09.2020	101	1521,997	1521,900	1522,571	1522,310	1518,902	1518,864	1518,850	1518,820	1518,809	1518,783	1518,794			
PW079	22.09.2020	101	1560,360	1560,300	1560,935	1560,730	1557,454	1557,423	1557,395	1557,374	1557,363	1557,330	1557,344			
PW082	22.09.2020	101	1499,742	1499,654	1499,708	1499,455	1496,632	1496,591	1496,576	1496,543	1496,529	1496,453	1496,514			
PW085	22.09.2020	101	1540,679	1540,600	1540,820	1540,550	1538,203	1538,170	1538,158	1538,105	1538,130	1538,088	1538,103			
PW088	22.09.2020	73	1521,120	1521,035	1521,397	1521,200	1518,292	1518,265	1518,224	1518,197	1518,200					
PW092	22.09.2020	73	1531,284	1531,237	1531,652	1531,441	1529,005	1528,988	1528,925	1528,937	1528,94					

Appendix Table 10-6: continued

Sample	m (dry)	m(PW) b.e.	m(PW) a.e.
	g	g	g
PW001	1549,414	2,646	2,826
PW004	1559,328	2,625	2,787
PW007	1517,382	2,618	2,948
PW010	1565,894	3,079	3,091
PW014	1551,418	2,347	2,722
PW016	1553,878	2,724	2,732
PW019	1558,406	2,842	2,899
PW022	1531,221	2,440	2,469
PW027	1544,475	2,553	2,537
PW028	1529,185	2,428	2,317
PW031	1534,168	2,637	2,515
PW034	1521,606	2,299	2,064
PW037	1517,048	2,114	2,154
PW040	1516,885	2,482	2,275
PW044	1501,115	2,429	2,676
PW046	1501,869	2,337	2,181
PW049	1552,371	3,308	3,409
PW052	1515,424	2,910	3,054
PW055	1535,166	2,402	2,478
PW058	1543,347	2,657	3,056
PW061	1529,410	2,109	2,560
PW064	1562,606	2,314	2,534
PW067	1547,077	1,953	2,533
PW070	1548,012	2,359	2,858
PW073	1515,663	3,137	3,307
PW076	1518,783	3,117	3,527
PW079	1557,330	2,970	3,400
PW082	1496,453	3,201	3,002
PW085	1538,088	2,512	2,462
PW088	1518,197	2,838	3,003
PW092	1528,925	2,312	2,516

DETERMINATION OF BULK WET AND DRY DENSITY: RAW DATA

Appendix Table 10-7: Determination of bulk wet and dry density; sample dimensions, weights and density results

Sample	m (core) wet	diameter core	height core	Volume core	bulk, wet density
	g	cm	cm	ccm	g/ccm
IG_BH04_PW003 (AQ)	399,070	6,10	5,15	150,51	2,65
IG_BH04_PW006 (AQ)	345,965	6,09	4,50	131,08	2,64
IG_BH04_PW009 (AQ)	372,194	6,07	4,84	140,06	2,66
IG_BH04_PW011 (AQ)	473,354	6,12	6,09	179,15	2,64
IG_BH04_PW015 (AQ)	398,423	6,12	5,24	154,14	2,58
IG_BH04_PW018 (AQ)	349,423	6,10	4,50	131,51	2,66
IG_BH04_PW021 (AQ)	312,984	6,11	4,05	118,75	2,64
IG_BH04_PW024 (AQ)	411,189	6,10	5,26	153,72	2,67
IG_BH04_PW026 (AQ)	344,120	6,09	4,45	129,62	2,65
IG_BH04_PW030 (AQ)					
IG_BH04_PW033 (AQ)	not determined				
IG_BH04_PW036 (AQ)	339,415	6,08	4,51	130,94	2,59
IG_BH04_PW039 (AQ)	734,120	6,01	9,74	276,31	2,66
IG_BH04_PW042 (AQ)	358,542	6,09	4,70	136,91	2,62
IG_BH04_PW045 (AQ)	388,700	6,06	5,23	150,85	2,58
IG_BH04_PW048 (AQ)	344,098	6,05	4,62	132,81	2,59
IG_BH04_PW051 (AQ)	405,296	6,10	5,29	154,60	2,62
IG_BH04_PW054 (AQ)	642,825	6,09	8,35	243,23	2,64
IG_BH04_PW057 (AQ)	313,507	6,09	4,06	118,26	2,65
IG_BH04_PW060 (AQ)	275,897	6,08	3,60	104,52	2,64
IG_BH04_PW063 (AQ)	400,009	6,07	5,22	151,06	2,65
IG_BH04_PW066 (AQ)	1431,255	6,11	18,32	537,15	2,66
IG_BH04_PW069 (AQ)	486,617	6,14	6,25	185,06	2,63
IG_BH04_PW072 (AQ)	470,115	6,14	6,06	179,43	2,62
IG_BH04_PW075 (AQ)	323,966	6,03	4,30	122,80	2,64
IG_BH04_PW078 (AQ)	297,272	6,07	3,90	112,86	2,63
IG_BH04_PW081 (AQ)	379,392	6,07	5,01	144,98	2,62
IG_BH04_PW084 (AQ)	436,244	6,06	5,74	165,56	2,64
IG_BH04_PW087 (AQ)	358,303	6,07	4,63	133,98	2,67
IG_BH04_PW090 (AQ)	983,372	6,05	12,68	364,52	2,70
IG_BH04_PW093 (AQ)	750,289	6,09	9,63	280,51	2,67

Appendix Table 10-7: continued

Sample	m (core a.e.) wet	m (core a.e.) dry	diameter core	height core	Volume core	bulk, wet density	bulk, dry density
	g	g	cm	cm	ccm	g/ccm	g/ccm
IG_BH04_PW001	1552,240	1549,414	6,11	19,85	582,01	2,67	2,66
IG_BH04_PW004	1562,115	1559,328	6,10	20,05	585,95	2,67	2,66
IG_BH04_PW007	1520,330	1517,382	6,07	19,87	575,00	2,64	2,64
IG_BH04_PW010	1568,985	1565,894	6,11	20,04	587,58	2,67	2,66
IG_BH04_PW014	1554,140	1551,418	6,13	19,87	586,42	2,65	2,65
IG_BH04_PW016	1556,610	1553,878	6,11	19,89	583,19	2,67	2,66
IG_BH04_PW019	1561,305	1558,406	6,12	19,87	584,51	2,67	2,67
IG_BH04_PW022	1533,690	1531,221	6,11	19,53	572,63	2,68	2,67
IG_BH04_PW027	1547,012	1544,475	6,12	19,77	581,57	2,66	2,66
IG_BH04_PW028	1531,502	1529,185	6,07	19,95	577,31	2,65	2,65
IG_BH04_PW031	1536,683	1534,168	6,09	19,96	581,41	2,64	2,64
IG_BH04_PW034	1523,670	1521,606	6,08	19,64	570,21	2,67	2,67
IG_BH04_PW037	1519,202	1517,048	6,03	19,87	567,44	2,68	2,67
IG_BH04_PW040	1519,160	1516,885	6,04	19,91	570,47	2,66	2,66
IG_BH04_PW044	1503,266	1501,115	6,02	19,71	561,01	2,68	2,68
IG_BH04_PW046	1504,050	1501,869	6,05	19,61	563,74	2,67	2,66
IG_BH04_PW049	1555,780	1552,371	6,11	19,94	584,65	2,66	2,66
IG_BH04_PW052	1518,478	1515,424	6,08	19,70	571,96	2,65	2,65
IG_BH04_PW055	1537,644	1535,166	6,04	19,87	569,33	2,70	2,70
IG_BH04_PW058	1546,403	1543,347	6,07	19,98	578,18	2,67	2,67
IG_BH04_PW061	1531,970	1529,410	6,09	19,70	573,84	2,67	2,67
IG_BH04_PW064	1565,140	1562,606	6,10	20,03	585,37	2,67	2,67
IG_BH04_PW067	1549,610	1547,077	6,11	19,70	577,62	2,68	2,68
IG_BH04_PW070	1550,870	1548,012	6,11	19,90	583,48	2,66	2,65
IG_BH04_PW073	1518,970	1515,663	6,03	20,09	573,73	2,65	2,64
IG_BH04_PW076	1522,310	1518,783	6,07	19,80	572,97	2,66	2,65
IG_BH04_PW079	1560,730	1557,330	6,06	20,41	588,68	2,65	2,65
IG_BH04_PW082	1499,455	1496,453	6,06	19,60	565,32	2,65	2,65
IG_BH04_PW085	1540,550	1538,088	6,05	19,92	572,65	2,69	2,69
IG_BH04_PW088	1521,200	1518,197	6,06	19,96	575,70	2,64	2,64
IG_BH04_PW092	1531,441	1528,925	6,07	19,7	570,08	2,69	2,68

AQUEOUS EXTRACTION EXPERIMENTS: RAW DATA

Appendix Table 10-8: Determination of bulk wet and dry density; sample dimensions, weights and density results

Sample	Depth	m (bottle)	m (bottle + rock)	m (rock)	m (H2O)	m (tot)	water:rock
	m a.b.	g	g	g	g	g	
IG_BH04_PW003 (AQ)	163,7	18,468	112,342	93,874	74,600	186,942	0,79
IG_BH04_PW006 (AQ)	168,1	18,232	119,621	101,389	63,536	183,157	0,63
IG_BH04_PW009 (AQ)	213,9	18,423	128,197	109,774	64,328	192,525	0,59
IG_BH04_PW011 (AQ)	238,0	18,240	121,269	103,029	62,902	184,171	0,61
IG_BH04_PW015 (AQ)	268,0	18,174	101,487	83,313	74,765	176,252	0,90
IG_BH04_PW018 (AQ)	294,5	18,454	113,548	95,094	76,367	189,915	0,80
IG_BH04_PW021 (AQ)	318,1	18,506	123,819	105,313	74,585	198,404	0,71
IG_BH04_PW024 (AQ)	348,2	18,202	107,314	89,112	75,000	182,314	0,84
IG_BH04_PW026 (AQ)	372,0	18,507	100,858	82,351	64,550	165,408	0,78
IG_BH04_PW030 (AQ)	397,1	19,970	127,792	107,822	65,021	192,813	0,60
IG_BH04_PW033 (AQ)	424,2	17,981	98,350	80,369	62,230	160,580	0,77
IG_BH04_PW036 (AQ)	451,5	18,681	124,530	105,849	56,974	181,504	0,54
IG_BH04_PW039 (AQ)	478,8	17,978	124,942	106,964	73,152	198,094	0,68
IG_BH04_PW042 (AQ)	505,7	17,985	124,606	106,621	64,957	189,563	0,61
IG_BH04_PW045 (AQ)	532,5	18,158	130,161	112,003	57,224	187,385	0,51
IG_BH04_PW048 (AQ)	561,9	18,697	121,849	103,152	69,217	191,066	0,67
IG_BH04_PW051 (AQ)	585,9	18,130	137,585	119,455	72,915	210,500	0,61
IG_BH04_PW054 (AQ)	615,4	17,976	114,314	96,338	70,424	184,738	0,73
IG_BH04_PW057 (AQ)	637,5	17,936	109,226	91,290	69,456	178,682	0,76
IG_BH04_PW060 (AQ)	666,1	18,178	102,514	84,336	67,747	170,261	0,80
IG_BH04_PW063 (AQ)	693,1	18,454	94,183	75,729	69,544	163,727	0,92
IG_BH04_PW066 (AQ)	712,1	18,139	111,751	93,612	66,925	178,676	0,71
IG_BH04_PW069 (AQ)	747,0	18,107	121,050	102,943	57,784	178,834	0,56
IG_BH04_PW072 (AQ)	772,3	18,412	93,800	75,388	73,662	167,462	0,98
IG_BH04_PW075 (AQ)	796,0	18,128	102,604	84,476	70,519	173,123	0,83
IG_BH04_PW078 (AQ)	825,9	18,373	116,207	97,834	60,346	176,553	0,62
IG_BH04_PW081 (AQ)	850,1	18,240	120,170	101,930	59,776	179,946	0,59
IG_BH04_PW084 (AQ)	878,4	18,527	116,846	98,319	62,128	178,974	0,63
IG_BH04_PW087 (AQ)	904,7	18,213	102,168	83,955	70,068	172,236	0,83
IG_BH04_PW090 (AQ)	932,1	18,098	117,129	99,031	59,998	177,127	0,61
IG_BH04_PW093 (AQ)	959,3	18,107	103,947	85,84	73,062	177,009	0,85

ISOTOPE DIFFUSIVE EXCHANGE EXPERIMENTS: RAW DATA

Appendix Table 10-9: Analytical raw data of isotope diffusive exchange experiments

Sample		Date Experiment Start	Date Experiment End	Weight container	Weight container and rock	Cryst. dish	Cryst Dish + H2O	Total weight container	Weight rock	Weight test solution	Total weight container after experiment	Weight test solution after experiment	Weight container and rock after experiment	Weight test solution after experiment	Weight rock after experiment	mass (PW)	mass TW+PW after exp.	Δ total weight before & after	Δ weight rock before & after	Δ weight test solution before & after	Δ weight rock and test solution	Δ weight rock and test solution - Δ total weight before and after	Δ weight rock and test solution	Δ water loss (total weight)	remaining water fraction
				g	g	g	g	g	g	g	g	g	g	g	g	g	g	g	g	g	g	g	% of TW	% of TW+PW	
PW001	LAB	15.01.2020	18.03.2020	527,096	1007,740	14,914	16,732	1024,464	480,644	1,818	1024,441	16,731	1007,701	1,817	480,605	0,692	2,509	-0,023	-0,039	-0,001	-0,040	-0,017	2,2	0,9	0,99
PW004	LAB	15.01.2020	18.03.2020	526,404	881,108	13,390	15,194	896,298	354,704	1,804	896,280	15,156	881,118	1,766	354,714	0,555	2,321	-0,018	0,010	-0,038	-0,028	-0,010	1,6	0,8	0,99
PW007	LAB	15.01.2020	18.03.2020	524,171	880,098	15,041	16,848	896,936	355,927	1,807	896,911	16,805	880,102	1,764	355,931	0,535	2,299	-0,025	0,004	-0,043	-0,039	-0,014	2,2	1,1	0,99
PW010	LAB	15.01.2020	18.03.2020	525,786	964,239	15,001	16,804	981,030	438,453	1,803	981,015	16,781	964,225	1,780	438,439	0,715	2,495	-0,015	-0,014	-0,023	-0,037	-0,022	2,1	0,6	0,99
PW014	LAB	15.01.2020	18.03.2020	523,240	981,814	15,730	17,534	999,416	458,574	1,804	999,401	17,516	981,881	1,786	458,641	0,632	2,418	-0,015	0,067	-0,018	0,049	0,064	-2,7	0,6	0,99
PW016	LAB	15.01.2020	18.03.2020	516,369	992,804	14,897	16,708	1009,499	476,435	1,811	1009,484	16,626	992,855	1,729	476,486	0,728	2,457	-0,015	0,051	-0,082	-0,031	-0,016	1,7	0,6	0,99
PW019	LAB	15.01.2020	18.03.2020	518,090	941,454	12,910	14,721	956,163	423,364	1,811	956,147	14,639	941,503	1,729	423,413	0,972	2,701	-0,016	0,049	-0,082	-0,033	-0,017	1,8	0,6	0,99
PW022	LAB	15.01.2020	18.03.2020	513,743	967,266	12,966	14,778	982,037	453,523	1,812	982,023	14,706	967,307	1,740	453,564	0,596	2,336	-0,014	0,041	-0,072	-0,031	-0,017	1,7	0,6	0,99
PW027	LAB	24.04.2020	30.06.2020	523,937	894,470	14,839	16,649	911,106	370,533	1,810	911,131	16,567	894,561	1,728	370,624	0,479	2,207	0,025	0,091	-0,082	0,009	-0,016	-0,5	-1,1	1,01
PW028	LAB	07.02.2020	15.04.2020	522,806	965,346	12,944	14,966	980,305	442,540	2,022	980,266	14,993	965,273	2,049	442,467	0,525	2,574	-0,039	-0,073	0,027	-0,046	-0,007	2,3	1,5	0,98
PW031	LAB	07.02.2020	15.04.2020	526,183	931,491	14,631	16,441	947,929	405,308	1,810	947,888	16,462	931,424	1,831	405,241	0,496	2,327	-0,041	-0,067	0,021	-0,046	-0,005	2,5	1,8	0,98
PW034	LAB	07.02.2020	15.04.2020	524,932	932,663	13,425	15,231	947,875	407,731	1,806	947,841	15,269	932,571	1,844	407,639	0,433	2,277	-0,034	-0,092	0,038	-0,054	-0,020	3,0	1,5	0,99
PW037	LAB	07.02.2020	15.04.2020	525,718	983,191	14,789	16,484	999,664	457,473	1,695	999,637	16,430	983,204	1,641	457,486	0,606	2,247	-0,027	0,013	-0,054	-0,041	-0,014	2,4	1,2	0,99
PW040	LAB	07.02.2020	15.04.2020	523,648	909,434	15,275	17,090	926,511	385,786	1,815	926,515	17,124	909,360	1,849	385,712	0,423	2,272	0,004	-0,074	0,034	-0,040	-0,044	2,2	-0,2	1,00
PW044	LAB	08.02.2020	15.04.2020	523,790	906,009	12,971	14,765	920,765	382,219	1,794	920,732	14,831	905,896	1,860	382,106	0,41	2,270	-0,033	-0,113	0,066	-0,047	-0,014	2,6	1,5	0,99
PW046	LAB	08.02.2020	15.04.2020	525,628	931,637	13,572	15,379	947,012	406,009	1,807	946,979	15,423	931,554	1,851	405,926	0,448	2,299	-0,033	-0,083	0,044	-0,039	-0,006	2,2	1,4	0,99
PW049	LAB	06.03.2020	07.05.2020	518,096	875,376	14,677	16,462	891,831	357,280	1,785	891,787	16,422	875,374	1,745	357,278	0,594	2,339	-0,044	-0,002	-0,040	-0,042	0,002	2,4	1,9	0,98
PW052	LAB	06.03.2020	07.05.2020	516,310	939,999	13,335	15,131	954,121	423,689	1,796	954,081	15,219	939,873	1,884	423,563	0,47	2,354	-0,040	-0,126	0,088	-0,038	0,002	2,1	1,7	0,98
PW055	LAB	18.03.2020	18.05.2020	522,803	986,603	13,413	15,221	1001,812	463,800	1,808	1001,806	15,119	986,690	1,706	463,887	0,683	2,389	-0,006	0,087	-0,102	-0,015	-0,009	0,8	0,3	1,00
PW058	LAB	18.03.2020	18.05.2020	525,139	933,139	14,922	16,728	949,855	408,000	1,806	949,852	16,659	933,185	1,737	408,046	0,488	2,225	-0,003	0,046	-0,069	-0,023	-0,020	1,3	0,1	1,00
PW061	LAB	18.03.2020	18.05.2020	527,637	955,831	13,951	15,774	971,591	428,194	1,823	971,580	15,658	955,918	1,707	428,281	0,618	2,325	-0,011	0,087	-0,116	-0,029	-0,018	1,6	0,5	1,00
PW064	LAB	18.03.2020	18.05.2020	524,141	984,096	14,877	16,684	1000,761	459,955	1,807	1000,753	16,600	984,151	1,723	460,010	0,511	2,234	-0,008	0,055	-0,084	-0,029	-0,021	1,6	0,4	1,00
PW067	LAB	26.03.2020	29.05.2020	521,097	983,287	12,982	14,772	998,046	462,190	1,790	998,048	14,668	983,383	1,686	462,286	0,557	2,243	0,002	0,096	-0,104	-0,008	-0,010	0,4	-0,1	1,00
PW070	LAB	26.03.2020	29.05.2020	514,968	924,241	13,893	15,707	939,938	409,273	1,814	939,939	15,607	924,333	1,714	409,365	0,574	2,288	0,001	0,092	-0,100	-0,008	-0,009	0,4	0,0	1,00
PW073	LAB	26.03.2020	29.05.2020	514,641	845,862	14,380	16,174	862,030	331,221	1,794	862,024	16,112	845,910	1,732	331,269	0,63	2,362	-0,006	0,048	-0,062	-0,014	-0,008	0,8	0,3	1,00
PW076	LAB	26.03.2020	29.05.2020	524,482	905,080	14,712	16,501	921,574	380,598	1,789	921,573	16,463	905,106	1,751	380,624	0,622	2,373	-0,001	0,026	-0,038	-0,012	-0,011	0,7	0,0	1,00
PW079	LAB	26.03.2020	29.05.2020	524,044	834,548	14,890	16,685	851,228	310,504	1,795	851,225	16,613	834,607	1,723	310,563	0,512	2,235	-0,003	0,059	-0,072	-0,013	-0,010	0,7	0,1	1,00
PW082	LAB	26.03.2020	29.05.2020	523,518	951,040	15,001	16,784	967,817	427,522	1,783	967,805	16,781	951,022	1,780	427,504	0,635	2,415	-0,012	-0,018	-0,003	-0,021	-0,009	1,2	0,5	1,00
PW085	LAB	26.03.2020	29.05.2020	512,563	1012,972	14,376	16,172	1029,132	500,409	1,796	1029,126	16,098	1013,025	1,722	500,462	0,647	2,369	-0,006	0,053	-0,074	-0,021	-0,015	1,2	0,3	1,00
PW088	LAB	26.03.2020	29.05.2020	520,002	1003,431	13,895	15,669	1019,097	483,429	1,774	1019,095	15,545	1003,554	1,650	483,552	0,700	2,350	-0,002	0,123	-0,124	-0,001	0,001	0,1	0,1	1,00
PW092	LAB	26.03.2020	29.05.2020	522,704	1003,032	14,917	16,718	1019,728	480,328	1,801	1019,731	16,620	1003,115	1,703	480,411	0,605	2,308	0,003	0,083	-0,098	-0,015	-0,018	0,8	-0,1	1,00
PW001	ICE	15.01.2020	18.03.2020	521,292	1004,784	15,373	17,176	1021,948	483,492	1,803	1021,918	17,133	1004,781	1,760	483,489	0,646	2,406	-0,030	-0,003	-0,043	-0,046	-0,016	2,6	1,2	0,99
PW004	ICE	15.01.2020	18.03.2020	526,610	884,861	14,755	16,566	901,413	358,251	1,811	901,394	16,483	884,860	1,728	358,250	0,560	2,288	-0,019	-0,001	-0,083	-0,084	-0,065	4,6	0,8	0,99
PW007	ICE	15.01.2020	18.03.2020	523,164	878,164	12,984	14,805	892,954	355,000	1,821	892,939	14,749	878,182	1,765	355,018	0,528	2,293	-0,015	0,018	-0,056	-0,038	-0,023	2,1	0,7	0,99
PW010	ICE	15.01.2020	18.03.2020	523,209	969,306	15,162	16,958	986,235	446,097	1,796	986,219	16,928	969,287	1,766	446,078	0,720	2,486	-0,016	-0,019	-0,030	-0,049	-0,033	2,7	0,6	0,99
PW014	ICE	15.01.2020	18.03.2020	525,641	984,794	15,026	16,833	1001,618	459,153	1,807	1001,595	16,791	984,800	1,765	459,159	0,627	2,392	-0,023	0,006	-0,042	-0,036	-0,013	2,0	1,0	0,99
PW016	ICE	15.01.2020	18.03.2020	516,385	992,406	14,820	16,620	1009,019	476,021	1,800	1009,001	16,545	992,453	1,725	476,068	0,675	2,400	-0,018	0,047	-0,075	-0,028	-0,010	1,6	0,8	0,99
PW019	ICE	15.01.2020	18.03.2020	517,051	937,086	13,787	15,592	952,669	420,035	1,805	952,656	15,524	937,127	1,737	420,076	1,030	2,767	-0,013	0,041	-0,068	-0,027	-0,014	1,5	0,5	1,00
PW022	ICE	15.01.2020	18.03.2020	518,600	970,743	14,267	16,065	986,798	452,143	1,798	986,782	15,979	970,797	1,712	452,197	0,616	2,328	-0,016	0,054	-0,086	-0,032	-0,016	1,8	0,7	0,99
PW027	ICE	24.04.2020	30.06.2020	525,086	895,473	13,572	15,391	910,851	370,387	1,819	910,876	15,330	895,544	1,758	370,458	0,488	2,246	0,025	0,071	-0,061	0,010	-0,015	-0,5	-1,1	1,01
PW028	ICE	07.02.2020	15.04.2020	523,608	969,602	16,545	18,366	987,959	445,994	1,821	987,928	18,389	969,539	1,844	445,931	0,524	2,368	-0,031	-0,063	0,023	-0,040	-0,009	2,2	1,3	0,99
PW031	ICE	07.02.2020	15.04.2020	522,609	925,113	14,117	15,926	941,034	402,504	1,809	941,001	15,953	925,048	1,836	402,439	0,528	2,364	-0,033	-0,065	0,027	-0,038	-0,005	2,1	1,4	0,99
PW034	ICE	07.02.2020	15.04.2020	524,663	932,708	14,435	16,233	948,929	408,045	1,798	948,903	16,290	932,612	1,855	407,949	0,439	2,294	-0,026	-0,096	0,057	-0,039	-0,013	2,2	1,1	0,99
PW037	ICE	07.02.2020	15.04.2020	525,614	985,016	14,760	16,559	1001,57	459,402	1,799	1001,517	16,553	984,965	1,793	459,351	0,656	2,449	-0,053	-0,051	-0,006	-0,057	-0,004	3,2	2,2	0,98
PW040	ICE	07.02.2020	15.04.2020	524,955	908,092	13,794	15,584	923,669	383,137	1,790	923,639	15,653	907,981	1,859	383,026	0,431	2,290	-0,030	-0,111	0,069	-0,042	-0,012	2,3	1,3	0,99
PW044	ICE	08.02.2020	15.04.2020	521,915	902,628	14,911	16,722	919,340	380,713	1,811	919,310	16,779	902,527	1,868	380,612	0,457	2,325	-0,030	-0,101	0,057	-0,044	-0,014	2,4	1,3	0,99
PW046	ICE	08.02.2020	15.04.2020	524,320	933,544	14,481	16,292	949,830	409,224	1,811	949,797	16,313	933,487	1,832	409,167	0,463	2,295	-0,033	-0,057	0,021	-0,036	-0,003	2,0	1,4	0,99
PW049	ICE	06.03.2020	07.05.2020	514,141	875,611	12,321	14,128	889,730	361,470	1,807	889,692	14,077	875,623	1,756	361,482	0,618	2,374	-0,038	0,012	-0,051	-0,039	-0,001	2,2	1,6	0,98
PW052	ICE	06.03.2020	07.05.2020	516,310	938,078	15,068	16,884	954,925	421,768	1,816	954,882	16,915	937,978	1,847	421,668	0,488	2,335	-0,043	-0,100	0,031	-0,069	-0,026	3,8	1,8	0,98
PW055	ICE	18.03.2020	18.05.2020	514,562	978,208	14,653	16,468	994,662	463,646	1,815	994,656	16,364	978,289	1,711	463,727	0,683	2,394	-0,006	0,081	-0,104	-0,023	-0,017	1,3	0,3	1,00
PW058	ICE	18.03.2020	18.05.2020	517,909	925,524	13,419	15,225	940,735	407,615	1,806	940,727	15,137	925,587	1,718	407,678	0,491	2,209	-0,008	0,063	-0,088	-0,025	-0,017	1,4	0,4	1,00
PW061	ICE	18.03.2020	18.05.2020	523,474	952,169	13,024	14,836	966,992	428,695	1,812	966,986	14,716	952,262	1,692	428,788	0,661	2,353	-0,006	0,093	-0,12	-0,027	-0,021	1,5	0,3	1,00
PW064	ICE	18.03.2020	18.05.2020	523,960	979,048	13,508	15,322	994,355	455,088	1,814	994,352	15,254	979,094	1,746	455,134	0,513	2,259	-0,003	0,046	-0,068	-0,022	-0,019	1,2	0,1	1,00
PW067	ICE	26.03.2020	29.05.2020	514,488	973,163	14,059	15,859	989,012	458,675	1,800	989,014	15,763	973,258	1,704	458,770	0,498	2,202	0,002	0,095	-0,096	-0,001	-0,003	0,1	-0,1	1,00
PW070	ICE	26.03.2020	29.05.2020	523,029	934,418	12,910	14,705	949,110	411,389	1,795	949,114	14,603	934,510	1,693	411,481	0,526	2,219	0,004	0,092	-0,102	-0,01	-0,014	0,6	-0,2	1,00
PW073	ICE	26.03.2020	29.05.2020	514,834	847,715	12,068	14,761	862,468	332,881	2,693	862,464	14,685	847,779	2,617	332,945	0,602	3,219	-0,004	0,064	-0,076	-0,012	-0,008	0,4	0,1	1,00
PW076	ICE	26.03.2020	29.05.2020	514,004	895,589	14,434	16,248	911,831	381,585	1,814	911,828	16,196	895,634	1,762	381,630	0,603	2,365	-0,003	0,045	-0,052	-0,007	-0,004	0,4	0,1	1,00
PW079	ICE	26.03.2020	29.05.2020	520,442	831,240	14,345	16,128	847,359	310,798	1,783	847,353	16,045	831,308	1,700	310,866	0,520	2,220	-0,006	0,068	-0,083	-0,015	-0,009	0,8	0,3	1,00
PW082	ICE	26.03.2020	29.05.2020	514,779	942,561	13,995	15,784	958,324	427,782	1,789	958,310	15,787	942,519	1,792	427,740	0,617	2,409	-0,014	-0,042	0,003	-0,039	-0,025	2,2	0,6	0,99
PW085	ICE	26.03.2020	29.05.2020	517,195	1016,439	13,144	14,930	1031,355	499,244	1,786	1031,354	14,849	1016,500	1,705	499,305	0,609	2,314	-0,001	0,061	-0,081	-0,02	-0,019	1,1	0,0	1,00
PW088	ICE	26.03.2020	29.05.2020	527,785	1010,445	14,102	15,925	1026,318	482,660	1,823	1026,320	15,794	1010,529	1,692	482,744	0,757	2,449	0,002	0,084	-0,131	-0,047	-0,049	2,6	-0,1	1,00
PW092	ICE	26.03.2020	29.05.2020	521,667	1003,828	13,826	15,615	1019,435	482,161	1,789	1019,438	15,542	1003,899	1,716	482,232	0,603	2,319	0,003	0,071	-0,073	-0,002	-0,005	0,1	-0,1	1,00

Appendix Table 10-10: Analytical data of isotope diffusive exchange experiments

Sample	Test water	Initial $\delta^{18}O$ TW	Initial $\delta^{2}H$ TW	Final $d^{18}O$ TW	Final $\delta^{2}H$ TW
		‰ VSMOW	‰ VSMOW	‰ VSMOW	‰ VSMOW
PW001	LAB	-10,32	-73,6	-11,18	-82,2
PW004	LAB	-10,32	-73,6	-11,50	-85,0
PW007	LAB	-10,32	-73,6	-10,40	-78,8
PW010	LAB	-10,32	-73,6	-11,09	-82,4
PW014	LAB	-10,32	-73,6	-10,63	-77,6
PW016	LAB	-10,32	-73,6	-10,92	-79,0
PW019	LAB	-10,32	-73,6	-11,31	-82,6
PW022	LAB	-10,32	-73,6	-10,89	-79,7
PW027	LAB	-10,18	-73,0	-10,28	-74,8
PW028	LAB	-10,25	-73,0	-10,45	-78,1
PW031	LAB	-10,25	-73,0	-10,35	-78,4
PW034	LAB	-10,25	-73,0	-9,76	-73,1
PW037	LAB	-10,25	-73,0	-10,82	-80,0
PW040	LAB	-10,25	-73,0	-9,65	-71,4
PW044	LAB	-10,25	-73,0	-9,97	-75,4
PW046	LAB	-10,25	-73,0	-10,12	-76,6
PW049	LAB	-10,21	-73,1	-10,63	-77,0
PW052	LAB	-10,21	-73,1	-9,84	-73,3
PW055	LAB	-10,22	-72,8	-10,53	-76,5
PW058	LAB	-10,22	-72,8	-9,93	-72,5
PW061	LAB	-10,22	-72,8	-9,86	-71,9
PW064	LAB	-10,22	-72,8	-9,74	-71,5
PW067	LAB	-10,24	-73,1	-10,03	-71,8
PW070	LAB	-10,24	-73,1	-10,07	-71,4
PW073	LAB	-10,24	-73,1	-9,94	-71,0
PW076	LAB	-10,24	-73,1	-9,77	-69,9
PW079	LAB	-10,24	-73,1	-9,73	-69,7
PW082	LAB	-10,24	-73,1	-9,50	-69,5
PW085	LAB	-10,24	-73,1	-9,35	-68,4
PW088	LAB	-10,24	-73,1	-9,73	-70,1
PW092	LAB	-10,24	-73,1	-9,72	-70,7

Appendix Table 10-10: continued

Sample	Test water	Initial δ^{18}O TW	Initial δ^{2}H TW	Final d^{18}O TW	Final δ^{2}H TW
		‰ VSMOW	‰ VSMOW	‰ VSMOW	‰ VSMOW
PW001	ICE	-31,82	-245,4	-25,95	-200,7
PW004	ICE	-31,82	-245,4	-26,42	-204,3
PW007	ICE	-31,82	-245,4	-26,76	-207,8
PW010	ICE	-31,82	-245,4	-25,55	-199,4
PW014	ICE	-31,82	-245,4	-25,92	-200,5
PW016	ICE	-31,82	-245,4	-25,48	-196,4
PW019	ICE	-31,82	-245,4	-24,31	-188,1
PW022	ICE	-31,82	-245,4	-26,25	-203,4
PW027	ICE	-31,62	-246,5	-25,49	-201,8
PW028	ICE	-31,50	-243,9	-25,51	-199,4
PW031	ICE	-31,50	-243,9	-25,34	-198,1
PW034	ICE	-31,50	-243,9	-25,98	-203,8
PW037	ICE	-31,50	-243,9	-25,70	-200,4
PW040	ICE	-31,50	-243,9	-25,08	-196,4
PW044	ICE	-31,50	-243,9	-25,05	-196,4
PW046	ICE	-31,50	-243,9	-24,98	-196,0
PW049	ICE	-31,38	-245,2	-25,90	-200,8
PW052	ICE	-31,38	-245,2	-25,47	-200,1
PW055	ICE	-31,53	-245,3	-25,36	-197,7
PW058	ICE	-31,53	-245,3	-26,61	-207,2
PW061	ICE	-31,53	-245,3	-25,99	-203,0
PW064	ICE	-31,53	-245,3	-25,87	-203,2
PW067	ICE	-31,29	-244,6	-26,36	-205,6
PW070	ICE	-31,29	-244,6	-26,41	-205,3
PW073	ICE	-31,29	-244,6	-25,97	-201,9
PW076	ICE	-31,29	-244,6	-25,26	-197,0
PW079	ICE	-31,29	-244,6	-25,95	-202,3
PW082	ICE	-31,29	-244,6	-24,43	-192,4
PW085	ICE	-31,29	-244,6	-24,56	-193,3
PW088	ICE	-31,29	-244,6	-24,13	-188,5
PW092	ICE	-31,29	-244,6	-25,07	-196,5

OUT-DIFFUSION EXPERIMENTS: RAW DATA

Appendix Table 10-11: Experimental data of out-diffusion experiments

Sample		IG_BH03_Blank	IG_BH04_PW001	IG_BH04_PW004	IG_BH04_PW007	IG_BH04_PW010	IG_BH04_PW014	IG_BH04_PW016	IG_BH04_PW019	IG_BH04_PW022	IG_BH04_PW027	IG_BH04_PW028
Depth	m		162,5	167,4	213,2	236,4	267,7	293,4	317,4	347,4	372,2	397,8
start experiment		03.09.2019	15.01.2020	15.01.2020	15.01.2020	15.01.2020	15.01.2020	15.01.2020	15.01.2020	15.01.2020	24.04.2020	07.02.2020
Initial Rock Mass (as received, +/- mountain wet)	g		1552,100	1561,972	1520,128	1569,103	1553,836	1556,613	1561,256	1533,689	1547,140	1531,650
Initial Rock Mass (start experiment)	g		1552,060	1561,953	1520,000	1568,973	1553,765	1556,602	1561,248	1533,661	1547,028	1531,613
Final Rock Mass (resaturated)	g		1552,240	1562,115	1520,330	1568,985	1554,140	1556,610	1561,305	1533,690	1547,012	1531,502
Uptake of water	g		0,14	0,14	0,20	-0,12	0,30	0,00	0,05	0,00	-0,13	-0,15
Saturation	%		99,991	99,991	99,987	100,008	99,980	100,000	99,997	100,000	100,008	100,010
Core Diametre	cm		6,11	6,1	6,07	6,11	6,13	6,11	6,12	6,11	6,12	6,07
Core Length	cm		19,85	20,05	19,87	20,04	19,87	19,89	19,87	19,53	19,77	19,95
Volume of Rock Sample	cm3		582,01	585,95	575,00	587,58	586,42	583,19	584,51	572,63	581,57	577,31
Density (calculated from volume & mass)	g/cm3		2,67	2,67	2,64	2,67	2,65	2,67	2,67	2,68	2,66	2,65
Mass of Rock (calculated from volume and density)			1552,10	1561,97	1520,13	1569,10	1553,84	1556,61	1561,26	1533,69	1547,14	1531,65
Masses before experiment												
Mass cylinder	g	356,319	382,730	380,310	380,829	379,840	356,029	381,245	380,285	382,244	356,763	380,406
Mass cylinder + core	g		1934,799	1942,264	1900,831	1948,808	1909,791	1937,844	1941,547	1915,929	1903,808	1911,990
Mass cylinder + core + H2O	g	921,227	2065,286	2063,272	2027,882	2071,756	2039,623	2069,874	2064,979	2040,549	2027,149	2052,187
Mass tot start	g	921,227	2065,266	2063,269	2027,872	2071,739	2039,616	2069,855	2064,961	2040,523	2027,136	2052,208
Initial Water Mass	ml	564,908	130,487	121,008	127,051	122,948	129,832	132,030	123,432	124,620	123,341	140,197
Ratio Exp.Water : Rock			0,084	0,077	0,084	0,078	0,084	0,085	0,079	0,081	0,080	0,092
End Experiment		22.01.2020	09.06.2020	09.06.2020	09.06.2020	09.06.2020	09.06.2020	09.06.2020	09.06.2020	09.06.2020	22.09.2020	04.08.2020
Mass cylinder + core + H2O final	g		2058,023	2050,979	2014,715	2060,762	2031,467	2058,786	2057,507	2027,934	2016,132	2042,090
Final Water Mass (measured, not all recoverable)	ml	112,774	120,351	105,982	110,547	108,479	118,216	117,961	113,119	108,809	109,120	128,010
Time Experiment	days	141	146	146	146	146	146	146	146	146	151	179
Volume of samples for Cl-measurements												
sample A	ml	0,5	0,5	0,5	0,5	0,5	0,7	0,5	0,6	0,5	0,5	0,5
sample B	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample C	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample D	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample E	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample F	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample G	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample H	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample I	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample K	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample L	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample M	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample N	ml		0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
total volume subsamples		6,0	6,5	6,5	6,5	6,5	6,7	6,5	6,6	6,5	6,5	6,5
Volumen TS calculated cyl (ini-final)	ml		7,243	12,290	13,157	10,977	8,149	11,069	7,454	12,589	11,004	10,118
Difference V(ss) - V(calc)	ml		0,043	5,090	5,957	3,777	0,749	3,869	0,154	5,389	3,804	2,918
Difference % of TS	%		0,0	4,2	4,7	3,1	0,6	2,9	0,1	4,3	3,1	2,1

Appendix Table 10-11: continued

Sample		IG_BH04_PW031	IG_BH04_PW034	IG_BH04_PW037	IG_BH04_PW040	IG_BH04_PW044	IG_BH04_PW046	IG_BH04_PW049	IG_BH04_PW052	IG_BH04_PW055	IG_BH04_PW058	IG_BH04_PW061
Depth	m	423,6	450,9	478,1	505,1	531,9	561,3	586,2	614,4	636,8	665,4	692,4
start experiment		07.02.2020	07.02.2020	07.02.2020	07.02.2020	08.02.2020	08.02.2020	06.03.2020	06.03.2020	06.03.2020	06.03.2020	06.03.2020
Initial Rock Mass (as received, +/- mountain wet)	g	1536,922	1524,063	1519,176	1519,733	1503,821	1504,325	1555,679	1518,550	1537,588	1546,038	1531,521
Initial Rock Mass (start experiment)	g	1536,805	1523,905	1519,162	1519,367	1503,544	1504,206	1555,679	1518,334	1537,568	1546,004	1531,519
Final Rock Mass (resaturated)	g	1536,683	1523,670	1519,202	1519,160	1503,266	1504,050	1555,780	1518,478	1537,644	1546,403	1531,970
Uptake of water	g	-0,24	-0,39	0,03	-0,57	-0,55	-0,28	0,10	-0,07	0,06	0,37	0,45
Saturation	%	100,016	100,026	99,998	100,038	100,037	100,018	99,994	100,005	99,996	99,976	99,971
Core Diametre	cm	6,09	6,08	6,03	6,04	6,02	6,05	6,11	6,08	6,09	6,07	6,09
Core Length	cm	19,96	19,64	19,87	19,91	19,71	19,61	19,94	19,70	19,87	19,98	19,70
Volume of Rock Sample	cm3	581,41	570,21	567,44	570,47	561,01	563,74	584,65	571,96	578,79	578,18	573,84
Density (calculated from volume & mass)	g/cm3	2,64	2,67	2,68	2,66	2,68	2,67	2,66	2,66	2,66	2,67	2,67
Mass of Rock (calculated from volume and density)		1536,92	1524,06	1519,18	1519,73	1503,82	1504,33	1555,68	1518,55	1537,59	1546,04	1531,52
Masses before experiment												
Mass cylinder	g	382,598	382,401	382,266	381,080	381,484	381,357	356,913	357,127	357,744	357,013	358,014
Mass cylinder + core	g	1919,389	1906,279	1901,483	1900,458	1888,025	1885,530	1912,601	1875,434	1895,313	1903,004	1889,575
Mass cylinder + core + H2O	g	2049,778	2042,459	2046,308	2044,897	2042,505	2025,623	2036,893	2006,925	2021,656	2032,417	2027,707
Mass tot start	g	2049,801	2042,448	2046,314	2044,919	2039,522	2025,616	2036,886	2006,935	2021,671	2032,432	2027,677
Initial Water Mass	ml	130,389	136,180	144,825	144,439	154,480	140,093	124,292	131,491	126,343	129,413	138,132
Ratio Exp.Water : Rock		0,085	0,089	0,095	0,095	0,103	0,093	0,080	0,087	0,082	0,084	0,090
End Experiment		04.08.2020	04.08.2020	04.08.2020	04.08.2020	11.08.2020	11.08.2020	14.08.2020	14.08.2020	22.09.2020	22.09.2020	22.09.2020
Mass cylinder + core + H2O final	g	2041,883	2035,413	2039,057	2037,750	2032,360	2018,341	2024,592	1993,274	2014,415	2024,997	2020,448
Final Water Mass (measured, not all recoverable)	ml	117,670	122,769	131,795	131,077	139,965	126,140	106,701	109,061	115,395	118,182	127,246
Time Experiment	days	179	179	179	179	185	185	161	161	200	200	200
Volume of samples for Cl-measurements												
sample A	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,7	0,6
sample B	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample C	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample D	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample E	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample F	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample G	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample H	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample I	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample K	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample L	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample M	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample N	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
total volume subsamples		6,5	6,5	6,5	6,5	6,5	6,5	6,5	6,5	6,5	6,7	6,6
Volumen TS calculated cyl (ini-final)	ml	7,918	7,035	7,257	7,169	7,162	7,275	12,294	13,661	7,256	7,435	7,229
Difference V(ss) - V(calc)	ml	0,718	-0,165	0,057	-0,031	-0,038	0,075	5,094	6,461	0,056	0,035	-0,071
Difference % of TS	%	0,6	-0,1	0,0	0,0	0,0	0,1	4,1	4,9	0,0	0,0	-0,1

Table 10-11: continued

Sample		IG_BH04_PW064	IG_BH04_PW067	IG_BH04_PW070	IG_BH04_PW073	IG_BH04_PW076	IG_BH04_PW079	IG_BH04_PW082	IG_BH04_PW085	IG_BH04_PW088	IG_BH04_PW092
Depth	m	711,3	746,3	771,6	795,3	825,3	849,3	877,8	904,0	931,1	959,0
start experiment		06.03.2020	26.03.2020	26.03.2020	26.03.2020	26.03.2020	26.03.2020	26.03.2020	26.03.2020	26.03.2020	26.03.2020
Initial Rock Mass (as received, +/- mountain wet)	g	1564,960	1549,043	1550,393	1518,842	1521,997	1560,360	1499,742	1540,679	1521,120	1531,284
Initial Rock Mass (start experiment)	g	1564,920	1549,030	1550,371	1518,800	1521,900	1560,300	1499,654	1540,600	1521,035	1531,237
Final Rock Mass (resaturated)	g	1565,140	1549,610	1550,870	1518,970	1522,310	1560,730	1499,455	1540,550	1521,200	1531,441
Uptake of water	g	0,18	0,57	0,48	0,13	0,31	0,37	-0,29	-0,13	0,08	0,16
Saturation	%	99,988	99,963	99,969	99,992	99,979	99,976	100,019	100,008	99,995	99,990
Core Diametre	cm	6,10	6,11	6,11	6,03	6,07	6,06	6,06	6,05	6,06	6,07
Core Length	cm	20,03	19,70	19,90	20,09	19,80	20,41	19,60	19,92	19,96	19,70
Volume of Rock Sample	cm3	585,37	577,62	583,48	573,73	572,97	588,68	565,32	572,65	575,70	570,08
Density (calculated from volume & mass)	g/cm3	2,67	2,68	2,66	2,65	2,66	2,65	2,65	2,69	2,64	2,69
Mass of Rock (calculated from volume and density)		1564,96	1549,04	1550,39	1518,84	1522,00	1560,36	1499,74	1540,68	1521,12	1531,28
Masses before experiment											
Mass cylinder	g	357,729	357,825	356,334	356,070	356,897	356,798	362,949	376,371	363,246	359,892
Mass cylinder + core	g	1922,570	1906,840	1906,719	1874,860	1878,794	1917,072	1862,576	1916,950	1884,240	1891,112
Mass cylinder + core + H2O	g	2058,218	2031,797	2028,466	2013,765	2012,424	2049,261	1996,614	2046,197	2015,469	2025,833
Mass tot start	g	2058,260	2031,776	2028,455	2013,752	2012,426	2049,277	1993,836	2051,672	2018,250	2020,353
Initial Water Mass	ml	135,648	124,957	121,747	138,905	133,630	132,189	134,038	129,247	131,229	134,721
Ratio Exp.Water : Rock		0,087	0,081	0,079	0,091	0,088	0,085	0,089	0,084	0,086	0,088
End Experiment		22.09.2020	22.09.2020	22.09.2020	22.09.2020	22.09.2020	22.09.2020	22.09.2020	22.09.2020	22.09.2020	22.09.2020
Mass cylinder + core + H2O final	g	2049,514	2024,458	2020,596	2006,054	2004,956	2041,835	1986,052	2042,938	2010,825	2012,901
Final Water Mass (measured, not all recoverable)	ml	123,380	113,855	110,452	127,502	122,258	120,235	120,307	122,243	123,038	118,659
Time Experiment	days	200	180	180	180	180	180	180	180	180	180
Volume of samples for Cl-measurements											
sample A	ml	0,8	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample B	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample C	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample D	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample E	ml	0,8	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample F	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample G	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample H	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample I	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample K	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample L	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample M	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
sample N	ml	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5	0,5
total volume subsamples		7,1	6,5	6,5	6,5	6,5	6,5	6,5	6,5	6,5	6,5
Volumen TS calculated cyl (ini-final)	ml	8,746	7,318	7,859	7,698	7,470	7,442	7,784	8,734	7,425	7,452
Difference V(ss) - V(calc)	ml	0,946	0,118	0,659	0,498	0,270	0,242	0,584	1,534	0,225	0,252
Difference % of TS	%	0,7	0,1	0,5	0,4	0,2	0,2	0,4	1,2	0,2	0,2

Table 10-12: Chemical composition of time series samples taken during out-diffusion experiments

Sample			IG_BH04_PW001											IG_BH04_PW004										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		15.01.2020																						
A	1	16.01.2020	7,6	2,2	4,3	0,38	<1	<1	5,8	1	0,22	0,47	81	8	1,9	5,2	0,33	<1	<1	3,4	0,83	0,21	0,28	82
B	2	17.01.2020	8	2,8	4,8	0,37	<1	<1	7,3	1,2	<0,2	0,96	132	8,8	2,3	5,4	0,27	<1	<1	3,8	0,94	<0,2	0,49	129
C	4	19.01.2020	11,4	3	5,8	0,22	<1	<1	9,9	1,3	<0,2	1,4	141	14	2,4	6,5	0,21	<1	<1	5,1	1,1	<0,2	0,78	153
D	7	22.01.2020	14,2	3,3	6,5	<0,2	<1	<1	11,8	1,5	<0,2	1,6	136	15	2,8	6,8	<0,2	<1	<1	6,5	1,3	<0,2	1	154
E	11	26.01.2020	17,3	3,5	7,3	<0,2	<1	<1	13,7	1,9	<0,2	1,9	139	18	3,2	7,5	0,2	<1	<1	7,5	1,8	<0,2	1,1	147
F	14	29.01.2020	18,4	3,9	7,9	0,21	<1	<1	14,6	2,3	<0,2	2,1	144	19,2	3,5	8,3	0,25	<1	<1	7,8	2,1	<0,2	1,2	154
G	21	05.02.2020	22,7	4,1	8,5	0,27	<1	<1	15,7	2,6	<0,2	2,2	140	22,5	3,7	9,8	0,36	<1	<1	8,5	2,7	<0,2	1,3	153
H	29	13.02.2020	24,1	4,2	9	0,24	<1	<1	16,6	2,8	0,25	2,3	139	26,5	3,8	10,5	0,39	<1	<1	9	3,2	<0,2	1,4	156
I	48	03.03.2020	28	4,4	10,7	0,29	<1	<1	17,2	3,3	<0,2	2,4	140	29,6	4	11,2	0,43	<1	<1	9,4	4,1	<0,2	1,4	149
K	61	16.03.2020	30	4,5	11,4	0,33	<1	<1	17,4	3,7	<0,2	2,4	138	30,9	4	12,2	0,42	<1	<1	9,6	4,6	<0,2	1,4	146
L	74	29.03.2020	31,8	4,6	12,5	0,29	<1	<1	17,4	4,1	<0,2	2,4	138	32,6	4	12,7	0,39	<1	<1	9,7	4,9	<0,2	1,4	144
M	91	15.04.2020	33,4	4,6	12,8	0,34	<1	<1	17,4	4,5	<0,2	2,4	138	34,3	4	13	0,41	<1	<1	9,7	5,2	0,29	1,4	144
N	120	14.05.2020	34,1	4,6	13,4	0,36	<1	<1	17,4	5,1	<0,2	2,4	138	34,7	4	13,1	0,34	<1	<1	9,7	5,6	<0,2	1,4	144
FINAL	146	09.06.2020	35,3	4,6	14	0,32	0,17	1,4	17,4	5,8	<0,2	2,4	138	34,5	4	12,7	0,25	0,11	0,31	9,7	6,6	<0,2	1,4	144

Sample			IG_BH04_PW007											IG_BH04_PW010										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		15.01.2020																						
A	1	16.01.2020	14,4	2,3	4,7	0,22	<1	<1	13,2	0,62	0,38	0,26	20	11,7	2	5,1	0,2	<1	<1	6,6	0,78	<0,2	0,62	94
B	2	17.01.2020	16,3	2,6	5,7	<0,2	<1	<1	15,9	0,77	<0,2	0,46	29	12,2	2,2	5,6	0,2	<1	<1	7,4	0,98	<0,2	1,2	162
C	4	19.01.2020	25,3	2,9	6,9	<0,2	<1	<1	26	0,81	<0,2	0,67	26	16,7	2,4	6,1	<0,2	<1	<1	10,2	1,2	<0,2	1,6	157
D	7	22.01.2020	31,1	3,1	8,4	<0,2	<1	<1	31	1,3	<0,2	0,93	30	21,3	2,7	6,6	<0,2	<1	<1	11,5	1,7	<0,2	2	174
E	11	26.01.2020	38,6	3,7	9,4	<0,2	<1	<1	37,3	1,9	<0,2	1,02	27	25,5	2,9	7	<0,2	<1	<1	13,5	2	<0,2	2,3	170
F	14	29.01.2020	40,1	4	10,5	<0,2	<1	<1	38,4	2,3	<0,2	1,1	29	26,7	3	7,4	<0,2	<1	<1	14,1	2,3	<0,2	2,44	173
G	21	05.02.2020	44,4	4,1	11,9	<0,2	<1	<1	40,8	2,7	<0,2	1,2	29	31,4	3,1	8,9	<0,2	<1	<1	15,4	2,9	<0,2	2,6	169
H	29	13.02.2020	49,8	4,2	12,5	<0,2	<1	<1	42,8	3,8	<0,2	1,2	28	36,1	3,3	9,8	<0,2	<1	<1	16,2	3,4	<0,2	2,8	173
I	48	03.03.2020	54	4,4	14,2	<0,2	<1	<1	44,4	4,9	<0,2	1,2	27	43,9	3,6	11	<0,2	<1	<1	18	5	<0,2	3	167
K	61	16.03.2020	55,6	4,4	14,4	<0,2	<1	<1	44,4	5,4	<0,2	1,2	27	46	3,7	11,2	<0,2	<1	<1	18,5	5,5	<0,2	3,1	168
L	74	29.03.2020	56,9	4,4	14,5	<0,2	<1	<1	44,4	6,2	<0,2	1,2	27	48,4	3,7	11,3	<0,2	<1	<1	18,7	6,4	<0,2	3,1	166
M	91	15.04.2020	57,9	4,4	14,7	<0,2	<1	<1	44,4	6,6	<0,2	1,2	27	50,1	3,7	11,5	<0,2	<1	<1	18,7	6,8	<0,2	3,1	166
N	120	14.05.2020	63,5	4,4	14,8	<0,2	<1	<1	44,4	8,4	<0,2	1,2	27	50,3	3,7	11,6	<0,2	<1	<1	18,7	7,7	<0,2	3,1	166
FINAL	146	09.06.2020	60	4,4	14,9	<0,2	0,11	0,66	44,4	10,1	<0,2	1,2	27	50,9	3,7	11,6	<0,2	0,09	0,53	18,7	9,2	<0,2	3,1	166

Sample			IG_BH04_PW014											IG_BH04_PW016										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		15.01.2020																						
A	1	16.01.2020	9	1,7	3,8	<0,2	<1	<1	4,9	0,58	<0,2	0,63	129	9,3	1,1	3,6	<0,2	<1	<1	2,7	0,37	<0,2	0,27	100
B	2	17.01.2020	10,9	2	4,8	<0,2	<1	<1	6,4	1	<0,2	1,6	250	12,6	1,3	4,1	<0,2	<1	<1	3,9	0,56	<0,2	0,56	144
C	4	19.01.2020	14,8	2,2	5,4	<0,2	<1	<1	9,3	1,3	<0,2	2,2	237	15,9	1,7	4,6	<0,2	<1	<1	5,8	1	1,6	0,77	133
D	7	22.01.2020	18,5	2,5	5,8	<0,2	<1	<1	11,1	1,4	<0,2	2,7	243	18,4	1,8	4,7	<0,2	<1	<1	6,4	1,2	<0,2	0,98	153
E	11	26.01.2020	23,1	2,8	6,4	<0,2	<1	<1	13,2	1,8	<0,2	3,2	242	22,7	1,9	4,7	<0,2	<1	<1	7,5	1,3	<0,2	1,1	147
F	14	29.01.2020	24,6	3,1	6,6	<0,2	<1	<1	14,1	2,1	<0,2	3,4	241	24,6	2	4,8	<0,2	<1	<1	8	1,4	<0,2	1,2	150
G	21	05.02.2020	27,9	3,3	8	<0,2	<1	<1	15,5	2,5	<0,2	3,7	239	27,4	2	4,9	<0,2	<1	<1	8,6	1,6	<0,2	1,3	151
H	29	13.02.2020	32,4	3,5	8,5	0,21	<1	<1	16,8	3,2	<0,2	3,9	232	31,4	2	5	<0,2	<1	<1	9,1	2	<0,2	1,4	154
I	48	03.03.2020	36,7	3,6	9,2	0,25	<1	<1	17,4	4,2	<0,2	4,1	236	35,6	2,2	5,1	<0,2	<1	<1	10,3	2,8	<0,2	1,55	150
K	61	16.03.2020	39,3	3,6	9,9	0,26	<1	<1	17,7	4,5	<0,2	4,1	232	38,6	2,2	5,2	<0,2	<1	<1	10,6	3,4	<0,2	1,6	151
L	74	29.03.2020	41	3,6	10,1	0,25	<1	<1	17,8	4,8	<0,2	4,1	230	40,8	2,2	5,3	<0,2	<1	<1	10,9	4	<0,2	1,6	147
M	91	15.04.2020	43,6	3,6	10,5	0,3	<1	<1	17,8	5	0,24	4,1	230	41,1	2,2	5,4	<0,2	<1	<1	10,9	4,3	<0,2	1,6	147
N	120	14.05.2020	44,9	3,6	11,2	0,36	<1	<1	17,8	5,8	<0,2	4,1	230	42,6	2,2	5,6	<0,2	<1	<1	10,9	5	<0,2	1,6	147
FINAL	146	09.06.2020	48	3,6	11,4	0,34	0,13	0,51	17,8	7	<0,2	4,1	230	43,1	2,2	5,6	<0,2	0,05	0,42	10,9	6,3	<0,2	1,6	147

Table 10-12: continued

Sample			IG_BH04_PW019											IG_BH04_PW022										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		15.01.2020																						
A	1	16.01.2020	11,8	2,1	5,2	<0,2	<1	<1	4,1	0,27	<0,2	<0,1		9,5	1,8	4,2	<0,2	<1	<1	2,4	0,25	0,38	<0,1	
B	2	17.01.2020	14,2	2,4	6	<0,2	<1	<1	5	0,4	<0,2	<0,1		13,6	2	5,1	<0,2	<1	<1	2,9	0,41	<0,2	<0,1	
C	4	19.01.2020	20,5	3,5	8,1	0,21	<1	<1	6,6	0,89	<0,2	0,1	15	15,3	2,5	6,1	<0,2	<1	<1	3,6	0,65	<0,2	<0,1	
D	7	22.01.2020	25,8	4,4	12,1	<0,2	<1	<1	7,5	1,1	<0,2	0,13	17	18,9	3,2	6,3	<0,2	<1	<1	4,1	0,78	<0,2	<0,1	
E	11	26.01.2020	31,8	4,7	14,1	<0,2	<1	<1	8,6	1,3	<0,2	0,18	21	23,1	3,5	6,8	<0,2	<1	<1	4,8	0,97	<0,2	<0,1	
F	14	29.01.2020	33,9	5	15,2	<0,2	<1	<1	9,3	1,5	<0,2	0,20	22	24,3	3,6	7,3	<0,2	<1	<1	5	1,1	<0,2	<0,1	
G	21	05.02.2020	38,8	5,2	15,9	<0,2	<1	<1	9,7	1,7	<0,2	0,22	23	28,3	3,7	8,1	<0,2	<1	<1	5,4	1,4	<0,2	<0,1	
H	29	13.02.2020	44,3	5,3	16,6	<0,2	<1	<1	10,4	1,9	<0,2	0,22	21	31,9	3,7	8,7	<0,2	<1	<1	5,7	1,7	<0,2	<0,1	
I	48	03.03.2020	51,9	5,4	17,6	<0,2	<1	<1	11,5	2,6	<0,2	0,22	19	36,7	3,7	8,8	<0,2	<1	<1	6,2	2,4	<0,2	<0,1	
K	61	16.03.2020	55,7	5,4	19	0,22	<1	<1	11,8	3,4	<0,2	0,22	19	37,8	3,7	8,9	<0,2	<1	<1	6,4	2,8	<0,2	<0,1	
L	74	29.03.2020	59,7	5,4	19,3	<0,2	<1	<1	12,1	3,8	<0,2	0,22	18	38,7	3,7	9	<0,2	<1	<1	6,5	3	<0,2	<0,1	
M	91	15.04.2020	61,3	5,4	19,9	0,27	<1	<1	12,1	4,2	<0,2	0,22	18	39,3	3,7	9,1	<0,2	<1	<1	6,5	3,4	<0,2	<0,1	
N	120	14.05.2020	65,3	5,4	20,4	0,29	<1	<1	12,1	5,2	<0,2	0,22	18	39,7	3,7	9,3	<0,2	<1	<1	6,5	3,8	<0,2	<0,1	
FINAL	146	09.06.2020	69,6	5,4	21,9	0,27	0,19	0,34	12,1	6,1	<0,2	0,22	18	40,3	3,7	9,5	<0,2	0,07	0,25	6,5	4,5	<0,2	0,12	18

Sample			IG_BH04_PW028											IG_BH04_PW031										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		07.02.2020																						
A	1	08.02.2020	6,2	2,3	4,3	<0,2	<1	<1	4	0,64	0,5	0,17	43	5,1	2,2	4,8	<0,2	<1	<1	2,2	0,41	0,23	<0,1	
B	2	09.02.2020	7,1	2,4	4,8	<0,2	<1	<1	5	0,83	0,28	0,21	42	5,7	2,7	5,6	<0,2	<1	<1	2,6	0,48	0,2	<0,1	
C	4	11.02.2020	9,3	2,5	6,2	<0,2	<1	<1	6,5	1,1	0,23	0,28	43	8,5	2,9	7,2	<0,2	<1	<1	3,1	0,71	0,2	<0,1	
D	7	14.02.2020	11,3	2,8	7	<0,2	<1	<1	7,7	1,3	<0,2	0,35	45	9,5	3,3	8,5	<0,2	<1	<1	3,5	0,8	<0,2	<0,1	
E	12	19.02.2020	13,4	3,1	7,3	<0,2	<1	<1	8,7	1,5	<0,2	0,44	51	10,4	3,5	9,2	<0,2	<1	<1	4	0,86	<0,2	<0,1	
F	14	21.02.2020	14,1	3,3	7,9	<0,2	<1	<1	9,1	1,7	<0,2	0,45	49	10,7	3,6	9,5	<0,2	<1	<1	4,5	0,99	<0,2	<0,1	
G	21	28.02.2020	15,8	3,6	8,4	<0,2	<1	<1	9,8	1,9	0,21	0,46	47	12,3	3,8	10	<0,2	<1	<1	4,8	1,2	<0,2	<0,1	
H	28	06.03.2020	17,6	3,8	9,3	<0,2	<1	<1	10,2	2,1	<0,2	0,46	45	13,4	4,1	10,7	<0,2	<1	<1	4,9	1,3	<0,2	<0,1	
I	48	26.03.2020	20,7	3,9	10,7	<0,2	<1	<1	10,3	2,4	<0,2	0,46	45	16,8	4,5	13,6	<0,2	<1	<1	5,1	1,5	<0,2	<0,1	
K	60	07.04.2020	22,5	3,9	11,4	<0,2	<1	<1	10,3	2,5	<0,2	0,46	45	18,1	4,7	15,2	<0,2	<1	<1	5,2	1,6	<0,2	<0,1	
L	74	21.04.2020	23,7	3,9	11,8	<0,2	<1	<1	10,3	2,8	<0,2	0,46	45	19,9	4,8	16,1	<0,2	<1	<1	5,2	1,9	<0,2	<0,1	
M	91	08.05.2020	24,8	3,9	12	0,23	<1	<1	10,3	3,2	<0,2	0,46	45	20,2	4,75	16,1	<0,2	<1	<1	5,2	2,4	<0,2	<0,1	
N	120	06.06.2020	26,6	3,9	12	<0,2	<1	<1	10,3	3,8	<0,2	0,46	45	22,5	4,8	16,1	<0,2	<1	<1	5,2	2,8	<0,2	<0,1	
FINAL	179	04.08.2020	29,6	3,9	12	<0,2		0,63	10,3	5,1	<0,2	0,46	45	25,9	4,8	16,1	<0,2		0,62	5,2	3,1	<0,2	0,08	15

Sample			IG_BH04_PW034											IG_BH04_PW037										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		07.02.2020																						
A	1	08.02.2020	5,8	2,3	4,7	<0,2	<1	<1	6,2	0,69	<0,2	0,24	39	4,2	3	4,1	<0,2	<1	<1	3,3	0,57	<0,2	0,1	30
B	2	09.02.2020	6,7	2,8	5,9	<0,2	<1	<1	6,8	0,72	<0,2	0,38	56	5,5	3,2	5	<0,2	<1	<1	4,5	0,62	<0,2	0,14	31
C	4	11.02.2020	8,5	3,4	7,8	<0,2	<1	<1	8,7	0,8	0,22	0,47	54	6,7	3,2	7,5	<0,2	<1	<1	5,6	0,73	<0,2	0,22	39
D	7	14.02.2020	10,2	3,5	9,4	<0,2	<1	<1	10,2	0,95	<0,2	0,55	54	7,9	3,2	9,1	<0,2	<1	<1	6,6	0,91	<0,2	0,27	41
E	12	19.02.2020	11,7	3,6	10,6	<0,2	<1	<1	11,2	1,1	<0,2	0,63	56	9,5	3,2	10,3	<0,2	<1	<1	7,9	1,2	<0,2	0,32	41
F	14	21.02.2020	12,1	3,7	11,1	<0,2	<1	<1	11,9	1,3	<0,2	0,67	56	9,8	3,2	10,6	<0,2	<1	<1	8,5	1,3	<0,2	0,33	39
G	21	28.02.2020	13,3	3,8	11,8	<0,2	<1	<1	12,7	1,7	<0,2	0,77	61	10,7	3,2	11,6	<0,2	<1	<1	9,3	1,6	<0,2	0,35	38
H	28	06.03.2020	15	3,8	12	<0,2	<1	<1	13,7	2,1	<0,2	0,8	58	11,6	3,2	12	<0,2	<1	<1	9,9	1,8	<0,2	0,37	37
I	48	26.03.2020	16,6	3,8	12,9	<0,2	<1	<1	14,2	2,7	<0,2	0,84	59	13,4	3,2	13,3	<0,2	<1	<1	10,8	2,2	<0,2	0,38	35
K	60	07.04.2020	17,5	3,8	13,3	<0,2	<1	<1	14,4	3,1	<0,2	0,86	60	14,1	3,2	13,8	<0,2	<1	<1	10,8	2,5	<0,2	0,38	35
L	74	21.04.2020	18,3	3,8	13,8	<0,2	<1	<1	14,4	3,7	<0,2	0,86	60	14,8	3,2	14,4	<0,2	<1	<1	10,8	2,7	<0,2	0,38	35
M	91	08.05.2020	18,7	3,8	14,1	<0,2	<1	<1	14,4	4,2	<0,2	0,86	60	15,2	3,2	14,5	<0,2	<1	<1	10,8	2,9	<0,2	0,38	35
N	120	06.06.2020	20,2	3,8	14,1	<0,2	<1	<1	14,4	5,2	<0,2	0,86	60	16,8	3,2	14,6	<0,2	<1	<1	10,8	3,5	<0,2	0,38	35
FINAL	179	04.08.2020	20,9	3,8	14,4	<0,2		0,2	14,4	5,5	<0,2	0,86	60	17,8	3,2	14,8	<0,2		0,13	10,8	3,8	<0,2	0,38	35

Table 10-12: continued

Sample			IG_BH04_PW040										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		07.02.2020											
A	1	08.02.2020	7,1	3,1	7	<0,2	<1	<1	12,6	0,63	<0,2	0,32	25
B	2	09.02.2020	9,5	3,6	8,1	<0,2	<1	<1	17,6	0,83	<0,2	0,47	27
C	4	11.02.2020	12,1	4,3	10,7	<0,2	<1	<1	22,3	1	<0,2	0,63	28
D	7	14.02.2020	13,2	4,4	13,2	<0,2	<1	<1	26	1,3	<0,2	0,77	30
E	12	19.02.2020	15,8	4,5	15,5	<0,2	<1	<1	28,6	1,9	<0,2	0,83	29
F	14	21.02.2020	16	4,6	16,1	<0,2	<1	<1	29,3	2,2	<0,2	0,86	29
G	21	28.02.2020	17,3	4,8	17,6	<0,2	<1	<1	30,9	2,8	<0,2	0,92	30
H	28	06.03.2020	18,5	5	18,4	<0,2	<1	<1	32	3,1	<0,2	0,94	29
I	48	26.03.2020	20	5,2	21,8	<0,2	<1	<1	32,8	4	<0,2	0,95	29
K	60	07.04.2020	21	5,2	24,2	<0,2	<1	<1	33,2	4,4	<0,2	0,95	29
L	74	21.04.2020	21,1	5,2	25,1	<0,2	<1	<1	33,2	4,8	<0,2	0,95	29
M	91	08.05.2020	21,6	5,2	25,3	<0,2	<1	<1	33,2	5	<0,2	0,95	29
N	120	06.06.2020	22,6	5,2	26,3	<0,2	<1	<1	33,2	5,8	<0,2	0,95	29
FINAL	179	04.08.2020	23,4	5,2	27,8	<0,2		<0,1	33,2	6,7	<0,2	0,95	29

Sample			IG_BH04_PW044											IG_BH04_PW046										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		08.02.2020																						
A	1	09.02.2020	7	3,9	6,8	<0,2	<1	<1	11,8	0,5	<0,2	1,5	127	7,9	3,3	6,5	<0,2	<1	<1	12,7	0,96	<0,2	0,55	43
B	2	10.02.2020	8,3	4,4	8	<0,2	<1	<1	14,1	0,63	<0,2	1,7	121	8,8	3,6	7,9	<0,2	<1	<1	14,9	1,04	<0,2	0,65	44
C	4	12.02.2020	10,2	4,7	11,5	<0,2	<1	<1	17,9	0,83	<0,2	2,1	117	11,9	3,7	11,8	<0,2	<1	<1	20,3	1,1	<0,2	0,95	47
D	6	14.02.2020	11,2	4,7	12,3	<0,2	<1	<1	19,7	0,92	<0,2	2,5	127	12,9	3,8	12,9	<0,2	<1	<1	22,3	1,2	<0,2	1,1	49
E	11	19.02.2020	12,9	4,7	12,9	<0,2	<1	<1	23	1,15	<0,2	3,1	135	15,7	3,9	13,3	<0,2	<1	<1	26,7	1,4	<0,2	1,3	49
F	13	21.02.2020	13,2	4,7	13,6	<0,2	<1	<1	24,1	1,2	<0,2	3,3	137	16,1	4	13,5	<0,2	<1	<1	27,5	1,6	<0,2	1,4	51
G	20	28.02.2020	14,4	4,7	14	<0,2	<1	<1	26,1	1,4	<0,2	3,5	134	17,4	4	13,8	<0,2	<1	<1	29,5	2	<0,2	1,4	47
H	27	06.03.2020	15,3	4,7	14,9	<0,2	<1	<1	27,2	1,5	<0,2	3,6	132	18,6	4	14,3	<0,2	<1	<1	30,8	2,2	<0,2	1,4	45
I	47	26.03.2020	16,8	4,7	17,1	<0,2	<1	<1	28,5	1,65	<0,2	3,7	130	19,9	4	15	<0,2	<1	<1	31,7	2,5	0,21	1,4	44
K	59	07.04.2020	17,2	4,7	18	<0,2	<1	<1	29	1,7	<0,2	3,7	128	21,2	4	15,4	<0,2	<1	<1	32	2,7	<0,2	1,4	44
L	73	21.04.2020	17,5	4,7	18,3	<0,2	<1	<1	29	1,9	<0,2	3,7	128	21,4	4	15,7	<0,2	<1	<1	32	3	<0,2	1,4	44
M	90	08.05.2020	17,6	4,7	18,4	<0,2	<1	<1	29	2	<0,2	3,7	128	21,9	4	16	<0,2	<1	<1	32	3	<0,2	1,4	44
N	119	06.06.2020	19,1	4,7	18,7	<0,2	<1	<1	29	2,4	<0,2	3,7	128	23,3	4	16,4	<0,2	<1	<1	32	3,9	<0,2	1,4	44
FINAL	185	11.08.2020	19,4	4,7	19,6	<0,2	0,12	<1	29	3,6	<0,2	3,7	128	24	4	17,7	<0,2	0,14	<1	32	4,4	<0,2	1,4	44

Sample			IG_BH04_PW049											IG_BH04_PW052										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		06.03.2020																						
A	1	07.03.2020	6,9	2,5	6,6	0,24	<1	<1	10,1	0,94	<0,2	0,44	44	7,1	3,2	12,7	<0,2	<1	<1	15,7	1,3	<0,2	2,8	178
B	2	08.03.2020	7,2	2,7	7,6	<0,2	<1	<1	10,8	1,3	<0,2	0,59	55	8,1	3,3	13,3	<0,2	<1	<1	18,3	1,6	<0,2	3,4	186
C	4	10.03.2020	8,8	3,3	9,1	<0,2	<1	<1	13,1	1,5	<0,2	0,77	59	10,1	3,5	15,4	<0,2	<1	<1	22,5	1,9	<0,2	4,1	182
D	6	12.03.2020	10,5	3,8	11,1	<0,2	<1	<1	15,1	1,7	<0,2	0,86	57	12	3,9	16,3	<0,2	<1	<1	25,9	2,3	0,29	4,6	178
E	11	17.03.2020	13,5	4,5	13,7	<0,2	<1	<1	18,8	2,1	<0,2	1,05	56	13,6	3,9	17,8	<0,2	<1	<1	28,6	3	0,23	5,3	185
F	13	19.03.2020	14,4	4,8	14,4	0,27	<1	<1	19,3	2,2	<0,2	1,1	57	14,7	3,9	18,1	<0,2	<1	<1	29	3,3	<0,2	5,4	186
G	20	26.03.2020	16,7	5,2	16,2	<0,2	<1	<1	21,6	2,6	<0,2	1,2	56	15,8	3,9	18,4	<0,2	<1	<1	30,7	3,6	<0,2	5,5	179
H	28	03.04.2020	18,7	5,3	17,9	0,22	<1	<1	22,3	3,1	<0,2	1,3	58	16,7	3,9	18,7	<0,2	<1	<1	32	3,8	0,36	5,5	172
I	47	22.04.2020	20,1	5,3	19,3	0,28	<1	<1	22,6	3,7	<0,2	1,3	58	16,9	3,9	18,7	<0,2	<1	<1	32	4,2	<0,2	5,5	172
K	59	04.05.2020	20,8	5,3	20	0,26	<1	1,1	22,7	4	<0,2	1,3	57	17,1	3,9	18,7	<0,2	<1	<1	32	4,7	0,23	5,5	172
L	73	18.05.2020	21,5	5,3	20,4	0,24	<1	1,1	22,8	4,5	<0,2	1,3	57	17,3	3,9	19,3	<0,2	<1	<1	32	5,2	0,21	5,5	172
M	90	04.06.2020	22,6	5,3	20,3	<0,2	<1	1,8	22,7	5,4	<0,2	1,3	57	17,8	3,9	19,1	0,68	<1	<1	32	5,9	<0,2	5,5	172
N	119	03.07.2020	23,3	5,3	20,4	0,24	<1	2	22,7	6	<0,2	1,3	57	17,9	3,9	19,3	<0,2	<1	<1	32	6,3	<0,2	5,5	172
FINAL	161	14.08.2020	23,9	5,3	20,6	0,25	<1	2,4	22,7	6,4	<0,2	1,3	57	18,1	3,9	19,4	<0,2	<1	<1	32	6,6	0,29	5,5	172

Table 10-12: continued

Sample			IG_BH04_PW055											IG_BH04_PW058										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		18.03.2020																						
A	1	19.03.2020	5,4	2,9	9,7	<0,2	<1	<1	5,5	0,58	<0,2	<0,1		7	3,5	13,7	<0,2	<1	<1	18,5	0,98	0,53	0,78	42
B	2	20.03.2020	6,5	3,05	10,1	<0,2	<1	<1	6,7	0,77	<0,2	<0,1		9,1	3,9	16,1	<0,2	<1	<1	24,4	1,2	0,21	0,97	40
C	4	22.03.2020	8,3	3,3	10,7	<0,2	<1	<1	8,5	0,82	<0,2	<0,1		11,9	4,1	19,7	<0,2	<1	<1	33,4	1,4	0,26	1,4	40
D	6	24.03.2020	9,5	3,5	11,7	<0,2	<1	<1	9,9	0,9	<0,2	<0,1		13,3	4,3	21,7	<0,2	<1	<1	39	1,7	0,2	1,7	40
E	11	29.03.2020	10,9	3,7	12,7	<0,2	<1	<1	11,2	0,98	<0,2	<0,1		16,3	4,7	26,3	<0,2	<1	<1	51,7	2,6	<0,2	2,2	40
F	13	31.03.2020	11,8	3,8	13,9	<0,2	<1	<1	12,4	1,05	<0,2	0,17	14	17,5	4,9	27,5	<0,2	<1	<1	53,5	2,8	0,85	2,3	40
G	20	07.04.2020	13,5	3,9	15,7	<0,2	<1	<1	14	1,3	<0,2	0,21	15	19,1	5,1	30,6	<0,2	<1	<1	58	3,2	<0,2	2,5	40
H	28	15.04.2020	14,5	3,9	17,1	<0,2	<1	<1	14,4	1,5	<0,2	0,24	17	20,6	5,1	32,5	<0,2	<1	<1	59,4	3,6	0,24	2,5	40
I	47	04.05.2020	16,2	3,9	18,3	<0,2	<1	<1	14,9	1,7	0,29	0,27	18	22,2	5,1	33,7	<0,2	<1	<1	62,2	4,4	0,29	2,5	40
K	59	16.05.2020	17,9	3,9	19,5	<0,2	<1	<1	15,1	1,9	0,24	0,27	18	23,1	5,1	34,6	<0,2	<1	<1	63,7	5,1	0,23	2,5	40
L	73	30.05.2020	18,3	3,9	19,8	<0,2	<1	<1	15,1	2,1	0,29	0,27	18	23,6	5,1	35,1	<0,2	<1	<1	65,3	5,5	0,21	2,5	40
M	90	16.06.2020	20,8	3,9	19,9	<0,2	<1	<1	15,1	2,2	<0,2	0,27	18	24,8	5,1	36,7	0,21	<1	<1	66,1	5,9	<0,2	2,5	40
N	119	15.07.2020	22,9	3,9	20,3	<0,2	<1	<1	15,1	2,4	0,28	0,27	18	25,7	5,1	37,5	0,21	<1	<1	66,1	6,8	<0,2	2,5	40
FINAL	188	22.09.2020	24,4	3,9	24,4	<0,2	0,328	0,4	15,1	2,9	0,28	0,27	18	27,5	5,1	40	0,25	0,684	0,4	66,1	8,5	0,23	2,5	40
Sample			IG_BH04_PW061											IG_BH04_PW064										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		18.03.2020																						
A	1	19.03.2020	5,2	3	10,5	<0,2	<1	<1	12,8	0,5	<0,2	0,69	54	7,4	3,8	13,6	<0,2	<1	<1	25,5	0,83	0,21	1,7	67
B	2	20.03.2020	6,7	3,2	12,4	<0,2	<1	<1	17,2	<0,5	<0,2	1,1	64	9,7	4,2	16,1	<0,2	<1	<1	32,8	1	<0,2	2	61
C	4	22.03.2020	9	3,5	16	<0,2	<1	<1	24,3	0,6	0,3	1,3	53	12,9	5,1	20,4	<0,2	<1	<1	44,8	1,2	<0,2	2,7	60
D	6	24.03.2020	10,2	3,6	17,9	<0,2	<1	<1	28	0,69	0,36	1,5	54	14,5	5,2	23,3	<0,2	<1	<1	51,1	1,4	<0,2	3,1	61
E	11	29.03.2020	12,4	3,7	21,6	<0,2	<1	<1	37,7	0,96	0,25	2	53	17,1	5,3	25,9	0,46	<1	<1	61,5	1,8	<0,2	3,8	62
F	13	31.03.2020	13,6	3,8	22,5	<0,2	<1	<1	39,2	1,1	0,91	2,2	56	18,1	5,3	26,8	<0,2	<1	<1	64,8	2	<0,2	4	62
G	20	07.04.2020	15,2	3,8	24,2	<0,2	<1	<1	44,1	1,3	0,25	2,4	54	19,8	5,3	27,8	<0,2	<1	<1	68,5	2,2	<0,2	4,3	63
H	28	15.04.2020	16,1	3,8	25,1	<0,2	<1	<1	44,8	1,6	<0,2	2,5	56	20,4	5,3	28,4	<0,2	<1	<1	69,2	2,3	<0,2	4,3	62
I	47	04.05.2020	17,4	3,8	26,8	0,24	<1	<1	46,9	2	0,43	2,7	58	21,3	5,3	29	<0,2	<1	<1	70,6	2,6	<0,2	4,3	61
K	59	16.05.2020	18,7	3,8	27,8	0,2	<1	<1	47,8	2,3	0,33	2,8	59	22,4	5,3	29,5	<0,2	<1	<1	71,2	2,9	<0,2	4,3	60
L	73	30.05.2020	18,8	3,8	28,3	0,2	<1	<1	49,7	2,7	0,43	2,8	56	22,5	5,3	31,2	<0,2	<1	<1	72,3	3,2	<0,2	4,3	59
M	90	16.06.2020	20,5	3,8	29	0,23	<1	<1	50,4	3,3	0,25	2,8	56	23,8	5,3	31,4	<0,2	<1	<1	72,3	3,4	<0,2	4,3	59
N	119	15.07.2020	21,2	3,8	30,1	0,22	<1	<1	50,4	3,6	0,45	2,8	56	24,6	5,3	31,6	<0,2	<1	<1	72,3	3,7	<0,2	4,3	59
FINAL	188	22.09.2020	23,3	3,8	30,5	0,25	0,511	<0,1	50,4	5,2	0,47	2,8	56	25,9	5,3	32,8	<0,2	0,511	<0,1	72,3	4,7	<0,2	4,3	59
Sample			IG_BH04_PW067											IG_BH04_PW070										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		26.03.2020																						
A	1	27.03.2020	7,9	3,8	13,6	<0,2	<1	<1	22,6	0,57	<0,2	0,95	42	7,5	3,1	17,2	<0,2	<1	<1	28,1	0,48	0,35	1,3	46
B	3	29.03.2020	11,9	4,8	19,9	<0,2	<1	<1	40,7	0,84	<0,2	2	49	11,1	3,6	26	<0,2	<1	<1	51,9	0,68	<0,2	2,5	48
C	4	30.03.2020	13,4	5	23,6	<0,2	<1	<1	52	1	0,88	2,8	54	12,4	3,9	30	<0,2	<1	<1	62,6	1	0,4	3,1	50
D	6	01.04.2020	16,1	5,5	27,3	<0,2	<1	<1	59,6	1,2	0,44	3,2	54	15,1	4,4	35,2	<0,2	<1	<1	72,9	1,2	0,7	3,5	48
E	11	06.04.2020	18,9	5,7	33,1	<0,2	<1	<1	72,3	1,8	<0,2	3,7	51	17,6	4,6	43,1	<0,2	<1	<1	91,9	1,4	0,32	4,2	46
F	13	08.04.2020	19,9	5,8	35	<0,2	<1	<1	75,9	2	<0,2	3,85	51	18,5	4,6	45,6	<0,2	<1	<1	96,4	1,6	0,41	4,4	46
G	20	15.04.2020	21,5	5,8	37,1	<0,2	<1	<1	80,2	2,6	<0,2	4,1	51	19,5	4,6	47,2	<0,2	<1	<1	101	1,8	0,42	4,75	47
H	28	23.04.2020	23,2	5,8	39,6	0,23	<1	<1	82,4	3,1	<0,2	4,3	52	20,9	4,6	48,6	0,21	<1	<1	103	2,3	0,48	4,9	48
I	47	12.05.2020	24,4	5,8	42,1	0,24	<1	<1	83,1	3,8	0,25	4,4	53	21,6	4,6	50,4	0,26	<1	<1	105	2,9	0,42	5,2	50
K	59	24.05.2020	24,8	5,8	43,1	0,22	<1	<1	84,2	4,4	0,61	4,5	53	21,7	4,6	51,4	0,21	<1	<1	107	3,3	0,45	5,3	50
L	73	07.06.2020	25,3	5,8	44,3	0,29	<1	<1	84,2	5,1	<0,2	4,5	53	22,3	4,6	53,7	0,24	<1	1,3	107	3,8	0,45	5,3	50
M	90	24.06.2020	26,1	5,8	45,2	0,27	<1	<1	84,2	5,6	<0,2	4,5	53	23,3	4,6	55,2	0,24	<1	1,5	107	4,4	0,57	5,3	50
N	119	23.07.2020	26,7	5,8	46,8	0,37	0,23	<1	84,2	6,7	<0,2	4,5	53	23,5	4,6	58,3	0,29	0,26	1,8	107	5,2	0,45	5,3	50
FINAL	180	22.09.2020	29,2	5,8	48,1	0,33	0,817	0,54	84,2	6,8	<0,2	4,5	53	25,3	4,6	58,8	0,29	1,09	1,9	107	5,5	0,5	5,3	50

Table 10-12: continued

Sample			IG_BH04_PW073											IG_BH04_PW076										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		26.03.2020																						
A	1	27.03.2020	6,4	3,3	20,6	<0,2	<1	<1	33,3	0,6	<0,2	1,4	42	8	4,1	27,5	<0,2	<1	<1	48,5	0,82	0,58	1,4	29
B	3	29.03.2020	9,1	3,9	28,3	<0,2	<1	<1	53	0,74	<0,2	2,1	40	11,9	4,9	37,3	<0,2	<1	<1	77,2	1	0,52	2,35	30
C	4	30.03.2020	9,9	4,1	31,3	<0,2	<1	<1	61,3	0,82	<0,2	2,6	42	13,2	5,3	41,9	<0,2	<1	<1	88,8	1,4	0,2	2,7	30
D	6	01.04.2020	11,9	4,4	35,4	<0,2	<1	<1	68,8	0,88	<0,2	2,9	42	16,4	5,7	46,2	<0,2	<1	<1	101	1,6	0,44	3	30
E	11	06.04.2020	13,7	4,6	41,8	<0,2	<1	1	84,2	1	<0,2	3,6	43	18,4	6,1	55,3	<0,2	<1	<1	122	2	0,43	3,5	29
F	13	08.04.2020	14,3	4,6	42,8	<0,2	<1	1,1	88	1,05	<0,2	3,7	42	19,2	6,2	57,1	<0,2	<1	<1	127	2,3	0,44	3,6	28
G	20	15.04.2020	15,4	4,6	43,8	<0,2	<1	1,1	91,7	1,2	<0,2	3,9	43	20,1	6,2	58,2	0,22	<1	<1	130	2,8	<0,2	3,7	28
H	28	23.04.2020	16,5	4,6	45	<0,2	<1	1,1	93,9	1,5	<0,2	4,05	43	20,8	6,2	59,8	0,21	<1	<1	132	3,2	0,75	3,7	28
I	47	12.05.2020	17,7	4,6	47,3	0,2	<1	1,3	97,6	2	<0,2	4,2	43	21,3	6,2	60,8	0,24	<1	<1	134	4,1	0,7	3,7	28
K	59	24.05.2020	18,2	4,6	48,8	<0,2	<1	1,4	99,1	2,2	<0,2	4,3	43	21,5	6,2	61,8	0,21	<1	<1	136	4,9	0,77	3,7	27
L	73	07.06.2020	20	4,6	49,5	0,33	<1	1,6	99,1	3	0,7	4,4	44	22,1	6,2	63	0,28	<1	1,4	138	5,5	<0,2	3,7	27
M	90	24.06.2020	20,6	4,6	49,9	<0,2	<1	1,8	99,1	3,8	<0,2	4,4	44	22,7	6,2	64,1	0,24	<1	1,6	138	6,3	0,74	3,7	27
N	119	23.07.2020	20,8	4,6	50,1	<0,2	0,26	2	99,1	4,7	<0,2	4,4	44	23,6	6,2	65,1	0,31	0,37	1,8	138	7,9	0,59	3,7	27
FINAL	180	22.09.2020	21,7	4,6	50,4	<0,2	0,915	2,2	99,1	4,9	<0,2	4,4	44	25	6,2	66,1	0,38	1,46	1,9	138	9,2	0,7	3,7	27
Sample			IG_BH04_PW079											IG_BH04_PW082										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		26.03.2020																						
A	1	27.03.2020	8,6	4,6	30,3	<0,2	<1	<1	55,4	0,41	0,28	1,8	32	9,9	4,7	31,7	<0,2	<1	<1	58	0,6	0,26	4	69
B	3	29.03.2020	12,8	5,7	45,5	<0,2	<1	<1	95,5	0,96	0,25	3,2	34	13,9	5,5	43,4	<0,2	<1	<1	84,7	0,77	<0,2	6	71
C	4	30.03.2020	14,2	6,2	51	<0,2	<1	<1	114	1,3	0,31	3,8	33	15,8	6,4	48,8	<0,2	<1	<1	101	1	<0,2	7	69
D	6	01.04.2020	17,1	6,5	59,1	<0,2	<1	<1	129	1,5	0,34	4,3	33	17	6,6	54,7	<0,2	<1	<1	110	1,2	<0,2	7,8	71
E	11	06.04.2020	19,7	6,8	71,2	<0,2	<1	<1	162	1,9	0,21	5,3	33	19,3	6,8	64,4	<0,2	<1	<1	128	1,6	<0,2	9	70
F	13	08.04.2020	20,3	6,8	73,2	<0,2	<1	<1	169	2,1	0,3	5,5	33	19,8	6,8	66,4	<0,2	<1	<1	133	1,8	<0,2	9,4	71
G	20	15.04.2020	21,4	6,8	75,1	<0,2	<1	<1	175	2,5	0,35	5,6	32	20,7	6,8	67,1	0,24	<1	<1	139	2,1	<0,2	9,7	70
H	28	23.04.2020	23,1	6,8	77	<0,2	<1	<1	176	3,2	0,38	5,7	32	22	6,8	68,6	0,23	<1	<1	141	2,7	<0,2	9,9	70
I	47	12.05.2020	23,3	6,8	81,8	0,25	<1	<1	177	4,3	0,55	6	34	22,6	6,8	70	0,25	<1	<1	143	4	<0,2	10,2	71
K	59	24.05.2020	23,5	6,8	83	0,21	<1	<1	177	4,9	0,45	6,1	34	23	6,8	70,8	0,2	<1	<1	145	4,9	<0,2	10,5	72
L	73	07.06.2020	24,7	6,8	86,7	0,31	<1	<1	177	5,3	0,32	6,1	34	not determined due to defect of IC										
M	90	24.06.2020	25,6	6,8	87,4	0,21	<1	1	177	5,8	0,26	6,1	34	24,1	6,8	73,9	0,26	<1	1,2	147	6,4	<0,2	10,7	73
N	119	23.07.2020	26,7	6,8	88	0,28	0,45	1,3	177	7	0,24	6,1	34	24,8	6,8	75,6	0,3	0,47	1,6	147	8,1	<0,2	10,7	73
FINAL	180	22.09.2020	27,4	6,8	88,8	0,28	1,82	1,4	177	8,2	0,36	6,1	34	26,8	6,8	77,3	0,37	1,69	1,8	147	10	<0,2	10,7	73
Sample			IG_BH04_PW085											IG_BH04_PW088										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		26.03.2020																						
A	1	27.03.2020	9,3	5,9	21,9	0,23	<1	<1	46,1	0,43	<0,2	2,2	48	10,1	2,8	17,7	<0,2	<1	<1	32,3	0,69	<0,2	0,74	23
B	3	29.03.2020	13,3	7,1	30,1	0,32	<1	<1	69,3	0,69	<0,2	3,4	49	15	3	24,1	<0,2	<1	<1	52,4	0,88	<0,2	1,3	25
C	4	30.03.2020	14,3	7,6	33,2	0,35	<1	<1	77,9	0,84	<0,2	3,8	49	17,1	3,4	26,3	<0,2	<1	<1	58,7	0,96	<0,2	1,7	29
D	6	01.04.2020	16,7	8,2	37,5	0,38	<1	<1	87,8	0,98	<0,2	4,2	48	20,3	3,7	31,2	0,2	<1	<1	69,4	1,05	0,5	1,9	27
E	11	06.04.2020	19,3	8,4	42,1	0,39	<1	<1	105	1,2	<0,2	4,9	47	25,4	4	37,4	0,22	<1	<1	88,9	1,2	0,23	2,2	25
F	13	08.04.2020	20	8,4	43,2	0,41	<1	<1	107	1,3	<0,2	5,1	48	26,8	4,1	39	0,22	<1	<1	93	1,3	0,25	2,3	25
G	20	15.04.2020	21,1	8,4	44,3	0,43	<1	<1	109	1,7	<0,2	5,2	48	29,8	4,1	40,2	0,23	<1	<1	100	1,5	0,27	2,4	24
H	28	23.04.2020	22,3	8,4	45,4	0,49	<1	<1	111	2	<0,2	5,2	47	33,6	4,1	40,9	0,3	<1	<1	101	1,7	0,27	2,4	24
I	47	12.05.2020	23,2	8,4	47,1	0,49	<1	<1	113	2,9	<0,2	5,2	46	37,4	4,1	41,8	0,32	<1	<1	104	2,4	0,39	2,4	23
K	59	24.05.2020	24	8,4	47,4	0,42	<1	<1	114	3,6	<0,2	5,2	46	39,6	4,1	42,4	0,27	<1	<1	106	3,2	0,33	2,4	23
L	73	07.06.2020	25,3	8,4	48,2	0,51	<1	<1	115	4,1	<0,2	5,2	45	42,6	4,1	42,6	0,32	<1	1,3	108	3,8	<0,2	2,4	22
M	90	24.06.2020	26,8	8,4	50,5	0,52	<1	<1	115	4,7	<0,2	5,2	45	42,7	4,1	42,8	0,32	<1	1,4	108	4,3	0,23	2,4	22
N	119	23.07.2020	27,2	8,4	52,3	0,51	0,29	<1	115	6,9	<0,2	5,2	45	42,7	4,1	43,9	0,35	0,23	1,6	108	5,7	0,24	2,4	22
FINAL	180	22.09.2020	27,8	8,4	52,9	0,6	0,887	0,62	115	7,6	<0,2	5,2	45	42,8	4,1	46,3	0,51	0,507	1,9	108	10,5	<0,2	2,4	22

Table 10-12: continued

Sample			IG_BH04_PW092										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		26.03.2020											
A	1	27.03.2020	8,9	5,2	15,3	0,22	<1	<1	32,6	0,64	<0,2	0,78	24
B	3	29.03.2020	13,4	6,7	21,8	0,3	<1	<1	52,9	0,81	<0,2	1,2	23
C	4	30.03.2020	15,1	7	24,1	0,28	<1	<1	61,4	1,2	<0,2	1,6	26
D	6	01.04.2020	17,6	7,4	26,4	0,34	<1	<1	68,3	1,6	<0,2	1,8	26
E	11	06.04.2020	20,9	7,6	30,3	0,34	<1	<1	81,8	1,9	<0,2	2	24
F	13	08.04.2020	22,2	7,7	not determined due to defect of IC								
G	20	15.04.2020	23,7	7,8	32,6	0,37	<1	<1	88,1	2,6	<0,2	2,1	24
H	28	23.04.2020	25,2	7,8	34,9	0,42	<1	<1	88,4	3,3	<0,2	2,1	24
I	47	12.05.2020	26,8	7,8	36	0,43	<1	<1	89,4	4,9	<0,2	2,1	23
K	59	24.05.2020	27,8	7,8	36,4	0,38	<1	<1	91,5	5,9	<0,2	2,1	23
L	73	07.06.2020	29,3	7,8	37,3	0,48	<1	1,1	92	7	<0,2	2,1	23
M	90	24.06.2020	30,5	7,8	38,5	0,47	<1	1,3	92	8,1	<0,2	2,1	23
N	119	23.07.2020	31,6	7,8	39,5	0,5	0,26	1,6	92	10,5	<0,2	2,1	23
FINAL	180	22.09.2020	33,5	7,8	40	0,62	0,794	1,7	92	14,2	<0,2	2,1	23

Sample			IG_BH04_PW027										
Sub-samples	Time	Date	Na	K	Ca	Mg	Sr	F	Cl	SO4	NO3	Br	Br/Cl
	days		mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	mg/l	
Preparation		24.04.2020											
A	1	25.04.2020	6,7	1,6	6,8	<0,2	<1	<1	6,8	1	<0,2	0,29	43
B	3	27.04.2020	9,3	1,9	7,7	0,28	<1	<1	8,9	1,2	<0,2	0,385	43
C	4	28.04.2020	10,4	2,1	8,1	0,21	<1	<1	9,8	1,3	<0,2	0,43	44
D	6	30.04.2020	11,9	2,1	8,5	0,22	<1	<1	10,9	1,45	<0,2	0,45	41
E	11	05.05.2020	14,4	2,1	9,2	<0,2	<1	<1	12,5	1,8	0,23	0,49	39
F	13	07.05.2020	15,2	2,1	9,5	<0,2	<1	<1	12,9	2	<0,2	0,5	39
G	20	14.05.2020	17,8	2,4	10,3	<0,2	<1	<1	14	2,5	<0,2	0,56	40
H	28	22.05.2020	21	3,1	10,6	<0,2	<1	<1	15,5	3,8	<0,2	0,61	39
I	47	10.06.2020	25,7	3,8	10,8	<0,2	<1	<1	16,1	4,6	<0,2	0,65	40
K	59	22.06.2020	27,7	4	11,1	<0,2	<1	<1	16,4	5,4	<0,2	0,66	40
L	73	06.07.2020	29,4	4	12	<0,2	<1	<1	16,7	6,7	<0,2	0,66	40
M	90	23.07.2020	31,4	4	12,3	<0,2	<1	<1	16,7	7,5	<0,2	0,66	40
N	119	21.08.2020	34,5	4	12,6	0,24	<1	<1	16,7	9,2	<0,2	0,66	40
FINAL	151	22.09.2020	35	4	12,9	<0,2	0,176	0,4	16,7	10,6	<0,2	0,66	40

APPENDIX C

Error Calculations

CALCULATION OF WATER CONTENT VALUES: RAW DATA

Appendix Table 10-3: Determination of gravimetric water content; sample weights, drying times and calculated water contents of core pieces used for aqueous extraction experiments

Sample	Date prepared	m (cryst.dish)	m (cryst+ rock)	16.03.2020	31.03.2020	13.04.2020				Sample	m (rock, wet)	m (rock, dry)
Drying times	days			61	76	89					g	g
PW003 (AQ)	15.01.2020	88,733	486,951	486,315	486,304	486,305				PW003 (AQ)	398,218	397,571
PW006 (AQ)	15.01.2020	91,306	428,810	428,269	428,271					PW006 (AQ)	337,504	336,963
PW009 (AQ)	15.01.2020	88,733	453,845	453,185	453,187					PW009 (AQ)	365,112	364,452
PW011 (AQ)	15.01.2020	87,323	478,430	477,790	477,790					PW011 (AQ)	391,107	390,467
PW015 (AQ)	15.01.2020	91,260	473,089	472,513	472,511					PW015 (AQ)	381,829	381,251
PW018 (AQ)	15.01.2020	87,788	418,429	417,870	417,870					PW018 (AQ)	330,641	330,082
PW021 (AQ)	15.01.2020	87,284	385,058	384,506	384,503	384,505				PW021 (AQ)	297,774	297,219
PW024 (AQ)	15.01.2020	90,804	478,448	478,054	478,053					PW024 (AQ)	387,644	387,249
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**08.05.2020**	**20.05.2020**							
Drying times	**days**			14	26							
PW026 (AQ)	24.04.2020	88,618	373,238	372,862	372,860					PW026 (AQ)	284,620	284,242
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**17.03.2020**	**31.03.2020**	**14.04.2020**						
Drying times	**days**			38	52	66						
PW030 (AQ)	08.02.2020	84,668	566,695	565,939	565,929	565,928				PW030 (AQ)	482,027	481,260
PW033 (AQ)	08.02.2020	86,535	458,137	457,585	457,577	457,579				PW033 (AQ)	371,602	371,042
PW036 (AQ)	08.02.2020	87,165	418,079	417,613	417,603	417,605				PW036 (AQ)	330,914	330,438
PW039 (AQ)	08.02.2020	86,413	446,867	446,387	446,378	446,380				PW039 (AQ)	360,454	359,965
PW042 (AQ)	08.02.2020	83,841	360,862	360,431	360,433					PW042 (AQ)	277,021	276,590
PW045 (AQ)	08.02.2020	84,543	395,362	394,926	394,929					PW045 (AQ)	310,819	310,383
PW048 (AQ)	08.02.2020	88,662	378,759	378,334	378,333					PW048 (AQ)	290,097	289,671
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**20.03.2020**	**03.04.2020**	**16.04.2020**						
Drying times	**days**			14	28	41						
PW051 (AQ)	06.03.2020	88,325	448,952	448,169	448,152	448,154				PW051 (AQ)	360,627	359,827
PW054 (AQ)	06.03.2020	92,195	450,616	450,071	450,06	450,061				PW054 (AQ)	358,421	357,865
PW057 (AQ)	06.03.2020	90,942	401,275	400,855	400,851	400,853				PW057 (AQ)	310,333	309,909
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**01.04.2020**	**15.04.2020**	**29.04.2020**	**13.05.2020**	**27.05.2020**	**10.06.2020**			
Drying times	**days**			14	28	42	56	70	84			
PW060 (AQ)	18.03.2020	89,833	400,297	399,929	399,927	399,934	399,923	399,916	399,92	PW060 (AQ)	310,464	310,083
PW063 (AQ)	18.03.2020	97,341	476,743	476,355	476,353	476,359	476,357			PW063 (AQ)	379,402	379,012
Sample	**Date prepared**	**m (cryst.dish)**	**m (cryst+ rock)**	**07.04.2020**	**21.04.2020**	**07.05.2020**	**20.05.2020**	**03.06.2020**	**17.06.2020**			
Drying times	**days**			12	26	42	55	69	83			
PW066 (AQ)	26.03.2020	92,806	431,321	430,863	438,870	438,855	438,853			PW066 (AQ)	338,515	338,057
PW069 (AQ)	26.03.2020	88,079	394,319	393,954	393,962	393,946	393,948			PW069 (AQ)	306,240	305,867
PW072 (AQ)	26.03.2020	86,346	409,470	409,113	409,117	409,108	409,108			PW072 (AQ)	323,124	322,762
PW075 (AQ)	26.03.2020	88,640	360,144	359,640	359,647	359,644	359,635	359,647	359,654	PW075 (AQ)	271,504	270,995
PW078 (AQ)	26.03.2020	86,232	372,586	372,032	372,046	372,020	372,033	372,035		PW078 (AQ)	286,354	285,788
PW081 (AQ)	26.03.2020	87,193	418,553	417,996	417,997	417,976	417,993	417,996	418,002	PW081 (AQ)	331,360	330,783
PW084 (AQ)	26.03.2020	89,126	354,349	353,905	353,901	353,895	353,903	353,91	353,92	PW084 (AQ)	265,223	264,769
PW087 (AQ)	26.03.2020	92,881	415,915	415,523	415,534	415,531	415,521	415,539	415,544	PW087 (AQ)	323,034	322,640
PW090 (AQ)	26.03.2020	89,010	436,348	435,940	435,954	435,937	435,943	435,945		PW090 (AQ)	347,338	346,927
PW093 (AQ)	26.03.2020	85,364	405,625	405,025	405,031	405,028	405,02	405,027	405,038	PW093 (AQ)	320,261	319,656

Appendix Table 10-3: continued

			m(dry surf)	16.03.2020	31.03.2020	14.04.2020	28.04.2020					Sample	m (rock, wet)	m (rock, dry)
Drying times	days			61	76	90	104						g	g
PW003 (AQ) A	15.01.2020		130,116	129,856	129,849	129,847						PW003 (AQ) A	130,116	129,847
PW003 (AQ) B	15.01.2020		187,054	186,678	186,674	186,672						PW003 (AQ) B	187,054	186,672
PW006 (AQ) A	15.01.2020		161,468	161,200	161,192	161,193						PW006 (AQ) A	161,468	161,192
PW006 (AQ) B	15.01.2020		130,691	130,464	130,459	130,457						PW006 (AQ) B	130,691	130,457
PW009 (AQ) A	15.01.2020		173,927	173,569	173,559	173,553	173,552					PW009 (AQ) A	173,927	173,552
PW009 (AQ) B	15.01.2020		152,018	151,712	151,703	151,697	151,696					PW009 (AQ) B	152,018	151,696
PW011 (AQ) A	15.01.2020		178,723	178,400	178,391	178,389						PW011 (AQ) A	178,723	178,389
PW011 (AQ) B	15.01.2020		191,008	190,671	190,661	190,653	190,653					PW011 (AQ) B	191,008	190,653
PW011 (AQ Frnc)	15.01.2020		312,851	312,027	312,017	312,017								
PW015 (AQ) A	15.01.2020		190,780	190,486	190,482	190,475	190,476					PW015 (AQ) A	190,780	190,475
PW015 (AQ) B	15.01.2020		208,305	207,954	207,946	207,945						PW015 (AQ) B	208,305	207,945
PW018 (AQ) A	15.01.2020		171,029	170,721	170,716	170,710	170,711					PW018 (AQ) A	171,029	170,710
PW018 (AQ) B	15.01.2020		167,961	167,637	167,631	167,618	167,618					PW018 (AQ) B	167,961	167,618
PW021 (AQ) A	15.01.2020		167,043	166,715	166,704	166,700	166,698					PW021 (AQ) A	167,043	166,698
PW021 (AQ) B	15.01.2020		172,362	172,047	172,037	172,034	172,035					PW021 (AQ) B	172,362	172,034
PW024 (AQ) A	15.01.2020		256,723	256,458	256,447	256,439	256,440					PW024 (AQ) A	256,723	256,439
PW024 (AQ) B	15.01.2020		273,257	272,956	272,948	272,942	372,941					PW024 (AQ) B	273,257	272,942
			m(dry surf)	08.05.2020	20.05.2020	03.06.2020								
Drying times	days			14	26	40								
PW026 (AQ) A	24.04.2020		183,765	183,509	183,509	183,506						PW026 (AQ) A	183,765	183,506
PW026 (AQ) B	24.04.2020		133,570	133,380	133,380	133,376						PW026 (AQ) B	133,570	133,376
			m(dry surf)	18.02.2020	03.03.2020	17.03.2020	31.03.2020	14.04.2020	28.04.2020	12.05.2020				
Drying times	days			10	24	38	52	66	80	94				
PW030 (AQ) A	08.02.2020		206,140	205,806	205,803	205,793	205,786	205,782	205,783			PW030 (AQ) A	206,140	205,782
PW030 (AQ) B	08.02.2020		178,408	178,124	178,124	178,115	178,108	178,103	178,098	178,100		PW030 (AQ) B	178,408	178,098
PW033 (AQ) A	08.02.2020		192,430	192,117	192,109	192,097	192,092	192,086	192,085			PW033 (AQ) A	192,430	192,085
PW033 (AQ) B	08.02.2020		174,586	174,289	174,281	174,271	174,264	174,258	174,259			PW033 (AQ) B	174,586	174,258
PW036 (AQ) A	08.02.2020		130,034	129,846	129,842	129,836	129,829	129,817	129,818			PW036 (AQ) A	130,034	129,817
PW036 (AQ) B	08.02.2020		131,960	131,779	131,772	131,766	131,755	131,751	131,749			PW036 (AQ) B	131,960	131,749
PW039 (AQ) A	08.02.2020		155,352	155,160	155,156	155,151	155,145	155,144				PW039 (AQ) A	155,352	155,144
PW039 (AQ) B	08.02.2020		171,300	171,046	171,042	171,036	171,031	171,026	171,026			PW039 (AQ) B	171,300	171,026
PW042 (AQ) A	08.02.2020		358,542	357,972	357,964	357,953	357,950	357,945	357,946			PW042 (AQ) A	358,542	357,945
PW042 (AQ) B	08.02.2020		156,199	155,927	155,915	155,906	155,901	155,899				PW042 (AQ) B	156,199	155,899
PW045 (AQ) A	08.02.2020		119,637	119,449	119,441	119,435	119,426	119,424				PW045 (AQ) A	119,637	119,424
PW045 (AQ) B	08.02.2020		204,391	204,073	204,068	204,054	204,042	204,040				PW045 (AQ) B	204,391	204,040
PW048 (AQ) A	08.02.2020		152,742	152,502	152,492	152,485	152,479	152,477				PW048 (AQ) A	152,742	152,477
PW048 (AQ) B	08.02.2020		133,910	133,686	133,676	133,670	133,660	133,656	133,656			PW048 (AQ) B	133,910	133,656
			m(dry surf)	20.03.2020	03.04.2020	16.04.2020	30.04.2020							
Drying times	days			14	28	41	55							
PW051 (AQ) A	06.03.2020		118,203	117,965	117,957	117,862	117,863					PW051 (AQ) A	118,203	117,862
PW051 (AQ) B	06.03.2020		155,562	155,246	155,237	155,236						PW051 (AQ) B	155,562	155,236
PW054 (AQ) A	06.03.2020		235,422	235,032	235,022	235,021						PW054 (AQ) A	235,422	235,021
PW054 (AQ) B	06.03.2020		207,669	207,316	207,303	207,301						PW054 (AQ) B	207,669	207,301
PW057 (AQ) A	06.03.2020		179,963	179,682	179,670	179,665	179,665					PW057 (AQ) A	179,963	179,665
PW057 (AQ) B	06.03.2020		257,109	256,750	256,734	256,736						PW057 (AQ) B	257,109	256,734
			m(dry surf)	01.04.2020	16.04.2020	29.04.2020								
Drying times	days			14	29	42								
PW060 (AQ) A	18.03.2020		161,160	160,965	160,958	160,959						PW060 (AQ) A	161,160	160,958
PW060 (AQ) B	18.03.2020		179,254	179,033	179,020	179,021						PW060 (AQ) B	179,254	179,020
PW063 (AQ) A	18.03.2020		224,256	224,018	224,009	224,011						PW063 (AQ) A	224,256	224,009
PW063 (AQ) B	18.03.2020		188,917	188,719	188,715	188,716						PW063 (AQ) B	188,917	188,715
			m(dry surf)	07.04.2020	22.04.2020	07.05.2020	20.05.2020							
Drying times	days			12	27	42	55							
PW066 (AQ) A	26.03.2020		296,948	296,528	296,511	296,510						PW066 (AQ) A	296,948	296,510
PW066 (AQ) B	26.03.2020		223,954	223,639	223,624	223,623						PW066 (AQ) B	223,954	223,623
PW069 (AQ) A	26.03.2020		230,755	230,344	230,337	230,335						PW069 (AQ) A	230,755	230,335
PW069 (AQ) B	26.03.2020		173,129	172,902	172,898	172,896						PW069 (AQ) B	173,129	172,896
PW072 (AQ) A	26.03.2020		199,441	199,208	199,205	199,205						PW072 (AQ) A	199,441	199,205
PW072 (AQ) B	26.03.2020		184,446	184,225	184,221	184,221						PW072 (AQ) B	184,446	184,221
PW075 (AQ) A	26.03.2020		198,442	197,985	197,975	197,971	197,971					PW075 (AQ) A	198,442	197,971
PW075 (AQ) B	26.03.2020		141,750	141,465	141,457	141,456						PW075 (AQ) B	141,750	141,456
PW078 (AQ) A	26.03.2020		116,211	115,993	115,985	115,984						PW078 (AQ) A	116,211	115,984
PW078 (AQ) B	26.03.2020		167,346	167,001	166,988	166,985	166,984					PW078 (AQ) B	167,346	166,984
PW081 (AQ) A	26.03.2020		143,810	143,554	143,546	143,544						PW081 (AQ) A	143,810	143,544
PW081 (AQ) B	26.03.2020		162,437	162,141	162,129	162,128						PW081 (AQ) B	162,437	162,128
PW084 (AQ) A	26.03.2020		210,949	210,461	210,447	210,446						PW084 (AQ) A	210,949	210,446
PW084 (AQ) B	26.03.2020		231,646	231,202	231,190	231,189						PW084 (AQ) B	231,646	231,189
PW087 (AQ) A	26.03.2020		176,989	176,775	176,767	176,766						PW087 (AQ) A	176,989	176,766
PW087 (AQ) B	26.03.2020		182,259	181,973	181,962	181,959	181,957					PW087 (AQ) B	182,259	181,957
PW090 (AQ) A	26.03.2020		265,511	265,081	265,078	265,076						PW090 (AQ) A	265,511	265,076
PW090 (AQ) B	26.03.2020		178,331	178,087	178,084	178,082						PW090 (AQ) B	178,331	178,082
PW093 (AQ) A	26.03.2020		221,257	220,848	220,843	220,840	220,840					PW093 (AQ) A	221,257	220,840
PW093 (AQ) B	26.03.2020		229,273	228,812	228,808	228,807						PW093 (AQ) B	229,273	228,807

Appendix Table 10-4: Determination of gravimetric water content; sample weights, drying times and calculated water contents of rim core pieces of samples used for out-diffusion and isotope diffusive exchange experiments

	Set-up date	m(dry surf)	16.03.2020	31.03.2020	15.04.2020			m wet	m dry
Drying time (days)			14	29	44			g	g
PW001 A	02.03.2020	168,713	168,435	168,429	168,320			168,713	168,32
PW001 B	02.03.2020	443,495	442,771	442,761	442,756			443,495	442,756
PW004 A	02.03.2020	111,799	111,609	111,607				111,799	111,607
PW004 B	02.03.2020	229,610	229,232	229,224	229,213			229,610	229,213
PW007 A	02.03.2020	230,246	229,812	229,803	229,785			230,246	229,785
PW007 B	02.03.2020	220,839	220,474	220,463	220,449			220,839	220,449
PW010 A	02.03.2020	243,542	243,076	243,070	243,058			243,542	243,058
PW010 B	02.03.2020	277,887	277,324	277,316	277,305			277,887	277,305
PW014 A	02.03.2020	238,333	237,966	237,955	237,890			238,333	237,89
PW014 B	02.03.2020	191,003	190,726	190,720	190,709			191,003	190,709
PW016 A	02.03.2020	258,065	257,368	257,627	257,619			258,065	257,368
PW016 B	02.03.2020	192,855	192,532	192,522	192,514			192,855	192,514
PW019 A	02.03.2020	208,736	208,270	208,261	208,256			208,736	208,256
PW019 B	02.03.2020	172,595	172,266	172,255	172,251			172,595	172,251
PW022 A	02.03.2020	252,485	252,135	252,119	252,108			252,485	252,108
PW022 B	02.03.2020	221,034	220,689	220,675	220,667			221,034	220,667
	Set-up date	m(dry surf)	08.05.2020	20.05.2020					
Drying time (days)			14	26					
PW027 A	24.04.2020	212,193	211,860	211,860				212,193	211,86
PW027 B	24.04.2020	161,354	161,101	161,099				161,354	161,099
	Set-up date	m(dry surf)	18.02.2020	03.03.2020	17.03.2020	31.03.2020	15.04.2020		
Drying time (days)			11	25	39	53	68		
PW028 A	07.02.2020	223,134	222,808	222,800	222,793	222,789	222,783	223,134	222,783
PW028 B	07.02.2020	107,715	107,547	107,541	107,535	107,531	107,522	107,715	107,522
PW031 A	07.02.2020	203,775	203,449	203,434	203,421	203,417	203,410	203,775	203,41
PW031 B	07.02.2020	194,217	193,865	193,850	193,837	193,824	193,814	194,217	193,814
PW034 A	07.02.2020	172,390	172,096	172,085	172,074	172,068	172,057	172,390	172,057
PW034 B	07.02.2020	190,891	190,603	190,591	190,583	190,578	190,568	190,891	190,568
PW037 A	07.02.2020	189,469	189,175	189,147	189,137	189,137		189,469	189,137
PW037 B	07.02.2020	133,384	133,221	133,217	133,201	133,198	133,191	133,384	133,191
PW040 A	07.02.2020	205,842	205,514	205,509	205,501	205,497	205,488	205,842	205,488
PW040 B	07.02.2020	182,463	182,183	182,169	182,159	182,156	182,148	182,463	182,148
PW044 A	08.02.2020	192,270	191,899	191,884	191,870	191,860	191,851	192,270	191,851
PW044 B	08.02.2020	174,217	173,919	173,915	173,904	173,900	173,857	174,217	173,857
PW046 A	08.02.2020	142,324	142,122	142,115	142,111	142,109		142,324	142,109
PW046 B	08.02.2020	229,676	229,325	229,319	229,311	229,281	229,271	229,676	229,271

Appendix Table 10-4: continued

	Set-up date	m(dry surf)	20.03.2020	03.04.2020	16.04.2020	30.04.2020			m wet	m dry
Drying time (days)			14	28	41	55			g	g
PW049 A	06.03.2020	201,429	201,037	201,029	201,027				201,429	201,027
PW049 B	06.03.2020	183,186	182,848	182,838	182,836				183,186	182,836
PW052 A	06.03.2020	288,580	288,127	288,115	288,110	288,112			288,580	288,11
PW052 B	06.03.2020	175,975	175,683	175,677	175,671	175,673			175,975	175,671
	Set-up date	**m(dry surf)**	**01.04.2020**	**15.04.2020**	**29.04.2020**	**12.05.2020**				
Drying time (days)			14	28	42	55				
PW055 A	18.03.2020	232,680	232,304	232,297	232,298				232,680	232,297
PW055 B	18.03.2020	128,611	128,393	128,379	128,376	128,374			128,611	128,374
PW058 A	18.03.2020	164,144	163,932	163,928	163,925	163,923			164,144	163,923
PW058 B	18.03.2020	245,474	245,118	245,107	245,109				245,474	245,107
PW061 A	18.03.2020	175,059	174,843	174,836	174,836				175,059	174,836
PW061 B	18.03.2020	227,645	227,299	227,291	227,292				227,645	227,291
PW064 A	18.03.2020	227,558	227,244	227,238	227,240				227,558	227,238
PW064 B	18.03.2020	174,514	174,290	174,281	174,283				174,514	174,281
	Set-up date	**m(dry surf)**	**08.04.2020**	**22.04.2020**	**07.05.2020**	**20.05.2020**	**03.06.2020**			
Drying time (days)			13	27	42	55	69			
PW067 A	26.03.2020	260,701	260,354	260,348	260,345	260,342	260,342		260,701	260,342
PW067 B	26.03.2020	178,264	178,033	178,030	178,027	178,024	178,024		178,264	178,024
PW070 A	26.03.2020	208,017	207,713	207,707	207,705				208,017	207,705
PW070 B	26.03.2020	208,643	208,353	208,349	208,347				208,643	208,347
PW073 A	26.03.2020	172,987	172,643	172,635	172,635				172,987	172,635
PW073 B	26.03.2020	168,397	168,029	168,027	168,022	168,021			168,397	168,021
PW076 A	26.03.2020	112,627	112,420	112,417	112,414	112,412			112,627	112,412
PW076 B	26.03.2020	170,257	169,923	169,916	169,914				170,257	169,914
PW079 A	26.03.2020	104,073	103,901	103,891	103,889				104,073	103,889
PW079 B	26.03.2020	162,269	162,001	161,997	161,995				162,269	161,995
PW082 A	26.03.2020	184,852	184,388	184,381	184,378	184,372	184,371		184,852	184,371
PW082 B	26.03.2020	162,878	162,505	162,494	162,492				162,878	162,492
PW085 A	26.03.2020	276,682	276,246	276,233	276,231				276,682	276,231
PW085 B	26.03.2020	149,218	148,970	148,964	148,961	148,958	148,956		149,218	148,956
PW088 A	26.03.2020	213,059	212,680	212,677	212,675				213,059	212,675
PW088 B	26.03.2020	129,712	129,467	129,464	129,464				129,712	129,464
PW092 A	26.03.2020	257,860	257,481	257,477	257,474	257,471	257,471		257,860	257,471
PW092 B	26.03.2020	255,948	255,485	255,481	255,478	255,476			255,948	255,476

Appendix Table 10-5: Determination of gravimetric water content; sample weights, drying times and calculated water contents of core pieces used for isotope-diffusive exchange experiments

Sample	Date start drying	Drying times (days)	m (cryst.dish)	m (cryst+ rock)	01.04.2020	14.04.2020	27.04.2020	12.05.2020	27.05.2020	mass dry	m rock wet	m rock dry
PW001 LAB	18.03.2020	27	86,252	566,673	565,981	565,983				565,981	480,421	479,729
PW001 ICE	18.03.2020	27	88,299	536,074	535,428	535,430				535,428	447,775	447,129
PW004 LAB	18.03.2020	27	90,021	444,589	444,034	444,035				444,034	354,568	354,013
PW004 ICE	18.03.2020	27	87,593	443,765	443,205	443,207				443,205	356,172	355,612
PW007 LAB	18.03.2020	27	86,230	441,555	441,020	441,022				441,020	355,325	354,790
PW007 ICE	18.03.2020	27	90,447	444,409	443,881	443,885				443,881	353,962	353,434
PW010 LAB	18.03.2020	70	88,295	522,100	521,391	521,385	521,397	521,388	521,386	521,385	433,805	433,090
PW010 ICE	18.03.2020	27	89,510	532,909	532,190	532,189				532,189	443,399	442,679
PW014 LAB	18.03.2020	27	89,350	547,687	547,057	547,055				547,055	458,337	457,705
PW014 ICE	18.03.2020	27	88,438	539,860	539,233	539,234				539,233	451,422	450,795
PW016 LAB	18.03.2020	27	86,927	550,570	549,842	549,845				549,842	463,643	462,915
PW016 ICE	18.03.2020	27	87,597	514,794	514,119	514,121				514,119	427,197	426,522
PW019 LAB	18.03.2020	70	90,904	510,381	509,412	509,409	509,427	509,419	509,420	509,409	419,477	418,505
PW019 ICE	18.03.2020	27	91,511	510,430	509,400	509,403				509,400	418,919	417,889
PW022 LAB	18.03.2020	55	88,390	520,766	520,178	520,170	520,178	520,170		520,170	432,376	431,780
PW022 ICE	18.03.2020	27	90,684	536,734	536,118	536,121				536,118	446,05	445,434
Sample	**Date start drying**	**Drying times (days)**	**m (cryst.dish)**	**m (cryst+ rock)**	**14.07.2020**	**28.07.2020**						
PW027 LAB	30.06.2020	28	87,228	457,475	456,996	459,994				456,996	370,247	369,768
PW027 ICE	30.06.2020	28	90,452	460,190	459,702	459,702				459,702	369,738	369,250
Sample	**Date start drying**	**Drying times (days)**	**m (cryst.dish)**	**m (cryst+ rock)**	**29.04.2020**	**13.05.2020**	**27.05.2020**	**10.06.2020**				
PW028 LAB	15.04.2020	28	89,356	531,622	531,097	531,097				531,097	442,266	441,741
PW028 ICE	15.04.2020	56	83,840	528,777	528,264	528,253	528,260	528,262		528,253	444,937	444,413
PW031 LAB	15.04.2020	42	90,805	495,717	495,224	495,221	495,223			495,221	404,912	404,416
PW031 ICE	15.04.2020	56	87,788	490,014	489,499	489,486	489,492	489,495		489,486	402,226	401,698
PW034 LAB	15.04.2020	42	91,261	498,625	498,197	498,192	498,192			498,192	407,364	406,931
PW034 ICE	15.04.2020	56	88,818	496,449	496,020	496,014	496,010	496,014		496,010	407,631	407,192
PW037 LAB	15.04.2020	42	88,663	545,829	545,233	545,226	545,223			545,223	457,166	456,560
PW037 ICE	15.04.2020	42	89,546	544,424	543,774	543,768	543,769			543,768	454,878	454,222
PW040 LAB	15.04.2020	42	90,679	476,093	475,678	475,670	475,672			475,670	385,414	384,991
PW040 ICE	15.04.2020	28	87,804	470,631	470,200	470,201				470,200	382,827	382,396
PW044 LAB	15.04.2020	42	91,195	473,128	472,724	472,720	472,718			472,718	381,933	381,523
PW044 ICE	15.04.2020	56	87,498	467,973	467,532	467,516	467,523	467,528		467,516	380,475	380,018
PW046 LAB	15.04.2020	56	91,786	497,494	497,050	497,046	497,051	497,058		497,046	405,708	405,260
PW046 ICE	15.04.2020	42	89,567	497,420	496,964	496,957	496,959			496,957	407,853	407,390

Appendix Table 10-5: continued

Sample	Date start drying	Drying times (days)	m (cryst.dish)	m (cryst+ rock)	28.05.2020	10.06.2020	24.06.2020			mass dry	m rock wet	m rock dry
PW049 LAB	07.05.2020	48	81,570	438,442	437,860	437,848	437,85			437,848	356,872	356,278
PW049 ICE	07.05.2020	34	86,422	447,013	446,395	446,397				446,395	360,591	359,973
PW052 LAB	07.05.2020	34	89,012	511,386	510,916	510,917				510,916	422,374	421,904
PW052 ICE	07.05.2020	34	92,197	512,650	512,162	512,163				512,162	420,453	419,965
Sample	**Date start drying**	**ying times (da**	**m (cryst.dish)**	**m (cryst+ rock)**	**02.06.2020**	**16.06.2020**	**01.07.2020**	**15.07.2020**	**29.07.2020**			
PW055 LAB	18.05.2020	44	87,823	550,713	550,030	550,048	550,05			550,030	462,89	462,207
PW055 ICE	18.05.2020	58	90,887	554,283	553,600	553,627	553,624	553,623		553,600	463,396	462,713
PW058 LAB	18.05.2020	72	84,302	491,835	491,347	491,367	491,36	491,355	491,354	491,347	407,533	407,045
PW058 ICE	18.05.2020	44	85,987	492,728	492,237	492,245	492,243			492,237	406,741	406,250
PW061 LAB	18.05.2020	44	86,108	513,403	512,792	512,787	512,785			512,785	427,295	426,677
PW061 ICE	18.05.2020	58	93,415	521,434	520,775	520,783	520,775	520,773		520,773	428,019	427,358
PW064 LAB	18.05.2020	44	91,127	550,530	550,019	550,025	550,024			550,019	459,403	458,892
PW064 ICE	18.05.2020	44	88,338	542,891	542,378	542,389	542,387			542,378	454,553	454,040
Sample	**Date start drying**	**Drying times (days)**	**m (cryst.dish)**	**m (cryst+ rock)**	**10.06.2020**	**24.06.2020**	**14.07.2020**	**28.07.2020**				
PW067 LAB	29.05.2020	26	88,793	550,630	550,073	550,075				550,073	461,837	461,280
PW067 ICE	29.05.2020	26	85,239	543,717	543,219	543,221				543,219	458,478	457,980
PW070 LAB	29.05.2020	46	88,914	498,046	497,477	497,474	497,472			497,472	409,132	408,558
PW070 ICE	29.05.2020	26	88,053	499,232	498,708	498,706				498,706	411,179	410,653
PW073 LAB	29.05.2020	46	90,745	421,556	420,935	420,928	420,926			420,926	330,811	330,181
PW073 ICE	29.05.2020	60	93,925	426,356	425,766	425,762	425,754	425,755		425,754	332,431	331,829
PW076 LAB	29.05.2020	60	88,468	468,639	468,029	468,026	468,017	468,017		468,017	380,171	379,549
PW076 ICE	29.05.2020	60	86,249	467,172	466,576	466,571	466,569	466,569		466,569	380,923	380,320
PW079 LAB	29.05.2020	60	89,364	399,671	399,169	399,165	399,16	399,159		399,159	310,307	309,795
PW079 ICE	29.05.2020	60	87,295	397,235	396,727	396,721	396,715	396,716		396,715	309,94	309,420
PW082 LAB	29.05.2020	26	91,407	518,621	517,987	517,986				517,986	427,214	426,579
PW082 ICE	29.05.2020	60	87,600	514,314	513,713	513,703	513,697	513,697		513,697	426,714	426,097
PW085 LAB	29.05.2020	60	90,420	590,139	589,493	589,5	589,492	589,495		589,492	499,719	499,072
PW085 ICE	29.05.2020	26	86,961	585,006	584,398	584,397				584,397	498,045	497,436
PW088 LAB	29.05.2020	26	84,663	566,916	566,216	566,216				566,216	482,253	481,553
PW088 ICE	29.05.2020	26	86,550	568,912	568,155	568,155				568,155	482,362	481,605
PW092 LAB	29.05.2020	60	86,266	566,140	565,536	565,548	565,537	565,535		565,535	479,874	479,269
PW092 ICE	29.05.2020	26	91,547	573,339	572,736	572,738				572,736	481,792	481,189

Appendix Table 10-6: Determination of gravimetric water content; sample weights, drying times and calculated water contents of core pieces used for out-diffusion experiments

			before experiment (b.e.)		after experiment (a.e.)											
Sample	**Date start drying**	**Drying times (days)**	**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**23.06.2020**	**08.07.2020**	**21.07.2020**	**04.08.2020**	**18.08.2020**	**01.09.2020**	**16.09.2020**	**29.09.2020**	**07.10.2020**	
			g	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	
Drying time (days)																
PW001	09.06.2020	120	1552,100	1552,060	1552,482	1552,240	1549,470	1549,467	1549,458	1549,453	1549,469	1549,433	1549,452	1549,414	1549,420	
PW004	09.06.2020	56	1561,972	1561,953	1562,281	1562,115	1559,364	15589,348	1559,330	1559,328						
PW007	09.06.2020	120	1520,128	1520,000	1520,561	1520,330	1517,444	1517,441	1517,432	1517,424	1517,439	1517,411	1517,422	1517,382	1517,386	
PW010	09.06.2020	120	1569,103	1568,973	1569,186	1568,985	1565,976	1565,968	1565,955	1565,948	1565,962	1565,924	1565,940	1565,894	1565,896	
PW014	09.06.2020	120	1553,836	1553,765	1554,344	1554,140	1551,472	1551,469	1551,460	1551,456	1551,478	1551,440	1551,463	1551,418	1551,420	
PW016	09.06.2020	120	1556,613	1556,602	1556,776	1556,610	1553,966	1553,952	1553,938	1553,927	1553,951	1553,908	1553,932	1553,878	1553,880	
PW019	09.06.2020	56	1561,256	1561,248	1561,485	1561,305	1558,484	1558,436	1558,408	1558,406						
PW022	09.06.2020	120	1533,689	1533,661	1533,862	1533,690	1531,353	1531,297	1531,272	1531,262	1531,581	1531,241	1531,261	1531,221	1531,222	
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**06.10.2020**	**20.10.2020**	**03.11.2020**	**17.11.2020**	**04.12.2020**	**18.12.2020**	**01.01.2021**			
			g	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**			
Drying time (days)																
PW027	22.09.2020	101	1547,140	1547,028	1547,172	1547,012	1544,649	1544,603	1544,526	1544,489	1544,524	1544,475	1544,524			
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**18.08.2020**	**01.09.2020**	**16.09.2020**	**29.09.2020**	**07.10.2020**	**21.10.2020**	**03.11.2020**	**10.11.2020**	**25.11.2020**	**11.12.2020**
			g	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**
Drying time (days)																
PW028	04.08.2020	64	1531,650	1531,613	1531,762	1531,502	1529,271	1529,223	1529,23	1529,187	1529,185					
PW031	04.08.2020	129	1536,922	1536,805	1536,910	1536,683	1534,356	1534,295	1534,298	1534,25	1534,243	1534,216	1534,204	1534,198	1534,170	1534,168
PW034	04.08.2020	64	1524,063	1523,905	1524,132	1523,670	1521,686	1521,643	1521,653	1521,608	1521,606					
PW037	04.08.2020	98	1519,176	1519,162	1519,515	1519,202	1517,175	1517,13	1517,136	1517,091	1517,086	1517,058	1517,048	1517,048		
PW040	04.08.2020	64	1519,733	1519,367	1520,041	1519,160	1516,964	1516,921	1516,933	1516,885	1516,887					
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**25.08.2020**	**08.09.2020**	**23.09.2020**	**06.10.2020**	**20.10.2020**	**03.11.2020**				
			g	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**				
Drying time (days)																
PW044	11.08.2020	84	1503,821	1503,544	1503,791	1503,266	1501,204	1501,167	1501,167	1501,142	1501,115	1501,115				
PW046	11.08.2020	84	1504,325	1504,206	1504,541	1504,050	1501,920	1501,984	1501,907	1501,891	1501,871	1501,869				
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**28.08.2020**	**16.09.2020**	**28.09.2020**	**15.10.2020**	**29.10.2020**	**12.11.2020**	**25.11.2020**	**11.12.2020**	**23.12.2020**	
			g	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	
Drying time (days)																
PW049	14.08.2020	119	1555,679	1555,679	1556,148	1555,780	1552,569	1552,578	1552,545	1552,413	1552,371	1552,495	1552,417	1552,415		
PW052	14.08.2020	131	1518,550	1518,334	1519,001	1518,478	1515,649	1515,641	1515,625	1515,5	1515,483	1515,553	1515,541	1515,424	1515,425	
Sample	**Date start drying**		**m wet surface**	**m dry surface**	**m wet surf**	**m dry surf**	**06.10.2020**	**20.10.2020**	**03.11.2020**	**17.11.2020**	**04.12.2020**	**18.12.2020**	**01.01.2021**			
			g	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**	**g**			
Drying time (days)																
PW055	22.09.2020	101	1537,588	1537,568	1537,786	1537,644	1535,369	1535,281	1535,260	1535,220	1535,185	1535,166	1535,175			
PW058	22.09.2020	101	1546,038	1546,004	1546,620	1546,403	1543,47	1543,436	1543,422	1543,389	1543,366	1543,347	1543,362			
PW061	22.09.2020	87	1531,521	1531,519	1532,210	1531,970	1529,535	1529,491	1529,458	1529,434	1529,410	1529,412				
PW064	22.09.2020	73	1564,960	1564,920	1565,362	1565,140	1562,706	1562,676	1562,666	1562,606	1562,608					
PW067	22.09.2020	87	1549,043	1549,030	1549,885	1549,610	1547,174	1547,145	1547,139	1547,105	1547,077	1547,080				
PW070	22.09.2020	73	1550,393	1550,371	1551,134	1550,870	1548,129	1548,099	1548,069	1548,012	1548,014					
PW073	22.09.2020	101	1518,842	1518,800	1519,220	1518,970	1515,798	1515,755	1515,745	1515,683	1515,673	1515,663	1515,684			
PW076	22.09.2020	101	1521,997	1521,900	1522,571	1522,310	1518,902	1518,864	1518,850	1518,820	1518,809	1518,783	1518,794			
PW079	22.09.2020	101	1560,360	1560,300	1560,935	1560,730	1557,454	1557,423	1557,395	1557,374	1557,363	1557,330	1557,344			
PW082	22.09.2020	101	1499,742	1499,654	1499,708	1499,455	1496,632	1496,591	1496,576	1496,543	1496,529	1496,453	1496,514			
PW085	22.09.2020	101	1540,679	1540,600	1540,820	1540,550	1538,203	1538,170	1538,158	1538,105	1538,130	1538,088	1538,103			
PW088	22.09.2020	73	1521,120	1521,035	1521,397	1521,200	1518,292	1518,265	1518,224	1518,197	1518,200					
PW092	22.09.2020	73	1531,284	1531,237	1531,652	1531,441	1529,005	1528,988	1528,925	1528,937	1528,94					

GRAVIMETRIC WATER CONTENT

The water content is calculated according to $$WC_{grav} = \frac{m_{pw}}{m_{core,wet}}$$

Where WC_{grav} = gravimetric water content, m_{pw} = mass of pore water, $m_{core,wet}$ = mass of the wet core sample

Error calculation after Gaussian error propagation

$$\sigma(WC_{grav}) = \sqrt{\left(dWC_{grav}dm_{PW} \times \sigma(m_{PW})\right)^2 + \left(dWC_{grav}dm_{core,wet} \times \sigma(m_{core,wet})\right)^2}$$

Analytical errors (error of measurement)

s(m_{pw}) = difference between $m_{core,dry\ surface}$ before and after drying + 0.05 g (=variations at end of drying); The constant of 0.05 g is the empirically derived uncertainty associated to the drying process of the surface, i.e. loss of water from the core surface.

s($m_{core,wet}$) = difference between $m_{core,dry\ surface}$ before and after experiment

Both uncertainties include the mass difference of the individual cores before and after the experiments (Appendix B).

Derivations

$$dWC_{grav}dm_{pw} = \frac{100}{m_{core,wet}}$$

$$dWC_{grav}dm_{core,wet} = \frac{-100 \times m_{pw}}{(m_{core,wet})^2}$$

WATER-LOSS POROSITY

The water-loss (connected porosity), ϕ_{WL}, is calculated according to

$$\phi_{WL} = WC_{wet} \times \frac{\rho_{bulk,wet}}{\rho_{water}}$$

where WC_{wet} is the water content based on the wet weight of the rock sample and $\rho_{bulk,wet}$ the bulk wet density of the rock. The density of water, ρ_{water}, is assumed to be 1 g/cm^3.

The conversion of the formula leads to

$$\phi_{WL} = \frac{m_{pw} \times 100}{r^2 \times h \times \pi \times \rho_{water}}$$

where *r* = radius of the core pieces, *h* = height of the core.

Error calculation after Gaussian error propagation

$$\sigma(\phi_{WL}) = \sqrt{\begin{aligned}&\left(d\phi_{WL} dm_{PW} \times \sigma(m_{PW})\right)^2 + \left(d\phi_{WL} dr \times \sigma(r)\right)^2 + \\ &\left(d\phi_{WL} dh \times \sigma(h)\right)^2 + \left(d\phi_{WL} d\rho_{water} \times \sigma(\rho_{water})\right)^2\end{aligned}}$$

Analytical errors (error of measurement)

s(m_{pw}) = difference between $m_{core,dry\ surface}$ before and after drying + 0.05 g (=variations

at end of drying)

s(r) = 0.02 cm

s(h) = 0.2 cm

s(r_{water}) = 0.03 g/cm^3

Derivations

$$d\phi dm_{pw} = \frac{100}{r^2 \times h \times \pi \times \rho_{water}}$$

$$d\phi dr = \frac{-m_{pw} \times 100 \times 2r \times h \times \pi \times \rho_{water}}{(r^2 \times h \times \pi \times \rho_{water})^2}$$

$$d\phi dh = \frac{-m_{pw} \times 100 \times r^2 \times \pi \times \rho_{water}}{(r^2 \times h \times \pi \times \rho_{water})^2}$$

$$d\phi dh = \frac{-m_{pw} \times 100 \times r^2 \times \pi \times h}{(r^2 \times h \times \pi \times \rho_{water})^2}$$

POREWATER CL- AND BR CONCENTRATION

Calculations

$$C_{PW} = \frac{(m_{PW} + m_{TWi} - \sum^{n} m_s) \times C_{TW\infty} - (m_{TWi} \times C_{TWi}) + \sum^{n} m_s \times C_s}{m_{PW}}$$

where C_{pw} = porewater concentration; m_{pw} = mass of porewater; m_{TWi} = initial mass of test water; C_{TWi} = initial Cl-concentration of test water; m_s = mass of sub sample used for time series; C_s = Cl concentration of sub sample used for time series.

Error calculation after Gaussian error propagation

$$\sigma(C_{PW}) = \sqrt{\begin{array}{l}(dC_{PW}dm_{PW} \times \sigma(m_{PW}))^2 + (dC_{PW}dm_{TWi} \times \sigma(m_{TWi}))^2 + \\ +(dC_{PW}dC_{TW\infty} \times \sigma(C_{TW\infty}))^2 + (dC_{PW}dC_{TWi} \times \sigma(C_{TWi}))^2 + \\ (\sigma(\sum m_S))^2 + (\sigma(\sum m_S \times c_S))^2\end{array}}$$

Analytical errors (error of measurement)

$\sigma(m_{PW})$ = difference between $m_{core,dry\ surface}$ before and after drying + 0.05 g (=variations at end of drying

$\sigma(m_{TWi})$ = difference between $m_{TWi} - m_S - m_{TW\infty}$-2 ml (2 ml = remaining water in the cylinder

$\sigma(C_{TWi})$ = 5 % (Cl) and 10 % (Br) of the analysed concentration

$\sigma(C_{TW\infty})$ = 5 % (Cl) and 10 % (Br) of the analysed concentration

$\sigma(m_S)$ = 0.05 ml

$\sigma(C_S)$ = 5 % (Cl) and 10 % (Br) of the analysed concentration

Derivations

$$dC_{PW}dm_{PW} = \frac{C_{TW\infty} * m_{PW} - [C_{TW\infty} * (m_{PW} + m_{TWi}) - C_{TW} * m_{TWi}]}{m_{PW}^{2}}$$

$$dC_{PW}dm_{TWi} = \frac{(C_{TW\infty} - C_{TWi}) * m_{PW}}{m_{PW}^{2}}$$

$$dC_{PW}dC_{TW\infty} = \frac{(m_{PW} - m_{TWi}) * m_{PW}}{m_{PW}^{2}}$$

$$dC_{PW}dC_{TWi} = \frac{-m_{TWi} * m_{PW}}{m_{PW}^{2}}$$

$$\sigma\left(\sum(m_s)\right) = \left(Nr_S \times \sigma(m_S)\right)$$

$$\sigma\left(\sum(m_S \times C_S)\right) = \left(Nr_S \times C_{S,ave} \times \sigma(m_S)\right) + \left(Nr_S \times m_S \times \sigma(C_S)\right)$$

BR*1000/CL MASS RATIO OF POREWATER

Br*1000/Cl porewater mass ratio = R

Error calculation after Gaussian error propagation

$$\sigma(R) = \sqrt{\left(dRdC_{Br} \times \sigma(C_{Br})\right)^2 + \left(dRdC_{Cl} \times \sigma(C_{Cl})\right)^2}$$

Analytical errors (error of measurement)

$\sigma(C_{Cl})$ = Error of porewater Cl concentration calculated according to *porewater Cl- and Br concentration*

$\sigma(C_{Br})$ = Error of porewater Br concentration calculated according to *porewater Cl- and Br concentration*

Derivations

$$dRdC_{Br} = \frac{1000}{C_{Cl}}$$

$$dRdC_{Cl} = \frac{-1000 \times C_{Br}}{C_{Cl}^2}$$

CALCULATION OF ISOTOPE SIGNATURES OF MATRIX POREWATER

Calculation

$$C_{PW} = \frac{C_{TW\infty(Std1)} \times m_{TW(Std2)} \times m_{Rock(Std1)} \times (C_{TW\infty(Std2)} - C_{TW^0(Std2)}) - C_{TW\infty(Std2)} \times m_{TW(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std1)} - C_{TW^0(Std1)})}{m_{TW(Std2)} \times m_{Rock(Std1)} \times (C_{TW\infty(Std2)} - C_{TW^0(Std2)}) - m_{TW(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std1)} - C_{TW^0(Std1)})}$$

m_{PW} = mass of porewater (g)

m_{TW} = mass of test water (g)

C_{TW} = isotopic signature of test water at the beginning of the experiment (‰)

$C_{TW\infty}$ = isotopic signature of test water after equilibration (‰)

Std 1 = Experiment 1 applying standard 1

Std 2 = Experiment 2 applying standard 2

Error calculation after Gaussian error propagation

$$\sigma(C_{PW}) = \sqrt{\begin{aligned}&\left(dC_{PW}dm_{TW(Std1)} \times \sigma(m_{TW(Std1)})\right)^2 + \left(dC_{PW}dm_{TW(Std2)} \times \sigma(m_{TW(Std2)})\right)^2 + \\ &+\left(dC_{PW}dC_{TW(Std1)} \times \sigma(C_{TW(Std1)})\right)^2 + \left(dC_{PW}dC_{TW(Std2)} \times \sigma(C_{TW(Std2)})\right)^2 + \\ &+\left(dC_{PW}dC_{TW\infty(Std1)} \times \sigma(C_{TW\infty(Std1)})\right)^2 + \left(dC_{PW}dC_{TW\infty(Std2)} \times \sigma(C_{TW\infty(Std2)})\right)^2\end{aligned}}$$

Analytical errors (error of measurement)

$\sigma(m_{TW(Std1)})$ = 0.002 g

$\sigma(m_{TW(Std2)})$ = 0.002 g

$\sigma(C_{TW(Std1)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

$\sigma(C_{TW(Std2)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

$\sigma(C_{TW\infty(Std1)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

$\sigma(C_{TW\infty(Std2)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

Derivations

$$dC_{PW}dm_{TW(Std1)} = \frac{\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)} -$$

$$-\frac{\left(\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}\times m_{TW(Std1)} - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)^2}$$

$$dC_{PW}dm_{TW(Std2)} = \frac{-\left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)} +$$

$$+\frac{\left(\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}\times m_{TW(Std1)} - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)\times\left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)^2}$$

$$dC_{PW}dC_{TW(Std1)} = \frac{C_{TW\infty(Std2)}\times m_{TW(Std1)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)} -$$

$$-\frac{\left(\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}\times m_{TW(Std1)} - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)\times m_{TW(Std1)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)^2}$$

$$dC_{PW}dC_{TW(Std2)} = \frac{-C_{TW\infty(Std1)}\times m_{TW(Std2)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)} +$$

$$+\frac{\left(\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}\times m_{TW(Std1)} - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)\times m_{TW(Std2)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)^2}$$

$$dC_{PW}dC_{TW\infty(Std1)} = \frac{-\left(C_{TW\infty(Std2)}\times m_{TW(Std1)} + \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)} +$$

$$+\frac{\left(\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}\times m_{TW(Std1)} - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)\times m_{TW(Std1)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)^2}$$

$$dC_{PW}dC_{TW\infty(Std1)} = \frac{-\left(C_{TW\infty(Std2)}\times m_{TW(Std1)} + \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)} +$$

$$+\frac{\left(\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}\times m_{TW(Std1)} - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)\times m_{TW(Std1)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)^2}$$

$$dC_{PW}dC_{TW\infty(Std2)} = \frac{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) + C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)} -$$

$$-\frac{\left(\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)\times C_{TW\infty(Std2)}\times m_{TW(Std1)} - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times C_{TW\infty(Std1)}\times m_{TW(Std2)}\right)\times m_{TW(Std2)}}{\left(m_{TW(Std1)}\times\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) - \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)\times m_{TW(Std2)}\right)^2}$$

CALCULATION OF MASS OF POREWATER BY ISOTOPE DIFFUSIVE EXCHANGE TECHNIQUE

Calculation

$$WC_{IsoEx} = \left[\frac{m_{TW(Std2)} \times m_{Rock(Std1)} \times (C_{TW^0(Std2)} - C_{TW\infty(Std2)}) + m_{TW(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std1)} - C_{TW^0(Std1)})}{m_{Rock(Std1)} \times m_{Rock(Std2)} \times (C_{TW\infty(Std2)} - C_{TW\infty(Std1)})} \right] \times 100$$

m_{PW} = mass of porewater (g)

m_{TW} = mass of test water (g)

C_{TW} = isotopic signature of test water at the beginning of the experiment (‰)

$C_{TW\infty}$ = isotopic signature of test water after equilibration (‰)

Std 1 = Experiment 1 applying standard 1

Std 2 = Experiment 2 applying standard 2

Error calculation after Gaussian error propagation

$$\sigma(m_{PW}) = \sqrt{\begin{aligned} &\left(dm_{PW} dm_{TW(Std1)} \times \sigma(m_{TW(Std1)})\right)^2 + \left(dm_{PW} dm_{TW(Std2)} \times \sigma(m_{TW(Std2)})\right)^2 + \\ &+\left(dm_{PW} dC_{TW(Std1)} \times \sigma(C_{TW(Std1)})\right)^2 + \left(dm_{PW} dC_{TW(Std2)} \times \sigma(C_{TW(Std2)})\right)^2 + \\ &+\left(dm_{PW} dC_{TW\infty(Std1)} \times \sigma(C_{TW\infty(Std1)})\right)^2 + \left(dm_{PW} dC_{TW\infty(Std2)} \times \sigma(C_{TW\infty(Std2)})\right)^2 \end{aligned}}$$

Analytical errors (error of measurement)

$\sigma(m_{TW(Std1)})$ = 0.002 g

$\sigma(m_{TW(Std2)})$ = 0.002 g

$\sigma(C_{TW(Std1)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

$\sigma(C_{TW(Std2)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

$\sigma(C_{TW\infty(Std1)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

$\sigma(C_{TW\infty(Std2)})$ = 0.1 ‰ for ^{18}O and 1.0 ‰ for ^{2}H

Derivations

$$dm_{PW}dm_{TW(Std1)} = \frac{\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)}$$

$$dm_{PW}dm_{TW(Std2)} = \frac{-\left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)}$$

$$dm_{PW}dC_{TW(Std1)} = \frac{m_{TW(Std1)}}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)}$$

$$dm_{PW}dC_{TW(Std2)} = \frac{-m_{TW(Std2)}}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)}$$

$$dm_{PW}dC_{TW\infty(Std1)} = \left(\frac{-1}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)} - \frac{\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right)}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)^2}\right) \times m_{TW(Std1)} + \left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right) \times m_{TW(Std2)}$$

$$dm_{PW}dC_{TW\infty(Std2)} = \left(\frac{\left(C_{TW(Std1)} - C_{TW\infty(Std1)}\right) \times m_{TW(Std1)}}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)^2} + \frac{1}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)^2} - \frac{\left(C_{TW(Std2)} - C_{TW\infty(Std2)}\right)}{\left(C_{TW\infty(Std1)} - C_{TW\infty(Std2)}\right)^2}\right) \times m_{TW(Std2)}$$

wsp.com

Hydroisotop