Supplement to "Controls of fluorescent tracer retention by soils and sediments" by Bork et. al

Marcus Bork[1,2], Jens Lange[2], Markus Graf-Rosenfellner[1], and Friederike Lang[1]

[1]Soil Ecology, Faculty of Environment and Natural Resources, University of Freiburg, Freiburg, Germany
[2]Hydrology, Faculty of Environment and Natural Resources, University of Freiburg, Freiburg, Germany

Table S1. Residual water contents of samples from top- and subsoil, sediment and clay mineral (difference between at 105 °C dried and air-dried sample. The values are the means of three repetitions +/- standard deviation.

Subtrate	Treatment	Water Content (wt% ± wt%)
Topsoil	high OC	2.16 ± 0.02
Topsoil	low OC	1.17 ± 0.03
Subsoil	high OC	2.11 ± 0.01
Subsoil	low OC	1.85 ± 0.36
Sediment	Clay0	0.14 ± 0.01
Montmorillonite	-	4.11 ± 0.04

Table S2. Mean concentrations and standard deviations (n = 3) from batch experiment of topsoil samples. Where the standard deviation is missing only on single measurement was performed. Data of treatment high OC at pH 5.5, 6.5 and 7.5 were used in Fig.2. Data from treatments high OC and low OC at pH 7.5 were used in Fig.4.

Subtrate	Treatment	pH (-)	c_{step} [a]	$c_{initial}$ ($\mu g \cdot L^{-1}$)		$c_{solution}$ ($\mu g \cdot L^{-1}$)		$q_{adsorbed}$ ($\mu g \cdot kg^{-1}$)	
				UR	SRB	UR	SRB	UR	SRB
Topsoil	high OC	5.5	c1	20	400	1.3 ± 0.1	135.1 ± 11.0	93 ± 0.6	1325 ± 55.2
Topsoil	high OC	5.5	c2	25	500	1.7	194.2	116	1529
Topsoil	high OC	5.5	c3	30	600	2.1	243.1	139	1784
Topsoil	high OC	5.5	c4	35	700	2.4	283.9	163	2081
Topsoil	high OC	5.5	c5	40	800	2.8	338.6	186	2307
Topsoil	high OC	5.5	c6	45	900	2.6 ± 0.4	378.5 ± 18.5	212 ± 2.1	2608 ± 92.4
Topsoil	high OC	6.5	c1	20	400	3.4 ± 0.5	165.8 ± 3.1	83 ± 2.4	1171 ± 15.6
Topsoil	high OC	6.5	c2	25	500	3.6	230.7	107	1347
Topsoil	high OC	6.5	c3	30	600	3.6	266.7	132	1666
Topsoil	high OC	6.5	c4	35	700	4.3 ± 0.1	331.8 ± 2.5	153 ± 0.6	1841 ± 12.5
Topsoil	high OC	6.5	c5	40	800	5.1	389.5	174	2053
Topsoil	high OC	6.5	c6	45	900	5.5 ± 0.9	435.0 ± 24.6	198 ± 4.3	2325 ± 123.0
Topsoil	high OC	7.5	c1	20	400	13.5 ± 0.8	229.6 ± 8.8	33 ± 4.2	871 ± 44.2
Topsoil	high OC	7.5	c2	25	500	15.9 ± 0.5	289.9 ± 14.5	47 ± 2.5	1074 ± 72.3
Topsoil	high OC	7.5	c3	30	600	18.5 ± 0.6	369.3 ± 7.0	59 ± 3.1	1179 ± 35.1
Topsoil	high OC	7.5	c4	35	700	23.0 ± 2.6	425.0 ± 14.5	62 ± 13.1	1406 ± 72.5
Topsoil	high OC	7.5	c5	40	800	24.9 ± 0.5	503.6 ± 3.4	77 ± 2.3	1514 ± 16.9
Topsoil	high OC	7.5	c6	45	900	28.4 ± 1.8	540.0 ± 15.4	85 ± 9.0	1840 ± 77.1
Topsoil	low OC	7.5	c1	20	400	17.4 ± 0.6	128.2 ± 6.8	13 ± 2.8	1375 ± 33.8
Topsoil	low OC	7.5	c2	25	500	21.3 ± 0.2	149.6 ± 3.2	19 ± 0.9	1773 ± 15.9
Topsoil	low OC	7.5	c3	30	600	27.7 ± 0.7	201.9 ± 11.1	12 ± 3.3	2014 ± 55.3
Topsoil	low OC	7.5	c4	35	700	30.1 ± 0.6	231.7 ± 4.4	25 ± 3.2	2369 ± 21.9
Topsoil	low OC	7.5	c5	40	800	34.1 ± 0.1	274.7 ± 4.8	30 ± 0.5	2658 ± 24.1
Topsoil	low OC	7.5	c6	45	900	40.3 ± 0.1	308.1 ± 3.7	24 ± 0.3	2994 ± 18.7

[a] Concentration step of initial tracer addition.

Table S3. Mean concentrations and standard deviations (n = 3) from batch experiment of subsoil samples. Where the standard deviation is missing only on single measurement was performed. Data of treatment high OC at pH 5.5, 6.5 and 7.5 were used in Fig.2. Data from treatments high OC and low OC at pH 7.5 were used in Fig.4.

Subtrate	Treatment	pH (-)	c_{step} [a]	$c_{initial}$ ($\mu g \cdot L^{-1}$)		$c_{solution}$ ($\mu g \cdot L^{-1}$)		$q_{adsorbed}$ ($\mu g \cdot kg^{-1}$)	
				UR	SRB	UR	SRB	UR	SRB
Subsoil	high OC	5.5	c1	20	400	2.0	9.4	90	1953
Subsoil	high OC	5.5	c2	25	500	2.8	27.2	111	2364
Subsoil	high OC	5.5	c3	30	600	4.1	58.0	129	2710
Subsoil	high OC	5.5	c4	35	700	4.4	70.5	153	3148
Subsoil	high OC	5.5	c5	40	800	5.1	92.7	174	3536
Subsoil	high OC	5.5	c6	45	900	5.7	110.2	196	3949
Subsoil	high OC	6.5	c1	20	400	3.8 ± 0	26.9 ± 0.9	81 ± 0.01	1865 ± 4.3
Subsoil	high OC	6.5	c2	25	500	5.5 ± 0.02	60.3 ± 0.8	97 ± 0.1	2199 ± 4.0
Subsoil	high OC	6.5	c3	30	600	7.3	91.8	114	2541
Subsoil	high OC	6.5	c4	35	700	7.4	107.0	138	2965
Subsoil	high OC	6.5	c5	40	800	9.9	146.9	151	3265
Subsoil	high OC	6.5	c6	45	900	9.9	161.5	176	3692
Subsoil	high OC	7.5	c1	20	400	12.0 ± 0.8	86.7 ± 5.9	41 ± 4.0	1600 ± 29.7
Subsoil	high OC	7.5	c2	25	500	15.1 ± 0.2	116.5 ± 1.9	50 ± 1.0	1959 ± 9.3
Subsoil	high OC	7.5	c3	30	600	18.8 ± 0.3	149.9 ± 3.2	57 ± 1.3	2299 ± 15.9
Subsoil	high OC	7.5	c4	35	700	23.1 ± 0.7	193.0 ± 8.4	61 ± 3.5	2590 ± 42.0
Subsoil	high OC	7.5	c5	40	800	25.3 ± 1.0	224.3 ± 7.7	75 ± 4.8	2940 ± 38.7
Subsoil	high OC	7.5	c6	45	900	29.2 ± 0.2	261.5 ± 0.5	80 ± 1.2	3261 ± 2.5
Subsoil	low OC	7.5	c1	20	400	12.7 ± 0.2	54.1 ± 2.8	37 ± 0.8	1762 ± 13.8
Subsoil	low OC	7.5	c2	25	500	16.7 ± 0.7	77.6 ± 3.8	42 ± 3.5	2152 ± 18.8
Subsoil	low OC	7.5	c3	30	600	20.4 ± 0.3	99.7 ± 1.5	49 ± 1.7	2549 ± 7.7
Subsoil	low OC	7.5	c4	35	700	24.0 ± 0.3	124.3 ± 0.6	56 ± 1.3	2933 ± 3.2
Subsoil	low OC	7.5	c5	40	800	25.3 ± 1.7	136.2 ± 9.6	75 ± 8.5	3382 ± 48.1
Subsoil	low OC	7.5	c6	45	900	30.6 ± 1.3	177.3 ± 15.0	73 ± 6.3	3682 ± 74.9

[a] Concentration step of initial tracer addition.

Table S4. Continuation: Mean concentrations and standard deviations (n = 3) from batch experiment of sediment samples. Where the standard deviation is missing only on single measurement was performed. Data of treatment Clay0 at pH 5.5, 6.5 and 7.5 were used in Fig.2. Data from treatments Clay0, Clay1 and Clay2 at pH 7.5 were used in Fig.4.

Subtrate	Treatment	pH (-)	c_{step} [a]	$c_{initial}$ ($\mu g \cdot L^{-1}$)		$c_{solution}$ ($\mu g \cdot L^{-1}$)		$q_{adsorbed}$ ($\mu g \cdot kg^{-1}$)	
				UR	SRB	UR	SRB	UR	SRB
Sediment	Clay0	5.5	c1	20	400	18.8 ± 0.8	321.7 ± 14.3	6 ± 3.8	391 ± 71.3
Sediment	Clay0	5.5	c2	25	500	23.9	447.0	5	265
Sediment	Clay0	5.5	c3	30	600	28.5	541.0	8	295
Sediment	Clay0	5.5	c4	35	700	33.2	638.1	9	309
Sediment	Clay0	5.5	c5	40	800	38.5	749.7	8	252
Sediment	Clay0	5.5	c6	45	900	41.4 ± 0.8	844.0 ± 20.7	18 ± 4.1	280 ± 103.3
Sediment	Clay0	6.5	c1	20	400	18.9 ± 0.1	343.5 ± 4.1	6 ± 0.6	283 ± 20.4
Sediment	Clay0	6.5	c2	25	500	24.8	463.8	1	181
Sediment	Clay0	6.5	c3	30	600	30.3	579.8	0	101
Sediment	Clay0	6.5	c4	35	700	34.1	660.1	5	199
Sediment	Clay0	6.5	c5	40	800	40.0	759.4	0	203
Sediment	Clay0	6.5	c6	45	900	44.4 ± 1.9	890.7 ± 35.5	3 ± 9.3	46 ± 177.5
Sediment	Clay0	7.5	c1	20	400	20.6 ± 0.2	343.1 ± 5.2	0	285 ± 26.2
Sediment	Clay0	7.5	c2	25	500	25.7 ± 0.4	453.7 ± 13.0	0	232 ± 65.2
Sediment	Clay0	7.5	c3	30	600	31.2 ± 0.5	540.9 ± 12.0	0	296 ± 60.0
Sediment	Clay0	7.5	c4	35	700	34.8 ± 0.5	587.3 ± 14.0	1 ± 2.4	564 ± 70.1
Sediment	Clay0	7.5	c5	40	800	39.1 ± 0.1	675.0 ± 6.2	4 ± 0.6	626 ± 30.8
Sediment	Clay0	7.5	c6	45	900	45.1 ± 0.7	748.4 ± 5.0	0 ± 3.3	759 ± 24.9

[a] Concentration step of initial tracer addition.

Table S4. Continuation: Mean concentrations and standard deviations (n = 3) from batch experiment of sediment samples. Where the standard deviation is missing only on single measurement was performed. Data of treatment Clay0 at pH 5.5, 6.5 and 7.5 were used in Fig.2. Data from treatments Clay0, Clay1 and Clay2 at pH 7.5 were used in Fig.4.

Subtrate	Treatment	pH	c_{step} [a]	$c_{initial}$		$c_{solution}$		$q_{adsorbed}$	
		(-)		($\mu g \cdot L^{-1}$)		($\mu g \cdot L^{-1}$)		($\mu g \cdot kg^{-1}$)	
				UR	SRB	UR	SRB	UR	SRB
Sediment	Clay1	7.5	c1	20	400	13.6 ± 0.2	138.9 ± 2.5	32 ± 0.8	1308 ± 12.3
Sediment	Clay1	7.5	c2	25	500	18.5 ± 0.5	200.0 ± 9.3	33 ± 2.3	1503 ± 46.4
Sediment	Clay1	7.5	c3	30	600	22.1 ± 0.8	241.8 ± 6.3	39 ± 4.1	1794 ± 31.4
Sediment	Clay1	7.5	c4	35	700	26.2 ± 0.3	287.5 ± 3.4	44 ± 1.7	2066 ± 16.9
Sediment	Clay1	7.5	c5	40	800	30.9 ± 0.7	348.1 ± 14.6	45 ± 3.5	2264 ± 72.8
Sediment	Clay1	7.5	c6	45	900	36.4 ± 0.4	409.8 ± 1.0	43 ± 2.1	2455 ± 4.8
Sediment	Clay2	7.5	c1	20	400	3.8 ± 0.1	47.5 ± 0.9	81 ± 0.5	1767 ± 4.7
Sediment	Clay2	7.5	c2	25	500	5.5 ± 0.2	64.1 ± 3.1	98 ± 1.1	2184 ± 15.5
Sediment	Clay2	7.5	c3	30	600	8.3 ± 0.8	92.9 ± 12.3	109 ± 4.2	2541 ± 61.5
Sediment	Clay2	7.5	c4	35	700	10.4 ± 0.6	108.9 ± 3.5	123 ± 3.2	2962 ± 17.7
Sediment	Clay2	7.5	c5	40	800	13.5 ± 1.1	140.1 ± 4.8	133 ± 5.6	3307 ± 23.8
Sediment	Clay2	7.5	c6	45	900	16.3 ± 0.5	169.2 ± 7.4	144 ± 2.4	3662 ± 37.2

[a] Concentration step of initial tracer addition.

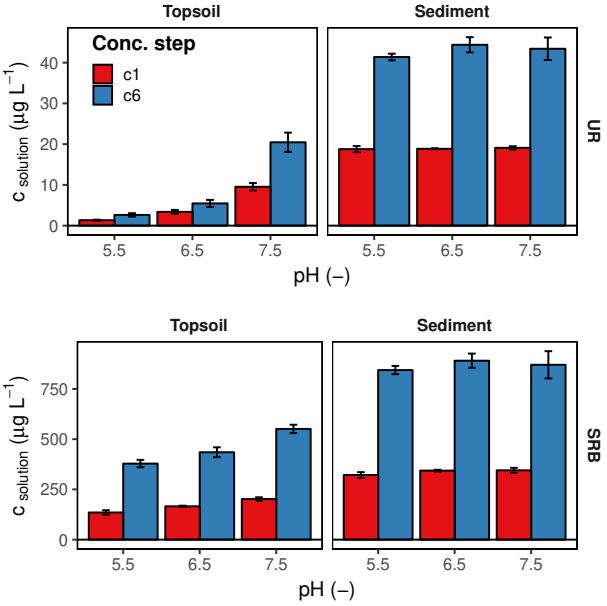

Figure S1. Measured concentrations in solution after separation of solid and liquid phase in dependence of pH for the concentration steps 1 and 6 (20 and 50 µg · L^{-1} for UR and 400 and 1000 µg · L^{-1} for SRB) for topsoil and sediment and the tracers UR and SRB. The error bars represent the standard deviation of three repeated measurements.

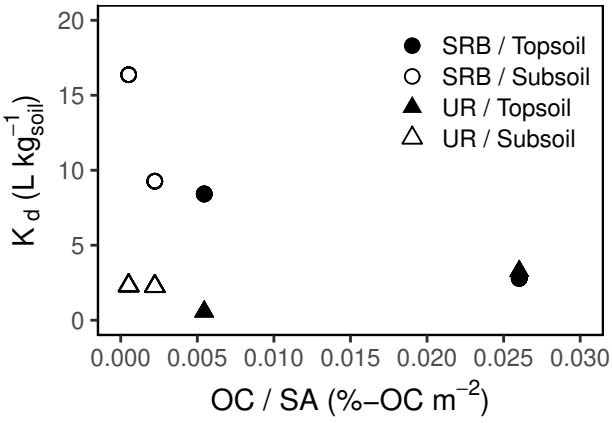

Figure S2. K_d-values as function of OC related to the surface area SA ($\% - \mathrm{OC} \cdot \mathrm{m}^{-2}$) for UR (triangles) and SRB (circles) in topsoil (filled symbols) and subsoil (open symbols). For each tracer and type of substrate (top- or subsoil) the K_d-value at lower OC-value result from the H_2O_2-treatment and the K_d at higher OC from the untreated samples. Each K_d-value was derived as the slope from linear regression of the sorption isotherms (six concentrations times three replications).

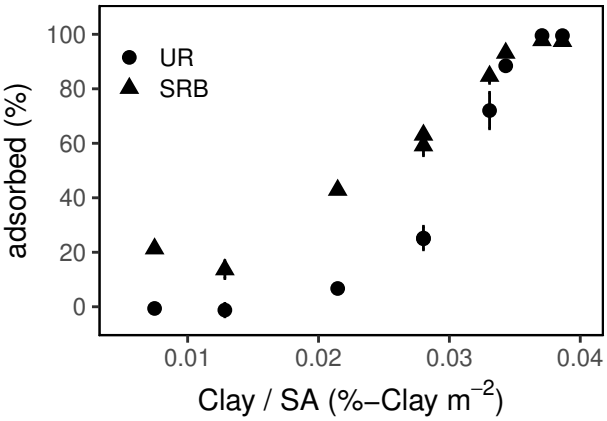

Figure S3. Adsorbed percentage as a function of the clay content related to the surface area SA ($\% - \mathrm{OC} \cdot \mathrm{m}^{-2}$) for UR (triangles) and SRB (circles) in the sediment. The data points at 0.14, 1 and 2 $\%$ clay- addition contain 18 single measurements consisting of the six tracer concentrations and each in triplicate preparation. The errorbars represent the standard deviation. The other data-points (without errorbars) are single measurements of tracer adsorption at 0.1, 0.5, 2.5, 5.0 and 10.0 $\%$ clay- addition.