

Supplementary material

Corresponding article: ‘Geochemical modelling to assess the consequences of an increase in pH for an in-situ experiment at the Mont Terri Rock Laboratory, Switzerland’

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Tab. SM1: Overview of the in-situ tests performed within the Bitumen-Nitrate-Clay interaction (BN) experiment. The pH value and the indicated concentrations of nitrate, nitrite, acetate, dissolved H₂ and selenate are the start concentrations after injection of the interval with a fresh solution and equilibration with the remaining interval solution in the downhole equipment. Note that in some injection tests, bromide or deuterated water was co-injected to assess diffusion coefficients (not indicated here). These tests have been discussed in the following references of the main paper: Bleyen et al. (2017, 2019, 2021, 2024).

Interval	Test code	Start date	Initial concentrations* and pH						Time of e ⁻ donor (acetate or H ₂) pulse**
			NO ₃ ⁻ (mM)	NO ₂ ⁻ (mM)	acetate (mM)	H ₂ (aq) (mM)	Se(VI) (μM)	pH	
1	INT1_2011	2011-03-16	1.5	—	—	—	—	7.8	No pulse injection
	INT1_2014	2014-10-01	16	—	—	2.3	—	7.8	54 days
	INT1_2015	2015-09-23	16	—	—	1.6	—	8.0	48 days
	INT1_2022	2022-02-22	—	—	—	—	60	7.4	No pulse injection
	INT1_2024	2024-05-30	5	—	—	—	126	7.4	No pulse injection
2	INT2_2011a	2011-03-16	1.1	0.8	0.8	—	—	7.8	0 days
	INT2_2011b	2011-05-31	1.1	—	0.3	—	—	7.7	0 days
	INT2_2013	2013-11-05	25	—	5	—	—	7.8	70 days
	INT2_2022a	2022-02-23	—	—	—	—	58	7.7	No pulse injection
	INT2_2022b	2022-10-17	—	—	—	—	60	7.5	No pulse injection
	INT2_2024	2024-05-29	3	—	—	—	80	7.5	No pulse injection
3	INT3_2012	2012-05-24	44	—	—	—	—	7.1	No pulse injection
	INT3_2019a	2019-02-21	—	—	—	—	6	7.6	No pulse injection
	INT3_2019b	2019-06-06	—	—	—	—	60	7.3	No pulse injection
	INT3_2019c	2019-10-15	3	—	—	—	52	7.3	No pulse injection
	INT3_2020	2020-06-15	3	—	—	—	115	7.4	No pulse injection
	INT3_2021	2021-07-09	—	—	—	—	75	7.3	No pulse injection

* The initial concentration was calculated based on the measured concentration injected into the surface equipment, the known dilution caused by the solution in the downhole equipment and, if applicable, by the dilution due to the addition of new artificial Opalinus Clay pore water during the first sampling. Note that the calculated values match the concentrations measured in the intervals after equilibration, except for test INT3_2019c, which may be due to insufficient equilibration time before a water sample was taken. For tests in 2011, the injection was performed by completely replacing the interval solution with a new solution; thus, the initial concentration was the measured concentration in the injected solution.

** Number of days since start of injection test when electron donor was introduced in the interval.