Supplementary information for:

Organic matters, but inorganic matters too: column examination of elevated mercury sorption on low organic matter aquifer material using concentrations and stable isotopes ratios.

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S1. Preliminary experiments & column packing.

Packing Methods

All packing methods utilised glass beads and quartz wool below and above the solid-phase materials to minimise material and particle transport (see Figure 1 of main paper). The outlet for the liquid was located in or above the quartz wool. The plunger of the syringe was placed as a mechanical barrier on top of the syringe to prevent the layers from slipping. Finally, tubing was attached to the outlet (just below the plunger) to transport eluate away from the column. This tubing was glued from the outside to prevent leaks.

Filling with dried material and layer-by-layer flooding of the column

Layers of ≈18 g of aquifer material were added layer by layer into the column and then dry compacted before flooding each layer from below. The 18.09 g of the initial layer of material could be compressed to a volume of about 11 cm³, resulting in a bulk density of 1.64 g/cm³. To further compact the layers and remove trapped air bubbles, the first layer was flooded from the bottom and the water was drained. To ensure hydraulic connection between the layers, the surface was scratched and lightly loosened. The second layer, consisting of another 18.03 g, was then added and compressed to a volume of 11 cm³. After flooding the column again from the bottom, the two layers separated from each other. Attempting to reassemble the layers was unsuccessful, thus this packing method experiment was terminated.

Dry packing of the column

Figure S1.1: dry packed soil column

The next method involved the addition of layers of ≈16 g of aquifer material were added. 16.03 g of the first layer added could be compressed to a volume of 11.5 cm³, resulting in a storage density of 1.39 g/cm³. The surface of the layer was then slightly loosened to achieve hydraulic connection between the layers. After flooding the entire column, some small pockets were observed (Figure S1.1). Therefore, another packing method was considered.

Packing the column with 7 wt.% water

In this method, the sieved aquifer material was mixed with 7 wt.% tap water to avoid gradation of the material during filling and to prevent possible air inclusions. The lower structure of the column S2 is identical to the first and second packing experiments. For every 9-10 cm³, a dry mass of about 15 g was filled. The surface of each layer was loosened again to ensure a better connection between the layers. A bulk density of 1.56 g/cm³ was achieved.

The distribution of the material appeared more even and fewer air inclusions were visible compared to the second packing experiment.

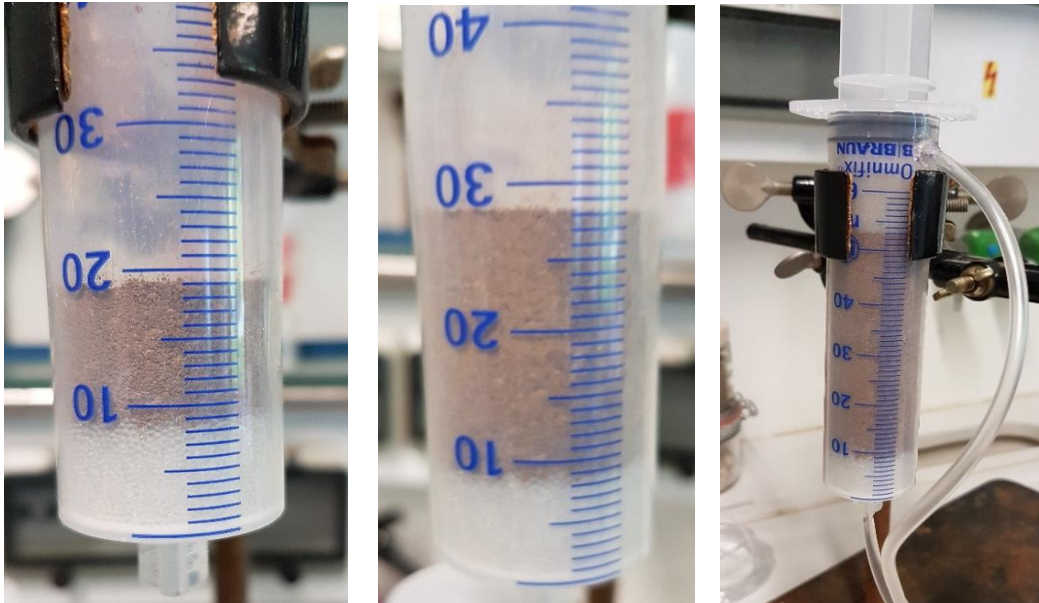



Figure S1.2: Presentation of the layered introduction of the material mixed with 7% water

Preliminary flow-through column experiments

Three columns using 7% water volume and one column dry packed were tested under flow conditions. These columns were flushed with tap water for one week prior to the start of the preliminary test. During the testing phase, there was separation of the lower layers in columns S2 to S4 (Appendix A 3), indicating that this occurred in columns with higher bulk density and 7% water addition. S1 did not have this problem and showed similar results to the other columns in the preliminary test, which led to the decision to use the drying packing method for actual experiments (EXP1 and EXP2).

Table S1.1: Summary of the setup of the pre-test columns S1 to S4.

	Dry mass [g]	Volume [cm³]	Bulk density [g/cm³]	Packing Methode
S1	72.21	51.00	1.42	Dry packing
S2	67.10	43.50	1.54	With 7 % water
S3	74.34	49.25	1.51	With 7 % water
S4	74.42	47.00	1.58	With 7 % water

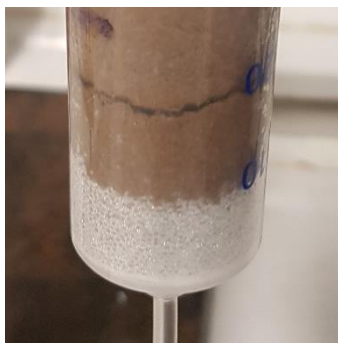



Figure S1.3: Example of layer separation during the flushing process using the 7% water packing method.

Background Investigations

Upon connecting the first columns, discoloration of the eluate was observed (see Appendix A4). This slight yellowish to brownish discoloration decreased with increasing water flow. Filtering the fluid with a 0.45 µm nylon syringe filter did not change the coloration. Subsequently, the fresh eluate was analysed for dissolved organic carbon (DOC) and other constituents immediately after connecting the column to the system and after a 24-hour flushing period. Table S2.2 (in Section S2 below) shows the DOC and other constituents of the two solutions. The origin of the DOC was somewhat surprising, as the determination of organic material showed a low value of only 0.16 ± 0.02%. Additionally, the syringe, glass beads, and quartz wool were tested for DOC in separate experiments to investigate their origin. This confirmed our decision to allow the columns to equilibrate for 7 days, flowing with tap water.

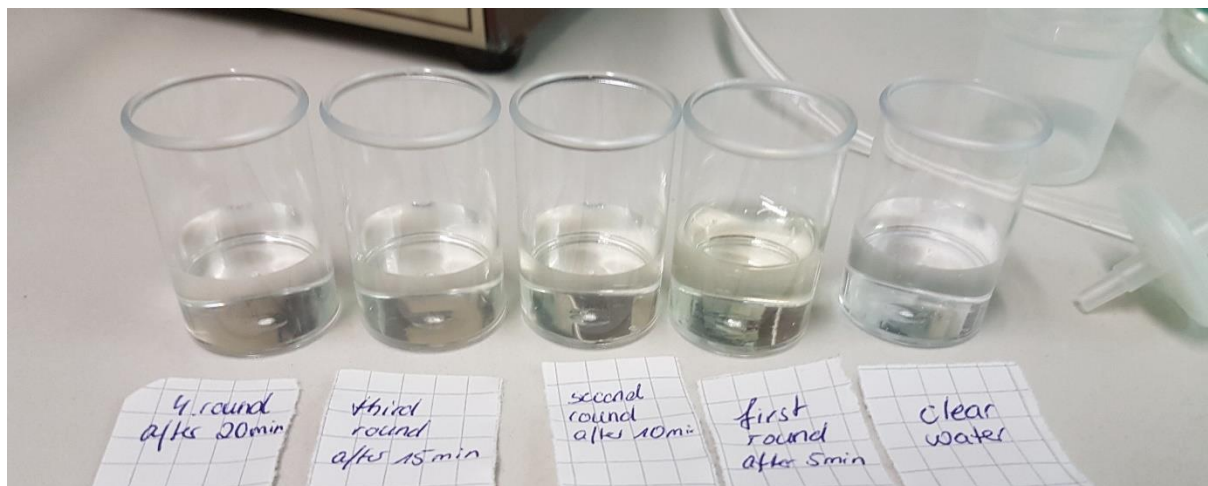



Figure S1.4. Coloration of the eluate after the start of the column experiment at 5 min, 10 min, 15 min, and after 20 min.

Tracer experiments

In order to test the usability of the chloride tracer, theoretical calculations for the required time of the water front were made and real-time measurements (stop watch) were taken during preliminary experiments on column S4 listed above (as listed above). For the theoretical calculations, the volumes were determined based on the lengths and diameters of the hoses, and a range between 0.2 and 0.4 effective porosity was assumed based on the bulk density of 1.58 g/cm³. The volumetric flow rate to be set via the pump was determined in advance with a measuring cylinder and stopwatch and averaged 1.17 ml min^{-1} for S4. Based on these assumed effective porosities, a flow-through time of 12.8 min to 25.7 min was calculated for the column. Timed measurements determined the water front to pass through the column in 16.1 min .

These estimates were compared to tracer experiments based on NaCl addition and measurements of eluate conductivity observed over time using a hand-help electronic conductivity probe. Baseline values were set by measuring the conductivity of tap water before NaCl addition and compared to the conductivity of the initial salt solution used. The average time for the tracer to pass through was determined at 50% of the resulting cumulative curve. The chloride tracer indicates the time it takes for the chloride ions to pass through the entire system. Subtracting the hose volumes resulted in a required time of 15.6 ± 0.4 min (n=3) for column S4. It is evident that the theoretical considerations, the visual measurement, and the chloride tracer show similar values. Based on this, it is assumed that the chloride tracer is not reactive in the system and can thus be used to calculate the water front.

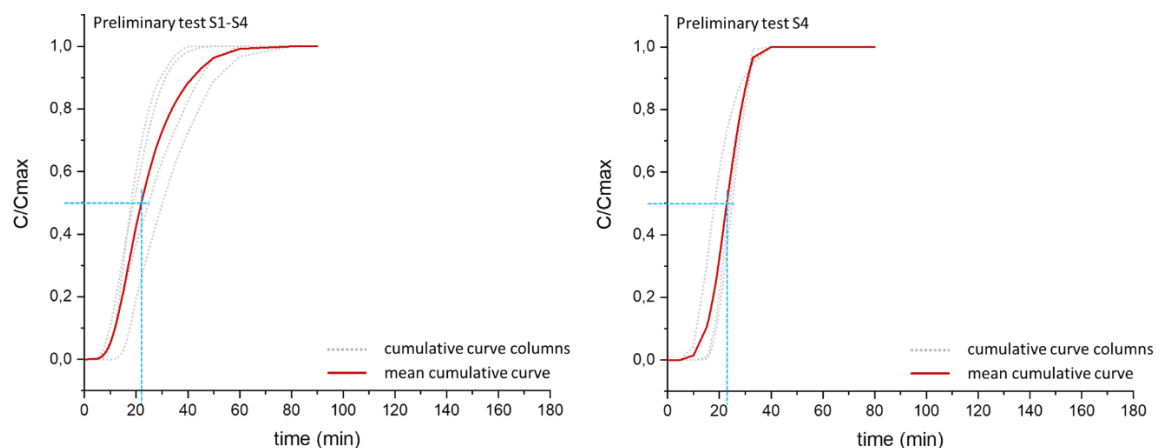



Figure S1.5: On the left side, the cumulative curves of the chloride tracer for the columns from the preliminary test and the corresponding averaged cumulative curve are displayed. The right figure shows the multiple measurements of the chloride tracer for column 4 and its averaged cumulative curve. The cumulative curves indicate the time required for the water front to pass through the entire system at C/Cmax = 0.5.

Reaction time of BrCl

According to US EPA method 1631, a reaction time of 24 hours is recommended for complete extraction of Hg using BrCl for organic-rich samples. To obtain a better overview of the concentration changes during the experiment, a lower reaction time of 1 hour was tested. To detect any concentration differences resulting from the shortened BrCl reaction time in the liquid phase, samples were examined after 1 hour and 24 hours during the pre-experiment. For this purpose, the entire sample amount was divided into two subsamples, and each was treated with BrCl and measured 1 hour and 24 hours after BrCl additions (samples were refrigerated at 4 °C until analysis). It is evident that there is no difference between the samples with a BrCl reaction time of 1 hour and 24 hours (Table S1.2). The recovery rate of the samples with 1 hour reaction time was 101.5 ± 7.2% compared to the samples that reacted with BrCl for 24 hours. Thus, the reaction time could be shortened to 1 hour.

Table S1.2 Summary of mercury concentrations in the liquid phase after reaction times of 1 h and 24 h with BrCl. Several time intervals are depicted during which samples were taken for analysis. RPD represents the relative percent difference between samples with a reaction time of 24 h and samples with a reaction time of 1 h.

Sampling period /min after start of the experiment	Column	concentration [µg L^{-1}]		RPD [%]
		Reaction time [24 h]	Reaction time [1 h]	
200-220	S1	0.7	0.7	2.4%
	S2	88.0	85.0	3.4%
	S3	1.3	1.3	-1.1%
	S4	2.7	2.4	11.9%
220-280	S1	1.2	1.2	-3.0%
	S2	95.5	87.1	8.7%
	S3	1.8	1.7	9.0%
	S4	3.6	3.4	4.9%
1360-1420	S1	30.8	31.1	-0.8%
	S2	199.9	214.0	-7.1%
	S3	45.2	47.8	-5.8%
	S4	45.1	44.3	1.8%
1570-1610	S1	29.5	32.1	-8.8%
	S2	221.2	218.8	1.1%
	S3	55.7	60.6	-8.7%
	S4	47.6	52.6	-10.6%
1570-1610 filtered	S1	23.2	23.8	-2.6%
	S2	156.4	174.2	-11.3%
	S3	40.7	46.4	-14.1%
	S4	35.5	35.0	1.3%
			Recovery rate 1 h	101.5%
			S.D.	7.2%
			Number of samples	20

Results of the preliminary test

Concentration curve in the liquid phase

The average concentration trend was depicted as a function of the volume of the $HgCl_2$-spiked solution passing through the columns (see Figure S1.6). A total of 15.5 ± 0.27 L passed through each column, and the displayed points were averaged from the four columns. The whiskers in the x and y directions represent the standard deviations of the volume and concentration, respectively. The pre-experiment was divided into three sections, where the initial solution had different concentrations (1.7 ± 0.2 mg L^{-1}, 7.5 ± 0.8 mg L^{-1}, and 49.3 ± 4.4 mg L^{-1}). At this stock solution concentration, the increase in the liquid phase THg concentration was very little after 10 days. Hence it was deemed too low, and the stock solution increased. At 7.5 ± 0.8 mg L^{-1}, the concentration in the liquid phase reached 32.8% of the maximum possible concentration of 7.5 ± 0.8 mg L^{-1} of the initial solution after four more days, despite 9 L of 1.7 ± 0.2 mg L^{-1} already being added to the columns. Thus, the stock solution concentration was increased again to 49.3 ± 4.4 mg L^{-1}. Within two days (≈ 2 L of solution), the concentration in the eluate liquid phase rose to 26.73 ± 0.62 mg L^{-1}. Additionally, at the beginning of the newly introduced concentration, a linear increase in the concentration in the liquid phase was observed. At a volume of 14.5 ± 0.25 L, the concentration trend turned nonlinear. The experiment was terminated at 15.5 L. The pre-experiment served solely for assessing the starting concentrations and optimizing the methods.

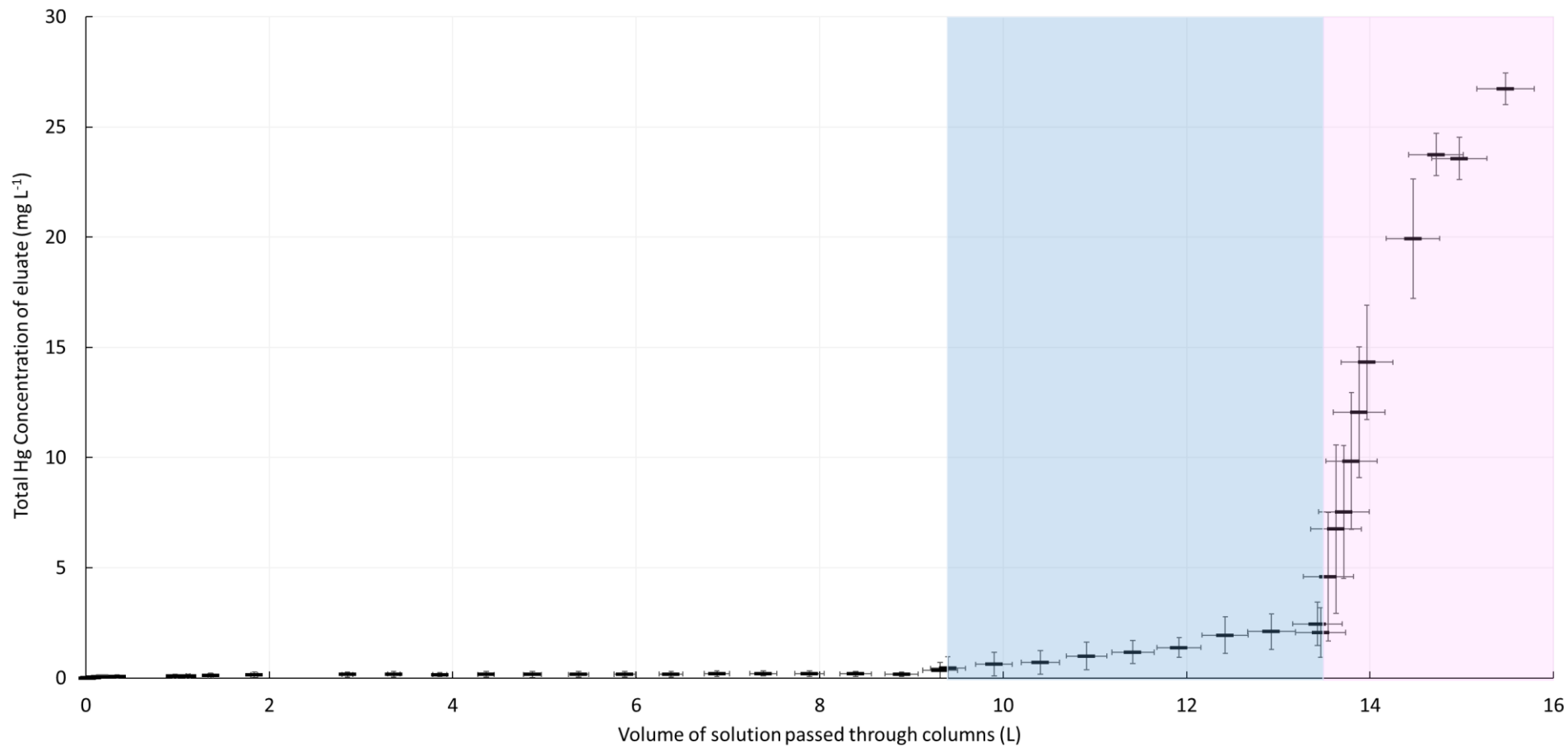



Figure S1.6 : Concentration curve of the preliminary test. Three different initial solutions were tested. In the first section (white), a solution with 1.7 ± 0.2 mg L^{-1} was used, in the second section (blue) 7.5 ± 0.8 mg L^{-1} and in the last section (violet) 49.3 ± 4.4 mg L^{-1}.

S2. Properties of solid- and liquid-phase materials used in column experiments.

Table S2.1 Results of the particle size distribution of the sieved aquifer material (< 2 mm). The grain size was determined by pipette method according to DIN EN ISO 11277 (2002).

Grain Size	Grain size range [μm]		percentage [%]
	from	until	
Coarse sand	2000	630	34.04
Middle sand	630	200	22.79
Fine sand	200	63	6.44
Coarse silt	63	20	16.03
Middle silt	20	6.3	3.87
Fine silt	6.3	2	3.33
Clay	2	0	13.50

Table S2.2 Results of the ICP-OES analysis for the tap water that was also used to mix the $HgCl_2$ solution. The eluate shown here describes the tap water used to rinse the columns. After a rinse of 24 h, this eluate was analyzed as well as at a rinse time of 48 h. These results lead to us using a minimum equilibration time of tapwater within the columns of 7 days for the actual experiments.

Element	Unit	Tap Water	Eluate after 24 h rinse	Eluate after 48 h rinse
DOC	mg L^{-1}	2.29	3.25	2.68
Ca 317.933	mg L^{-1}	34.82	61.52	154.19
Ca 315.887	mg L^{-1}	34.76	61.55	154.28
Fe 238.204	μg L^{-1}	0.52	2.91	14.03
Fe 259.940	μg L^{-1}	0.21	2.54	15.38
K 766.491	mg L^{-1}	1.18	1.92	3.20
K 769.897	mg L^{-1}	1.32	2.02	3.04
Mg 280.270	mg L^{-1}	3.98	3.23	6.66
Mg 285.213	mg L^{-1}	3.92	3.18	6.27
Mn 257.610	μg L^{-1}	3.91	177.24	16.83
Mn 259.372	μg L^{-1}	3.71	175.99	16.60
Na 589.592	mg L^{-1}	16.23	19.76	44.15
Na 588.995	mg L^{-1}	14.98	18.61	41.85
Si 251.611	mg L^{-1}	3.06	5.61	4.48
Si 288.158	mg L^{-1}	3.08	5.64	4.52
Sr 407.771	μg L^{-1}	132.96	128.76	326.80
Sr 421.552	μg L^{-1}	131.51	126.07	329.92
Zn 202.548	μg L^{-1}	112.09	3.21	5.03
Zn 206.200	μg L^{-1}	117.65	18.06	7.87
Zn 213.857	μg L^{-1}	106.33	6.53	8.05

Table S2.3 Results of the study of the following parameters: pH, electrical conductivity, oxygen content and concentration, and redox potential for the tap water used to prepare the $HgCl_2$ solution, as well as the $HgCl_2$ solutions used to contaminate the columns and the eluates collected after the columns.

	pH	Electrical Conductivity	Oxygen	Oxygen conc.	Redox potential
	[-]	[µS]	[%]	[mg L^{-1}]	[mV]
$HgCl_2$-Solution [46.1 ± 1.1 mg L^{-1}]	7.7	218.4	97.7	9.42	249.4
$HgCl_2$-Solution [143.72 ± 6.17 mg L^{-1}]	7.8	342.3	99.8	9.86	324
Tap Water	7.9	421	95.4	9.09	309
Eluate [46.1 ± 1.1 mg L^{-1}]	7.9	337.1	98.9	9.78	195
Eluate [143.72 ± 6.17 mg L^{-1}]	8.1	327.6	99.9	9.89	193

Table S2.4: Initial data of the columns. Listed is the filled dry mass of the sieved aquifer material, the volume as well as the resulting bulk density divided into EXP1 (46.1 ± 1.1 mg L^{-1}) and EXP2 (143.72 ± 6.17 mg L^{-1}).

	EXP1 (46.1 ± 1.1 mg L^{-1})			EXP2 (143.72 ± 6.17 mg L^{-1})		
Column	Dry mass [g]	Volume [ml]	Bulk density [g/cm³]	Dry mass [g]	Volume [ml]	Bulk density [g/cm³]
C1.1/C2.1	70.10	49.5	1.43	70.04	49.0	1.42
C1.2/C2.2	70.06	50.0	1.40	70.05	48.5	1.44
C1.3/C2.3	70.18	50.5	1.40	70.09	49.0	1.43
C1.4/C2.4	70.10	50.0	1.40	70.01	49.0	1.43
C1.5/C2.5	70.05	49.0	1.43	70.02	49.0	1.43
C1.6/C2.6	70.07	49.5	1.42	70.07	49.5	1.42
C1.7/C2.7	70.04	49.5	1.42	70.04	49.5	1.42
C1.8/C2.8	70.08	49.5	1.42	70.05	49.0	1.43

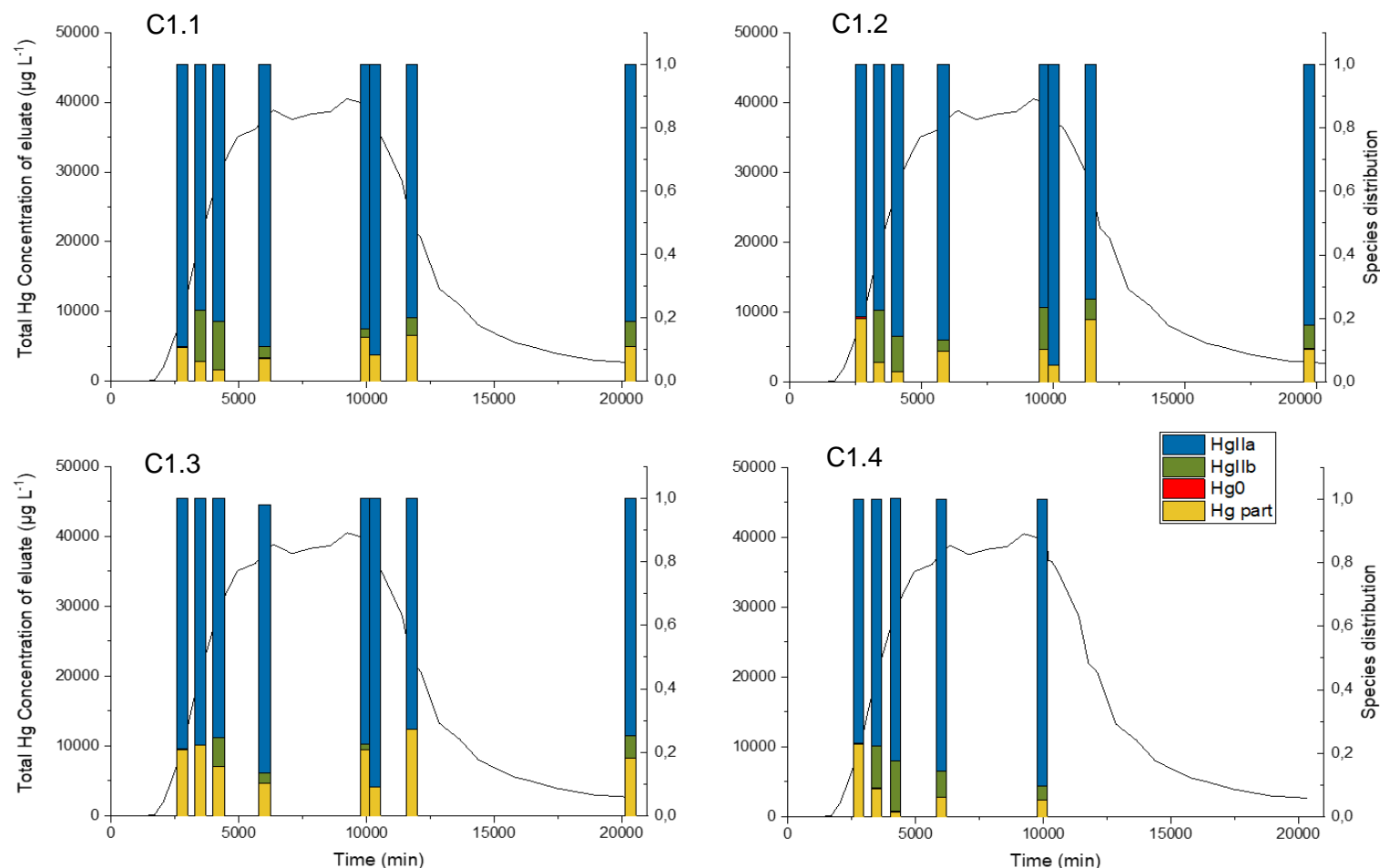
Table S1.5: Summary of the volumetric flow of the peristaltic pump for EXP1 and EXP2 measured via volume collections over time before and after each experiment.

Column	EXP1 (46.1 ± 1.1 mg L^{-1})		EXP2 (143.72 ± 6.17 mg L^{-1})	
	Flowrate		Flowrate	
	Mean value [ml min^{-1}]	Standard deviation [ml min^{-1}]	Mean value [ml min^{-1}]	Standard deviation [ml min^{-1}]
C1.1/C2.1	0.64	0.00	0.60	0.01
C1.2/C2.2	0.63	0.01	0.61	0.01
C1.3/C2.3	0.60	0.00	0.58	0.00
C1.4/C2.4	0.62	0.00	0.60	0.00
C1.5/C2.5	0.66	0.01	0.63	0.03
C1.6/C2.6	0.63	0.01	0.63	0.01
C1.7/C2.7	0.61	0.01	0.64	0.00
C1.8/C2.8	0.63	0.07	0.66	0.00

S3. Sorbed quantities of Hg in column experiments.

Table S3.1: Summary of the quantities of mercury added and sorbed as well as the quantities of mercury that could be desorbed again.

	Added Hg amount	sorbed Hg amount		Desorbed Hg amount	
	[mg]	*[mg]*	*[%]*	*[mg]*	*[%]*
EXP1 (46.1 ± 1.1 mg L⁻¹)					
C1.1	294.2	132.7	45.1	75.3	56.7
C1.2	294.1	138.3	47.0	76.0	55.0
C1.3	275.7	131.6	47.7	72.1	54.8
C1.4	284.9	131.4	46.1	-	-
C1.5	303.3	134.0	44.2	-	-
C1.6	289.5	130.8	45.2	-	-
C1.7	97.9	92.5	94.5	-	-
C1.8	101.1	91.4	90.4	-	-
EXP2 (143.72 ± 6.17 mg L⁻¹)					
C2.1	801.1	193.5	24.1	98.4	50.9
C2.2	814.5	188.6	23.2	97.2	51.6
C2.3	774.4	202.8	26.2	98.4	48.5
C2.4	86.2	72.2	83.8	-	-
C2.5	90.5	80.1	88.5	-	-
C2.6	841.2	194.0	23.1	-	-
C2.7	854.5	199.8	23.4	-	-
C2.8	881.2	197.7	22.4	-	-

S4. Liquid-phase speciation analyses.

FigureS4.1: Representation of the Hg speciation in the liquid phase of EXP1 with columns C1.1 to C1.4. Each column is shown separately. The averaged concentration curve of the entire experiment is shown in the background. The speciation at ¼, ½, and ¾ breakthrough as well as at the beginning and end of the sorption maximum, at the beginning and at the end of the desorption was investigated. Columns C1.1 to C1.3 reached the end of desorption. C1.4 to C1.6 were separated from the system after reaching the specified sorption maximum, while C1.7 and C1.8 were already separated from the system at half of the sorption curve. "Hg part" = Hg associated with particulates, referred to as Hg(II)P in the main manuscript.

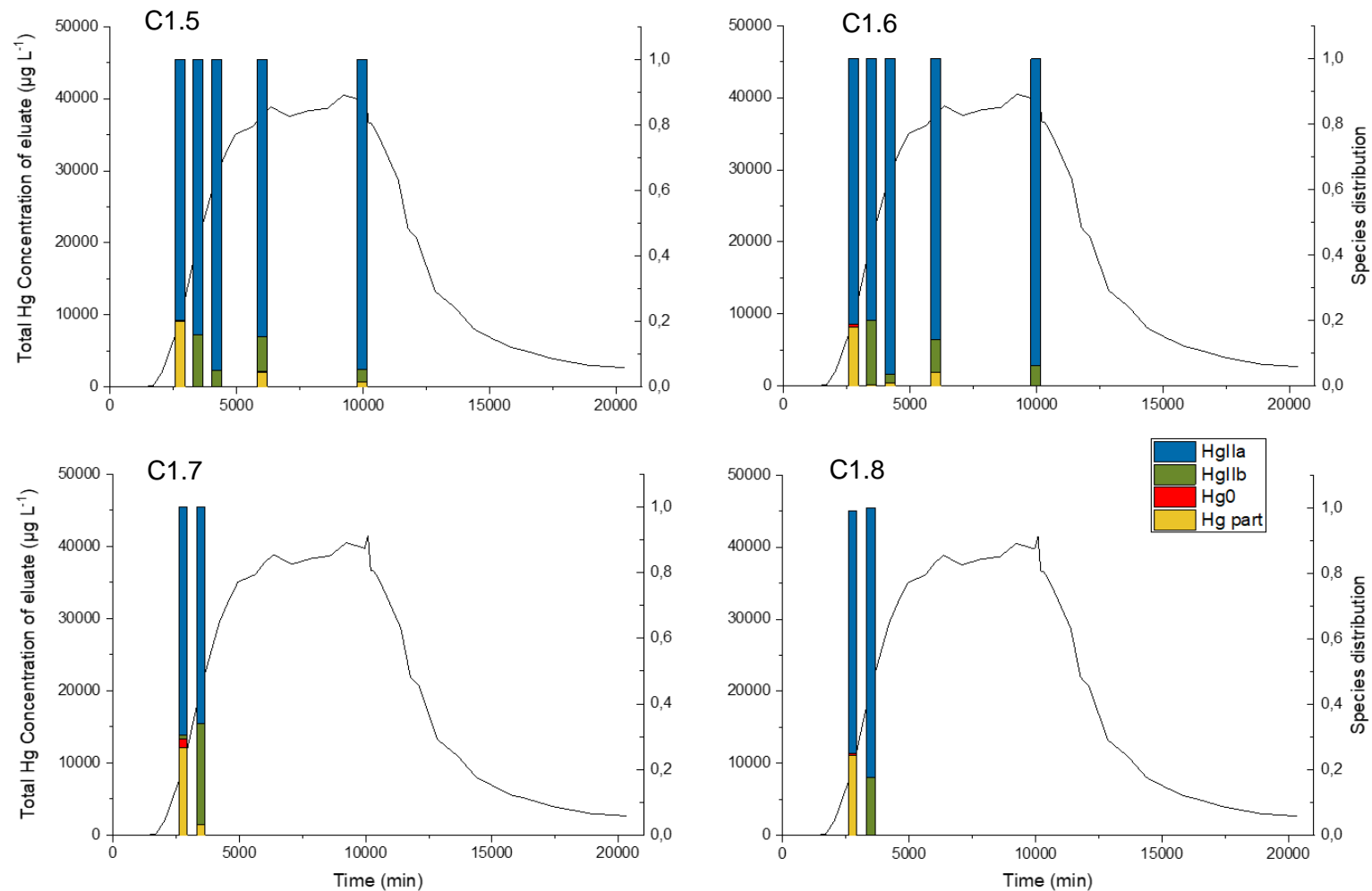



Figure S4.2: Plot of Hg speciation in the liquid phase of EXP1 (46.1 ± 1.1 mg L^{-1}) with columns C1.5 to C1.8. Each column is shown separately. The averaged concentration curve of the entire experiment is shown in the background. The speciation at ¼, ½, and ¾ breakthrough as well as at the beginning and end of the sorption maximum, at the beginning and at the end of the desorption was investigated. Columns C1.1 to C1.3 reached the end of desorption. C1.4 to C1.6 were separated from the system after reaching the specified sorption maximum, while C1.7 and C1.8 were already separated from the system at half of the sorption curve. "Hg part" = Hg associated with particulates, referred to as Hg(II)P in the main manuscript.

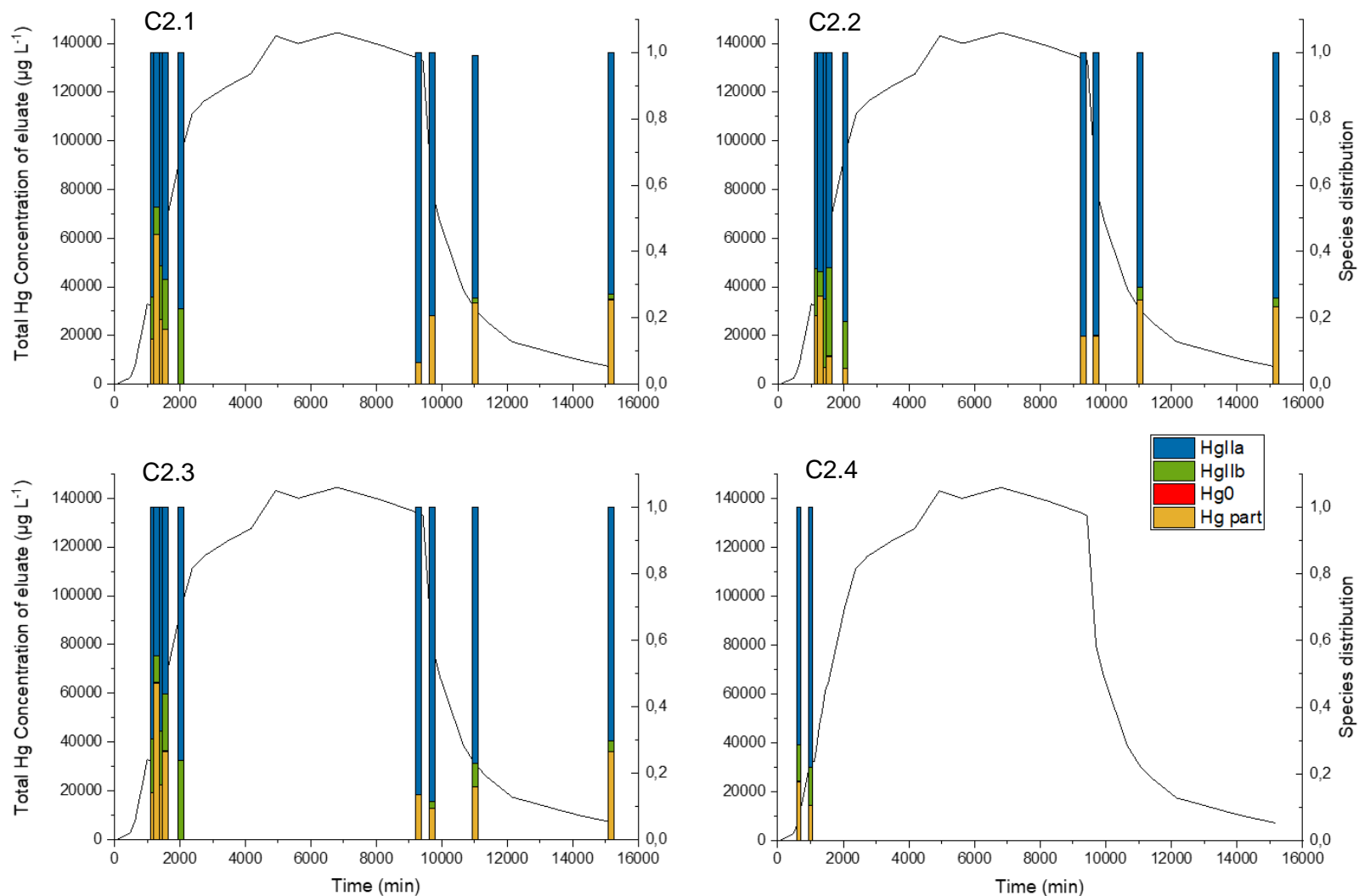



Figure S1.3: Plot of Hg speciation of columns C2.1 to C2.4 in the liquid phase of EXP2 (143.72 ± 6.17 mg L^{-1}). The columns show the species distribution, while the mean concentration curve is shown in the background. C2.1 to C2.3 underwent the sorption and desorption process. Shown here are ¼, ½, ¾ breakthrough, the sorption maximum, ¼ of desorption, ½ of desorption, and the end of the experiment. C2.4 was separated from the system halfway through the sorption process. "Hg part" = Hg associated with particulates, referred to as Hg(II)P in the main manuscript.

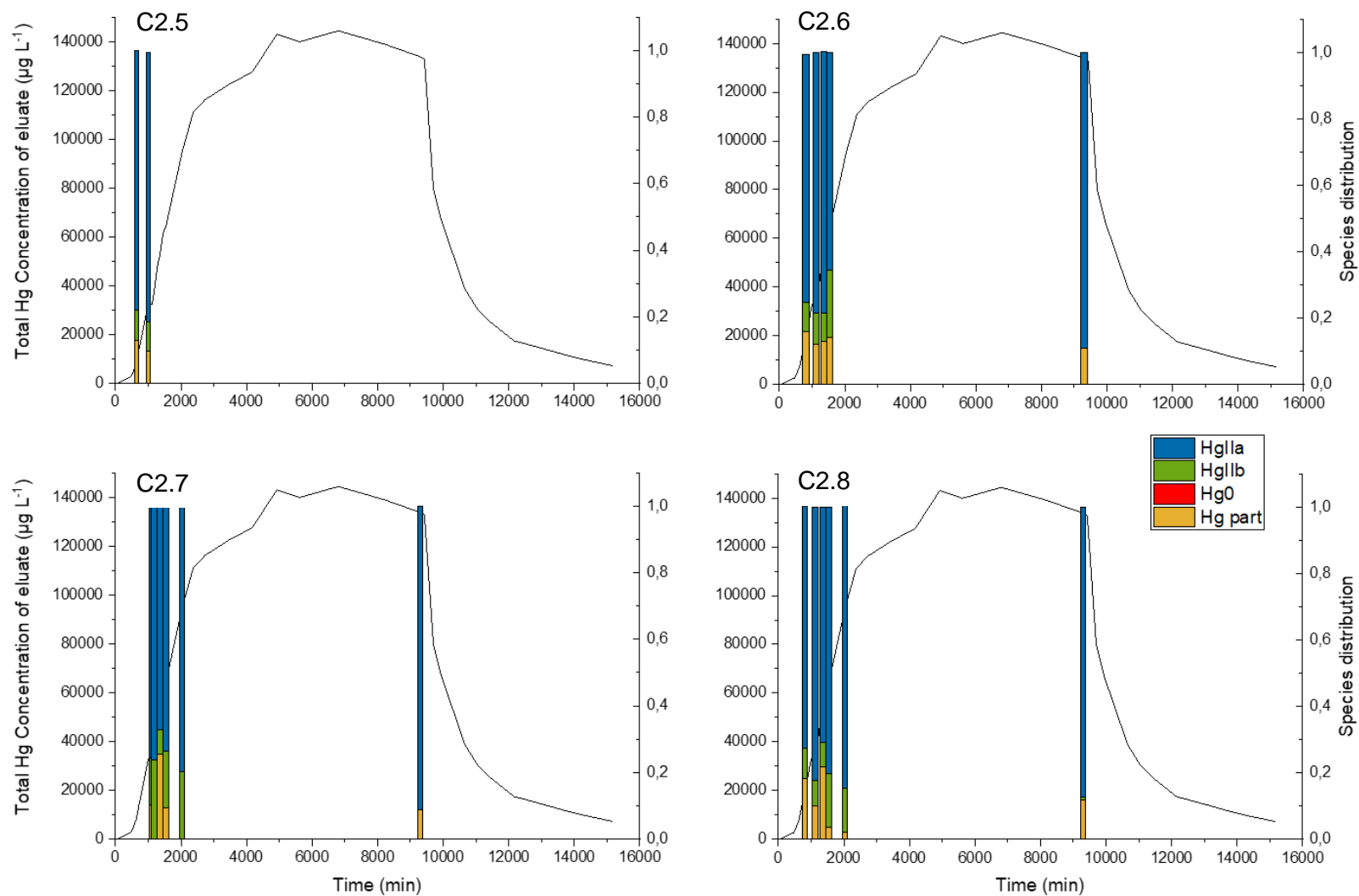



Figure S4.4: Shown is the distribution of Hg species of EXP2 (143.72 ± 6.17 mg L^{-1}) in columns C2.5 to C2.8. C2.5 was separated from the system at half sorption, while C2.6 to C2.8 extend to the sorption maximum. "Hg part" = Hg associated with particulates, referred to as Hg(II)P in the main manuscript.

Table S4.1 Summary of percent species distribution in EXP1 (46.1 ± 1.1 mg L^{-1}). Stock solution was measured (purged) for Hg(0) and the mean fraction of Hg(0) was 0.011 ± 0.003 %.

	Sorption					Desorption		
Experiment Duration [min]	2770	3480	4205	6005	9965	10325	11770	20350
Mean THg conc. in eluate [µg L^{-1}]	9125.8	20380.8	29453.2	37809.2	39755.8	36577.3	21943.5	2667.5
Standard Deviation [µg L^{-1}]	4086.0	2038.0	2124.1	1485.4	685.9	476.9	886.7	183.9
C1.1								
Hg(II)P	10.6%	-	3.5%	7.2%	13.9%	8.2%	14.3%	10.8%
Hg(0)	0.4%	-	0.0%	0.1%	0.0%	0.0%	0.1%	0.1%
Hg(II)$_b$	0.0%	-	15.2%	3.6%	2.6%	0.0%	5.6%	8.0%
Hg(II)$_a$	89.0%	-	81.2%	89.1%	83.6%	91.7%	80.0%	81.1%
C1.2								
Hg(II)P	19.8%	6.1%	3.3%	9.6%	10.3%	5.3%	19.7%	10.4%
Hg(0)	0.6%	0.1%	0.0%	0.1%	0.0%	0.0%	0.0%	0.2%
Hg(II)$_b$	0.0%	16.3%	11.1%	3.4%	13.1%	0.0%	6.2%	7.2%
Hg(II)$_a$	79.6%	77.5%	85.5%	86.9%	76.5%	94.7%	74.0%	82.3%
C1.3								
Hg(II)P	20.9%	22.2%	15.6%	10.1%	20.8%	9.1%	27.3%	18.0%
Hg(0)	0.2%	0.1%	0.1%	0.1%	0.0%	0.0%	0.0%	0.1%
Hg(II)$_b$	0.0%	0.0%	9.1%	3.3%	1.8%	0.0%	0.0%	7.1%
Hg(II)$_a$	78.9%	77.7%	75.3%	84.5%	77.3%	90.9%	72.6%	74.8%
C1.4								
Hg(II)P	23.0%	8.9%	1.6%	6.1%	5.2%	-	-	-
Hg(0)	0.3%	0.1%	0.1%	0.1%	0.0%	-	-	-
Hg(II)$_b$	0.0%	13.4%	16.0%	8.3%	4.6%	-	-	-
Hg(II)$_a$	76.8%	77.6%	82.7%	85.5%	90.3%	-	-	-
C1.5								
Hg(II)P	19.9%	0.0%	0.0%	4.5%	1.5%	-	-	-
Hg(0)	0.3%	0.1%	0.1%	0.0%	0.0%	-	-	-
Hg(II)$_b$	0.0%	15.7%	4.9%	10.6%	3.7%	-	-	-
Hg(II)$_a$	79.8%	84.2%	95.0%	84.8%	94.8%	-	-	-
C1.6								
Hg(II)P	18.0%	0.2%	0.8%	4.1%	0.0%	-	-	-
Hg(0)	0.7%	0.1%	0.0%	0.0%	0.0%	-	-	-
Hg(II)$_b$	0.0%	19.6%	2.6%	10.0%	6.2%	-	-	-
Hg(II)$_a$	81.3%	80.1%	96.6%	85.9%	93.6%	-	-	-
C1.7								
Hg(II)P	26.5%	3.1%	-	-	-	-	-	-
Hg(0)	2.8%	0.1%	-	-	-	-	-	-
Hg(II)$_b$	1.2%	30.9%	-	-	-	-	-	-
Hg(II)$_a$	69.5%	65.9%	-	-	-	-	-	-
C1.8								
Hg(II)P	24.5%	0.0%	-	-	-	-	-	-
Hg(0)	0.4%	0.1%	-	-	-	-	-	-
Hg(II)$_b$	0.0%	17.4%	-	-	-	-	-	-
Hg(II)$_a$	74.1%	82.4%	-	-	-	-	-	-

Mean	25% Breakthrough	50 % Breakthrough	75 % Breakthrough	Begin equilibrium	End Sorption	Begin Desorption	50 % Desorption	End Desorption
Hg(II)P	20.4%	5.8%	4.1%	6.9%	8.6%	7.5%	20.4%	13.1%
Hg(0)	0.7%	0.1%	0.0%	0.1%	0.0%	0.0%	0.0%	0.1%
Hg(II)$_b$	0.1%	16.2%	9.8%	6.5%	5.3%	0.0%	3.9%	7.4%
Hg(II)$_a$	78.6%	77.9%	86.0%	86.1%	86.0%	92.4%	75.6%	79.4%
Standard Deviation								
Hg(II)P	4.8%	8.0%	5.8%	2.3%	8.0%	2.0%	6.5%	4.3%
Hg(0)	0.8%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Hg(II)$_b$	0.4%	9.1%	5.4%	3.2%	4.1%	0.0%	3.4%	0.5%
Hg(II)$_a$	5.6%	5.9%	8.3%	1.5%	8.1%	2.0%	3.9%	4.1%

Table S4.2: Summary of species concentrations in EXP1 (46.1 ± 1.1 mg L^{-1}). Values in red are negative concentrations caused by subtraction of two measured values. These are considered as zero and highlight why we consider these qualitative analyses. Stock solution was measured (purged) for Hg(0) and the mean concentration was 5.1 ± 1.3 µg L^{-1} (n = 3).

	Sorption					Desorption		
Experiment Duration [min]	*2770*	*3480*	*4205*	*6005*	*9965*	*10325*	*11770*	*20350*
Mean THg conc. in eluate [µg L^{-1}]	*9125.8*	*20380.8*	*29453.2*	*37809.2*	*39755.8*	*36577.3*	*21943.5*	*2667.5*
Standard Deviation [µg L^{-1}]	*4086.0*	*2038.0*	*2124.1*	*1485.4*	*685.9*	*476.9*	*886.7*	*183.9*
C1.1								
Hg$_{(part)}$	564.2	-	1264.0	2757.7	5645.8	3058.0	2982.3	271.1
Hg(0)	29.8	-	15.8	24.3	13.0	10.3	10.6	2.5
Hg(II)$_b$	-1109.0	-	4973.6	1390.7	1043.5	-2438.9	1169.4	200.4
Hg(II)$_a$	7356.1	-	27233.1	34219.7	34052.1	36569.8	16657.2	2036.6
C1.2								
Hg$_{(part)}$	1632.7	1228.5	990.2	3761.8	4144.5	1928.8	4529.2	265.9
Hg(0)	50.3	16.3	0.3	23.7	14.2	11.2	10.5	4.0
Hg(II)$_b$	-732.4	3290.8	3294.1	1347.3	5271.7	-807.5	1429.9	185.9
Hg(II)$_a$	7292.6	15645.7	25309.3	34015.2	30708.7	35359.5	17017.5	2112.5
C1.3								
Hg$_{(part)}$	2846.9	4297.6	4172.8	3523.8	8249.9	3162.3	6017.0	527.3
Hg(0)	31.1	16.7	17.9	18.6	10.7	10.1	9.1	3.4
Hg(II)$_b$	-2432.4	-281.9	2431.0	1149.7	718.7	-2285.3	-271.7	207.3
Hg(II)$_a$	13276.1	15292.7	20144.0	29414.8	30618.6	35222.6	16269.4	2187.7
C1.4								
Hg$_{(part)}$	3507.0	1933.2	338.6	2251.3	2064.8	-	-	-
Hg(0)	39.3	24.2	19.0	35.5	13.8	-	-	-
Hg(II)$_b$	-2479.3	2907.8	4288.5	3087.0	1819.7	-	-	-
Hg(II)$_a$	14208.2	16844.8	22201.0	31764.1	36086.3	-	-	-
C1.5								
Hg$_{(part)}$	2561.5	-625.0	-1323.8	1761.9	580.8	-	-	-
Hg(0)	36.2	25.5	15.4	19.3	9.3	-	-	-
Hg(II)$_b$	-1117.8	3503.2	1471.7	4128.8	1458.9	-	-	-
Hg(II)$_a$	11362.4	19475.8	29678.7	32902.5	37505.5	-	-	-
C1.6								
Hg$_{(part)}$	964.7	43.0	248.6	1594.5	-323.8	-	-	-
Hg(0)	39.8	16.1	12.7	16.3	7.5	-	-	-
Hg(II)$_b$	-301.1	4128.5	805.8	3852.9	2386.6	-	-	-
Hg(II)$_a$	4664.8	16852.1	29891.6	33181.4	36819.1	-	-	-
C1.7								
Hg$_{(part)}$	736.8	503.2	-	-	-	-	-	-
Hg(0)	76.7	21.3	-	-	-	-	-	-
Hg(II)$_b$	-43.0	5007.1	-	-	-	-	-	-
Hg(II)$_a$	2005.4	10671.6	-	-	-	-	-	-
C1.8								
Hg$_{(part)}$	1966.4	-0.8	-	-	-	-	-	-
Hg(0)	30.3	23.6	-	-	-	-	-	-
Hg(II)$_b$	-424.5	4015.9	-	-	-	-	-	-
Hg(II)$_a$	6457.5	18986.3	-	-	-	-	-	-

Mean	25% Breakthrough	50 % Breakthrough	75 % Breakthrough	Begin equilibrium	End Sorption	Begin Desorption	50 % Desorption	End Desorption
Hg$_{(part)}$	1847.5	1054.2	948.4	2608.5	3393.7	2716.4	4509.5	354.8
Hg(0)	41.7	20.5	13.5	23.0	11.4	10.6	10.1	3.3
Hg(II)$_b$	-1079.9	3224.5	2877.5	2492.7	2116.5	-1843.9	775.9	197.9
Hg(II)$_a$	8327.9	16252.7	25742.9	32583.0	34298.4	35717.3	16648.1	2112.3
Standard Deviation								
Hg$_{(part)}$	1067.9	1662.4	1817.8	822.9	3247.0	684.0	1517.4	149.4
Hg(0)	15.7	4.1	6.8	6.3	2.7	0.6	0.8	0.8
Hg(II)$_b$	927.5	1688.1	1614.0	1239.0	1652.5	900.8	916.5	10.9
Hg(II)$_a$	4262.4	2915.8	3975.0	1627.8	3043.8	741.4	374.1	75.5

Table S4.3 Summary of percent species distribution in EXP2 (143.72 ± 6.17 mg L^{-1}). Stock solution was measured (purged) for Hg(0) and the mean fraction of Hg(0) was 0.0051 ± 0.008 %.

	Sorption											Desorption		
Experiment Duration [min]	640	815	1000	1120	1180	1270	1360	1450	1540	2035	9290	9700	11020	15170
Mean THg conc. in eluate [µg L^{-1}]	8381.1	20279.2	32932.3	32135.3	37621.6	47215.2	52939.8	61529.6	64319.0	94838.0	133889.9	79981.8	30877.0	7176.2
Standard Deviation [µg L^{-1}]	10551.8	17215.3	19884.0	18026.7	16249.2	15531.0	16775.5	14506.1	12549.8	6224.5	1388.9	1229.8	1124.1	355.5
C2.1														
Hg(II)P	-	-	-	-	13.7%	45.1%	-	19.5%	16.6%	0.0%	6.5%	20.5%	24.4%	25.5%
Hg(0)	-	-	-	-	0.0%	0.1%	-	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%	0.1%
Hg(II)$_b$	-	-	-	-	12.4%	8.1%	-	16.2%	14.9%	22.7%	0.0%	0.0%	1.5%	1.6%
Hg(II)$_a$	-	-	-	-	73.8%	46.7%	-	64.3%	68.4%	77.2%	93.5%	79.4%	73.2%	72.8%
C2.2														
Hg(II)P	-	-	-	-	20.8%	26.5%	-	5.0%	8.4%	4.9%	14.6%	14.6%	25.5%	23.3%
Hg(0)	-	-	-	-	0.0%	0.1%	-	0.0%	0.1%	0.0%	0.0%	0.1%	0.0%	0.1%
Hg(II)$_b$	-	-	-	-	14.1%	7.3%	-	20.8%	26.7%	14.0%	0.0%	0.0%	3.6%	2.6%
Hg(II)$_a$	-	-	-	-	65.1%	66.0%	-	74.2%	64.7%	81.1%	85.4%	85.3%	70.9%	74.1%
C2.3														
Hg(II)P	-	-	-	-	14.0%	47.2%	-	16.5%	26.6%	0.0%	13.4%	9.5%	16.0%	26.4%
Hg(0)	-	-	-	-	0.1%	0.1%	-	0.1%	0.1%	0.1%	0.0%	0.0%	0.0%	0.1%
Hg(II)$_b$	-	-	-	-	16.3%	8.2%	-	16.1%	17.2%	23.7%	0.0%	1.9%	7.0%	3.2%
Hg(II)$_a$	-	-	-	-	69.7%	44.6%	-	67.3%	56.1%	76.2%	86.6%	88.6%	77.0%	70.4%
C2.4														
Hg(II)P	17.7%	-	10.7%	-	-	-	-	-	-	-	-	-	-	-
Hg(0)	0.1%	-	0.0%	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_b$	11.0%	-	11.3%	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_a$	71.2%	-	78.0%	-	-	-	-	-	-	-	-	-	-	-
C2.5														
Hg(II)P	12.8%	-	9.5%	-	-	-	-	-	-	-	-	-	-	-
Hg(0)	0.2%	-	0.0%	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_b$	9.1%	-	8.9%	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_a$	77.9%	-	80.9%	-	-	-	-	-	-	-	-	-	-	-
C2.6														
Hg(II)P	-	15.9%	-	12.1%	-	-	13.0%	-	14.0%	-	10.8%	-	-	-
Hg(0)	-	0.0%	-	0.1%	-	-	0.1%	-	0.1%	-	0.0%	-	-	-
Hg(II)$_b$	-	8.7%	-	9.2%	-	-	8.3%	-	20.3%	-	0.0%	-	-	-
Hg(II)$_a$	-	74.7%	-	78.6%	-	-	78.9%	-	65.6%	-	89.1%	-	-	-
C2.7														
Hg(II)P	-	-	-	10.3%	0.0%	-	25.6%	-	9.2%	0.0%	8.8%	-	-	-
Hg(0)	-	-	-	0.0%	0.0%	-	0.0%	-	0.0%	0.0%	0.0%	-	-	-
Hg(II)$_b$	-	-	-	14.0%	23.6%	-	7.3%	-	17.0%	20.3%	0.0%	-	-	-
Hg(II)$_a$	-	-	-	75.9%	76.4%	-	67.1%	-	73.7%	79.7%	91.2%	-	-	-
C2.8														
Hg(II)P	-	18.3%	-	9.9%	-	-	21.6%	-	3.5%	2.0%	11.9%	-	-	-
Hg(0)	-	0.0%	-	0.0%	-	-	0.0%	-	0.0%	0.0%	0.0%	-	-	-
Hg(II)$_b$	-	8.9%	-	7.7%	-	-	7.6%	-	16.1%	13.3%	0.6%	-	-	-
Hg(II)$_a$	-	73.1%	-	82.4%	-	-	70.8%	-	80.3%	85.4%	87.5%	-	-	-

Mean					25% Breakthrough				50 % Breakthrough	75 % Breakthrough	End Sorption/ Begin Desorption	50 % Desorption	75 % Desorption	Ende Desorption
Hg(II)P	-	-	-	-	20.0%	-	-	-	10.1%	2.3%	11.0%	14.9%	22.0%	25.1%
Hg(0)	-	-	-	-	0.1%	-	-	-	0.0%	0.0%	0.0%	0.0%	0.0%	0.1%
Hg(II)$_b$	-	-	-	-	12.0%	-	-	-	18.9%	16.7%	0.1%	0.6%	4.0%	2.5%
Hg(II)$_a$	-	-	-	-	67.9%	-	-	-	70.9%	81.2%	88.9%	84.4%	73.7%	72.4%
Standard Deviation														
Hg(II)P	-	-	-	-	13.6%	-	-	-	8.9%	2.4%	3.0%	5.5%	5.2%	1.6%
Hg(0)	-	-	-	-	0.0%	-	-	-	0.0%	0.0%	0.0%	0.0%	0.0%	0.0%
Hg(II)$_b$	-	-	-	-	5.9%	-	-	-	6.8%	5.3%	0.3%	1.1%	2.8%	0.8%
Hg(II)$_a$	-	-	-	-	10.1%	-	-	-	6.0%	4.1%	3.0%	4.6%	3.1%	1.9%

Table S4.4: Summary of species concentrations in EXP1 (143.72 ± 6.17 mg L^{-1}). Values in red are negative concentrations caused by subtraction of two measured values. These are considered as zero and highlight why we consider these qualitative analyses. Stock solution was measured (purged) for Hg(0) and the mean concentration was 7.3 ± 1.1 µg L^{-1} (n = 3).

	Sorption											Desorption		
Experiment Duration [min]	640	815	1000	1120	1180	1270	1360	1450	1540	2035	9290	9700	11020	15170
Mean THg conc. in eluate [µg L^{-1}]	8381.1	20279.2	32932.3	32135.3	37621.6	47215.2	52939.8	61529.6	64319.0	94838.0	133889.9	79981.8	30877.0	7176.2
Standard Deviation [µg L^{-1}]	10551.8	17215.3	19884.0	18026.7	16249.2	15531.0	16775.5	14506.1	12549.8	6224.5	1388.9	1229.8	1124.1	355.5
C2.1														
Hg$_{(part)}$	-	-	-	-	4276.2	18185.3	-	12145.2	10175.9	-120.4	8646.2	16372.3	7691.3	1812.3
Hg(0)	-	-	-	-	5.0	23.3	-	25.5	21.8	19.3	24.2	21.3	8.0	7.4
Hg(II)$_b$	-	-	-	-	3872.2	3270.5	-	10091.3	9136.3	22484.3	-11913.4	-585.7	464.5	115.3
Hg(II)$_a$	-	-	-	-	23015.6	18823.2	-	40070.2	41918.1	76463.4	138402.6	63936.3	23028.3	5172.2
C2.2														
Hg$_{(part)}$	-	-	-	-	4348.1	11039.6	-	3163.8	5835.9	5025.8	19805.2	11895.6	7462.1	1576.9
Hg(0)	-	-	-	-	4.3	40.3	-	19.8	62.0	44.9	25.8	75.9	13.4	5.8
Hg(II)$_b$	-	-	-	-	2947.5	3053.2	-	13265.3	18519.3	14523.5	-5579.3	-596.3	1050.6	173.4
Hg(II)$_a$	-	-	-	-	13630.2	27491.6	-	47335.0	44823.3	83870.7	121821.9	70217.4	20776.4	5023.1
C2.3														
Hg$_{(part)}$	-	-	-	-	2631.6	11268.9	-	5721.0	10863.3	-2332.8	17824.4	7501.2	5081.3	2017.0
Hg(0)	-	-	-	-	10.2	26.3	-	17.5	35.0	43.6	22.3	14.5	13.3	5.4
Hg(II)$_b$	-	-	-	-	3054.9	1948.6	-	5576.1	7041.1	20558.0	-6508.7	1478.5	2219.5	242.1
Hg(II)$_a$	-	-	-	-	13091.8	10656.3	-	23297.9	22932.9	68403.5	121825.4	69614.2	24540.2	5377.3
C2.4														
Hg$_{(part)}$	5501.0	-	5856.2	-	-	-	-	-	-	-	-	-	-	-
Hg(0)	39.7	-	11.5	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_b$	3428.1	-	6201.7	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_a$	22146.4	-	42912.6	-	-	-	-	-	-	-	-	-	-	-
C2.5														
Hg$_{(part)}$	2446.9	-	5020.3	-	-	-	-	-	-	-	-	-	-	-
Hg(0)	33.9	-	6.4	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_b$	1741.6	-	4684.4	-	-	-	-	-	-	-	-	-	-	-
Hg(II)$_a$	14903.1	-	42539.7	-	-	-	-	-	-	-	-	-	-	-
C2.6														
Hg$_{(part)}$	-	4748.5	-	6391.4	-	-	9065.5	-	10324.2	-2302.3	14620.9	-	-	-
Hg(0)	-	14.8	-	31.0	-	-	33.3	-	55.6	50.2	31.5	-	-	-
Hg(II)$_b$	-	2594.9	-	4876.4	-	-	5760.9	-	14927.7	-19530.5	-6599.4	-	-	-
Hg(II)$_a$	-	22347.1	-	41527.8	-	-	54839.0	-	48206.2	116799.9	126886.1	-	-	-
C2.7														
Hg$_{(part)}$	-	-	-	3345.9	-641.2	-	13150.7	-	5582.6	-5987.7	11581.4	-	-	-
Hg(0)	-	-	-	8.1	6.9	-	13.9	-	21.8	26.1	25.2	-	-	-
Hg(II)$_b$	-	-	-	4550.1	8785.7	-	3767.1	-	10284.2	17696.7	-2932.2	-	-	-
Hg(II)$_a$	-	-	-	24662.9	29110.2	-	34466.9	-	44623.5	75505.6	122948.0	-	-	-
C2.8														
Hg$_{(part)}$	-	6513.3	-	5688.5	-	-	16951.9	-	2856.6	2023.9	15869.8	-	-	-
Hg(0)	-	8.2	-	10.9	-	-	13.5	-	17.8	17.9	28.0	-	-	-
Hg(II)$_b$	-	3168.0	-	4432.9	-	-	5922.5	-	12967.6	11220.5	866.0	-	-	-
Hg(II)$_a$	-	26040.7	-	47317.7	-	-	55443.2	-	64681.2	84475.1	116941.1	-	-	-

Mean					25% Breakthrough				50 % Breakthrough	75 % Breakthrough	End Sorption/ Begin Desorption	50 % Desorption	75 % Desorption	Ende Desorption
Hg$_{(part)}$	-	-	-	-	7295.3	-	-	-	5827.9	2309.8	14724.7	11923.0	6744.9	1802.1
Hg(0)	-	-	-	-	21.5	-	-	-	37.1	27.4	26.2	37.3	11.5	6.2
Hg(II)$_b$	-	-	-	-	4268.1	-	-	-	14460.1	16076.1	-5444.5	98.8	1244.9	177.0
Hg(II)$_a$	-	-	-	-	24179.6	-	-	-	55716.7	81603.1	124804.2	67922.6	22781.6	5190.9
Standard Deviation														
Hg$_{(part)}$	-	-	-	-	5893.4	-	-	-	8591.5	2585.0	4088.3	4435.6	1445.3	220.3
Hg(0)	-	-	-	-	13.8	-	-	-	19.6	15.2	3.2	33.7	3.1	1.0
Hg(II)$_b$	-	-	-	-	2210.1	-	-	-	5754.8	5790.2	4253.6	1194.8	893.5	63.5
Hg(II)$_a$	-	-	-	-	3552.1	-	-	-	13550.7	4461.4	7379.6	3465.4	1894.0	177.8

S5. Liquid-phase THg concentrations over time across all columns

Table S5.1: Summary of the measured THg concentrations for each column at the different times after the start of the sorption and desorption experiments and the corresponding volume of contaminated solution flowed through (EXP1, 46.1 ± 1.1 mg L^{-1}).

		C1.1		C1.2		C1.3		C1.4		C1.5		C1.6		C1.7		C1.8	
Time		Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate
[min]		[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]
70	Sorption	0.04	0.6	0.04	0.7	0.04	0.8	0.04	0.8	0.05	0.5	0.04	0.6	0.04	0.4	0.04	0.5
250		0.16	1.1	0.16	1.0	0.15	1.2	0.16	1.2	0.17	0.8	0.16	0.9	0.15	0.8	0.16	1.0
430		0.28	1.7	0.27	20.6	0.26	1.8	0.27	2.4	0.28	1.3	0.27	1.3	0.26	1.2	0.27	1.7
610		0.39	2.4	0.38	2.2	0.37	2.9	0.38	3.0	0.40	2.3	0.38	2.2	0.37	2.2	0.38	2.6
1330		0.85	7.5	0.84	7.8	0.80	130.3	0.82	14.3	0.88	8.8	0.84	7.4	0.81	7.0	0.84	7.7
1690		1.08	13.1	1.06	83.8	1.01	656.1	1.05	338.0	1.12	13.6	1.06	11.9	1.03	11.5	1.06	13.1
2050		1.31	361.7	1.29	614.5	1.23	2691.6	1.27	1543.6	1.35	2758.1	1.29	2319.8	1.25	2919.4	1.29	2728.5
2770		1.77	6140.8	1.75	7399.5	1.66	12235.9	1.72	13711.6	1.83	11527.8	1.75	4818.6	1.69	2491.8	1.75	7207.8
3130		2.00	12772.4	1.97	13136.0	1.88	16137.7	1.94	15866.1	2.07	18432.0	1.97	13903.5	1.91	8732.6	1.97	16788.8
3480		2.23	19182.7	2.19	20181.3	2.09	19325.1	2.16	21710.0	2.30	22379.5	2.19	21039.6	2.12	16203.3	2.19	23025.0
4205		2.69	32711.8	2.65	29593.9	2.52	26765.7	2.61	26847.1	2.78	29842.0	2.65	30958.6				
4560		2.92	32757.7	2.87	34475.5	2.74	30631.5	2.83	29127.2	3.01	33092.1	2.87	33961.0				
4945		3.16	38471.7	3.12	35948.8	2.97	29869.3	3.07	32329.7	3.26	36178.4	3.12	37665.9				
5640		3.61	36366.2	3.55	37784.3	3.38	34740.4	3.50	35247.6	3.72	36106.1	3.55	36531.7				
6005		3.84	38309.3	3.78	39147.9	3.60	34802.5	3.72	37138.0	3.96	38812.4	3.78	38645.0				
6355		4.07	38765.9	4.00	38427.0	3.81	37034.8	3.94	41792.8	4.19	38488.9	4.00	38567.4				
7075		4.53	42074.6	4.46	36360.8	4.25	35517.0	4.39	35337.5	4.67	37859.7	4.46	38178.0				
7835		5.01	37373.1	4.94	38178.0	4.70	36917.7	4.86	38477.6	5.17	39359.7	4.94	39615.2				
8585		5.49	39361.4	5.41	38339.5	5.15	37795.0	5.32	37936.9	5.67	39796.9	5.41	38836.1				
9235		5.91	40305.7	5.82	39768.3	5.54	40675.8	5.73	40418.9	6.10	40418.9	5.82	41459.9				
9965		6.38	40754.5	6.28	40139.1	5.98	39597.8	6.18	39984.5	6.58	39551.8	6.28	38507.0				

Time		Volume of water	THg conc. in eluate	Volume of water	THg conc. in eluate	Volume of water	THg conc. in eluate
[min]		[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]
10095	Desorption	0.08	41899.5	0.08	41027.1	0.08	41550.2
10200		0.15	37276.7	0.15	36359.6	0.14	36386.4
10325		0.23	37199.2	0.23	36492.0	0.22	36040.5
10495		0.34	35843.4	0.33	36361.0	0.32	34554.7
10675		0.45	36176.9	0.45	35620.6	0.43	31156.9
11395		0.92	28473.2	0.90	30185.5	0.86	27354.8
11770		1.16	20819.5	1.14	22987.1	1.08	22023.9
12115		1.38	23198.4	1.35	18589.8	1.29	20282.4
12840		1.84	12770.1	1.81	12888.0	1.73	14124.0
13655		2.36	9145.9	2.32	11086.9	2.21	11530.7
14375		2.82	7012.9	2.78	8112.7	2.65	8981.1
15095		3.28	5974.3	3.23	7379.4	3.08	6839.8
15815		3.74	5185.6	3.69	5162.1	3.51	6228.2
16315		4.06	4765.2	4.00	5090.0	3.81	5445.0
17455		4.79	3737.1	4.72	3897.4	4.49	4172.2
18895		5.72	2827.2	5.63	2975.3	5.36	3198.3
20350		6.65	2510.6	6.54	2566.3	6.23	2925.7

Table S5.2: Summary of the measured THg concentrations for each column at the different times after the the start of the sorption and desorption experiments and the corresponding volume of contaminated solution flowed through (143.72 ± 6.17 mg L-1).

Sorption

		C2.1		C2.2		C2.3		C2.4		C2.5		C2.6		C2.7		C2.8	
Time		Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate	Volume of HgCl$_2$ solution	THg conc. in eluate
[min]		[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]
60		0.04	2.0	0.04	2.1	0.03	3.3	0.04	4.5	0.04	2.8	0.04	2.4	0.04	1.7	0.04	2.7
470		0.28	70.2	0.29	6.2	0.27	42.4	0.28	15443.7	0.30	4643.1	0.30	919.7	0.30	10.6	0.31	242.7
550		0.33	170.3	0.34	7.1	0.32	213.0	0.33	24172.9	0.35	10842.5	0.35	3726.1	0.35	57.2	0.36	1357.3
640		0.38	339.3	0.39	12.4	0.37	617.8	0.38	31115.2	0.40	19125.5	0.40	8652.8	0.41	631.1	0.42	6554.5
725		0.44	1133.6	0.44	30.9	0.42	1592.5	0.44	38162.9	0.46	29956.4	0.46	20936.0	0.46	2842.6	0.48	21838.8
815		0.49	2655.0	0.50	129.1	0.47	2761.3	0.49	44441.0	0.51	37801.8	0.51	29899.3	0.52	9085.6	0.54	35603.5
905		0.54	6430.3	0.55	777.7	0.52	5511.7	0.54	52330.6	0.57	46709.3	0.57	38507.2	0.58	16900.1	0.60	42662.8
1000		0.60	13677.3	0.61	2873.6	0.58	10407.1	0.60	54982.1	0.63	52597.5	0.63	44364.0	0.64	33074.0	0.66	52069.8
1120	Sorption	0.67	26657.0	0.68	8971.2	0.65	14412.9					0.71	52826.6	0.72	32494.2	0.74	57450.1
1180		0.71	31169.0	0.72	20930.1	0.68	18788.0					0.74	56251.2	0.76	37261.5	0.78	61330.0
1270		0.76	40302.4	0.77	41624.3	0.74	23900.1					0.80	62602.2	0.81	43662.5	0.84	71199.6
1360		0.82	47210.6	0.83	50096.7	0.79	27474.9					0.86	69545.8	0.87	51398.6	0.90	78331.1
1450		0.87	62332.2	0.88	63783.8	0.84	34612.4					0.91	74942.2	0.93	54550.5	0.96	78956.6
1540		0.92	61252.1	0.94	69240.5	0.89	40872.3					0.97	73513.8	0.99	60512.0	1.02	80523.2
2035		1.22	98846.6	1.24	103464.8	1.18	86672.3					1.28	93883.0	1.30	87240.7	1.34	98920.9
2375		1.43	115743.5	1.45	112668.5	1.38	108960.6					1.50	105180.7	1.52	113634.1	1.57	110991.7
2735		1.64	115933.8	1.67	118378.5	1.59	116450.8					1.72	111155.7	1.75	122557.2	1.81	113447.0
3455		2.07	120829.6	2.11	120869.2	2.00	122724.6					2.18	116947.6	2.21	129888.1	2.28	123361.9
4175		2.51	129316.7	2.55	130339.3	2.42	130397.9					2.63	125466.9	2.67	128924.3	2.76	121406.2
4925		2.96	144013.9	3.00	143324.3	2.86	147228.9					3.10	140397.0	3.15	146304.2	3.25	137545.3
5615		3.37	120309.2	3.43	118834.8	3.26	117071.0					3.54	126508.4	3.59	118991.6	3.71	123639.7
6805		4.08	143498.9	4.15	153098.7	3.95	140312.9					4.29	144131.0	4.36	141779.0	4.49	144131.0
8195		4.92	139125.6	5.00	139262.0	4.75	136533.9					5.16	138289.1	5.24	142606.0	5.41	138825.2
9290		5.57	133836.1	5.67	136073.5	5.39	133163.4					5.85	134939.2	5.95	131622.5	6.13	133704.9

Desorption

		Volume of water	THg conc. in eluate	Volume of water	THg conc. in eluate	Volume of water	THg conc. in eluate
		[L]	[µg L^{-1}]	[L]	[µg L^{-1}]	[L]	[µg L^{-1}]
9425		0.08	139816.9	0.08	139631.0	0.08	138821.8
9700		0.25	79744.4	0.25	81592.6	0.24	78608.4
9935		0.39	62344.6	0.39	67895.9	0.37	71020.8
10655		0.82	38428.8	0.83	37432.7	0.79	40584.6
11020	Desorption	1.04	31474.2	1.06	29302.4	1.00	31854.3
11375		1.25	26123.7	1.27	24603.6	1.21	26701.7
12155		1.72	17810.8	1.75	16304.9	1.66	18192.9
12815		2.12	17810.8	2.15	12510.0	2.04	14822.8
13625		2.60	11834.3	2.64	11239.5	2.51	12904.7
14255		2.98	9361.4	3.03	9311.3	2.88	10799.4
15170		3.53	7107.3	3.59	6779.3	3.41	7641.9

S6. Model fitting for liquid-phase sorption and desorption curves.

Table S6.1: Model fitting for liquid-phase sorption and desorption experiments for EXP1

EXP1 Sorption	
Model	Freundlich
Equation	y = a*x^(b*x^(-c))
Plot	C mean
a	1366.35747 ± 456.84715
b	5.29409 ± 0.60819
c	0.57616 ± 0.03746
Reduced Chi-Sqr	12.26486
R-Square (COD)	0.99442
Adj. R-Square	0.9938

EXP1 Desorption	
Model	Exponential decay
Equation	y = A1*exp(-x/t1) + y0
Plot	C mean
y0	2053.32898 ± 367.5216
A1	2.59719e6 ± 676227.00532
t1	1.50833 ± 0.0942
Reduced Chi-Sqr	3.71419
R-Square (COD)	0.99894
Adj. R-Square	0.99879

Table S6.2: Model fitting for liquid-phase sorption and desorption experiments for EXP2

EXP2 Sorption		
Model	FreundlichEXT	
Equation	y = a*x^(b*x^(-c))	
Plot	C mean	
a	67537.02358 ± 4269.52802	
b	1.47832 ± 0.1398	
c	0.75874 ± 0.03538	
Reduced Chi-Sqr		2.07179
R-Square (COD)		0.99878
Adj. R-Square		0.99867

EXP2 Desorption		
Model	Exponential Decay	
Equation	y = y0 + A1*exp(-(x-x0)/t1) + A2*exp(-(x-x0)/t2)	
Plot	C mean	
y0	5561.52218 ± 1303.39439	
x0	5.79595 ± 14079.54274	
A1	93048.54603 ± 1.08768e10	
t1	0.12045 ± 0.03325	
A2	72737.1491 ± 1.06232e9	
t2	0.96403 ± 0.18122	
Reduced Chi-Sqr		1.87912
R-Square (COD)		0.99993
Adj. R-Square		0.99986

S7. Liquid-phase stable isotope data.

Table S7.1: Liquid-phase Hg stable isotope data.

Column	Sample time [Minutes]	Sample time [Hours]	MCICPMS Session Date	Conc. Level for MCICPMS run	$\delta^{202/198}$Hg [‰]	2SD [‰]	Δ^{199}Hg [‰]	2SD [‰]	Δ^{200}Hg [‰]	2SD [‰]	Δ^{201}Hg [‰]	2SD [‰]	Δ^{204}Hg [‰]	2SD [‰]
C2.1	1180	19.7	03/05/2022	10 ppb	-0.39	0.05	0.06	0.05	0.02	0.03	0.03	0.03	-0.04	0.04
C2.1	1270	21.17	03/05/2022	10 ppb	-0.46	0.05	0.06	0.05	0.01	0.03	0.01	0.03	-0.03	0.04
C2.1	1450	24.17	04/05/2022	5 ppb	-0.53	0.08	0.06	0.07	0.03	0.03	0.05	0.02	-0.02	0.02
C2.1	1540	25.7	04/05/2022	5 ppb	-0.51	0.08	0.06	0.07	-0.02	0.03	0.02	0.02	-0.04	0.02
C2.1	4005	66.75	04/05/2022	5 ppb	-0.55	0.08	0.04	0.07	-0.01	0.03	-0.03	0.02	-0.06	0.02
C2.1	4005	66.75	04/05/2022	5 ppb	-0.60	0.08	0.01	0.07	-0.02	0.03	0.00	0.02	-0.04	0.02
C2.1	9290	154.8	03/05/2022	10 ppb	-0.53	0.05	0.05	0.05	0.03	0.03	0.01	0.03	-0.03	0.04
C2.1	9700	161.7	03/05/2022	10 ppb	-0.57	0.05	0.04	0.05	0.01	0.03	0.00	0.03	0.00	0.04
C2.1	11020	183.7	03/05/2022	10 ppb	-0.54	0.05	0.04	0.05	0.03	0.03	-0.01	0.03	0.01	0.04
C2.1	15190	253.2	03/05/2022	10 ppb	-0.55	0.05	0.01	0.05	-0.01	0.03	-0.01	0.03	0.02	0.04
C2.2	1180	19.7	03/05/2022	10 ppb	-0.11	0.05	0.07	0.05	0.01	0.03	0.01	0.03	-0.03	0.04
C2.2	1270	21.2	04/05/2022	5 ppb	-0.16	0.08	0.10	0.07	0.06	0.03	0.03	0.02	0.01	0.02
C2.2	1450	24.2	03/05/2022	10 ppb	-0.45	0.05	0.05	0.05	0.01	0.03	0.01	0.03	-0.06	0.04
C2.2	1540	25.7	03/05/2022	10 ppb	-0.47	0.05	0.04	0.05	0.00	0.03	0.00	0.03	-0.04	0.04
C2.2	4005	66.8	04/05/2022	5 ppb	-0.56	0.08	0.04	0.07	0.03	0.03	0.02	0.02	0.01	0.02
C2.2	9290	154.8	03/05/2022	10 ppb	-0.60	0.05	0.04	0.05	-0.01	0.03	-0.01	0.03	-0.03	0.04
C2.2	9700	161.7	03/05/2022	10 ppb	-0.56	0.05	0.05	0.05	0.00	0.03	0.01	0.03	0.00	0.04
C2.2	11020	183.7	03/05/2022	10 ppb	-0.61	0.05	0.03	0.05	0.01	0.03	0.00	0.03	0.04	0.04
C2.2	15190	253.2	03/05/2022	10 ppb	-0.51	0.05	0.02	0.05	0.02	0.03	-0.02	0.03	0.01	0.04
C2.3	1180	19.7	03/05/2022	10 ppb	-0.40	0.05	0.01	0.05	-0.02	0.03	0.02	0.03	-0.01	0.04
C2.3	1270	21.2	03/05/2022	10 ppb	-0.33	0.05	0.06	0.05	0.01	0.03	0.01	0.03	-0.04	0.04
C2.3	1450	24.2	04/05/2022	5 ppb	-0.51	0.08	0.05	0.07	0.01	0.03	0.06	0.02	-0.05	0.02
C2.3	1540	25.7	04/05/2022	5 ppb	-0.52	0.08	0.05	0.07	-0.01	0.03	0.01	0.02	-0.03	0.02
C2.3	4005	66.8	04/05/2022	5 ppb	-0.55	0.08	0.02	0.07	0.00	0.03	-0.01	0.02	-0.01	0.02
C2.3	9290	154.8	04/05/2022	10 ppb	-0.60	0.03	0.03	0.02	0.03	0.03	0.01	0.02	0.01	0.03
C2.3	9700	161.7	04/05/2022	10 ppb	-0.57	0.03	0.04	0.02	0.01	0.03	0.01	0.02	0.01	0.03
C2.3	11020	183.7	04/05/2022	10 ppb	-0.57	0.03	0.04	0.02	0.02	0.03	0.01	0.02	0.03	0.03
C2.3	15470	257.8	04/05/2022	5 ppb	-0.51	0.08	0.02	0.07	0.01	0.03	0.00	0.02	0.03	0.02
Stock Solution			03/05/2022	10 ppb	-0.60	0.05	0.01	0.05	0.00	0.03	0.01	0.03	0.00	0.04
Stock Solution			04/05/2022	10 ppb	-0.62	0.03	0.03	0.02	0.01	0.03	0.00	0.02	-0.02	0.03
Stock Solution			04/05/2022	5 ppb	-0.62	0.08	0.02	0.07	0.01	0.03	-0.01	0.02	-0.01	0.02

S8. Hg stable isotope, THg concentration & moisture content data for solid-phase materials including column sections.

Table S8.1: Solid-phase THg concentrations and Hg stable isotope data.

Column	Section	Sorption period	THg Conc. [mg kg-1]	MCICPMS Session Date	Concentration Level for MCICPMS run	δ²⁰²/¹⁹⁸Hg [‰]	2SD [‰]	Δ¹⁹⁹Hg [‰]	2SD [‰]	Δ²⁰⁰Hg [‰]	2SD [‰]	Δ²⁰¹Hg [‰]	2SD [‰]	Δ²⁰⁴Hg [‰]	2SD [‰]
C1.7	T	50% brkth.	1076	15/12/2021	5 ppb	-0.57	0.15	0.04	0.01	0.00	0.02	0.03	0.05	0.01	0.07
C1.7	M	50% brkth.	1843	15/12/2021	10 ppb	-0.71	0.07	0.03	0.02	0.03	0.02	0.00	0.02	-0.05	0.08
C1.7	B	50% brkth.	1490	15/12/2021	10 ppb	-0.76	0.07	0.02	0.02	0.00	0.02	0.00	0.02	0.00	0.08
C1.8	T	50% brkth.	356	15/12/2021	10 ppb	-0.59	0.07	0.05	0.02	0.02	0.02	0.00	0.02	-0.03	0.08
C1.8	M	50% brkth.	1280	15/12/2021	10 ppb	-0.66	0.07	0.02	0.02	0.00	0.02	0.01	0.02	0.01	0.08
C1.8	B	50% brkth.	1245	15/12/2021	10 ppb	-0.75	0.07	0.02	0.02	-0.01	0.02	0.00	0.02	-0.04	0.08
C1.4	T	Equilib.	1432	14/12/2021	10 ppb	-0.73	0.03	0.01	0.01	-0.01	0.02	-0.03	0.01	-0.04	0.03
C1.4	M	Equilib.	1183	14/12/2021	10 ppb	-0.77	0.03	0.03	0.01	0.03	0.02	0.03	0.01	-0.01	0.03
C1.4	B	Equilib.	1698	14/12/2021	10 ppb	-0.88	0.03	0.16	0.01	0.11	0.02	0.08	0.01	-0.05	0.03
C1.4	B	Equilib.	1575	14/12/2021	10 ppb	-0.77	0.03	-0.01	0.01	-0.02	0.02	-0.05	0.01	0.11	0.03
C1.4	B	Equilib.	369	15/12/2021	10 ppb	-0.84	0.07	0.00	0.02	0.00	0.02	0.00	0.02	0.02	0.08
C1.5	T	Equilib.	1261	15/12/2021	5 ppb	-0.69	0.15	0.03	0.01	-0.02	0.02	-0.01	0.05	-0.01	0.07
C1.5	M	Equilib.	2031	15/12/2021	10 ppb	-0.76	0.07	0.05	0.02	0.03	0.02	0.04	0.02	-0.03	0.08
C1.5	B	Equilib.	1594	15/12/2021	10 ppb	-0.62	0.07	0.13	0.02	0.06	0.02	0.04	0.02	-0.96	0.08
C1.6	T	Equilib.	1364	15/12/2021	10 ppb	-0.73	0.07	0.03	0.02	0.01	0.02	0.01	0.02	-0.01	0.08
C1.6	M	Equilib.	1541	15/12/2021	10 ppb	-0.77	0.07	0.04	0.02	0.02	0.02	0.01	0.02	-0.03	0.08
C1.6	B	Equilib.	1410	15/12/2021	10 ppb	-0.76	0.07	0.02	0.02	0.00	0.02	0.00	0.02	-0.04	0.08
C1.1	T	Desorp.	816	14/12/2021	10 ppb	-0.88	0.03	0.03	0.01	0.01	0.02	0.00	0.01	-0.01	0.03
C1.1	M	Desorp.	716	14/12/2021	10 ppb	-1.00	0.03	0.02	0.01	0.00	0.02	-0.02	0.01	0.00	0.03
C1.1	B	Desorp.	634	14/12/2021	10 ppb	-1.02	0.03	0.05	0.01	0.00	0.02	0.01	0.01	-0.02	0.03
C1.2	T	Desorp.	948	14/12/2021	10 ppb	-0.91	0.03	0.01	0.01	0.01	0.02	0.01	0.01	0.00	0.03
C1.2	M	Desorp.	771	14/12/2021	10 ppb	-0.94	0.03	0.00	0.01	0.00	0.02	0.00	0.01	-0.01	0.03
C1.2	M	Desorp.	634	14/12/2021	10 ppb	-1.00	0.03	0.02	0.01	0.02	0.02	0.00	0.01	0.01	0.03
C1.2	M	Desorp.	850	14/12/2021	10 ppb	-0.92	0.03	0.01	0.01	0.03	0.02	-0.01	0.01	0.03	0.03
C1.2	B	Desorp.	1182	14/12/2021	10 ppb	-1.01	0.03	0.04	0.01	-0.02	0.02	0.01	0.01	-0.02	0.03
C1.3	T	Desorp.	804	14/12/2021	10 ppb	-0.88	0.03	0.01	0.01	-0.01	0.02	0.01	0.01	-0.04	0.03
C1.3	M	Desorp.	733	14/12/2021	10 ppb	-0.93	0.03	0.03	0.01	0.01	0.02	0.00	0.01	0.00	0.03
C1.3	B	Desorp.	968	14/12/2021	10 ppb	-0.92	0.03	-0.12	0.01	-0.12	0.02	-0.06	0.01	0.03	0.03
C2.4	T	50% brkth.	819	16/12/2021	5 ppb	-0.64	0.01	0.03	0.02	0.04	0.03	0.01	0.01	0.03	0.06
C2.4	M	50% brkth.	550	16/12/2021	5 ppb	-0.62	0.01	0.00	0.02	0.00	0.03	-0.01	0.01	0.03	0.06
C2.5	T	50% brkth.	987	17/12/2021	5 ppb	-0.62	0.01	0.02	0.02	-0.01	0.03	-0.02	0.01	0.00	0.06
C2.5	M	50% brkth.	953	17/12/2021	5 ppb	-0.72	0.15	0.02	0.01	0.04	0.02	0.01	0.05	0.00	0.07
C2.5	M	50% brkth.	495	17/12/2021	5 ppb	-0.69	0.15	0.02	0.01	0.03	0.02	0.01	0.05	0.05	0.07
C2.5	M	50% brkth.	479	17/12/2021	5 ppb	-0.58	0.01	0.04	0.02	0.00	0.03	0.00	0.01	-0.03	0.06
C2.5	B	50% brkth.	427	17/12/2021	10 ppb	-0.58	0.01	0.04	0.02	0.00	0.03	0.00	0.01	-0.02	0.06
C2.6	T	Equilib.	1157	17/12/2021	10 ppb	-0.70	0.03	0.15	0.02	0.03	0.01	0.00	0.00	-0.06	0.01
C2.6	M	Equilib.	2766	17/12/2021	10 ppb	-0.77	0.03	0.24	0.02	0.06	0.01	0.03	0.00	-0.01	0.01
C2.6	B	Equilib.	1885	17/12/2021	10 ppb	-0.70	0.03	0.11	0.02	0.02	0.01	0.02	0.00	0.00	0.01
C2.7	T	Equilib.	2500	17/12/2021	10 ppb	-0.68	0.03	0.03	0.02	0.00	0.01	0.00	0.00	-0.02	0.01
C2.7	M	Equilib.	1946	17/12/2021	10 ppb	-0.96	0.03	0.03	0.02	0.02	0.01	0.00	0.00	0.04	0.01
C2.7	B	Equilib.	2284	17/12/2021	10 ppb	-0.70	0.03	0.05	0.02	0.02	0.01	0.03	0.00	-0.01	0.01
C2.8	T	Equilib.	2720	17/12/2021	10 ppb	-0.75	0.03	0.05	0.02	0.02	0.01	0.01	0.00	-0.01	0.01
C2.8	T	Equilib.	1823	17/12/2021	10 ppb	-1.53	0.03	0.03	0.02	0.00	0.01	-0.03	0.00	0.01	0.01
C2.8	T	Equilib.	2175	17/12/2021	5 ppb	-1.52	0.03	0.04	0.02	0.01	0.01	0.01	0.00	0.01	0.01
C2.8	T	Equilib.	2414	17/12/2021	10 ppb	-0.65	0.03	0.02	0.02	0.02	0.01	0.05	0.00	-0.04	0.01
C2.8	M	Equilib.	2333	17/12/2021	10 ppb	-0.71	0.03	0.02	0.02	0.01	0.01	0.00	0.00	0.00	0.01
C2.8	B	Equilib.	2524	17/12/2021	10 ppb	-0.76	0.03	0.04	0.02	0.00	0.01	0.02	0.00	0.01	0.01
C2.1	T	Desorp.	1324	15/12/2021	10 ppb	-0.85	0.07	0.05	0.02	0.01	0.02	0.04	0.02	-0.01	0.08
C2.1	M	Desorp.	975	15/12/2021	5 ppb	-0.81	0.15	0.03	0.01	0.01	0.02	0.03	0.05	-0.02	0.07
C2.1	B	Desorp.	889	15/12/2021	10 ppb	-0.96	0.07	0.06	0.02	-0.01	0.02	0.01	0.02	0.02	0.08
C2.2	T	Desorp.	384	15/12/2021	10 ppb	-0.86	0.07	0.03	0.02	0.02	0.02	0.00	0.02	0.00	0.08
C2.2	M	Desorp.	1165	15/12/2021	10 ppb	-0.85	0.07	0.04	0.02	0.01	0.02	0.00	0.02	0.00	0.08
C2.2	B	Desorp.	808	15/12/2021	10 ppb	-0.93	0.07	0.03	0.02	0.00	0.02	0.00	0.02	-0.02	0.08
C2.3	T	Desorp.	1108	15/12/2021	10 ppb	-1.68	0.07	0.06	0.02	0.03	0.02	0.03	0.02	0.01	0.08
C2.3	T	Desorp.	1108	16/12/2021	5 ppb	-1.66	0.07	0.05	0.02	0.00	0.02	-0.01	0.02	0.02	0.08
C2.3	M	Desorp.	1030	16/12/2021	10 ppb	-0.79	0.07	0.04	0.02	0.01	0.02	0.00	0.02	-0.05	0.08
C2.3	B	Desorp.	996	16/12/2021	5 ppb	-0.88	0.01	0.04	0.02	0.00	0.03	0.00	0.01	0.00	0.06

Table S8.2: Moisture content of solid-phase samples.

sample	empty bowl [g]	bowl + wet [g]	bowl + dry [g]	wet [g]	dry [g]	Moisture content fraction [-]
C1.1 T	14.2399	16.1681	15.7769	1.9282	1.5370	0.25
C1.1 M	14.5923	16.8133	16.3516	2.2210	1.7593	0.26
C1.1 B	14.4404	16.2255	15.8688	1.7851	1.4284	0.25
C1.2 T	15.1776	17.2084	16.8279	2.0308	1.6503	0.23
C1.2 M	14.2865	16.5868	16.1434	2.3003	1.8569	0.24
C1.2 B	14.6072	16.7256	16.3260	2.1184	1.7188	0.23
C1.3 T	14.4939	16.7740	16.3102	2.2801	1.8163	0.26
C1.3 M	14.5032	16.6202	16.2059	2.1170	1.7027	0.24
C1.3 B	14.2353	16.9487	16.4914	2.7134	2.2561	0.20
C1.4 T	14.2520	16.6402	16.2112	2.3882	1.9592	0.22
C1.4 M	14.2428	16.4535	16.1166	2.2107	1.8738	0.18
C1.4 B	14.5614	16.7126	16.2810	2.1512	1.7196	0.25
C1.5 T	14.3377	16.6358	16.1890	2.2981	1.8513	0.24
C1.5 M	14.3580	16.5369	16.1098	2.1789	1.7518	0.24
C1.5 B	14.2582	16.9172	16.3734	2.6590	2.1152	0.26
C1.6 T	14.3407	16.4050	16.0082	2.0643	1.6675	0.24
C1.6 M	15.1316	17.5291	17.0667	2.3975	1.9351	0.24
C1.6 B	13.6881	16.2738	15.7482	2.5857	2.0601	0.26
C1.7 T	14.6466	16.9012	16.4728	2.2546	1.8262	0.23
C1.7 M	14.2800	16.7787	16.2839	2.4987	2.0039	0.25
C1.7 B	14.5585	17.1876	16.6729	2.6291	2.1144	0.24
C1.8 T	14.5288	16.5272	16.1569	1.9984	1.6281	0.23
C1.8 M	14.6245	17.0316	16.5597	2.4071	1.9352	0.24
C1.8 B	14.2253	16.9229	16.4047	2.6976	2.1794	0.24
C2.1 T	14.4793	16.4503	16.1304	1.9710	1.6511	0.19
C2.1 M	14.4759	16.3635	16.0722	1.8876	1.5963	0.18
C2.1 B	14.4480	17.3383	16.7690	2.8903	2.3210	0.25
C2.2 T	14.5447	16.7918	16.3792	2.2471	1.8345	0.22
C2.2 M	14.2621	16.5318	16.1551	2.2697	1.8930	0.20
C2.2 B	14.2837	16.3190	15.9553	2.0353	1.6716	0.22
C2.3 T	28.0688	30.2345	29.8495	2.1657	1.7807	0.22
C2.3 M	21.9693	24.2332	23.7923	2.2639	1.8230	0.24
C2.3 B	14.5411	16.7309	16.2667	2.1898	1.7256	0.27
C2.4 T	14.4307	16.4265	16.0489	1.9958	1.6182	0.23
C2.4 M	14.4250	16.4872	16.0988	2.0622	1.6738	0.23
C2.4 B	14.2458	16.7146	16.2126	2.4688	1.9668	0.26
C2.5 T	21.9291	24.2804	23.8550	2.3513	1.9259	0.22
C2.5 M	14.4951	16.2468	15.9168	1.7517	1.4217	0.23
C2.5 B	14.2588	16.9137	16.4452	2.6549	2.1864	0.21
C2.6 T	28.1416	30.3790	30.0203	2.2374	1.8787	0.19
C2.6 M	23.3120	25.5319	25.1501	2.2199	1.8381	0.21
C2.6 B	28.6517	31.0150	30.5710	2.3633	1.9193	0.23
C2.7 T	14.1971	16.3535	16.0053	2.1564	1.8082	0.19
C2.7 M	14.2804	16.5800	16.1495	2.2996	1.8691	0.23
C2.7 B	14.2438	16.5827	16.1254	2.3389	1.8816	0.24
C2.8 T	14.3536	16.3386	15.9580	1.9850	1.6044	0.24
C2.8 M	14.2856	16.4172	15.9998	2.1316	1.7142	0.24
C2.8 B	14.1807	17.0191	16.4126	2.8384	2.2319	0.27

S9. Pyrolytic Thermal Desorption (PTD) curves for solid-phase speciation analyses.

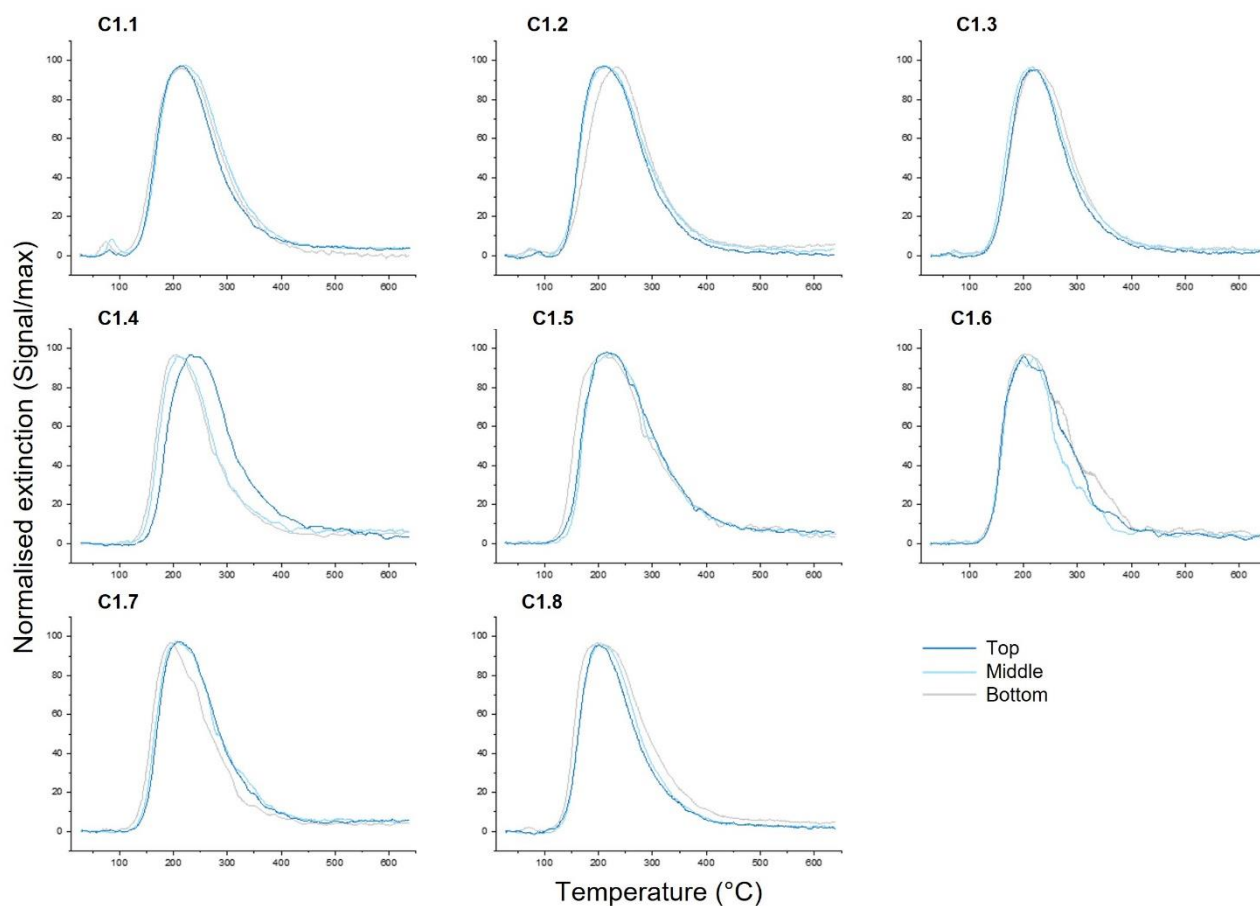



Figure S9.1: Full PTD curves for ≈0.1 g of solid-phase materials from EXP1

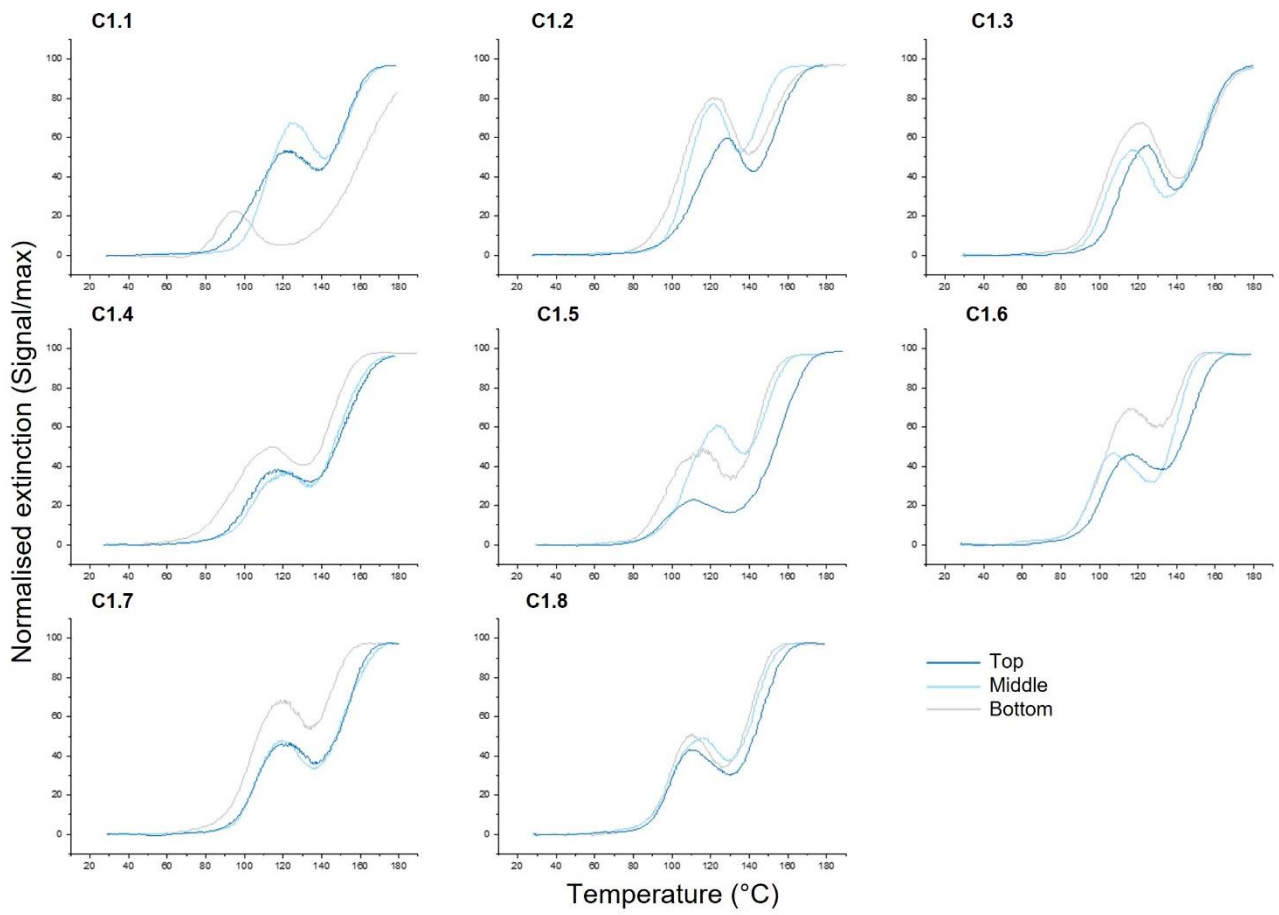



Figure S9.2: PTD curves up to 180°C for ≈2.0 g of solid-phase materials from EXP1 to assess the presence of Hg(0) produced during the experiments.

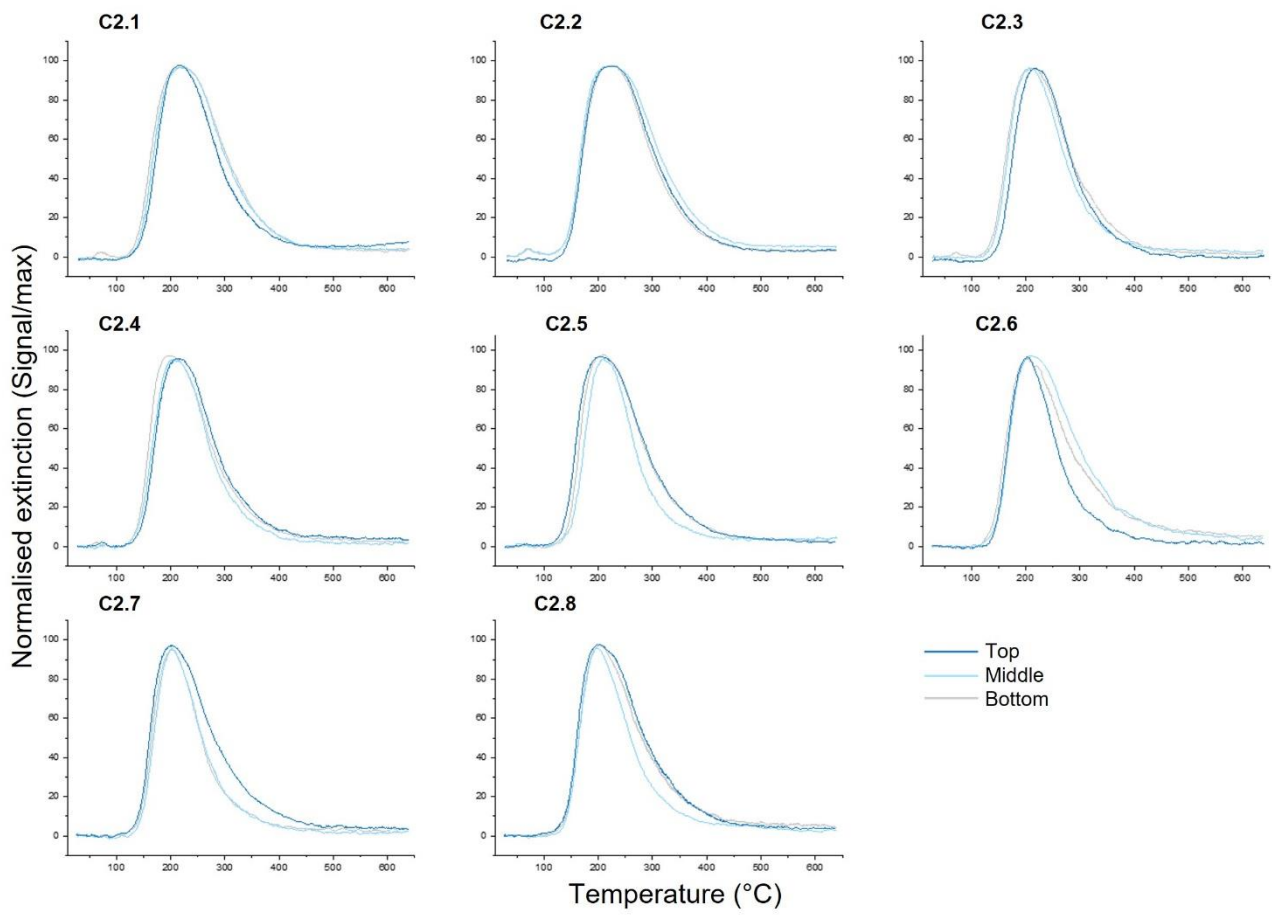



Figure S9.3: Full PTD curves for ≈0.1 g of solid-phase materials from EXP2

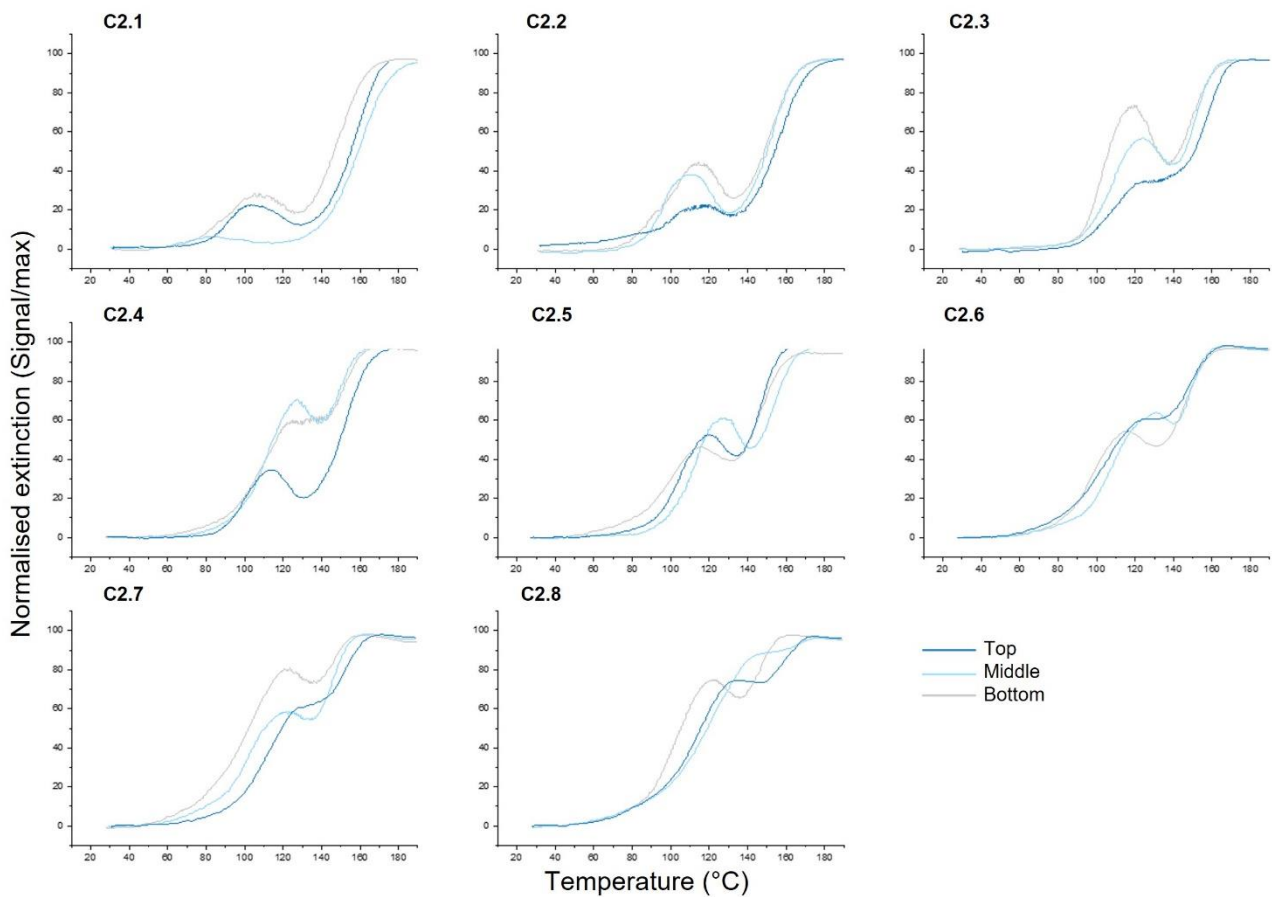



Figure S9.4: PTD curves up to 180°C for ≈2.0 g of solid-phase materials from EXP2 to assess the presence of Hg(0) produced during the experiments.

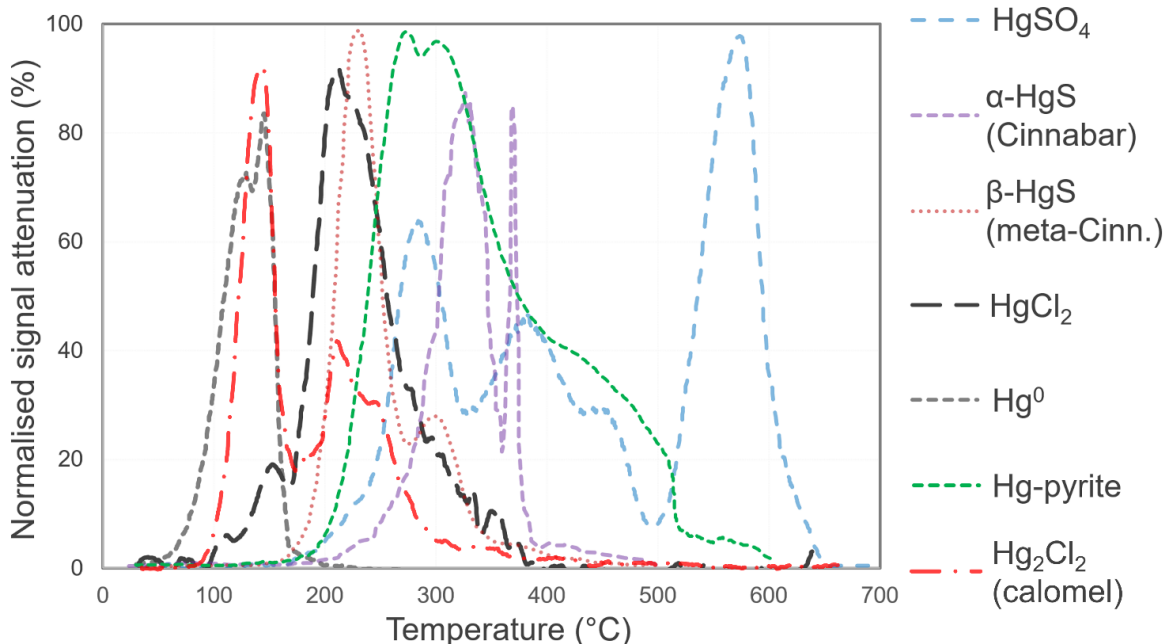



Figure S9.5: Mean (between 2 and 10 replications), normalised PTD release curves of standards for Hg species. All standards were prepared in silica (SiO2) matrix. Species are below 100% normalised maximum attenuation due to variability in signal of replicates (from McLagan et al., 2022). As discussed in McLagan et al. (2022), calomel is highly unstable in the environment and the conditions of these experiments; and hence peaks <175 °C are attributed to Hg(0).

S10. Modelling estimation of liquid-phase Hg speciation using Visual MINTEQ v3.1

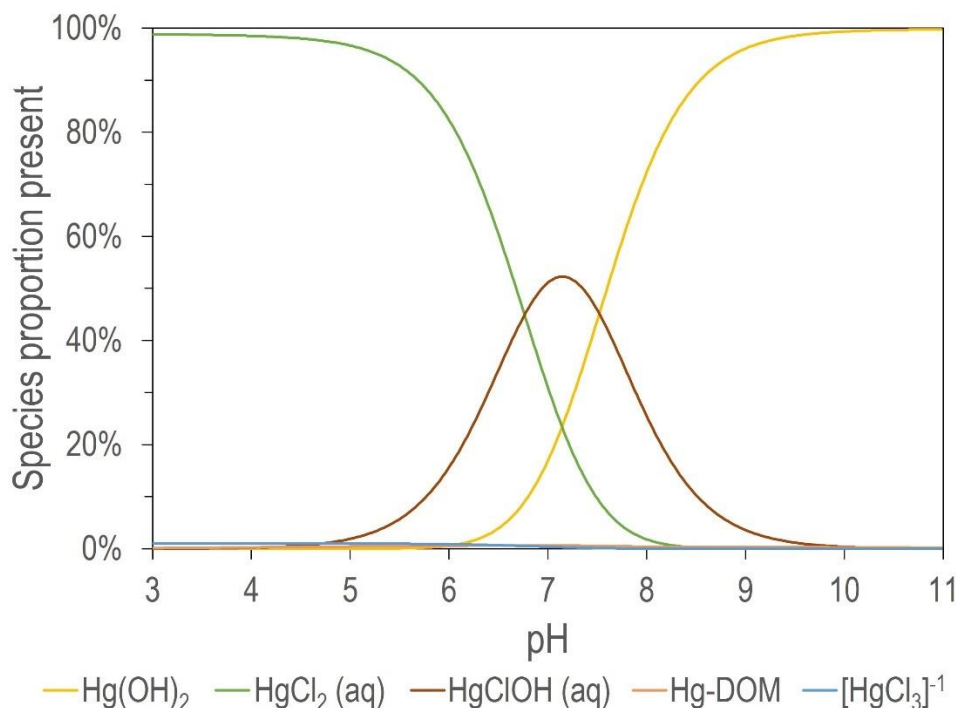



Figure S10.1: Species distribution for EXP1 (46.1 ± 1.1 mg L^{-1}) calculated with Visual Minteq ver. 3.1 (Gustafsson, 2014) using equilibrium constants from the thermo.vdb database and the "Stockholm Humic Model" (Gustafsson, 2001) without any changes. The input included ICP-OES and DOC results from tap water analysis (Table S2.2) and per mole Hg(II) two moles Cl$^-$ were included to account for the addition of Hg as HgCl$_2$. Additionally, Cl$^-$ concentration of 36 mg L^{-1} was added for tap water matrix based on published data for German tap water (Bergmann et al., 2015).

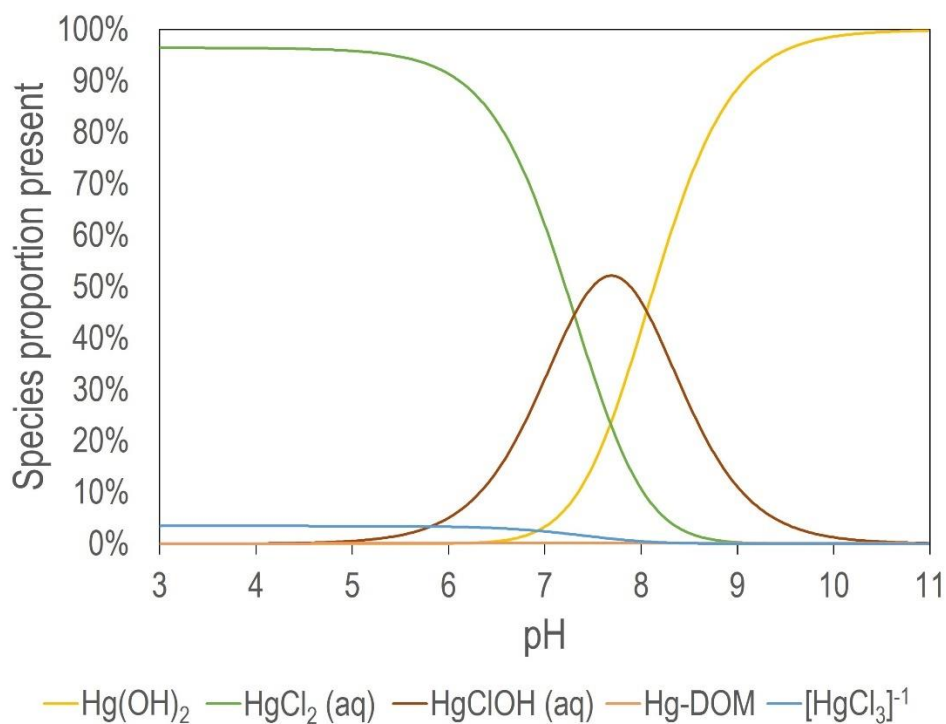



Figure S10.2: Species distribution for EXP2 (143.7 ± 6.2 mg L^{-1}) calculated with Visual Minteq ver. 3.1 (Gustafsson, 2014) using equilibrium constants from the thermo.vdb database and the "Stockholm Humic Model" (Gustafsson, 2001) without any changes. The input included ICP-OES and DOC results from tap water analysis (Table S2.2) and per mole Hg(II) two moles Cl$^-$ were included to account for the addition of Hg as HgCl$_2$. Additionally, Cl$^-$ concentration of 36 mg L^{-1} was added for tap water matrix based on published data for German tap water (Bergmann et al., 2015).

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