

Supplementary Information:

Modelling results of Phreeqc Interactive (USGS 2020)

Article Title Retention potential of a drained wetland in the Lusatian lignite mining district, Briesener Niedermoor, Germany, Europe

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Table 1 Modelling results of Phreeqc Interactive (USGS 2020) and comparison with reference measurements

		Groundwater			Surface water			
					Drainage stream			Downstream
site		000175	000509	000513	LaF50	LaF40	LaF20	GhF50
Measured / modelled E_H ^a	UH, 25°C [mV]	127 / 285		245 / 484	88 / 187	226 / 300	204 / 244	645 / 665
Measured / modelled ferrous iron Fe^{2+} ^b	[mg/L]	113 / 115	156 / 156	248 / 270	94 / 96	204 / 218	167 / 170	22 / 27
Measured / modelled ferric iron Fe^{3+} ^b	[mg/L]	2 / 0	0 / 0	21 / 0	2 / 0	14 / 0	3 / 1	12 / 7
Modelled ion balance error ^b	[]	-0.79	-4.12	-10.01	-7.74	-7.77	-10.76	-18.39
Modelled saturation index^b								
Ferrihydrite	$Fe(OH)_3$	0.51	-1.75	-1.28	1.60	0.77	2.28	-1.59
Goethite	$FeOOH$	5.90	3.63	4.14	7.28	6.56	8.11	4.18
Schwertmannite	$Fe_8O_8(OH)_6SO_4$	9.71	-4.71	-1.69	17.24	12.11	23.91	-0.03
K-Jarosite	$KFe_3(SO_4)_2(OH)_6$	-3.56	-4.95	-4.56	-1.65	-1.54	2.76	1.36
Calcite	$CaCO_3$	0.03	-3.91	-2.82	0.43	-0.56	-0.80	

Input parameters

^aModel 1 Measured ion concentration with ferrous and ferric iron, $E_H = 4$, alkalinity as hydrogen carbonate^bModel 2 Measured ion concentration with total dissolved iron, measured E_H , alkalinity as hydrogen carbonate