water

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Article -Supplementary material

The impact of river discharge and water temperature on manganese release from the riverbed during riverbank filtration – A case study from Dresden, Germany

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Supplementary material

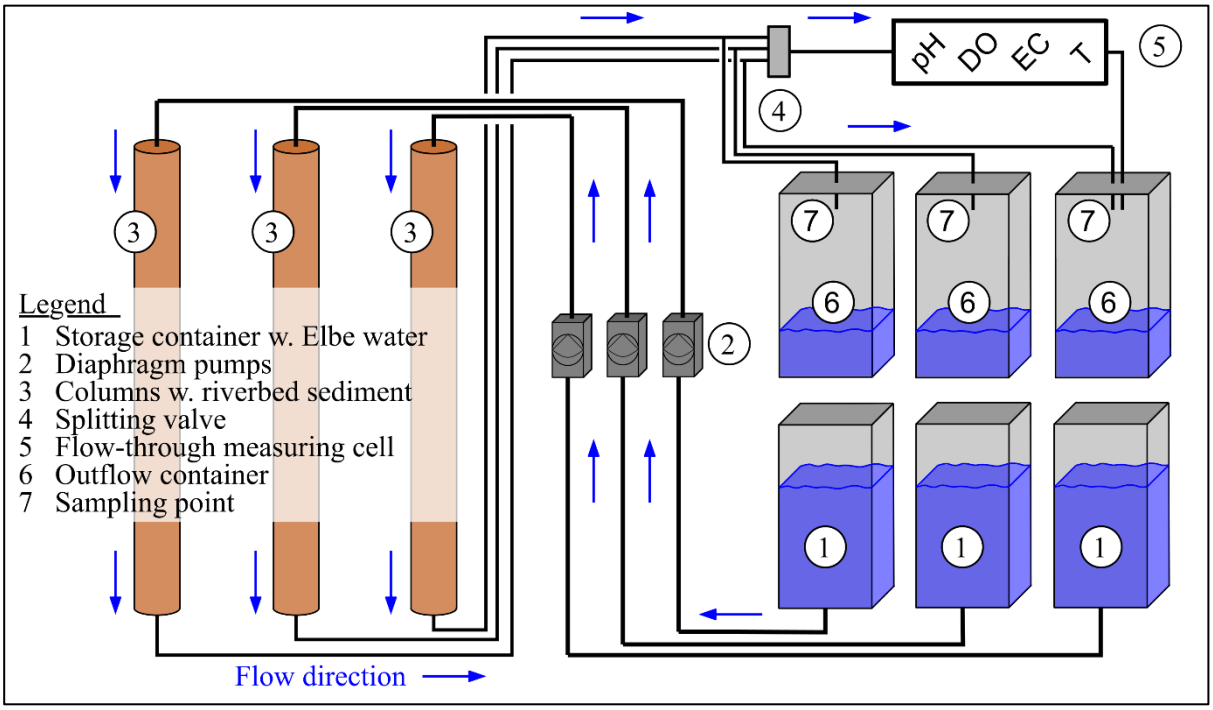

Figure S1: Flow scheme of the column experiments inside the thermostatic cabinets

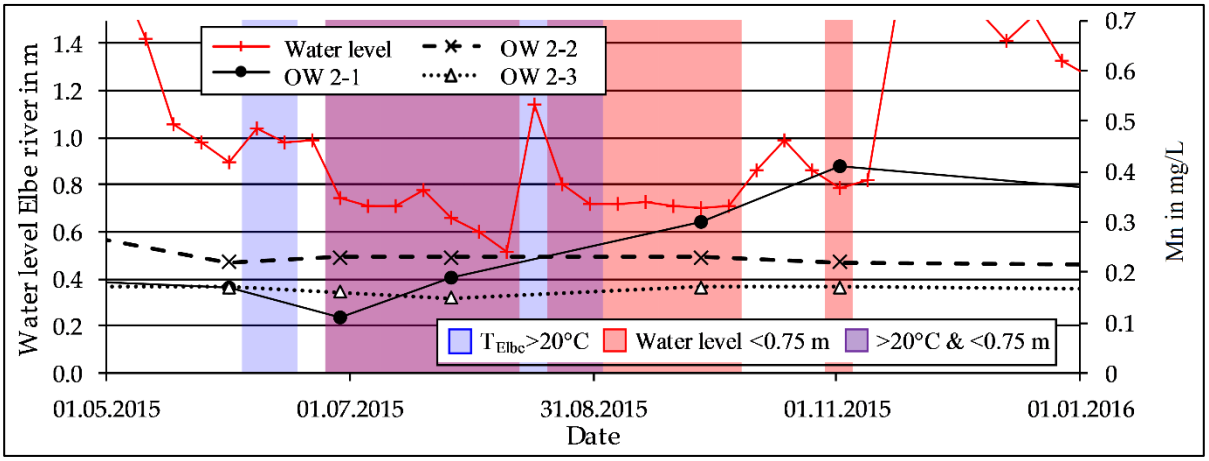

Figure S2: Mn concentration at OW 2 during a low discharge period in 2015

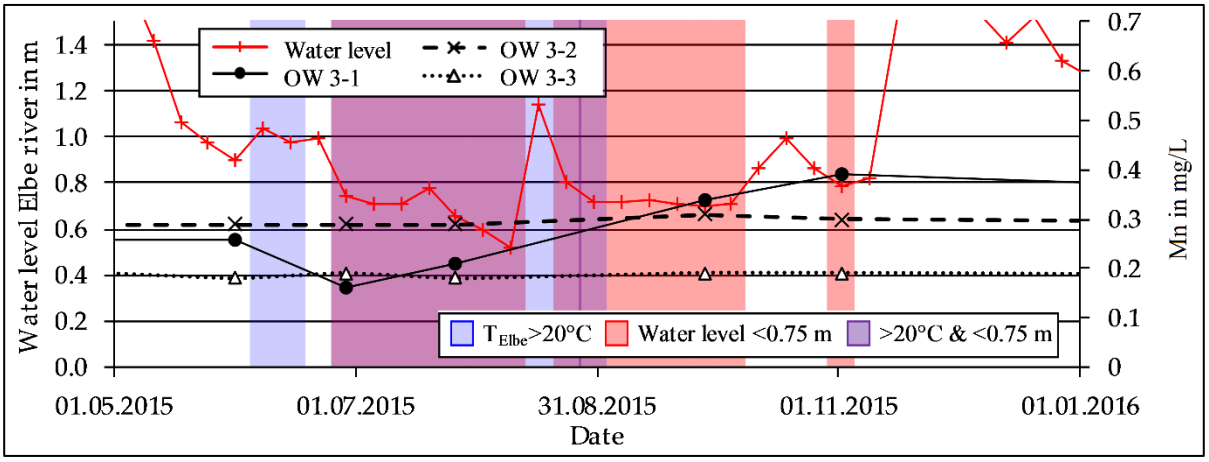

Figure S3: Mn concentration at OW 3 during a low discharge period in 2015

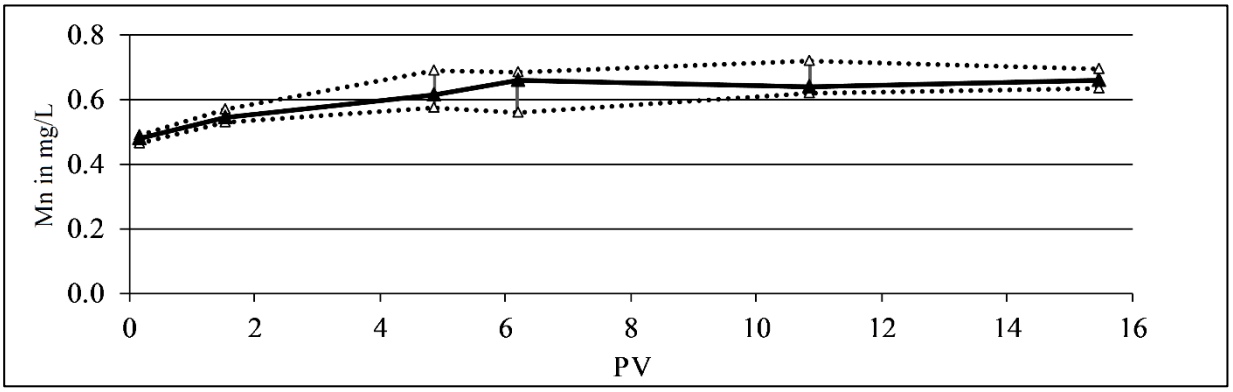

Figure S4: Increase of the Mn concentration within the first 5 PV at 30°C and 1 ml/min after lowering from 2 ml/min, Median, 10- and 90-%ile (each n=3)

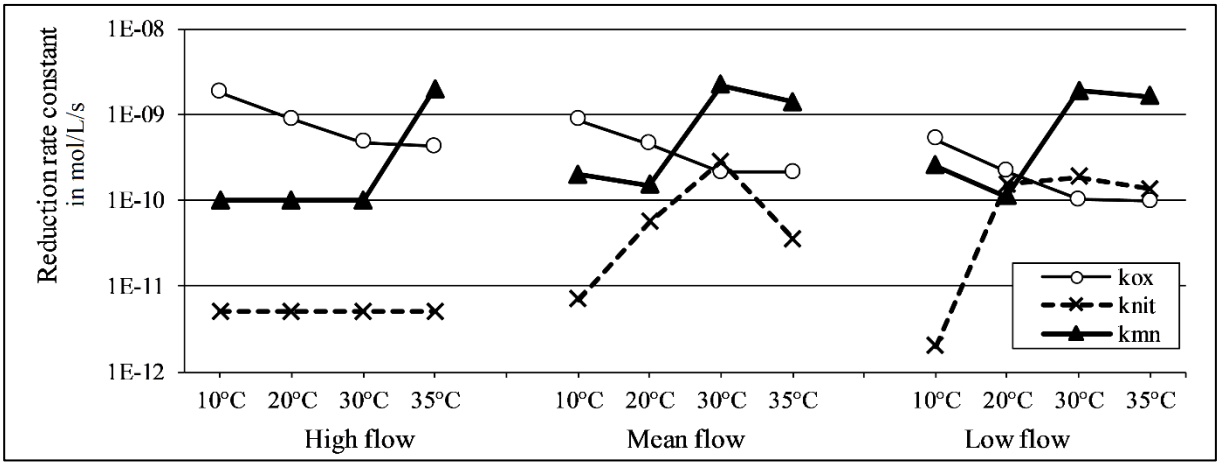

Figure S5: Calibrated reduction rate constants for the column experiment

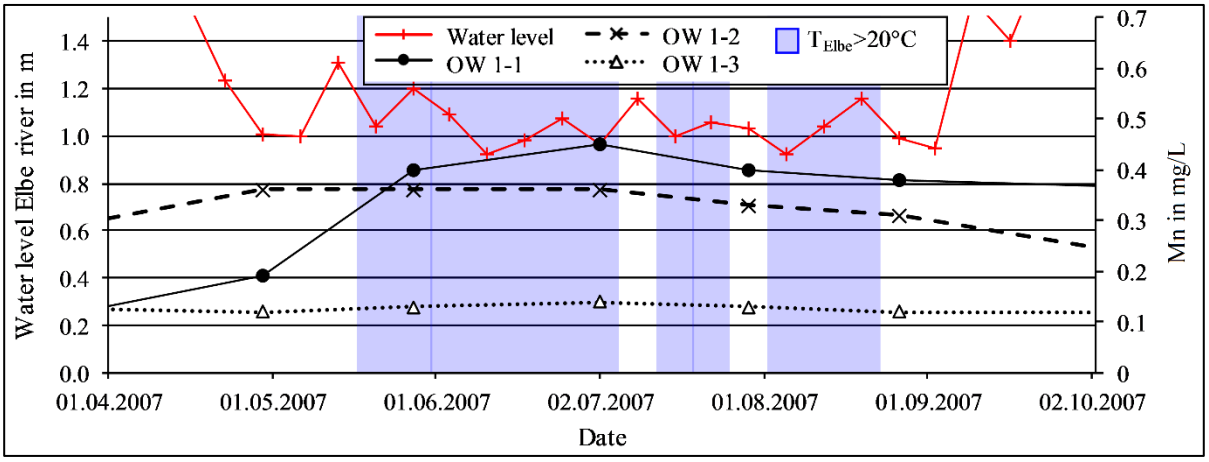

Figure S6: Mn concentration at OW 1 during a low discharge period in 2007

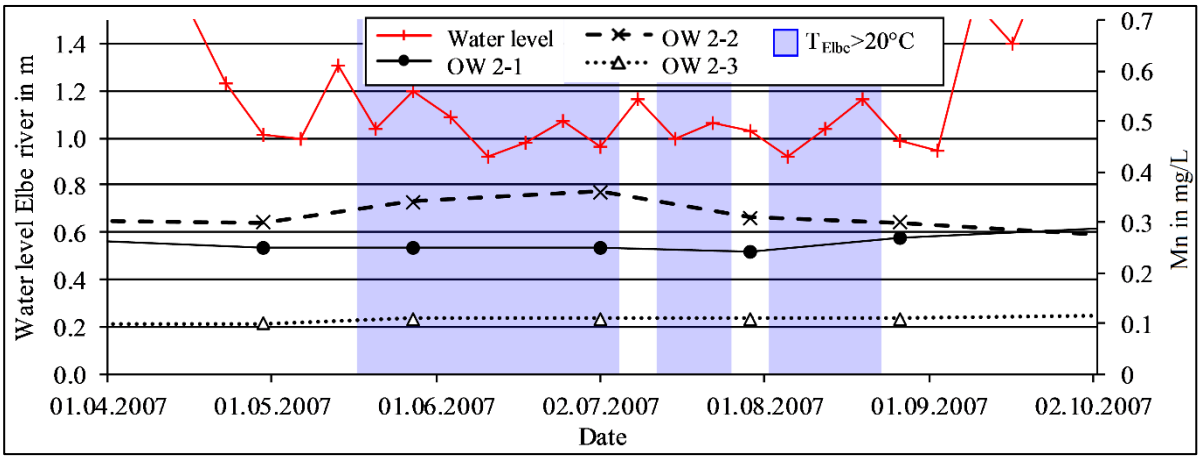

Figure S7: Mn concentration at OW 2 during a low discharge period in 2007

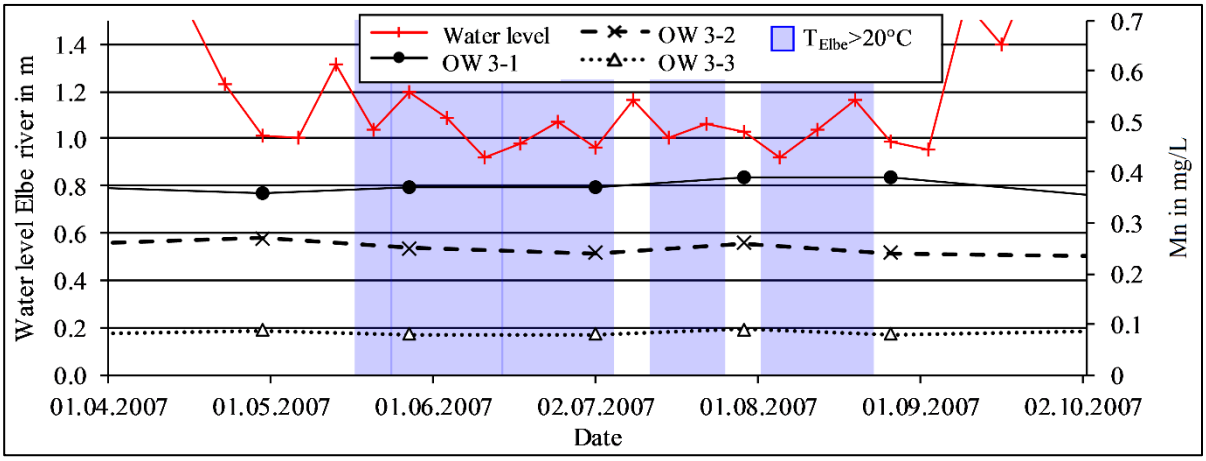

Figure S8: Mn concentration at OW 3 during a low discharge period in 2007

Table S1: Chemical reagents and analytical conditions for the optimized BCR sequential extraction procedure [27, 28]

Step	Extracted phase	Chemical reagents*1 and conditions
1	Acid extractable Exchangeable Carbonate	1 g aliquot, 40 ml 0.11 M CH_3COOH Shake for 16 h at 22±5 °C Separate extract from the solid by centrifugation at 3000 U/min for 20 min
2	Reducible	To step 1 residue: 40 ml 0.5 M $NH_2OH{\cdot}HCl$ (pH≈1.5) Shake for 16 h at 22±5 °C Centrifuge extract as per step 1
3	Oxidizable	To step 2 residue: 10 ml of 30 % H_2O_2 (pH 2–3) Keep at 85±2 °C for 1 h Add further 10 ml of 30 % H_2O_2 (pH 2–3) Keep at 85±2 °C for 1 h Add 50 ml; 1 M NH_4OAc (pH 2) Shake for 16 h at 22±5 °C Centrifuge extract as per step 1
4	Residual *2	To step 3 residue: 15 ml HNO_3 with 5 ml $HClO_4$ Keep at 70-80 °C for 1 h Add further 5 ml HNO_3 with 1 ml $HClO_4$ Keep at 120 °C for 1 h Centrifuge extract as per step 1

*1 CH_3COOH (Acetic acid), $NH_2OH{\cdot}HCl$ (Hydroxylammonium-hydrochloride), H_2O_2 (Hydrogen peroxide), NH_4OAc (Ammonium acetate), HNO_3 (Nitric acid), $HClO_4$ (Perchloric acid)

*2 Extraction of the residual phase differed slightly from Rauret et al. (1999) due to lab restrictions.

Note: Results were checked against a total extraction that was parallel conducted with separate samples by direct application of step 4.

Table S2: Input data of the column in PHREEQC

Parameter	Value
Cells	50
Lengths	0.02
Dispersivity	0.01
Diffusion coefficient	$1 \cdot 10^{-9}$
Porosities	0.34
Bcond	flux flux
Flow direction	forward
Shifts	depending on simulated infiltration rate
Time	depending on simulated infiltration rate

Table S3: Statistical data of the Elbe river at Dresden for the entire observation period 2006-2016 [25]

Month	EC	pH	T	DO	NO_3^-	DOC	TOC	Mn
Jan.	427	7.8	3.0	13.1	19.0	5.1	5.8	0.02
Feb.	443	7.8	3.0	13.0	19.0	4.9	5.6	0.03
Mar.	466	7.85	4.9	13.5	19.0	5.1	6.5	0.03
Apr.	365	7.9	9.5	12.1	18.0	4.9	6.2	0.01
May	413	8.9	14.9	11.8	13.0	5.0	7.4	0.01
June	429	7.9	19.0	9.7	14.0	5.1	7.1	0.01
July	427	7.9	21.6	8.5	12.0	5.2	6.3	0.01
Aug.	407	7.8	21.0	8.5	13.0	5.8	6.7	0.01
Sept.	447	7.7	17.7	8.4	13.0	5.4	6.0	0.01
Oct.	467	7.8	14.0	9.5	14.0	5.4	6.0	0.01
Nov.	446	7.8	9.7	10.6	15.0	5.4	6.1	0.01
Dec.	463	7.8	5.6	11.7	16.0	5.1	5.2	0.02
Min	255	7.5	0.0	7.0	9.7	4.0	4.4	<0.01
10%ile	355	7.7	3.0	8.4	12.0	4.5	5.2	0.01
Median	435	7.8	10.9	10.8	15.0	5.2	6.3	0.01
90%ile	492	8.6	21.3	13.8	20.0	6.0	8.2	0.03
Max	549	9.4	26.0	19.0	32.0	7.0	17.0	0.07
n	279	300	267	269	279	325	292	278

Table S4: Monthly median and 10-year median values of selected parameters along all three OW's of the transect in the WW Dresden-Tolkewitz for the entire observation period 2006-2016

Parameter	OW	Month												10-year
		Jan.	Feb.	Mar.	Apr.	May	June	July	Aug.	Sept.	Oct.	Nov.	Dec.	Median
EC in µS/cm	1-1	451	474	474	465	399	436	470	468	397	467	433	410	463
	1-2	470	449	486	478	423	428	464	446	407	465	435	410	464
	1-3	431	441	508	452	449	441	436	441	417	469	435	410	452
	2-1	471	465	468	526	415	436	458	448	396	462	429	414	460
	2-2	455	440	468	481	449	428	439	446	399	461	428	420	452
	2-3	420	442	509	447	443	448	434	434	417	467	470	413	449
	3-1	449	446	465	462	426	420	433	439	429	458	421	424	453
	3-2	415	439	456	438	441	447	429	433	430	458	459	396	453
	3-3	423	445	505	439	442	452	442	446	422	518	470	420	465
pH	1-1	6.8	6.9	6.8	7.0	7.0	7.1	7.0	6.9	7.0	7.0	7.1	6.9	7.0
	1-2	7.0	7.0	7.0	7.0	7.1	7.2	7.1	7.1	7.1	7.2	7.1	7.1	7.1
	1-3	7.1	7.0	7.1	7.1	7.1	7.0	7.1	7.0	6.9	7.1	7.1	7.0	7.0
	2-1	7.0	7.1	7.0	7.1	7.1	7.1	6.9	7.0	7.0	7.0	7.1	7.1	7.0
	2-2	7.2	7.2	7.2	7.2	7.2	7.2	7.1	7.1	7.1	7.1	7.1	7.1	7.1
	2-3	7.1	7.0	7.1	7.0	7.1	7.1	7.1	7.0	6.9	7.0	7.0	7.0	7.0
	3-1	7.0	7.0	7.0	7.1	7.1	7.1	7.1	7.0	7.0	7.0	7.1	7.0	7.0
	3-2	7.1	7.1	7.1	7.1	7.1	7.2	7.1	7.1	7.0	7.1	7.1	7.1	7.1
	3-3	7.1	6.9	7.1	7.0	7.1	7.1	7.1	7.0	6.8	7.0	7.0	7.0	7.0
T in °C	1-1	7.8	6.1	6.3	6.2	8.6	13.8	17.4	19.2	20.0	18.3	15.8	12.6	14.1
	1-2	10.5	7.8	7.3	6.5	8.3	10.9	14.2	16.0	19.2	17.2	16.5	14.5	12.1
	1-3	11.8	9.9	9.2	8.8	9.4	10.7	11.8	13.8	16.5	15.3	15.2	13.7	14.4
	2-1	11.7	8.3	8.6	6.1	7.8	10.6	14.2	16.3	19.9	17.6	17.1	15.1	12.6
	2-2	13.0	9.9	10.1	8.3	8.5	9.5	11.3	13.9	18.0	16.2	16.5	14.9	11.8
	2-3	12.8	10.8	10.7	9.4	9.7	10.1	11.0	12.7	15.9	14.6	15.0	14.1	11.7
	3-1	15.0	12.1	10.4	11.6	9.1	8.7	9.2	11.8	17.9	15.9	16.9	14.2	11.7
	3-2	15.2	12.9	10.8	12.2	10.2	9.4	8.8	10.8	15.6	13.1	15.7	12.8	11.5
	3-3	14.4	12.6	11.5	12.2	10.9	10.2	9.3	10.8	14.4	13.3	14.6	12.1	14.1
DO in mg/l	1-1	8.2	6.6	7.1	3.2	0.9	0.7	1.7	0.7	0.4	0.5	2.9	1.7	1.3
	1-2	2.0	2.7	2.2	1.1	0.4	0.3	0.4	0.3	0.3	0.4	1.6	0.3	0.4
	1-3	0.7	0.1	0.2	0.2	0.2	0.4	0.4	0.3	0.3	0.4	1.2	0.2	0.2
	2-1	2.9	1.3	2.2	1.2	0.5	0.5	0.5	0.3	0.6	0.4	1.3	0.2	0.5
	2-2	0.8	0.1	0.2	0.1	0.2	0.3	0.3	0.6	0.3	0.4	1.1	0.2	0.2
	2-3	1.0	0.1	0.2	0.1	0.2	0.3	0.4	0.3	0.4	0.4	1.1	0.3	0.3
	3-1	2.5	0.5	2.1	1.2	1.5	1.0	1.2	1.0	0.5	0.8	1.8	0.7	1.1
	3-2	0.8	0.1	0.1	0.1	0.2	0.3	0.4	0.3	0.3	0.4	1.2	0.2	0.2
	3-3	0.9	0.1	0.2	0.1	0.2	0.3	0.4	0.3	0.3	0.4	1.1	0.2	0.2
NO_3^- in mg/l	1-1	28.2	20.5	31.8	10.8	8.9	0.7	5.3	10.2	0.9	1.7	6.0	9.9	5.3
	1-2	5.9	7.6	11.6	4.8	2.0	0.3	0.3	0.3	0.3	0.3	0.3	1.1	0.3
	1-3	6.5	10.1	11.0	9.2	12.2	11.4	9.5	8.3	4.4	4.0	5.3	5.5	8.9
	2-1	18.9	13.5	13.4	5.6	7.2	2.2	2.9	5.5	2.6	3.1	4.0	4.1	4.1
	2-2	0.6	1.3	0.7	0.9	2.0	2.5	0.6	0.6	0.3	0.3	1.3	0.5	0.7
	2-3	8.4	11.5	13.4	10.7	14.8	13.6	11.4	10.6	5.7	6.8	6.3	7.9	10.8
	3-1	7.8	7.7	8.2	6.5	6.4	4.0	2.6	2.0	1.4	3.4	3.0	2.3	4.0
	3-2	3.7	9.0	5.2	9.9	6.9	5.9	7.0	3.3	1.9	1.6	3.8	4.7	5.2
	3-3	6.9	11.8	14.9	11.6	15.3	15.1	14.8	12.1	6.2	10.0	6.7	11.0	12.0

Continued: Table S4: Monthly median and 10-year median values of selected parameters along all three OW's of the transect in the WW Dresden-Tolkewitz for the entire observation period

Parameter	OW	Month												10-year
		Jan.	Feb.	Mar.	Apr.	May	June	July	Aug.	Sept.	Oct.	Nov.	Dec.	Median
DOC in mg/l	1-1	3.3	3.0	3.4	3.2	2.9	3.6	3.6	3.5	3.9	3.4	3.2	3.2	3.4
	1-2	3.4	2.8	3.1	3.4	3.1	3.6	3.7	3.9	3.9	3.6	3.3	3.7	3.5
	1-3	2.9	2.8	2.8	3.0	3.0	2.9	2.9	3.2	3.0	3.2	3.1	3.0	3.0
	2-1	3.4	3.0	3.1	2.8	3.0	3.5	3.1	3.6	3.7	3.5	3.3	3.6	3.4
	2-2	3.4	3.0	2.9	3.1	2.8	3.3	3.3	3.8	4.0	3.8	3.5	3.9	3.5
	2-3	2.7	2.5	2.7	2.9	2.7	2.8	2.9	2.8	2.7	2.9	3.0	3.0	2.8
	3-1	2.9	2.8	2.9	2.9	2.7	2.9	3.0	3.3	3.4	3.3	3.4	3.5	3.0
	3-2	3.3	3.1	3.1	3.4	3.1	3.0	3.0	3.2	3.3	3.4	3.4	3.4	3.2
	3-3	2.7	2.3	2.5	2.6	2.7	2.5	2.6	2.6	2.1	2.6	2.7	2.5	2.6
Mn in mg/l	1-1	0.01	0.04	0.01	0.14	0.05	0.05	0.08	0.18	0.42	0.31	0.04	0.22	0.06
	1-2	0.33	0.34	0.25	0.30	0.28	0.32	0.41	0.36	0.32	0.27	0.26	0.31	0.32
	1-3	0.20	0.18	0.24	0.19	0.19	0.18	0.25	0.21	0.15	0.21	0.20	0.17	0.20
	2-1	0.17	0.20	0.22	0.17	0.16	0.18	0.21	0.22	0.31	0.24	0.22	0.32	0.21
	2-2	0.30	0.32	0.35	0.33	0.29	0.28	0.30	0.28	0.30	0.28	0.25	0.31	0.30
	2-3	0.16	0.15	0.18	0.16	0.16	0.16	0.17	0.16	0.11	0.18	0.17	0.13	0.17
	3-1	0.22	0.32	0.31	0.35	0.29	0.24	0.28	0.23	0.39	0.30	0.33	0.43	0.30
	3-2	0.30	0.28	0.32	0.26	0.29	0.29	0.28	0.28	0.24	0.31	0.29	0.25	0.29
	3-3	0.22	0.15	0.21	0.15	0.19	0.18	0.20	0.20	0.18	0.24	0.19	0.13	0.19
n	1-1	1	2	2	2	4	4	5	4	2	5	5	2	38
	1-2	1	2	2	2	4	4	5	4	2	5	5	2	38
	1-3	1	2	2	2	4	4	5	4	2	5	5	2	38
	2-1	1	2	2	1	4	4	5	4	2	5	5	2	37
	2-2	1	2	2	2	4	4	5	4	2	5	5	2	38
	2-3	1	2	2	2	4	4	5	4	2	5	5	2	38
	3-1	1	2	2	2	4	4	5	4	2	5	5	2	38
	3-2	1	2	2	2	4	4	5	4	2	5	5	2	38
	3-3	1	2	2	2	4	4	5	4	2	5	5	2	38

Table S5: Statistical data for the low flow period in 2015

	Elbe river		OW 1-1	OW 1-2	OW 1-3	OW 2-1	OW 2-2	OW 2-3	OW 3-1	OW 3-2	OW 3-3
	T in °C	Water level in m	Mn in mg/l								
10%ile	11.0	0.62	0.06	0.20	0.18	0.14	0.22	0.16	0.19	0.29	0.18
Median	20.1	0.74	0.19	0.24	0.20	0.19	0.23	0.17	0.26	0.29	0.19
90%ile	24.6	1.05	0.61	0.28	0.21	0.36	0.25	0.17	0.37	0.31	0.19
n	153	153	6	6	6	6	6	6	6	6	6

Table S6: Statistical data for Mn release during the column experiment with riverbed sediment from the Elbe river in Dresden-Tolkewitz, Q_1 & Q_3 correspond to the 1st & 3rd quartile

Flow rate		10°C	20°C	30°C	35°C
4 ml/min (High flow)	Min.	0.001	0.000	0.000	0.457
	Q1	0.001	0.000	0.019	0.508
	Median	0.002	0.001	0.029	0.512
	Q3	0.008	0.006	0.045	0.526
	Max.	0.014	0.020	0.076	0.569
	n	9	12	21	12
2 ml/min (Mean flow)	Min.	0.002	0.005	0.410	0.537
	Q1	0.005	0.013	0.462	0.596
	Median	0.007	0.018	0.491	0.627
	Q3	0.007	0.029	0.496	0.670
	Max.	0.007	0.041	0.500	0.717
	n	9	9	9	15
1 ml/min (Low low)	Min.	0.000	0.005	0.465	0.564
	Q1	0.002	0.011	0.562	0.802
	Median	0.002	0.038	0.636	0.812
	Q3	0.002	0.057	0.658	0.847
	Max.	0.003	0.074	0.691	0.868
	n	6	21	18	15

Table S7: Comparison of the measured parameter values during the column experiment and the modeled parameters from PHREEQC

Temperature	Flow rate	% Error between the measured and the calibrated value			
		DO	NO_3^-	Mn^{2+}	pH
10°C	1 ml/min	0.1	0.3	8.7	6.2
	2 ml/min	0.2	0.4	6.9	1.6
	4 ml/min	-0.9	0.3	-1.4	-2.2
20°C	1 ml/min	0.2	-0.2	1.8	-2.8
	2 ml/min	-5.3	1.1	-36.6	0.2
	4 ml/min	-3.3	0.5	-17.3	1.5
30°C	1 ml/min	-6.7	4.4	0.1	-9.3
	2 ml/min	-16.6	-1.7	4.8	-8.7
	4 ml/min	-5.4	0.8	8.8	-5.1
35°C	1 ml/min	0.2	-0.7	0.3	-8.7
	2 ml/min	-1.6	-0.1	-1.5	1.2
	4 ml/min	-6.6	0.9	-1.6	1.7
10%ile		-6.7	-0.6	-15.7	-8.7
Median		**-2.4**	**0.4**	**0.2**	**-1.0**
90%ile		0.2	1.1	8.5	1.7
n		12	12	12	12

Table S8: Results and statistical data of the sequential extraction of the riverbed sediment after the column experiment (n=3 for each statistical data)

Column	Depth	Carb.	Easily red.	Organ.	Residual	Sum	Total Extr.
no.	in m	in mg/kg	in mg/kg	in mg/kg	in mg/kg	in mg/kg	in mg/kg
1	0.05	61	149	15	51	277	213
	0.3	30	55	8	53	146	98
	0.6	33	48	7	70	158	112
	0.9	28	36	7	55	125	110
2	0.05	79	115	9	46	249	251
	0.3	47	46	7	62	162	133
	0.6	57	42	7	63	168	331
	0.9	30	34	6	46	116	111
3	0.05	65	142	9	54	270	250
	0.3	37	44	6	64	151	106
	0.6	28	48	6	64	146	705
	0.9	21	38	6	64	129	476
10%ile	0.05	62	121	9	47	253	101
Median		65	142	9	51	270	112
90%ile		76	148	14	53	275	192
10%ile	0.3	32	45	6	54	147	114
Median		37	46	7	62	151	133
90%ile		45	53	8	64	160	228
10%ile	0.6	29	43	6	63	148	138
Median		33	48	7	64	158	250
90%ile		52	48	7	69	166	315
10%ile	0.9	22	34	6	48	118	180
Median		28	36	6	55	125	476
90%ile		30	38	7	62	128	659

Table S9: Median concentration of DO in the outflow during the column experiment

Flow	Residence time	Temperature			
		10°C	20°C	30°C	35°C
4 ml/min	8.1 h	5.4	1.8	0.2	0.2
		n=9	n=12	n=21	n=12
2 ml/min	16.2 h	5.1	0.6	0.2	0.2
		n=9	n=9	n=9	n=15
1 ml/min	32.4 h	4.2	0.2	0.2	0.2
		n=6	n=21	n=18	n=15