Supporting information

Uptake, translocation and elimination in sediment-rooted macrophytes: A model-supported analysis of whole sediment test data

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Table S1. Overview of chemical uptake, translocation and elimination routes in macrophytes, and possible mechanisms that might prevent this.

		Transport routes	Mechanisms
Roots	Mucigel	Apoplastic	Accumulation
	Epidermis	Apoplastic; Symplastic	Accumulation; blockage
	Cortex	Apoplastic; Symplastic	
	Endodermis	Apoplastic; Symplastic	Blockage by casparian strip and suberin deposition
	pericycle	Apoplastic; Symplastic	
Shoot	Xylem	Symplastic from roots to shoots	
	Phloem	Symplastic from shoots to roots	Blockage by sieve-tube elements
	Cell walls	Apoplastic	
Leaves	Lower or upper epidermis	Apoplastic; Symplastic	Accumulation; blockage
	Cutile	Apoplastic; Symplastic	Accumulation; blockage
	Stoma		Blockage

Materials and Methods

Chemicals and materials. PCBs standards IUPAC numbers 2, 3, 28, 29, 143 (internal standard), 149, 155, CPF (purity 98.0 %) and CPF-D10 (internal standard) were obtained from Dr. Ehrenstorfer. Other chemicals used were n-hexane and acetone (Promochem; picograde), methanol (Mallinckrodt Baker, Deventer, The Netherlands; HPLCgradient grade), acetonitrile (Lab-Scan, Dublin, Ireland; HPLC grade), Barnstead Nanopure water (Sybron-Barnstead, Dubuque, IA, USA), and calcium chloride (Merck; p.a), sodium azide (Merck; p.a.).
Polyoxymethylene sheets (POM; thickness 76 µm) were obtained from CS Hyde Company, Lake Villa, IL, USA.
For OECD sediment peat from Klasmann Deilmann Benelux BV, $CaCO_3$ powder from Sigma Aldrich, Germany, quartz sand from Geba 0.06-0.25 mm, Eurogrid, The Netherlands and kaolin from Sigma Aldrich, German was used.

Sediment and water medium. Standard sediment (OECD 218[1] with small modification described in ISO 16191) was prepared, in four batches of 10 kg dry weight, by mixing peat (5%), $CaCO_3$ powder (2%), and an aqueous nutrient ($Na_3PO_4 \bullet 12H_2O$ and NH_4Cl) medium of 0.36 g P/L and 0.30 g N/L to obtain a homogeneous slurry. After three batches were spiked with PCBs and CPF, and thoroughly mixed, quartz sand (75%), and kaolin clay (18%) were added to each of the four batches. Barko and Smart medium[2] consists of 91.7mg/L $CaCl_2.2H_2O$, 69.0mg/L $MgSO_4.7H_2O$, 58.4 mg/L $NaHCO_3$, 15.4 mg/L $KHCO_3$.
Sediment samples were taken at start and end of the experiment to determine wet weight, dry weight (24h at 105°C), organic matter (OM) (3h at 550°C) and organic carbon (OC) (2h at 950°C) content. Sediment had an average (standard deviation (SD)) pH of 6.12 (0.03), and OM content of 6.46 (0.14)% at the start of the experiment. The moisture content was 33.7 (0.7)%.

Table S2. Sediment characteristics at start of equilibrium period, start of the experiment, and per species end of the experiment.

	Water content (%)		OM (%)	
	average	SD	average	SD
t=-28 (n=12)	33.73	0.68	6.46	0.14
t=0 (n=12)	33.85	0.69	6.30 (n=11)	0.11
t=28 M (n=27)	31.72	1.95	5.59	0.71
t=28 E (n=27)	30.20	0.65	6.12	0.32

Spiking procedure.

Spiking of Sediment. Sediment was spiked with PCBs 3, 29, 155, and CPF in acetone to reach target concentrations of 20 µg/kg for these PCBs and 40 µg/kg for CPF. All concentrations are expressed on a sediment dry weight (DW) basis. These target concentrations have been shown to yield detectable concentrations in macrophytes.[3] The CPF spike target concentration was higher to compensate for possible degradation. PCB spike solution was added to the sediment in five portions of 1 mL with 30 minutes of vigorous agitation in between. The volume of acetone was less than 0.098% (v:v), well below the recommended level of ISO.[4] Polyoxymethylene (POM) passive samplers[5] were added to the sediment to acquire in situ pore water concentrations at start of exposure (see below). To assure a state of (pseudo-)equilibrium between chemicals and sediment prior to exposure[6], sediment with POM samplers were agitated for four weeks on a roller bank in the dark. After seven days, the solvent was allowed to evaporate in a fume hood. After two weeks, CPF stock solution was spiked into the sediment, thoroughly mixed, and the solvent was allowed to evaporate seven days later, after which CPF was equilibrated for one more week. Consequently, PCBs had a pre-equilibration of four weeks and CPF, which equilibrates faster, two weeks.

Macrophytes.

Table S3. Test species characteristics.

Species	Specific leaf area (mm^2/mg)[a]	Average lipid content (SD) (%)[b]	Water flow plant (SD) (µl H_2O g^{-1} plant DW h^{-1})[7]	Water flow shoot (SD) (µl H_2O g^{-1} shoot DW h^{-1})[7]	Water flow root (SD) (µl H_2O g^{-1} root DW h^{-1})[7]
Myriophyllum spicatum (Dicotyledonous)	15-33	0.2 (0.09)	16 (3)	18 (3)	165 (30)
Elodea canadensis (Monocotyledonous)	25.7-59	2.1 (0.54)	11 (4)	12 (4)	146 (12)

[a] TRYdatabase[8], [b] measured in this experiment, values are based on wet weight

Preparation of macrophytes. The macrophytes were gently rinsed with demineralized water, then cut off at 8 cm, and planted with three nodes in an aquarium (40 x 64 cm) containing a 7 cm sediment layer consisting of potting soil, and natural clay in a 1:1 ratio, and 25 L of Barko and Smart medium.[2] Macrophytes were pre-grown for seven days under conditions mimicking the experimental conditions. Afterwards, macrophytes were taken from the aquaria and carefully cleaned with demineralized water.

Macrophyte bioaccumulation test.

Test set up. Glass pots (370 mL) were filled with OECD sediment of 450 g (corresponding to 298 g dry weight) (160 g of each container in case of spiked sediment). A thin layer (30 g) of fine quartz sand was put on the top of the sediment in order to reduce suspension of sediment into the water. Three shoots were carefully planted in each pot. Pots were placed in 2 L beakers filled with 1.5 L Barko and Smart medium. Pot locations were randomly varied during the test to prevent influence from the light conditions. Water loss was compensated by adding demineralized water weekly. Lamps used were Philips 400 W HPI-T.

Impermeable layer. The impermeable layer existed of a Teflon plate with three holes (diameter of 2 mm). From each hole to the edge, a small incision was made, which enabled us to place the main stem into the hole without damaging the macrophyte. To cover the hole, sulphur free plasteline (NPS non-drying modelling clay medium Chavant^{TM}) was used on the sediment side of the Teflon. The layer was sealed onto the glass pot with Teflon tape.

Control treatments. To check if the test system (e.g. the Teflon layer) had any influence, a control and a solvent control spiked with appropriate amount of acetone were used. In order to quantify any potential leakage by the Teflon layer a control with spiked water and sediment but without macrophytes was used. An 8 cm stainless steel bar replaced each macrophyte.

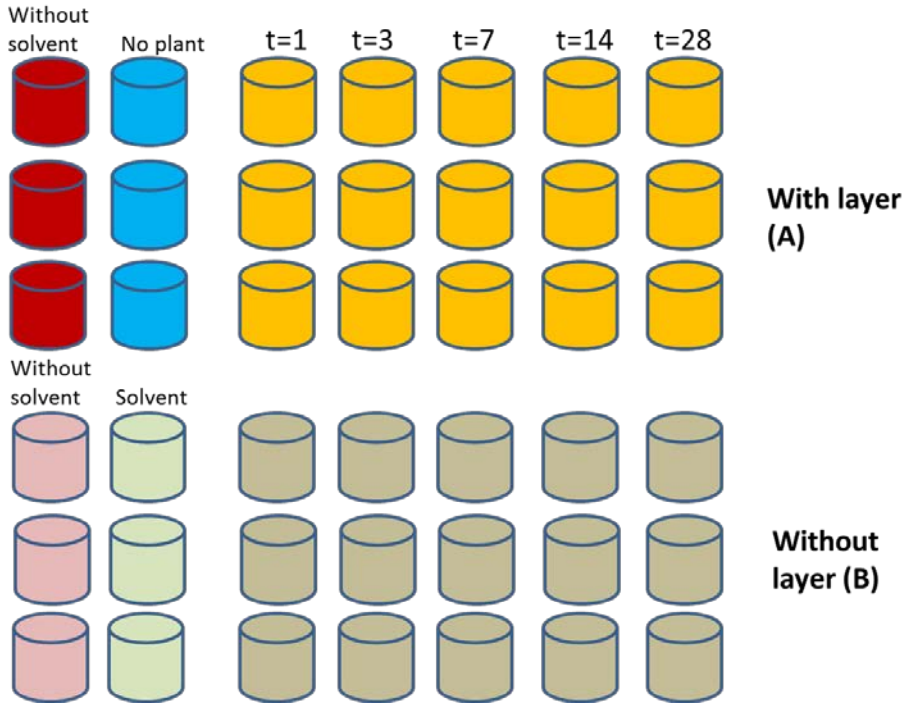


Figure S1. Overview of the experimental design

Water quality. Oxygen (Wissenschaftlich-Technische Werkstätten (WTW) Oxi 330), pH and temperature (WTW pH 323) and conductivity (WTW Cond 315i) were recorded weekly and each time when pots were taken out for chemical analyses. Algae growth (brown, green, blue) was determined by chlorophyll measurements (Phyto-pam, WAL2 mess and Regeltechiek) in a mixture of three separate samples (each 2 mL) from one test unit when pots were taken out for chemical analyses.

Extraction and analyses.

Analytical verification. Fifteen minutes after spiking the water phase, a water sample was taken and extracted. Samples of 25 mL with 2 mL n-hexane were shaken, and vortexed. At the end of each treatment, 750 mL of water was transferred into a dark green bottle, 50 ml of n-hexane was added and shaken for at least 45 minutes. In some bottles, no clear separation of water and hexane was achieved. Bottles, therefore, were sonicated for at least 15 minutes and stored at 4°C. The n-hexane was carefully transferred to a glass tube and evaporated under a gentle flow of nitrogen until approximately 200 µL. Then, 50 µL of internal standard (PCB 143) was added, mixed, and stored in an insert vial for subsequent analyses.

Macrophyte shoots and roots from one treatment were pooled (i.e. 3 shoots or roots from 1 pot) to obtain sufficient material for analysis. *M. spicatum* root samples at t=1, and t=3 were

pooled (i.e. 9 roots from 3 pots). Samples were transferred into a mortar and liquid nitrogen was added. The macrophytes were crushed to almost powder and the sample was transferred into a 100 mL centrifuge tube. A known volume of ± 30 mL acetone was added to the sample and the tubes were vigorously shaken for 30 minutes on a shaking apparatus at a speed of 175 r.p.m.. A known amount of acetone was transferred into a 25 ml test tube and the extract was evaporated to just dryness. The samples were redissolved in approximately 1.5 mL of hexane followed by a clean-up procedure on florisil according to Brock et al[9]. After chemical analysis, plant material was dried in an oven (70 °C for 24 h) to determine dry weight.

Sediment was extracted with ASE (accelerated solvent extraction) technique. Sediment samples were intensively homogenized with a small spoon. A subsample was transferred in a mortar and mixed with a sufficient amount of diatomeous earth. This mix was transferred into a 100 mL ASE cell and was extracted at a temperature of 100 °C with ± 75 mL hexane:acetone (6:1 v/v) mixture. The test tubes were evaporated to a volume between 10 and 20 ml by placing them without stopper in the fume hood. The extract was transferred into a graduated test tube of 25 mL and it was evaporated to a known volume of ± 2 mL. The samples were analysed without any clean-up.

Pore water concentrations at t=0 were measured using passive sampler polyoxymethylene sheets (POM; thickness 76 µm). POM was prepared by cutting sheet into pieces (approx. 400 mg), and cleaned with hexane (30 min) and methanol (3 times 30 min), following previously published procedures.[5] Air dried pieces were directly added to the spiked sediment (3 pieces to 10 kg DW). After equilibration, POM strips were dried with a tissue, and Soxhlet-extracted. Concentrations were calculated from concentrations in POM and POM-water equilibrium partition coefficients (Kpom).[10] Kpom values for CPF were calculated from the regression of the SP-LFER model provided by Endo et al[11].

Samples were analysed on a Hewlett Packard 6890N gas chromatograph equipped with a µ-ECD detector. Splitless injections were done at 225°C on a HP5MS column with a 0.25µm film thickness. The following temperature program was run: Initial temperature: 70°C; Initial time: 1 min; Rate A: 25°C/min; Final temperature A: 250°C; final time A: 0 min; Rate B: 3°C/min; Final temperature B: 280°C; Final time B: 5 min. The LOD for PCB's is 0.1 ng/l.

Quality assurance. Limit of quantification (LOQ) depended upon sample intake, typically this was <10 ng/L for water and pore water and <50 ng/L for shoots, roots and sediment for PCBs and < 200 ng/L for chloropyrifos.

Background concentrations in macrophytes were below detection limit except for PCB 28 with an average (SD) of 5.0 (1.2) µg/kg DW, and PCB 149 of 0.4 (0.4) µg/kg DW for *E. Canadensis*, and PCB 28 of 2.0 (0.4) µg/kg DW, and PCB 149 of 0.4 (0.1) µg/kg DW for *M.*

spicatum. Macrophytes concentrations were corrected for background concentrations. Background concentrations in sediment were below detection limit except for PCB 28, 29, 149 and 155 and CPF. The concentrations ranged between 0.04 µg/kg DW for PCB 29 and 2.9 µg/kg DW for PCB 28. Background concentrations in water were below detection limit except for PCB 2, 28 and CPF. The concentrations ranged between 0.43 ng/L for PCB 2, and 6.25 ng/L for CPF. Overlying water concentrations in controls were mainly below detection limit or very low with maximal concentration of 49 ng/L for CPF.

Table S4. Average (SD) recovery percentage per test chemical for sediment and macrophytes

Average (SD) %	**PCB 2**	**PCB 3**	**PCB 28**	**PCB 29**	**PCB 149**	**PCB 155**	**CPF (n=2)**
Sediment (n=2)	78 (8)	77 (8)	93 (12)	97 (12)	88 (13)	83 (12)	92 (8)
Macrophytes (n=5)	76 (10)	76 (10)	96 (9)	90 (9)	92 (11)	87 (8)	102 (36)

Table S5. Limit of quantification per test chemical for water, shoots, roots, sediment, and pore water in µg/kg after correction with internal standard

Average (SD)	**PCB 2**	**PCB 3**	**PCB 28**	**PCB 29**	**PCB 149**	**PCB 155**	**CPF (n=2)**
Water	0.01	0.01	0.01	0.01	0.01	0.01	0.2
Shoots	0.05	0.05	0.05	0.05	0.05	0.05	0.2
Roots	0.05	0.05	0.05	0.05	0.05	0.05	0.2
Sediment	0.05	0.05	0.05	0.05	0.05	0.05	0.2
Pore water	0.01	0.01	0.01	0.01	0.01	0.01	0.2

Table S6. Nominal and measured chemical concentrations in overlying water (µg/L) (n=60) and sediment (µg/kg) (n=3) at start of the experiment (t=0).

	Chemical	Nominal concentration	Measured concentration	% of nominal
Overlying Water (µg/L)	PCB 2	10	2.8 (0.7)	27
n=60	28	10	6.2 (2.6)	62
	149	1	0.6 (0.1)	59
Sediment (µg/kg)	3	20	13.1 (1.2)	66
n=3	29	20	15.2 (1.3)	76
	155	20	18.9 (1.6)	95
	Chlorpyrifos	40	27.1 (11.1)	68

Modelling chemical flows in sediment systems with rooted macrophytes.

Table S7. Overview of model parameters.

Symbol	Parameter	Unit
A_{SED}	surface of sediment water interface	m^2
$A_{S,t}$	surface of shoot in overlying water	m^2
$A_{R,t}$	surface of root in pore water	m^2
$A_{TR,t}$	stem cross-sectional area at the sediment-water interface	m^2
$A_{SP,S}$	shoot specific surface area	$m^{2/}kg$
$A_{SP,R}$	root specific surface area	$m^{2/}kg$
C_{OW}	chemical concentration in overlying water	$\mu g/m^3$
C_{PW}	chemical concentration in pore water	$\mu g/m^3$
C_S	chemical concentration in shoot	µg/kg
C_R	chemical concentration in root	µg/kg
K_L	benthic boundary layer mass transfer coefficient	m/d
K_S	shoot-water partition coefficient	m^3/kg
K_R	root-water partition coefficient	m^3/kg
$K_{P,SED}$	sediment-water partition coefficient	m^3/kg
k_{LOSS}	lumped first order loss (volatilization, degradation, photolysis) rate constant	d^{-1}
$k_{G,l}$	first order growth rate constant for growth of main stem	d^{-1}
$k_{G,R}$	first order growth rate constant for growth of root	d^{-1}
$k_{G,S}$	first order growth rate constant for growth of shoot	d^{-1}
l_t	length of the main stem	m
$M_{R,t}$	mass of roots	kg DW
$M_{S,t}$	mass of shoots	kg DW
M_{SED}	mass of sediment	kg DW
P_R	root chemical permeability coefficient	m/d
P_S	shoot chemical permeability coefficient	m/d
P_{TR}	translocation mass transfer coefficient	m/d
t	time	d
V_{OW}	volume of overlying water	m^3
V_{PW}	apparent pore water volume	m^3
V'_{PW}	sediment interstitial pore water volume	m^3

Model equations macrophyte growth. Macrophyte growth (eq. 6, 7) and change of shoot and root surface areas (eq. 8, 9) over time were accounted for through the following auxiliary functions. Mass (kg DW) of root ($M_{R,t}$) and shoot ($M_{S,t}$) were modelled exponentially, using first order growth rate constants (d^{-1}) for root ($k_{G,R}$) or shoot ($k_{G,S}$), which were based on measured data.

$$M_{R,t} = M_{R,t=0} e^{k_{G,R} t} \quad \text{(S1)}$$

$$M_{S,t} = M_{S,t=0} e^{k_{G,S} t} \quad \text{(S2)}$$

Surface area (m^2) for root ($A_{R,t}$) in pore water and shoot ($A_{S,t}$) in overlying water was determined by macrophyte growth, and specific surface area (m^2/kg) of root ($A_{SP,R}$) or shoot ($A_{SP,S}$). Specific surface area for roots and shoots were defined as 25 m^2/kg for *E. canadensis* and 40 m^2/kg for *M. spicatum*.[8]

$$A_{R,t} = A_{SP,R} M_{R,t} \quad \text{(S3)}$$

$$A_{S,t} = A_{SP,S} M_{S,t} \quad \text{(S4)}$$

Stem cross-sectional area ($A_{TR,t}$; m^2) was calculated from relative stem biomass growth, assuming a cylindrical shape and constant density of the stem:

$$A_{TR,t} = A_{t=0} \frac{l_{t=0}}{l_t} e^{k_{G,R} t} \quad \text{(S5)}$$

Length of the main stem (l_t; m) was modelled exponentially, with the first order length growth rate constant ($k_{g,l}$) deduced from measured data.

$$l_t = l_{t=0} e^{k_{g,l} t} \quad \text{(S6)}$$

Parameter estimation. For the optimisation of parameters, the Mathematica function *NMinimize* was used with the *SimulatedAnnealing* optimisation algorithm to find for each of the experiments a parameter set Θ^* for which the value of Pearson's Chi^2 statistic $X^*(Y, \Theta^*)$ was minimal. Options for *SimulatedAnnealing* included "*PerturbationScale= 3, SearchPoints =25, MaxIterations=200*".

Rough initial parameter estimates were used as starting values for the optimisation in order to take into account that various orders of magnitude of the parameter values are expected from theory.

Goodness-of-fit of the model was calculated using the Pearson's Chi2 statistic defined as:

$$\mathrm{Chi}^2(\mathrm{Y}, \Theta) = \sum_{\mathrm{Y} \in (\mathrm{C_W}, \mathrm{C_S}, \mathrm{C_R})} \sum_{\mathrm{i}=1}^{\mathrm{n}} \frac{(\mathrm{Y_i} - \mathrm{S_i}(\Theta))^2}{\mathrm{Y_i}} \quad \text{(S7)}$$

where there are n observations in time, Yi are the measured concentrations in overlying water (CW), in roots (CR), and shoots (CS), and Si are the corresponding model simulations at time points i using the parameter vector θ.

Calculation of the overall sediment-water mass transfer coefficient for linuron. The transfer parameters for linuron across the sediment bed can be a priori calculated based on established mass transfer theory.[12] In the linuron experiments, the contaminated sediment and overlying water phase were separated by a 0.5 cm clean layer of sediment. This means that this transfer experiences a resistance from the benthic boundary layer (BBL) as well as from the transfer through the sediment bed. Transfer across the sediment bed can be modelled as molecular diffusion retarded by sorption to the organic matter in the sediment, with corrections for the diffusion path of linuron in the sediment based on porosity and tortuosity.

The overall resistance to mass transport $1/K_L$ is:

$$\frac{1}{k_L} = \frac{1}{k_{L,BBL}} + \frac{1}{k_{L,SED}} \quad \text{(S8)}$$

in which $k_{L,BBL}$ is the BBL mass transfer coefficient (0.025 m/d) and $k_{L,SED}$ is the mass transfer coefficient in the sediment bed. The value for $k_{L,SED}$ can be calculated as:

$$k_{L,SED} = \frac{D_{eff}}{\delta} \quad \text{(S9)}$$

with D_{eff} is the effective diffusion coefficient for linuron in the sediment bed (m^2/d) and δ is the thickness of the sediment layer (m).

The effective diffusion coefficient D_{eff} can be calculated as:

$$D_{eff} = \frac{D_m \Phi}{(1-\Phi)\sigma K_D \tau} \quad \text{(S10)}$$

with D_m is the molecular diffusion coefficient for linuron in water (m^2/d), Φ is sediment porosity (-), σ is the density of the sediment (kg/L), K_D is the equilibrium distribution coefficient for sorption of linuron to the sediment (L/kg) and τ (-) is the tortuosity of the diffusion path.

$$K_D = K_{oc} f_{oc} \quad \text{(S11)}$$

The overall value for k_L (eq 1) was calculated by substitution of eq 2 and 3 in eq 1 and using the parameters as indicated in Table S9, which yields a value of $5.86*10^{-4}$ m/d.

Table S8. Parameters used for the calculation of the overall sediment-water mass transfer coefficient for linuron.

Parameter	Value	Unit	Reference
Density of the sediment (σ)	1.208	kg/L	[13]
Fraction of organic carbon (f_{oc})	0.02	-	[13]
Organic carbon - water equilibrium distribution coefficient (K_{oc})	406	L/kg	[13]
Equilibrium distribution coefficient (K_D)	8.12	L/kg	[13]
Tortuosity (τ)	1.5	-	[14]
Sediment porosity (Φ)	0.464	-	[13]
Thickness of the sediment layer (δ)	0.005	m	[13]
Molecular diffusion coefficient (D_m)	$5.90*10^{-6}$	cm^2/s	[15]
Benthic boundary layer mass transfer coefficient ($k_{L,BBL}$)	0.025	m/d	[16]

Calculation of Confidence Intervals. The calculation of the confidence intervals of 90% (α = 0.90) for the parameters was processed using the likelihood-profiling method as described previously.[17] In short, for one of the parameters (i.e. the one for which the confidence intervals should be calculated), values were changed in steps starting at the optimal parameter value. For each changed parameter value, all other parameters were optimised resulting in a new optimal parameter set Θ', and values for the Pearson's Chi^2 statistic $X'(Y,\Theta')$ were calculated for this changed parameter set. The procedure of changing the values of the parameter was repeated until either the condition:

$$\frac{X'}{X^*} = \frac{Chi(Y,\Theta')}{Chi(Y,\Theta^*)} \geq \frac{p}{n-p} F(p, n-p, 90\%) \qquad \text{(S12)}$$

was fulfilled or the parameter was varied to a value of more than two orders of magnitude below or above the optimal parameter value. In equation 13, *n* is the number of data used in the optimization (n=XX), *p* is the number of fitted parameters (3 or 4), and *F* (*p,n-p*,90%) is the *F* distribution.

Table S9. Overview of model parameters for the macrophyte model. Abbreviations are: A to E are different concentration levels, EC *Elodea canadensis* capped system, EO *Elodea canadensis* open system, MC *Myriophyllum spicatum* capped system, MO *Myriophyllum spicatum* open system, BDL below detection limit, PF parameter was fitted.

		LIN					CPF			
	Unit	**A**	**B**	**C**	**D**	**E**	**EC**	**EO**	**MC**	**MO**
A_{SED}	m^2	0.0050	0.0050	0.0050	0.0050	0.0050	0.0079	0.0079	0.0079	0.0079
M_{SED}	kg DW	0.200	0.200	0.200	0.200	0.200	0.298	0.298	0.298	0.298
V_{OW}	m^3	0.002	0.002	0.002	0.002	0.002	0.0015	0.0015	0.0015	0.0015
V'_{PW}	m^3	0.00170	0.00170	0.00170	0.00170	0.00170	0.04868	0.04868	0.04868	0.04868
K_L	m/d	0.00024	0.00024	0.00024	0.00024	0.00024	0	0.025	0	0.025
$A_{SP,S}$	m^2/kg	40	40	40	40	40	25	25	40	40
$A_{SP,R}$	m^2/kg	40	40	40	40	40	25	25	40	40
$M_{R,init}$	kg DW	2.36E-06	2.90E-06	4.76E-06	3.85E-06	3.4E-06	1.44E-05	1.22E-05	1.58E-05	2.25E-05
$M_{S,init}$	kg DW	3.27E-04	3.58E-04	2.51E-04	3.17E-04	2.48E-04	5.50E-05	7.76E-05	1.66E-04	2.30E-04
$k_{G,R}$	d^{-1}	1.62E-01	1.46E-01	1.40E-01	1.38E-01	9.82E-02	2.47E-02	5.42E-02	4.53E-02	1.88E-02
$k_{G,S}$	d^{-1}	5.02E-02	4.06E-02	7.02E-02	4.49E-02	3.25E-02	2.70E-02	4.14E-02	3.32E-02	3.09E-02
l_{init}	m	1.19E-01	1.03E-01	1.09E-01	1.01E-01	1.24E-01	6.24E-02	6.88E-02	1.01E-01	1.34E-01
$k_{G,l}$	m/d	2.32E-02	2.97E-02	3.00E-02	3.14E-02	4.07E-03	5.53E-03	3.41E-04	2.56E-02	1.15E-02
$A_{TR,init}$	m^2	1.13E-08	1.13E-08	1.13E-08	1.13E-08	1.13E-08	7.85E-09	7.85E-09	1.13E-08	1.13E-08
$C_{OW,init}$	$\mu g/m^3$	0	0	0	0	0	3.97	4.57	0	0
$C_{PW,init}$	$\mu g/m^3$	BDL	2545	33650	447000	1079500	3.22	3.22	3.22	3.22
K_S	m^3/kg	0.4	0.4	0.4	0.4	0.4	3	4	2	1
K_R	m^3/kg	0.19	0.19	0.19	0.19	0.19	5.5	6.4	3.6	4.7
k_{LOSS}	d^{-1}	0	0	0	0	0	0	0	0	0

Table S9 continued.

		PCB 2				PCB 3				PCB 28			
	Unit	**EC**	**EO**	**MC**	**MO**	**EC**	**EO**	**MC**	**MO**	**EC**	**EO**	**MC**	**MO**
A_{SED}	m^2	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079
M_{SED}	kg DW	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298
V_{OW}	m^3	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015
V'_{PW}	m^3	0.09027	0.09027	0.09027	0.09027	0.09027	0.09027	0.09027	0.09027	0.85504	0.85504	0.85504	0.85504
K_L	m/d	0	0.025	0	0.025	0	0.025	0	0.025	0	0.025	0	0.025
$A_{SP,S}$	m^2/kg	25	25	40	40	25	25	40	40	25	25	40	40
$A_{SP,R}$	m^2/kg	25	25	40	40	25	25	40	40	25	25	40	40
$M_{R,init}$	kg DW	1.44E-05	1.22E-05	1.58E-05	2.25E-05	1.44E-05	1.22E-05	1.58E-05	2.25E-05	1.44E-05	1.22E-05	1.58E-05	2.25E-05
$M_{S,init}$	kg DW	5.50E-05	7.76E-05	1.66E-04	2.30E-04	5.50E-05	7.76E-05	1.66E-04	2.30E-04	5.50E-05	7.76E-05	1.66E-04	2.30E-04
$k_{G,R}$	d^{-1}	2.47E-02	5.42E-02	4.53E-02	1.88E-02	2.47E-02	5.42E-02	4.53E-02	1.88E-02	2.47E-02	5.42E-02	4.53E-02	1.88E-02
$k_{G,S}$	d^{-1}	2.70E-02	4.14E-02	3.32E-02	3.09E-02	2.70E-02	4.14E-02	3.32E-02	3.09E-02	2.70E-02	4.14E-02	3.32E-02	3.09E-02
l_{init}	m	6.24E-02	6.88E-02	1.01E-01	1.34E-01	6.24E-02	6.88E-02	1.01E-01	1.34E-01	6.24E-02	6.88E-02	1.01E-01	1.34E-01
$k_{G,l}$	m/d	5.53E-03	3.41E-04	2.56E-02	1.15E-02	5.53E-03	3.41E-04	2.56E-02	1.15E-02	5.53E-03	3.41E-04	2.56E-02	1.15E-02
$A_{TR,init}$	m^2	7.85E-09	7.85E-09	1.13E-08	1.13E-08	7.85E-09	7.85E-09	1.13E-08	1.13E-08	7.85E-09	7.85E-09	1.13E-08	1.13E-08
$C_{OW,init}$	$\mu g/m^3$	2308.07	2137.07	3171.37	3106.15	0	0	0	0	1057	1826.76	3337.32	3542
$C_{PW,init}$	$\mu g/m^3$	0	0	0	0	4.29	4.29	4.29	4.29	0	0	0	0
K_S	m^3/kg	3	4	2	1	3	4	2	1	37	22	22	16
K_R	m^3/kg	2.7	2.7	5.3	4.8	2.7	2.7	5.3	4.8	34.8	71.0	4.0	5.9
k_{LOSS}	d^{-1}	PF	PF	PF	PF	PF	PF	PF	PF	0	0	0	0

Table S9 continued.

		PCB 29				PCB 149				PCB 155			
	Unit	**EC**	**EO**	**MC**	**MO**	**EC**	**EO**	**MC**	**MO**	**EC**	**EO**	**MC**	**MO**
A_{SED}	m^2	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079	0.0079
M_{SED}	kg												
	DW	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298	0.298
V_{OW}	m^3	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015	0.0015
V'_{PW}	m^3	0.85504	0.85504	0.85504	0.85504	10.34702	10.34702	10.34702	10.34702	7.15835	7.15835	7.15835	7.15835
K_L	m/d	0	0.025	0	0.025	0	0.025	0	0.025	0	0.025	0	0.025
$A_{SP,S}$	m^2/kg	25	25	40	40	25	25	40	40	25	25	40	40
$A_{SP,R}$	m^2/kg	25	25	40	40	25	25	40	40	25	25	40	40
$M_{R,init}$	kg												
	DW	1.44E-05	1.22E-05	1.58E-05	2.25E-05	1.44E-05	1.22E-05	1.58E-05	2.25E-05	1.44E-05	1.22E-05	1.58E-05	2.25E-05
$M_{S,init}$	kg												
	DW	5.50E-05	7.76E-05	1.66E-04	2.30E-04	5.50E-05	7.76E-05	1.66E-04	2.30E-04	5.50E-05	7.76E-05	1.66E-04	2.30E-04
$k_{G,R}$	d^{-1}	2.47E-02	5.42E-02	4.53E-02	1.88E-02	2.47E-02	5.42E-02	4.53E-02	1.88E-02	2.47E-02	5.42E-02	4.53E-02	1.88E-02
$k_{G,S}$	d^{-1}	2.70E-02	4.14E-02	3.32E-02	3.09E-02	2.70E-02	4.14E-02	3.32E-02	3.09E-02	2.70E-02	4.14E-02	3.32E-02	3.09E-02
l_{init}	m	6.24E-02	6.88E-02	1.01E-01	1.34E-01	6.24E-02	6.88E-02	1.01E-01	1.34E-01	6.24E-02	6.88E-02	1.01E-01	1.34E-01
$k_{G,l}$	m/d	5.53E-03	3.41E-04	2.56E-02	1.15E-02	5.53E-03	3.41E-04	2.56E-02	1.15E-02	5.53E-03	3.41E-04	2.56E-02	1.15E-02
$A_{TR,init}$	m^2	7.85E-09	7.85E-09	1.13E-08	1.13E-08	7.85E-09	7.85E-09	1.13E-08	1.13E-08	7.85E-09	7.85E-09	1.13E-08	1.13E-08
$C_{OW,init}$	µg/m^3	0	0	0	0	144.58	308.26	658.98	891.38	0	0	0	0
$C_{PW,init}$	µg/m^3	0.83	0.83	0.83	0.83	0	0	0	0	0.08	0.08	0.08	0.08
K_S	m^3/kg	37	22	22	16	58	23	36	18	58	23	36	18
K_R	m^3/kg	34.8	71.0	4.0	5.9	375.8	649.8	278.6	360.3	375.8	649.8	278.6	360.3
k_{LOSS}	d^{-1}	0	0	0	0	0	0	0	0	0	0	0	0

Results

Water quality. Average (SD) water quality values were water temperature 21.5 (1.7) ºC, pH 9.14 (0.86), oxygen 13.01 (3.44) mg/L, and conductivity 396 (98) µS/m for all treatments over all time points. Blue green algae were not measured at any time point. Brown algae developed slightly over time. At 28 days, average concentration ranged from 0 to 58 µg/l for *Elodea Canadensis*, and 0 to 25 µg/l for *Myriophyllum spicatum* treatments. Green algea concentrations followed the same trend and increased to max 76.42 µg/l for *M. spicatum* treatments.

Table S10. Average (SD) water quality parameters per treatment and species

Treatment/species		pH (-)	SD	Temp. (°C)	SD	O_2 (mg/L)	SD	Cond. (µS/cm)	SD
Capped	***Elodea canadenis***								
	Control	8.71	0.35	21.7	0.6	10.37	0.95	334	36
	Spiked	8.36	0.68	20.0	1.3	10.26	2.19	355	75
	Myriophyllum spicatum								
	Control	9.65	0.39	23.3	0.6	14.48	2.86	359	50
	Spiked	9.44	0.54	20.7	1.1	13.75	2.65	322	26
	No Macrophyte								
	Leakage control	8.39	0.48	21.9	1.0	9.84	2.32	342	33
Open	***Elodea canadenis***								
	Control	8.76	1.60	21.4	0.8	12.46	2.77	477	107
	Control solvent	9.23	0.58	21.7	0.8	12.40	2.82	481	92
	Spiked	8.64	0.70	20.1	0.9	11.63	2.45	442	119
	Myriophyllum spicatum								
	Control	9.79	0.32	23.3	0.8	15.44	2.44	464	89
	Control solvent	9.93	0.43	23.5	0.8	15.74	3.12	467	91
	Spiked	9.73	0.48	22.6	1.0	15.71	3.59	419	95

Macrophyte endpoints.

Table S11. Total length and biomass for *Elodea canadensis* and *Myriophyllum spicatum* in the control treatments (n=3) at t=28.

Treatment	Total Length (cm)			Total biomass (g DW)		
	Average	SD	CV (%)	Average	SD	CV (%)
Myriophyllum spicatum						
Capped control	42.1	10.7	25.4	0.1019	0.0134	13.1
Open control	40.1	0.8	2.1	0.1712	0.0575	33.6
Open solvent control	47.7	5.3	11.1	0.2180	0.0286	13.1
Elodea canadensis						
Capped control	14.4	3.5	24.2	0.0561	0.0086	15.3
Open control	16.3	3.6	21.9	0.0914	0.0099	10.8
Open solvent control	16.3	1.8	11.1	0.1151	0.0267	23.2

Table S12. Average (SD) specific growth rates (SGR) at day 28, and modelled growth rates (d^{-1}) based on exponential growth for *Elodea canadensis* and *Myriophyllum spicatum* for capped and open systems.

	Measured		Modelled		
	SGR total length	SGR total biomass	Growth rate main stem length (d^{-1})	Growth rate shoots (d^{-1})	Growth rate roots (d^{-1})
Elodea canadensis					
capped systems	0.025 (0.007)	0.029 (0.006)	0.006	0.027	0.025
open systems	0.053 (0.003)	0.044 (0.008)	0.0003	0.041	0.054
Myriophyllum spicatum					
capped systems	0.048 (0.011)	0.026 (0.008)	0.026	0.033	0.045
open systems	0.051 (0.006)	0.042 (0.013)	0.012	0.031	0.019

Chemical flows in sediment-water macrophyte systems.

Table S13. Average overlying water concentrations (ng/L) (n=3) for *Elodea canadensis.*[a]

Elodea canadensis			Average concentrations in overlying water (ng/L) (n=3)						
Treatment		**Time (d)**	**PCB 2**	**PCB 3**	**PCB 28**	**PCB 29**	**CPF**	**PCB 149**	**PCB 155**
Background	B&S	0	0.34	0.00	0.92	0.00	6.25	0.00	0.00
Controls	AC	0	0.00	BDL	0.00	BDL	9.04	BDL	BDL
	BC	0	0.50	BDL	1.66	BDL	49.49	BDL	BDL
	BS	0	0.33	BDL	1.83	BDL	18.35	BDL	BDL
	AC	28	0.05	BDL	0.28	0.03	0.42	BDL	0.04
	BC	28	0.03	BDL	0.35	BDL	0.48	0.05	0.01
	BS	28	0.03	0.02	0.34	1.68	0.69	0.05	0.68
Control layer	AP	0	2305.63	BDL	3330.81	BDL	0.00	457.47	BDL
	AP	28	0.98	0.16	30.17	1.81	0.24	9.59	0.57

[a]B&S Barko and Smart medium, BDL = below detection limit, , A=capped, B=open, C=non-spiked control, S=non-spiked solvent control

Table S13. Continued

Elodea canadensis			Average concentrations in overlying water (ng/L) (n=3)						
Treatment		**Time (d)**	**PCB 2**	**PCB 3**	**PCB 28**	**PCB 29**	**CPF**	**PCB 149**	**PCB 155**
Capped(A)	A1	0	2186.10	BDL	4037.88	BDL	3.77	430.08	BDL
	A3	0	2138.76	BDL	4986.71	BDL	3.82	438.94	BDL
	A7	0	2481.49	BDL	3412.32	BDL	5.03	467.16	BDL
	A14	0	2450.29	BDL	3278.02	BDL	1.68	461.80	BDL
	A28	0	2271.50	BDL	5482.16	BDL	5.53	578.40	BDL
	A1	1	563.92	BDL	936.14	0.02	BDL	86.37	0.03
	A3	3	251.91	BDL	307.98	0.03	0.47	24.41	0.03
	A7	7	32.54	BDL	105.34	0.01	0.33	14.84	0.01
	A14	14	6.80	BDL	71.91	0.01	0.39	11.34	0.04
	A28	28	1.07	0.05	39.29	0.04	1.65	9.63	0.03
Open (B)	B1	0	1816.51	BDL	4764.33	BDL	2.97	443.92	BDL
	B3	0	2119.32	BDL	2485.28	BDL	5.35	494.11	BDL
	B7	0	2355.93	BDL	3636.19	BDL	7.55	508.86	BDL
	B14	0	2543.47	BDL	3504.40	BDL	6.67	507.90	BDL
	B28	0	1850.11	BDL	4803.75	BDL	0.31	466.55	BDL
	B1	1	770.92	BDL	1557.96	0.28	5.17	120.03	0.09
	B3	3	161.93	BDL	307.18	0.18	3.13	40.08	0.05
	B7	7	19.60	0.68	167.49	0.47	21.76	20.59	0.25
	B14	14	3.66	0.54	69.95	0.42	6.34	16.01	0.24
	B28	28	0.58	0.35	18.72	0.45	0.76	13.27	0.58

Table S14. Average overlying water concentrations (ng/L) (n=3) for *Myriophyllum spicatum*[a]

Myriophyllum spicatum			Average concentrations in water (ng/L) (n=3)						
Treatment		**Time (d)**	**PCB 2**	**PCB 3**	**PCB 28**	**PCB 29**	**CPF**	**PCB 149**	**PCB 155**
Controls	AC	0	3.85	BDL	4.90	BDL	0.00	BDL	0.26
	BC	0	3.13	BDL	7.35	BDL	31.41	BDL	0.53
	BS	0	9.93	BDL	12.01	BDL	BDL	BDL	0.50
	AC	28	0.02	BDL	0.12	BDL	BDL	BDL	BDL
	BC	28	0.05	BDL	0.19	BDL	2.71	BDL	BDL
	BS	28	0.05	BDL	0.30	BDL	3.91	BDL	BDL
Capped (A)	A1	0	2982.01	0.17	8428.22	BDL	BDL	711.09	BDL
	A3	0	3820.51	BDL	9813.79	BDL	0.00	818.36	0.13
	A7	0	3431.20	BDL	9469.89	BDL	BDL	734.91	BDL
	A14	0	2894.01	BDL	8651.83	BDL	BDL	704.97	BDL
	A28	0	2666.00	BDL	8117.33	BDL	BDL	702.94	BDL
	A1	1	1453.29	BDL	1640.13	BDL	0.03	127.11	BDL
	A3	3	402.43	BDL	456.80	0.01	0.37	47.72	0.01
	A7	7	117.55	BDL	211.24	0.01	0.97	37.99	0.11
	A14	14	11.10	BDL	171.07	BDL	0.31	26.73	BDL
	A28	28	1.32	BDL	75.87	BDL	BDL	17.04	BDL
Open (B)	B1	0	2726.35	BDL	6529.20	BDL	1.12	631.09	0.40
	B3	0	3066.61	BDL	8354.93	BDL	BDL	680.03	BDL
	B7	0	3321.29	BDL	7832.13	BDL	BDL	606.61	BDL
	B14	0	3222.20	BDL	8385.37	BDL	BDL	735.71	BDL
	B28	0	3194.32	BDL	8581.06	BDL	BDL	700.17	0.16
	B1	1	1723.52	BDL	1855.77	0.04	1.83	139.83	0.02
	B3	3	464.03	BDL	265.37	0.05	3.05	48.84	0.02
	B7	7	68.00	BDL	243.82	0.10	2.51	33.08	0.02
	B14	14	10.90	0.43	169.28	0.31	4.02	27.17	0.10
	B28	28	1.01	0.30	71.50	0.32	0.35	20.29	0.12

[a] BDL = below detection limit, A=capped, B=open, C=non-spiked control, S=non-spiked solvent control

Table S15. Average sediment (µg/kg DW) (n=3) values spiked OECD sediment[a]

Treatment		Time (d)	Average concentration in sediment (µg/kg DW) (n=3) CPF	PCB 2	PCB 3	PCB 28	PCB 29	PCB 149	PCB 155
Control (ng/kg)		0	0.93	BDL	BDL	39.84	0.04	0.14	1.07
Spiked		0	26.96	BDL	13.07	0.00	15.14	0.00	18.85
Capped (A)	P	28	30.94	BDL	12.70	0.00	14.05	0.00	16.93
Capped (A)	M	28	25.33	BDL	11.99	0.00	15.55	0.00	17.94
Open (B)	M	28	22.20	0.17	14.66	0.72	17.40	0.06	19.82
Capped (A)	E	28	18.35	0.07	11.32	0.00	14.38	0.00	17.21
Open (B)	E	28	18.00	0.15	11.46	0.47	13.62	0.18	15.87

[a] BDL = below detection limit, A=capped, B=open, P=Cap control without macrophytes, M=*Myriophyllum spicatum*, E=*Elodea canadensis*

Table S16. Average pore water (ng/L) concentrations at t=0 for spiked OECD sediment (n=3)

	CPF	PCB 3	PCB 29	PCB 155
Pore water (ng/L)	12.76	4.29	0.83	0.08
Standard deviation	10.21	1.51	0.45	0.02

Table S17. Average shoot concentrations (µg/kg DW) (n=3) for *Elodea canadensis* and *Myriophyllum spicatum*[a]

		Average concentration in shoots (µg/kg DW) (n=3)						
Treatment	**Time (d)**	**PCB 2**	**PCB 3**	**PCB 28**	**PCB 29**	**CPF**	**PCB 149**	**PCB 155**
Elodea canadensis								
A1	1	1360.80	BDL	14685.73	BDL	BDL	1723.01	BDL
A3	3	266.53	BDL	10388.72	BDL	BDL	1753.61	BDL
A7	7	78.29	BDL	6502.05	BDL	BDL	1673.91	BDL
A14	14	15.56	BDL	5376.12	BDL	BDL	1289.81	BDL
A28	28	3.29	BDL	1490.69	BDL	BDL	560.54	BDL
B1	1	998.72	BDL	15199.19	1.26	BDL	1486.14	BDL
B3	3	207.54	BDL	12307.87	1.88	BDL	2128.59	1.49
B7	7	78.87	BDL	8419.53	5.86	17.35	1746.51	3.06
B14	14	13.18	BDL	3049.24	3.52	12.15	647.60	2.75
B28	28	2.18	0.84	404.43	4.27	5.75	299.67	5.52
Myriophyllum spicatum								
A1	1	2539.09	BDL	12987.17	0.75	8.56	3164.40	0.42
A3	3	1397.08	BDL	13555.18	BDL	BDL	3846.20	BDL
A7	7	306.13	BDL	6570.86	BDL	2.67	2284.70	BDL
A14	14	72.02	BDL	2713.18	BDL	BDL	1198.17	BDL
A28	28	2.70	BDL	1323.22	0.26	BDL	539.17	BDL
B1	1	1878.44	BDL	14899.39	BDL	BDL	3437.88	BDL
B3	3	1249.44	BDL	9997.61	1.72	4.34	2815.42	0.91
B7	7	254.35	BDL	6247.57	1.11	2.73	1995.52	0.60
B14	14	61.62	BDL	3882.01	2.85	5.18	987.43	2.06
B28	28	1.45	0.49	1070.91	1.82	1.66	371.52	2.62

[a] BDL = below detection limit, A=capped, B=open

Table S18. Average root concentrations (µg/kg DW) (n=3) for *Elodea canadensis* and *Myriophyllum spicatum*[a]

		Average concentration in root (µg/kg DW) (n=3)						
Treatment	**Time (d)**	**PCB 2**	**PCB 3**	**PCB 28**	**PCB 29**	**CPF**	**PCB 149**	**PCB 155**
Elodea canadensis								
A1	1	26.77	BDL	321.47	6.56	32.92	32.65	BDL
A3	3	6.76	BDL	256.08	6.76	24.14	39.98	BDL
A7	7	24.44	BDL	224.88	12.71	62.84	24.99	BDL
A14	14	9.25	6.77	187.19	15.74	49.25	12.71	7.04
A28	28	BDL	11.56	415.99	28.89	70.20	80.99	30.06
B1	1	59.49	BDL	950.47	6.21	BDL	69.56	BDL
B3	3	12.65	BDL	445.97	10.67	33.61	44.44	BDL
B7	7	16.46	BDL	1505.42	28.54	89.93	181.83	21.82
B14	14	14.68	9.03	675.30	30.95	69.29	68.73	29.80
B28	28	BDL	11.52	292.21	58.96	81.93	45.58	51.98
Myriophyllum spicatum								
A1	1	714.49	BDL	4767.92	9.01	43.68	776.49	3.45
A3	3	108.11	6.44	458.19	10.81	BDL	51.28	4.38
A7	7	29.43	19.52	301.89	28.51	43.68	16.79	11.17
A14	14	8.48	23.44	275.22	40.52	51.14	18.19	17.13
A28	28	BDL	22.74	317.42	3.33	46.00	22.98	22.29
B1	1	88.94	6.28	226.41	11.16	16.74	23.94	5.58
B3	3	187.85	6.85	3537.00	23.73	28.41	475.13	10.03
B7	7	60.23	16.07	1587.37	29.23	38.66	324.70	14.38
B14	14	17.61	27.01	124.02	48.93	64.10	32.06	18.18
B28	28	BDL	20.61	336.87	4.86	60.57	22.12	28.82

[a] BDL = below detection limit, A=capped, B=open

Mass distribution of test chemicals over the compartments.

Mass in overlying water for PCBs spiked in the water layer decreased rapidly with 0.92% (PCB 2 EB) to 5.17% (PCB 149 MA) of initial mass left after 7 days, to 0.03% (PCB 2 E and MB) to 3.02% (PCB 149 MB) of initial mass after 28 days. Mass decreased less for PCBs with a higher hydrophobicity.

Mass in sediment for PCBs and CPF spiked in the sediment layer was stable with 100% of initial mass left after 7 days, to 68% (CPF EA) to 114% (PCB 149 MB) of initial mass after 28 days. Mass decreased most for CPF in systems with *E. canadensis*. PCBs spiked in the water layer increased slowly over time, a maximum of 0.11% (PCB 149 EA) was found in the sediment on day 7, and 7.24% (PCB 149 EB) on day 28.

Mass in shoots for PCBs spiked in the water layer increased first rapidly, then started to decrease again with 0.21% (PCB 2 EB) to 62.87% (PCB 149 MB) of initial mass after 7 days to 0.02% (PCB 2 MA, E and MB) to 19.02% (PCB 149 MB) of initial mass after 28 days. Mass in shoots was higher and decreased less for PCBs with a higher hydrophobicity. Mass in *M. spicatum* was higher than mass in *E. Canadensis*. For PCBs and CPF spiked in the sediment layer, a maximum of 0.01% for PCBs (PCB 29 E and MB) and 0.02% CPF (EB) was found in shoots on day 7, and 0.02% for PCBs (PCB 2, 29, 155 MA, E and MB) and 0% for CPF on day 28.

Mass in roots for PCBs spiked in the water layer increased first, then started to decrease again with 0% (PCB 2 EB) to 1.51% (PCB 149 MB) of initial mass after 7 days to 0% (PCB 2) to 0.38% (PCB 149 EB) of initial mass after 28 days. Mass in roots was higher and decreased less for PCBs with a high hydrophobicity. For PCBs and CPF spiked in the sediment layer, a maximum of 0.03% for PCBs (PCB 29 MB) and 0.02% CPF (EB) was found in roots on day 7, and 0.07% for PCBs (PCB 29 EB) and 0.06% for CPF (EB) on day 28.

Table S19. Proportion of initial mass per day for *Elodea canadensis* in capped systems, based on measured concentrations

A/E	Proportion of initial mass (%)						
	Time (d)	**Water**	**Shoots**	**Roots**	**Sediment**	**Sum**	**Loss**
PCB 2	1	24.46	1.94	0.00	0.00	26.4	73.6
	3	10.93	0.52	0.00	0.00	11.4	88.6
	7	1.41	0.15	0.01	0.00	1.6	98.4
	14	0.29	0.04	0.00	0.00	0.3	99.7
	28	0.05	0.01	0.00	0.61	0.7	99.3
PCB 3	1	0.00	0.00	0.00	100.00	100.0	0.0
	3	0.00	0.00	0.00	100.00	100.0	0.0
	7	0.00	0.00	0.00	100.00	100.0	0.0
	14	0.00	0.00	0.00	100.00	100.0	0.0
	28	0.00	0.00	0.00	86.58	86.6	13.4
PCB 28	1	22.08	11.43	0.09	0.00	33.6	66.4
	3	7.26	10.93	0.06	0.00	18.3	81.7
	7	2.48	6.54	0.04	0.00	9.1	90.9
	14	1.70	6.92	0.08	0.00	8.7	91.3
	28	0.93	2.87	0.17	0.00	4.0	96.0
PCB 29	1	0.00	0.00	0.00	100.00	100.0	0.0
	3	0.00	0.00	0.00	100.00	100.0	0.0
	7	0.00	0.00	0.00	100.00	100.0	0.0
	14	0.00	0.00	0.01	100.00	100.0	0.0
	28	0.00	0.00	0.02	94.99	95.0	5.0
PCB 149	1	18.17	11.92	0.08	0.11	30.3	69.7
	3	5.14	16.63	0.07	0.11	21.9	78.1
	7	3.12	15.38	0.04	0.11	18.6	81.4
	14	2.39	14.76	0.05	0.11	17.3	82.7
	28	2.03	8.99	0.29	0.00	11.3	88.7
PCB 155	1	0.00	0.00	0.00	100.00	100.0	0.0
	3	0.00	0.00	0.00	100.00	100.0	0.0
	7	0.00	0.00	0.00	100.00	100.0	0.0
	14	0.00	0.00	0.00	100.00	100.0	0.0
	28	0.00	0.00	0.00	91.34	91.3	8.7
CPF	1	0.00	0.00	0.00	99.93	99.9	0.1
	3	0.01	0.00	0.00	99.93	99.9	0.1
	7	0.01	0.00	0.01	99.93	99.9	0.1
	14	0.01	0.00	0.01	99.93	99.9	0.1
	28	0.03	0.00	0.00	67.99	68.0	32.0

Table S20. Proportion of initial mass per day for *Elodea canadensis* in open systems, based on measured concentrations

B/E	Proportion of initial mass (%)						
	Time (d)	**Water**	**Shoots**	**Roots**	**Sediment**	**Sum**	**Loss**
PCB 2	1	36.07	2.26	0.00	0.00	38.3	61.7
	3	7.58	0.52	0.00	0.00	8.1	91.9
	7	0.92	0.21	0.00	0.00	1.1	98.9
	14	0.17	0.08	0.00	0.00	0.2	99.8
	28	0.03	0.02	0.00	1.41	1.5	98.5
PCB 3	1	0.00	0.00	0.00	100.00	100.0	0.0
	3	0.00	0.00	0.00	100.00	100.0	0.0
	7	0.00	0.00	0.00	100.00	100.0	0.0
	14	0.02	0.00	0.00	100.00	100.0	0.0
	28	0.01	0.00	0.02	87.64	87.7	12.3
PCB 28	1	40.58	19.23	0.31	0.00	60.1	39.9
	3	8.00	16.80	0.14	0.00	24.9	75.1
	7	4.36	12.59	0.46	0.00	17.4	82.6
	14	1.82	9.36	0.23	0.00	11.4	88.6
	28	0.49	1.64	0.30	2.42	4.8	95.2
PCB 29	1	0.01	0.00	0.00	100.00	100.0	0.0
	3	0.01	0.00	0.00	100.00	100.0	0.0
	7	0.02	0.01	0.01	100.00	100.0	0.0
	14	0.01	0.01	0.01	100.00	100.0	0.0
	28	0.01	0.02	0.07	89.91	90.0	10.0
PCB 149	1	24.79	14.85	0.18	0.10	39.9	60.1
	3	8.28	23.22	0.11	0.10	31.7	68.3
	7	4.25	20.75	0.44	0.10	25.5	74.5
	14	3.31	16.10	0.18	0.10	19.7	80.3
	28	2.74	9.58	0.38	7.24	19.9	80.1
PCB 155	1	0.00	0.00	0.00	100.00	100.0	0.0
	3	0.00	0.00	0.00	100.00	100.0	0.0
	7	0.01	0.00	0.01	100.00	100.0	0.0
	14	0.01	0.01	0.01	100.00	100.0	0.0
	28	0.02	0.02	0.05	84.23	84.3	15.7
CPF	1	0.10	0.00	0.00	100.00	100.1	-0.1
	3	0.06	0.00	0.01	100.00	100.1	-0.1
	7	0.41	0.02	0.02	100.00	100.4	-0.4
	14	0.12	0.00	0.02	100.00	100.1	-0.1
	28	0.00	0.00	0.06	66.76	66.8	33.2

Table S21. Proportion of initial mass per day for *Myriophyllum spicatum* in capped systems, based on measured concentrations

A/M	Proportion of initial mass (%)						
	Time (d)	**Water**	**Shoots**	**Roots**	**Sediment**	**Sum**	**Loss**
PCB 2	1	46.01	10.32	1.72	0.00	58.0	42.0
	3	12.74	4.80	0.13	0.00	17.7	82.3
	7	3.72	1.45	0.00	0.00	5.2	94.8
	14	0.35	0.37	0.01	0.00	0.7	99.3
	28	0.04	0.02	0.00	0.00	0.1	99.9
PCB 3	1	0.00	0.00	0.00	100.00	100.0	0.0
	3	0.00	0.00	0.01	100.00	100.0	0.0
	7	0.00	0.00	0.00	100.00	100.0	0.0
	14	0.00	0.00	0.03	100.00	100.0	0.0
	28	0.00	0.00	0.03	91.68	91.7	8.3
PCB 28	1	18.44	19.02	4.07	0.00	41.5	58.5
	3	5.13	15.48	0.20	0.00	20.8	79.2
	7	2.37	10.79	0.05	0.00	13.2	86.8
	14	1.92	4.99	0.09	0.00	7.0	93.0
	28	0.85	4.18	0.12	0.00	5.2	94.8
PCB 29	1	0.00	0.00	0.02	100.00	100.0	0.0
	3	0.00	0.00	0.01	100.00	100.0	0.0
	7	0.00	0.00	0.01	100.00	100.0	0.0
	14	0.00	0.00	0.04	100.00	100.0	0.0
	28	0.00	0.00	0.00	102.67	102.7	-2.7
PCB 149	1	17.31	56.71	8.04	0.07	82.1	17.9
	3	6.50	53.55	0.27	0.07	60.4	39.6
	7	5.17	45.87	0.03	0.07	51.1	48.9
	14	3.64	26.56	0.07	0.07	30.3	69.7
	28	2.32	20.25	0.10	0.00	22.7	77.3
PCB 155	1	0.00	0.00	0.01	100.00	100.0	0.0
	3	0.00	0.00	0.00	100.00	100.0	0.0
	7	0.00	0.00	0.00	100.00	100.0	0.0
	14	0.00	0.00	0.01	100.00	100.0	0.0
	28	0.00	0.00	0.02	95.18	95.2	4.8
CPF	1	0.00	0.00	0.06	100.00	100.1	-0.1
	3	0.01	0.00	0.00	100.00	100.0	0.0
	7	0.02	0.00	0.00	100.00	100.0	0.0
	14	0.01	0.00	0.03	100.00	100.0	0.0
	28	0.00	0.00	0.03	93.92	94.0	6.0

Table S22. Proportion of initial mass per day for *Myriophyllum spicatum* in open systems, based on measured concentrations

B/M		Proportion of initial mass (%)					
	Time (d)	**Water**	**Shoots**	**Roots**	**Sediment**	**Sum**	**Loss**
PCB 2	1	55.49	6.59	0.09	0.00	62.2	37.8
	3	14.94	6.76	0.40	0.00	22.1	77.9
	7	2.19	1.74	0.06	0.00	4.0	96.0
	14	0.35	0.54	0.00	0.00	0.9	99.1
	28	0.03	0.02	0.00	1.11	1.2	98.8
PCB 3	1	0.00	0.00	0.01	100.00	100.0	0.0
	3	0.00	0.00	0.02	100.00	100.0	0.0
	7	0.00	0.00	0.02	100.00	100.0	0.0
	14	0.02	0.00	0.00	100.00	100.0	0.0
	28	0.01	0.01	0.01	112.17	112.2	-12.2
PCB 28	1	23.38	20.63	0.09	0.00	44.1	55.9
	3	3.34	21.38	2.94	0.00	27.7	72.3
	7	3.07	16.63	0.62	0.00	20.3	79.7
	14	2.13	13.09	0.06	0.00	15.3	84.7
	28	0.90	4.75	0.08	1.79	7.5	92.5
PCB 29	1	0.00	0.00	0.01	100.00	100.0	0.0
	3	0.00	0.01	0.05	100.00	100.1	-0.1
	7	0.00	0.01	0.03	100.00	100.0	0.0
	14	0.01	0.03	0.00	100.00	100.0	0.0
	28	0.01	0.02	0.00	114.89	114.9	-14.9
PCB 149	1	20.85	55.91	0.11	0.07	76.9	23.1
	3	7.28	71.03	4.68	0.07	83.1	16.9
	7	4.93	62.87	1.51	0.07	69.4	30.6
	14	4.05	39.28	0.16	0.07	43.6	56.4
	28	3.02	19.02	0.06	1.83	23.9	76.1
PCB 155	1	0.00	0.00	0.00	100.00	100.0	0.0
	3	0.00	0.00	0.02	100.00	100.0	0.0
	7	0.00	0.00	0.01	100.00	100.0	0.0
	14	0.00	0.01	0.02	100.00	100.0	0.0
	28	0.00	0.02	0.01	105.18	105.2	-5.2
CPF	1	0.03	0.00	0.01	100.00	100.0	0.0
	3	0.06	0.00	0.04	100.00	100.1	-0.1
	7	0.05	0.00	0.02	100.00	100.1	-0.1
	14	0.08	0.03	0.04	100.00	100.1	-0.1
	28	0.01	0.00	0.02	82.33	82.4	17.6

Table S23. Shoot and root-water partition coefficient (K_S Kr; m^3/kg) and BSAF (-) normalized on dry weight (DW) as well as on and lipids and organic matter (OM).

		DW normalized			*Lipid and OM normalized*		
		K_S (m^3/kg)	**K_R (m^3/kg)**	**BSAF (-)**	**K_S (m^3/kg)**	**K_R (m^3/kg)**	**BSAF (-)**
E. canadensis	*CPF*		5.5	2.6		47.9	1.4
Capped	*PCB 2*	3			48		
	PCB 3		2.7	0.9		31.9	0.6
	PCB 28	37			510		
	PCB 29		34.8	1.9		337.6	1.1
	PCB 149	58			828		
	PCB 155		375.8	1.6		3268.7	0.8
E. canadensis	*CPF*		6.4	3.0		78.8	2.3
Open	*PCB 2*	4			45		
	PCB 3		2.7	0.9		31.9	0.6
	PCB 28	22			266		
	PCB 29		71.0	3.9		860.8	2.9
	PCB 149	23			276		
	PCB 155		649.8	2.8		7920.2	2.1
M. spicatum	*CPF*		3.6	1.7		221.4	5.9
Capped	*PCB 2*	2			138		
	PCB 3		5.3	1.7		325.5	6.0
	PCB 28	22			1398		
	PCB 29		4.0	0.2		243.8	0.7
	PCB 149	36			2336		
	PCB 155		278.6	1.2		16765.3	4.0
M. spicatum	*CPF*		4.7	2.2		252.8	6.7
Open	*PCB 2*	1			72		
	PCB 3		4.8	1.6		228.3	4.2
	PCB 28	16			742		
	PCB 29		5.9	0.3		336.4	1.0
	PCB 149	18			914		
	PCB 155		360.3	1.5		18023.1	4.3

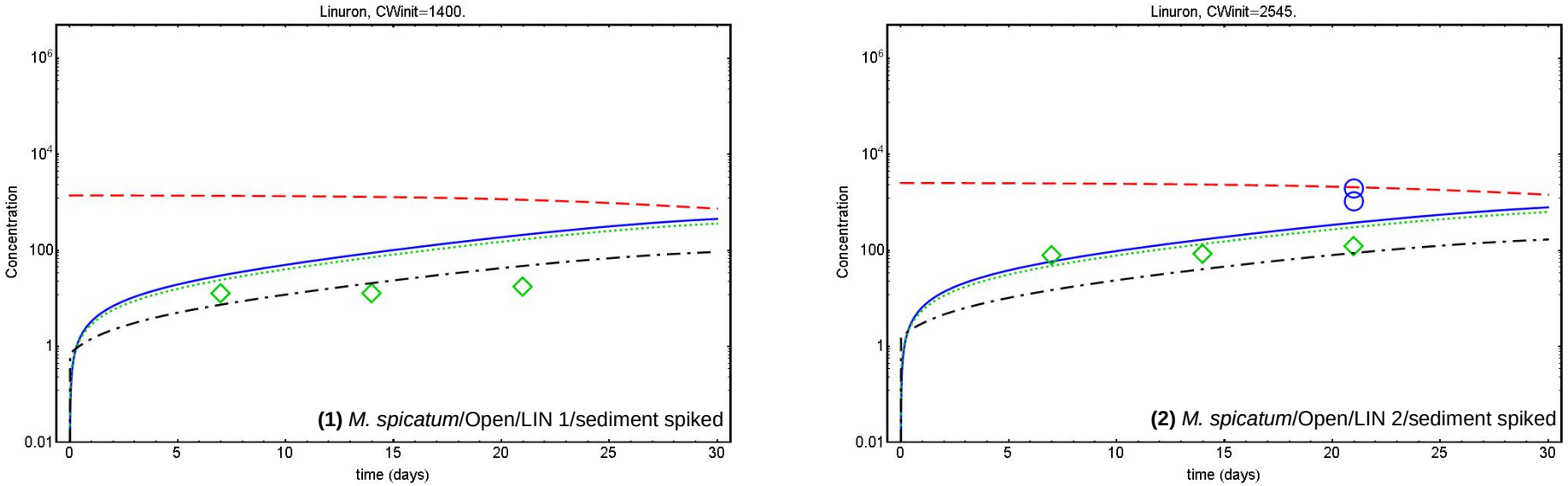
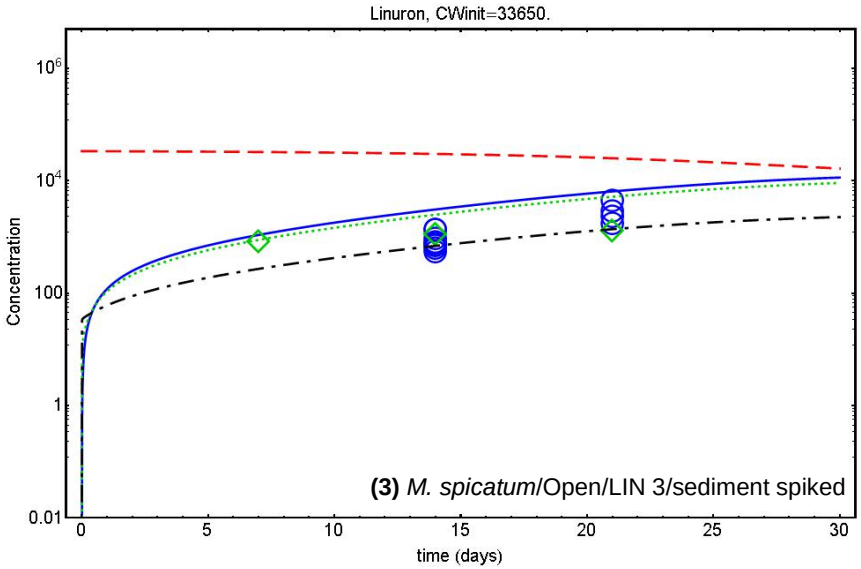
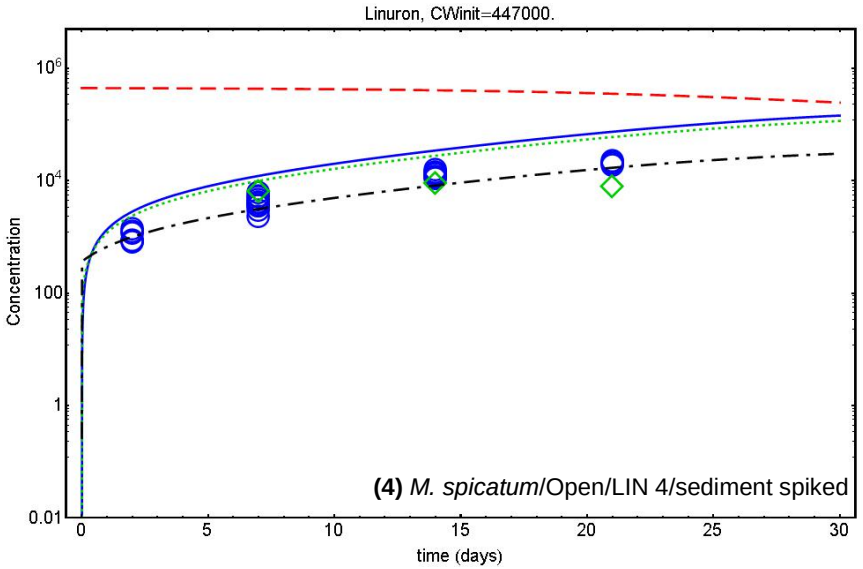


Figure S2. Measured (symbols) and modelled (curves) concentrations in overlying water (blue circles ○, solid line; µg/m^3), pore water (red dashed line; µg/m^3), shoots (green diamonds ◊, dotted line; µg/kg), and roots (black triangle Δ, dash dot line; µg/kg) for water spiked PCBs and sediment spiked PCBs, CPF, and LIN for *Elodea canadensis* and *Myriophyllum spicatum* in capped and open systems. Panels 1,2.





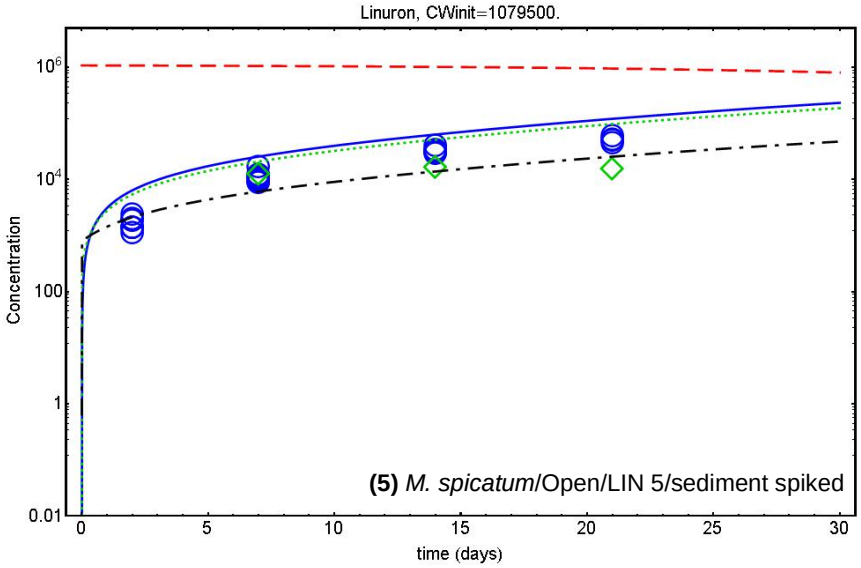
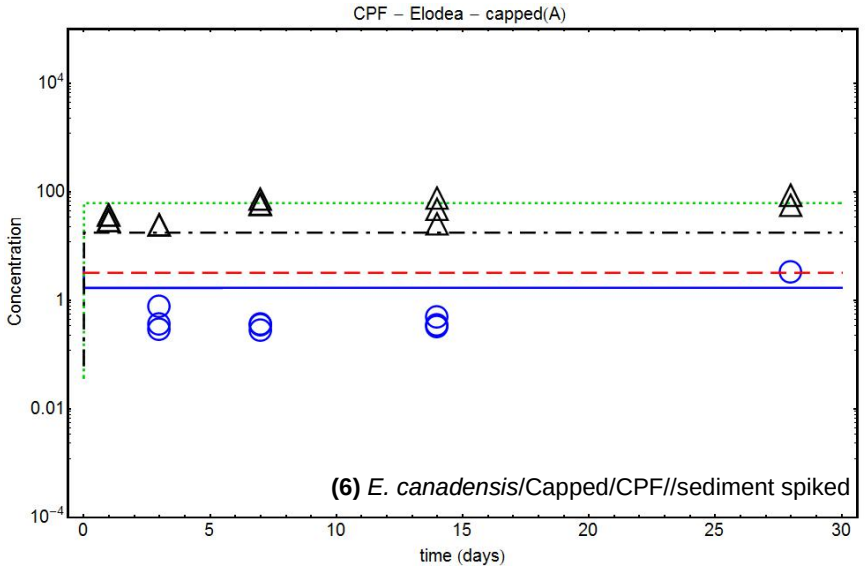
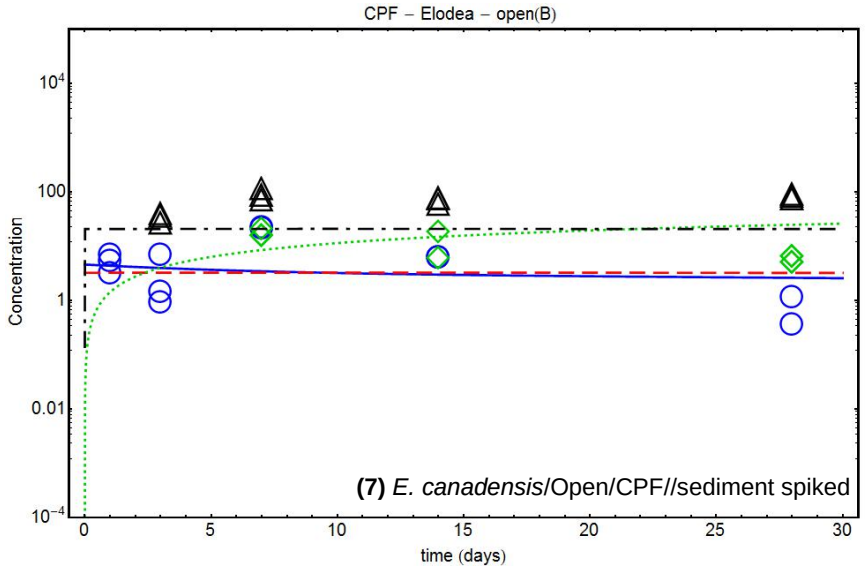
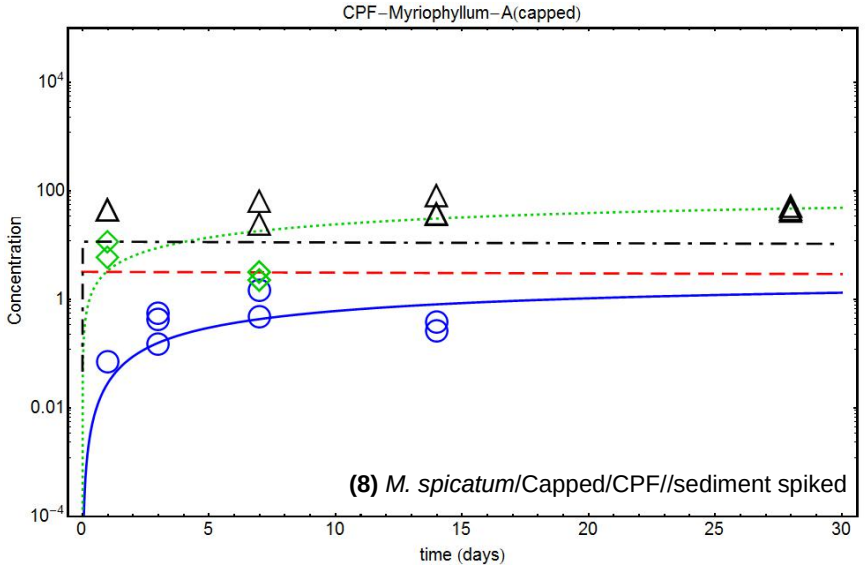
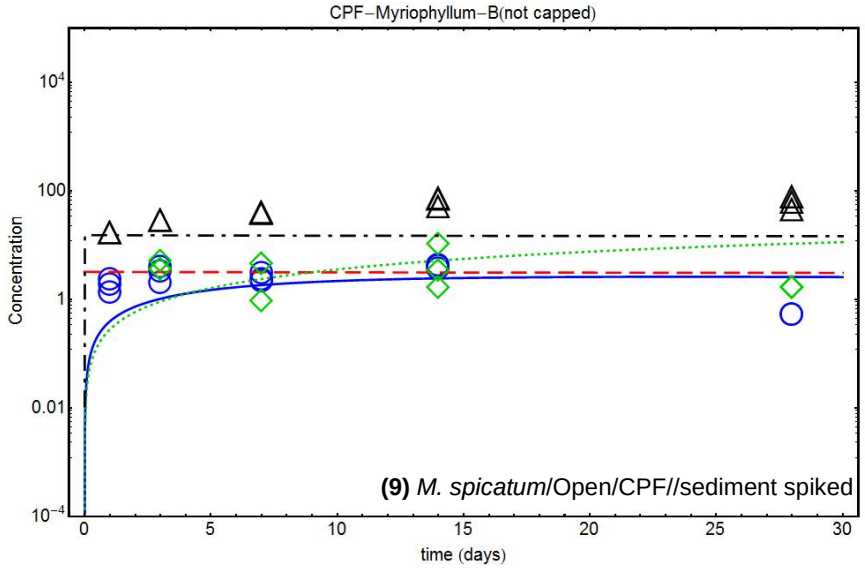


Figure S2 (Continued). Panels 3-5.









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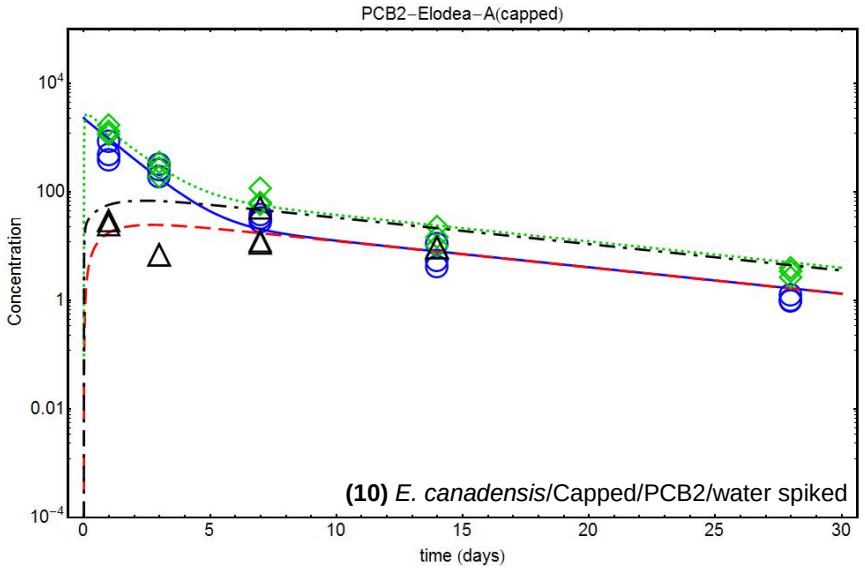
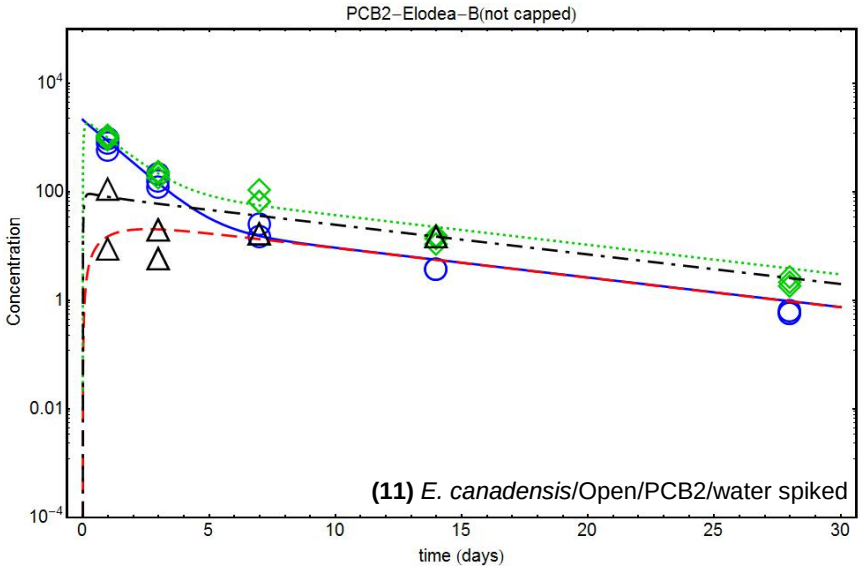
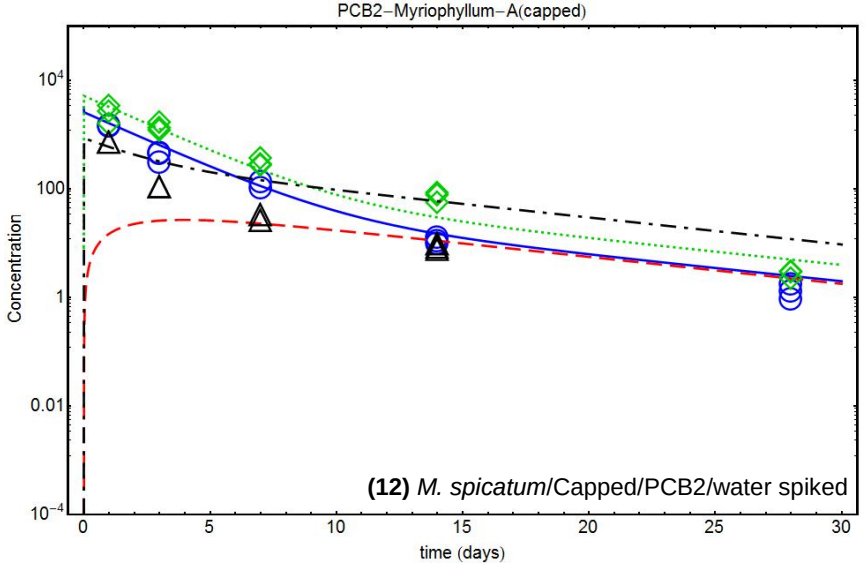






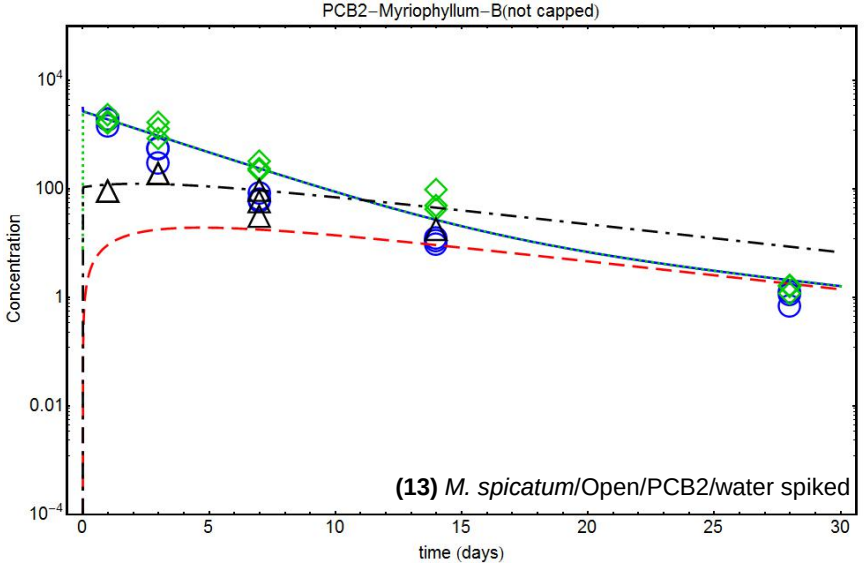
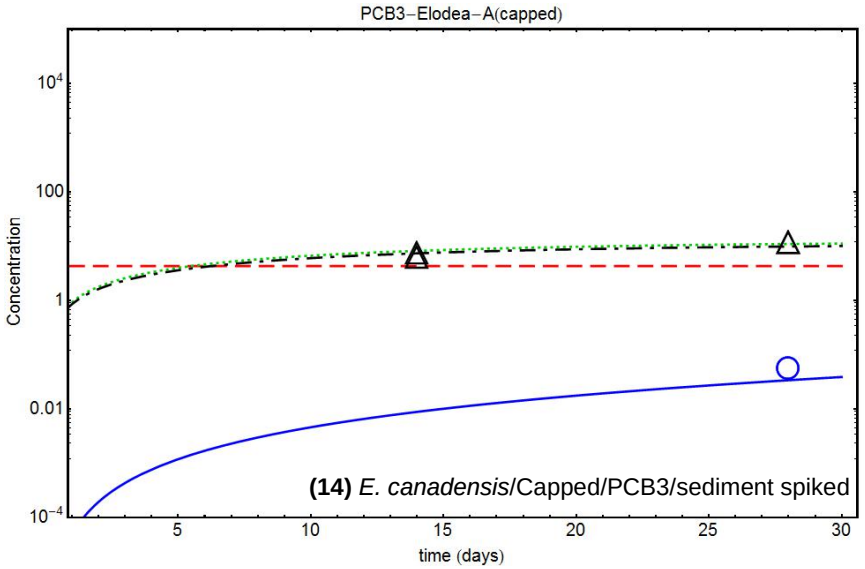
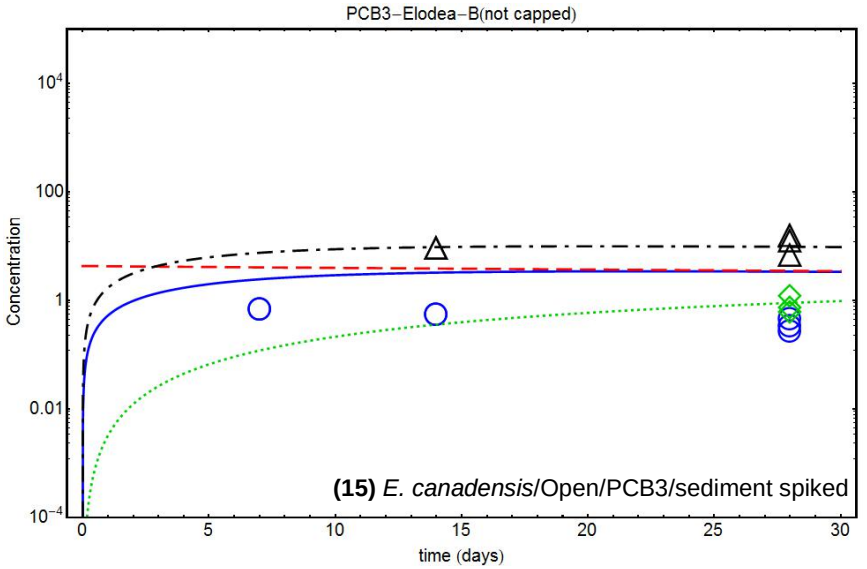
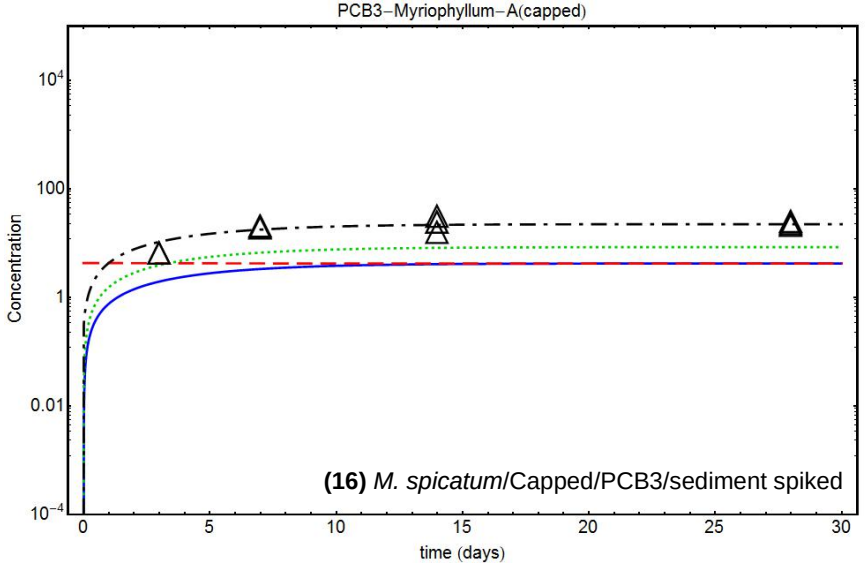


Figure S2 (Continued). Panels 10-13.







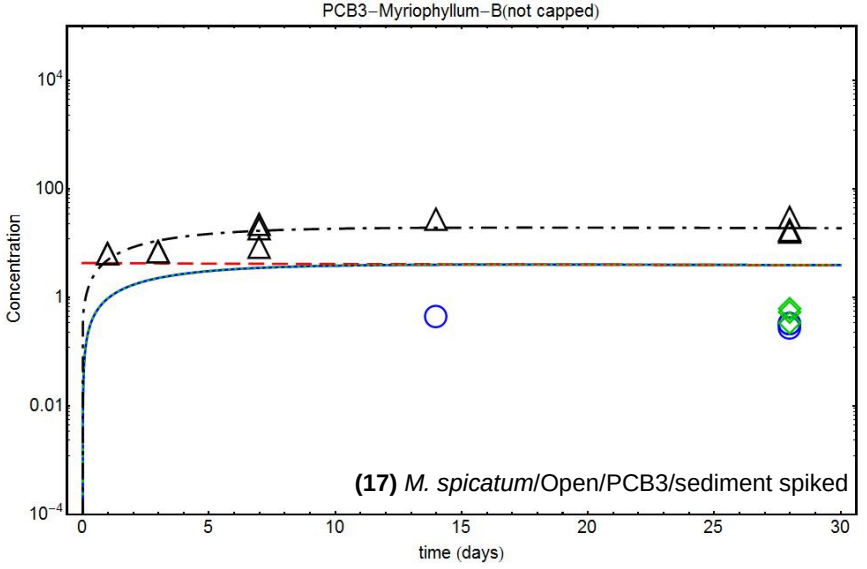
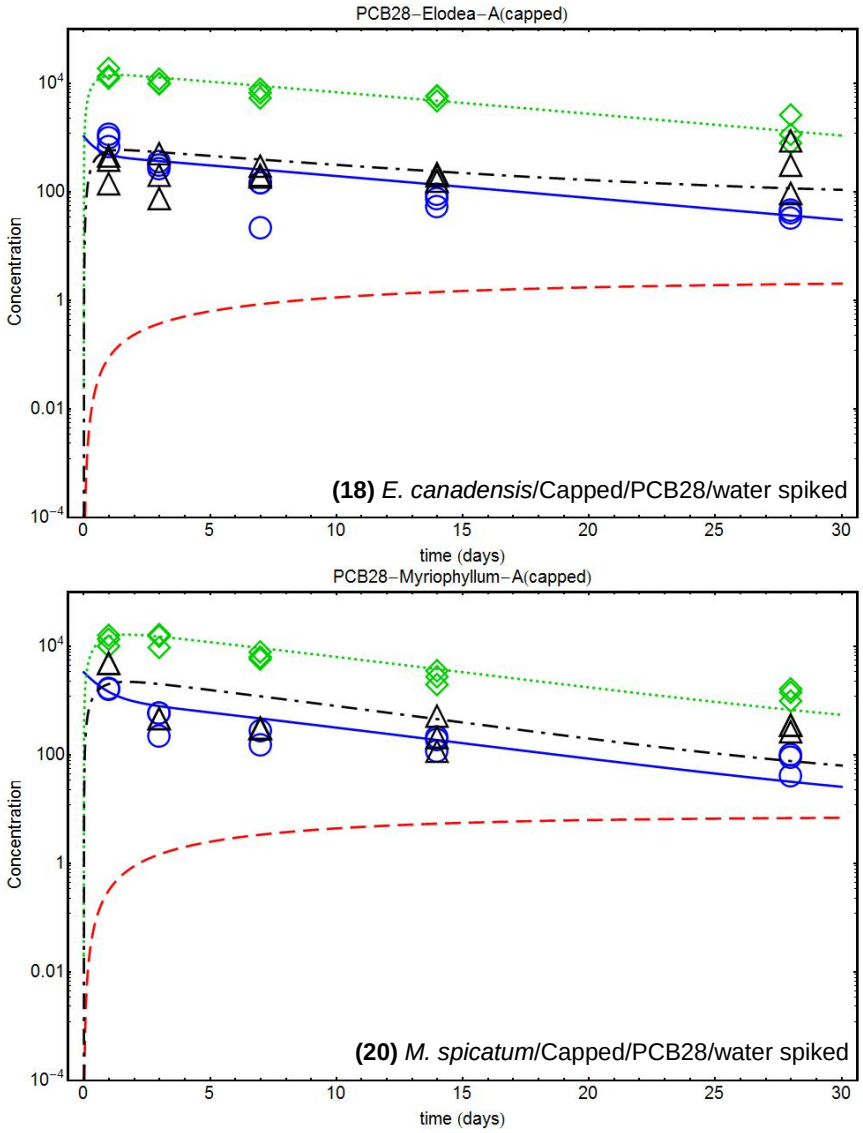


Figure S2 (Continued). Panels 14-17.



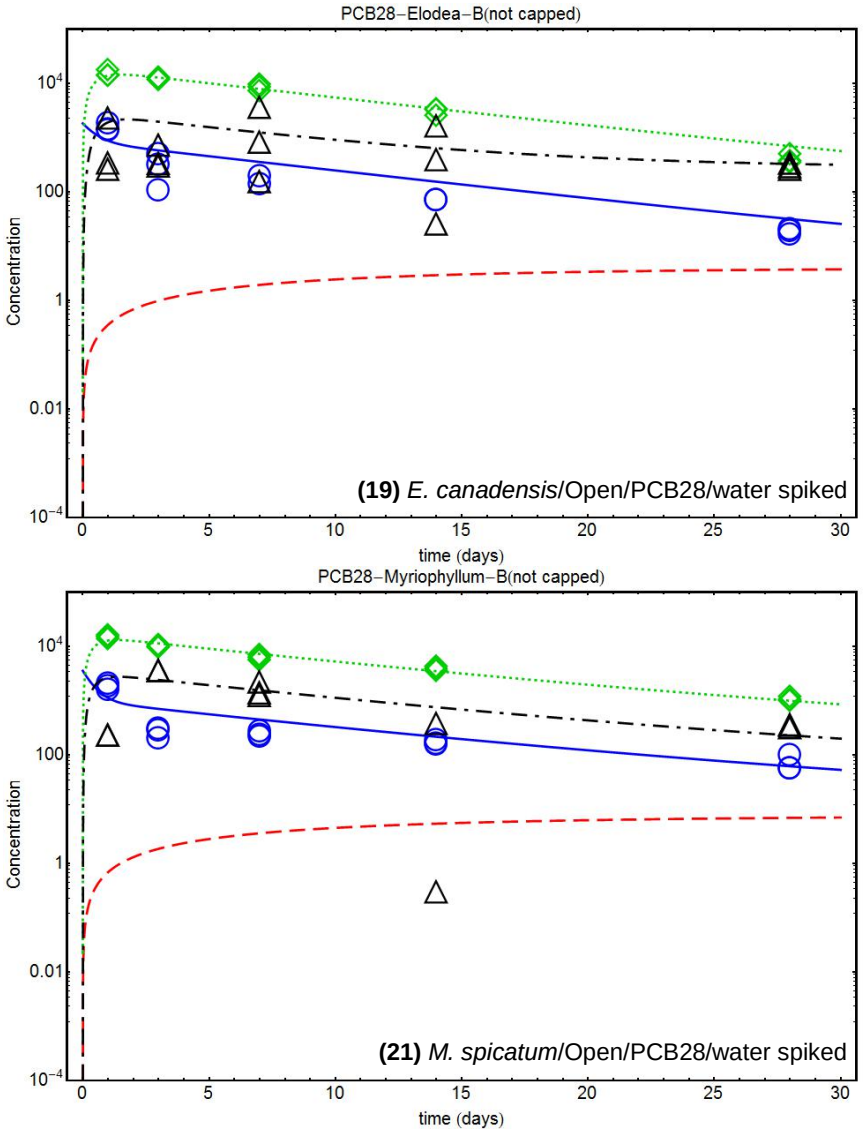
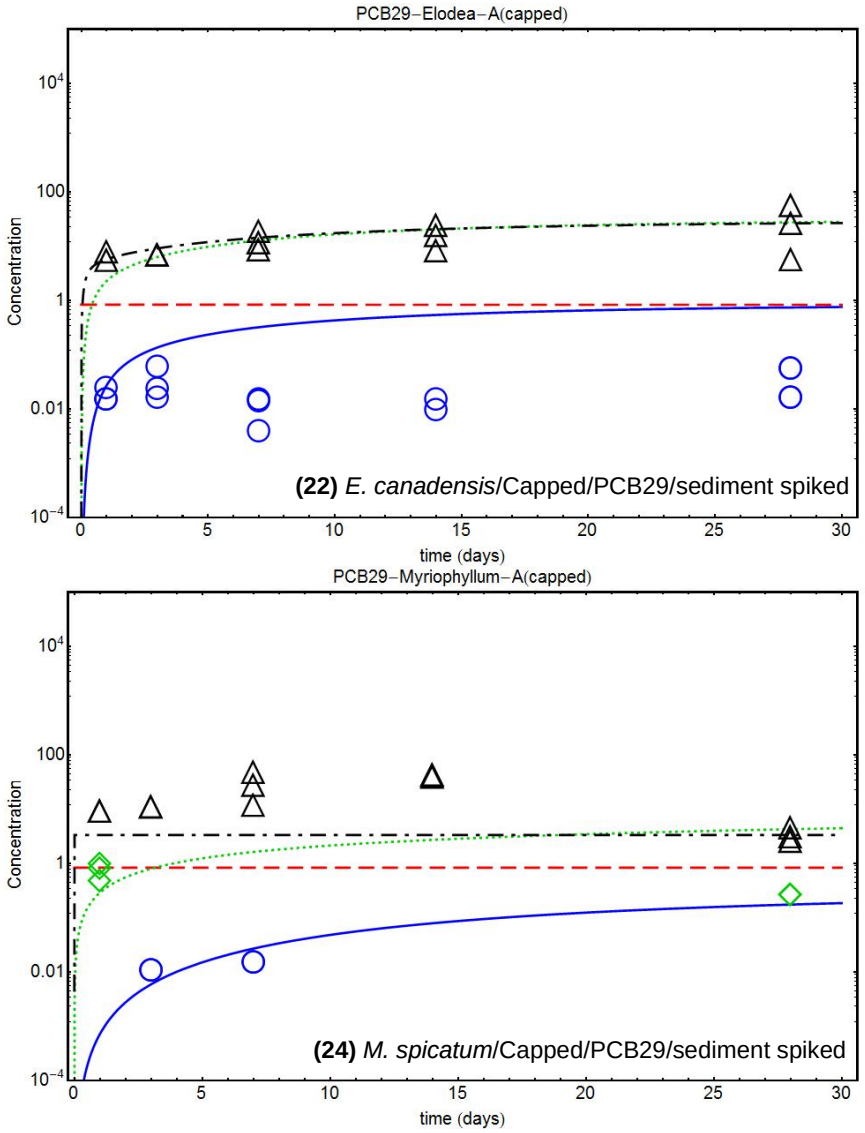


Figure S2 (Continued). Panels 18-21.



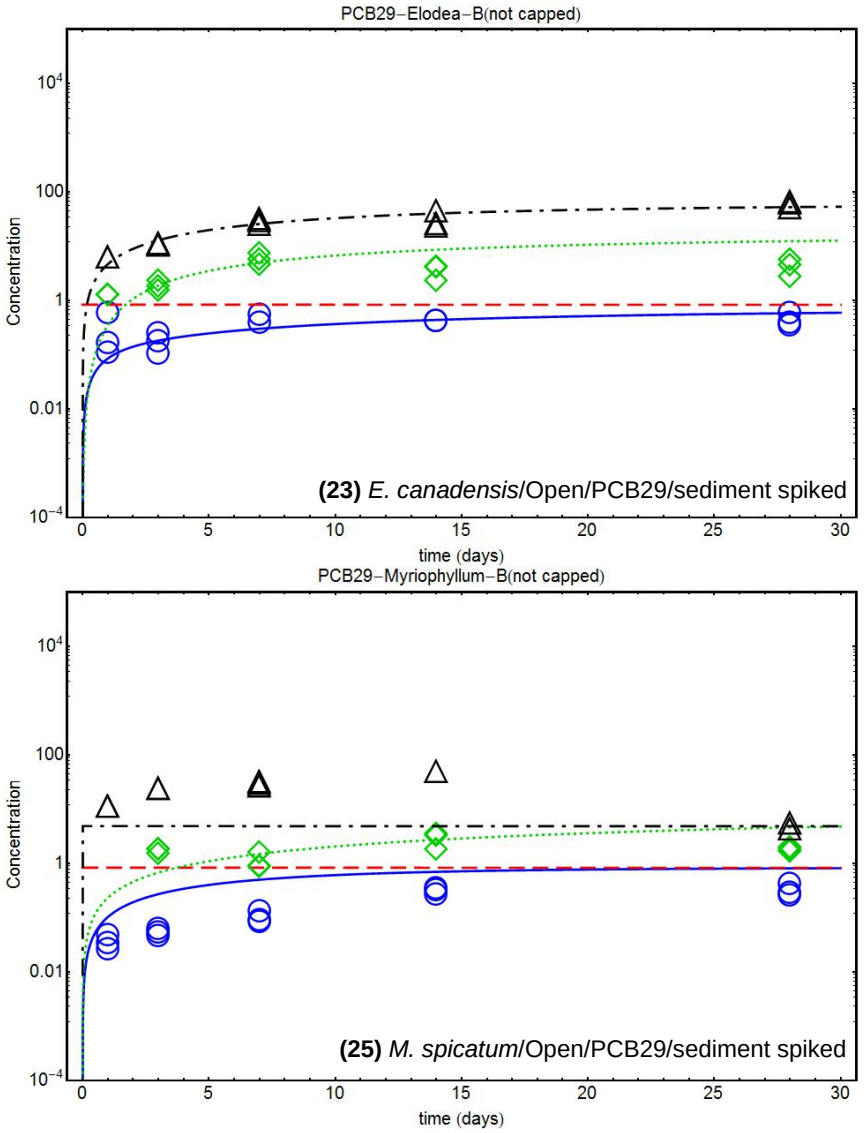
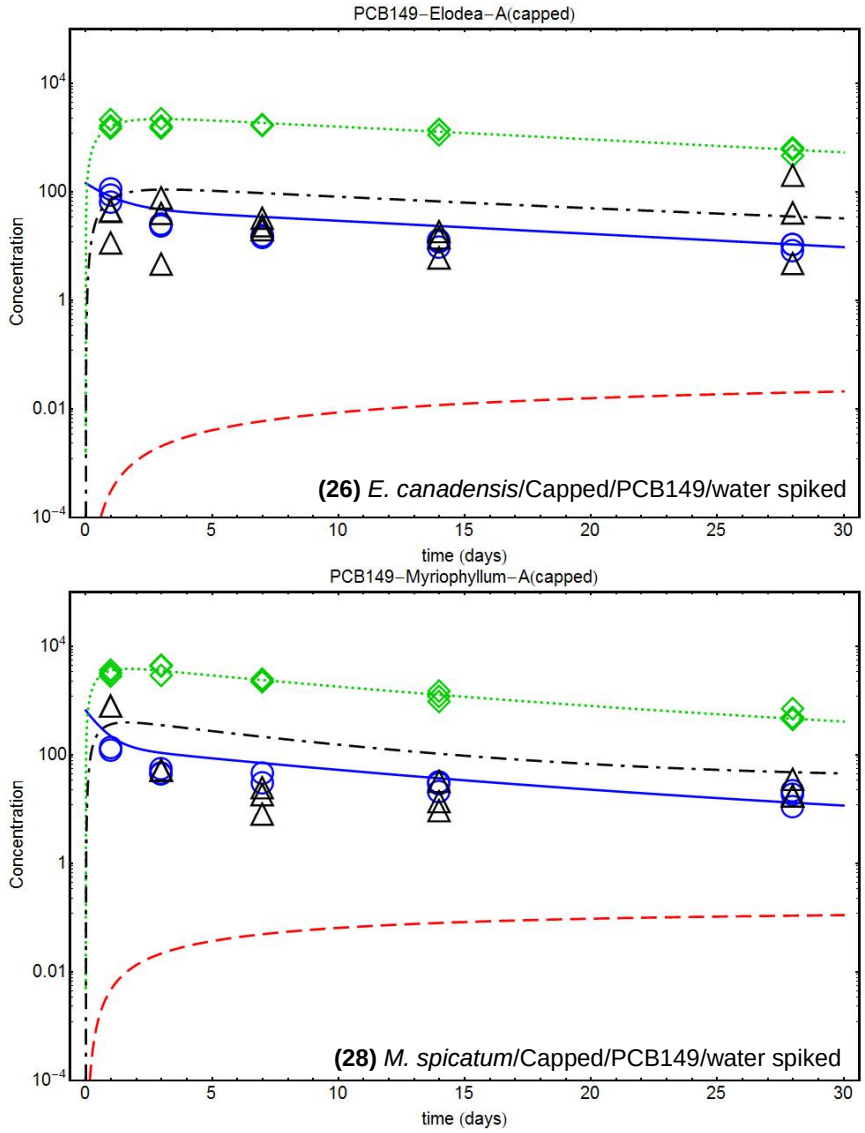


Figure S2 (Continued). Panels 22-25.



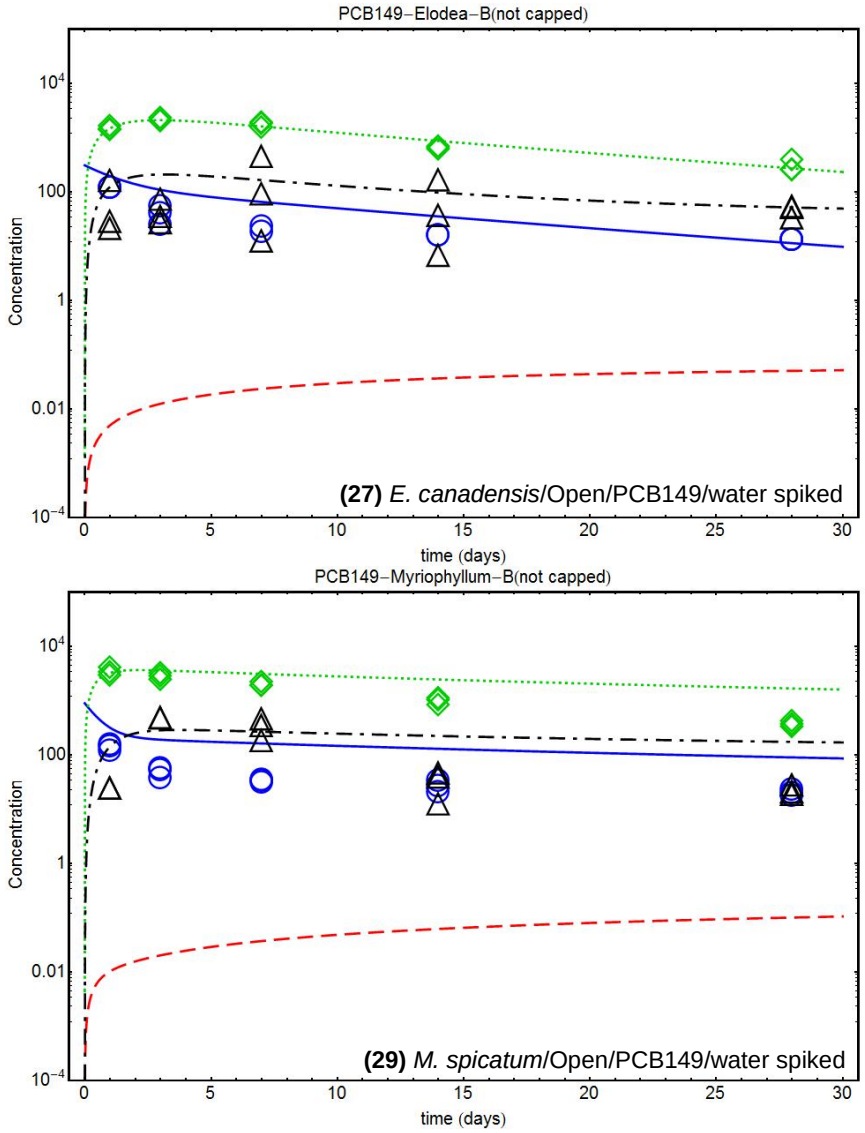
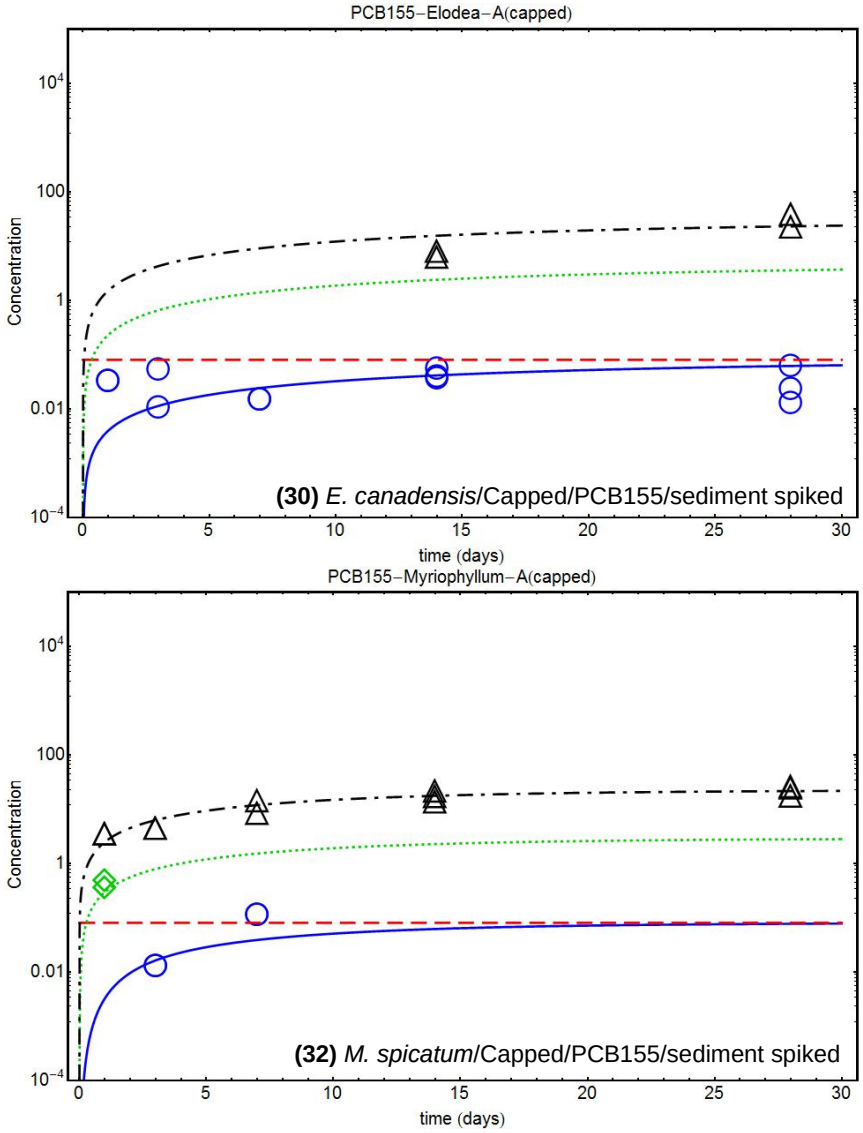


Figure S2 (Continued). Panels 26-29.



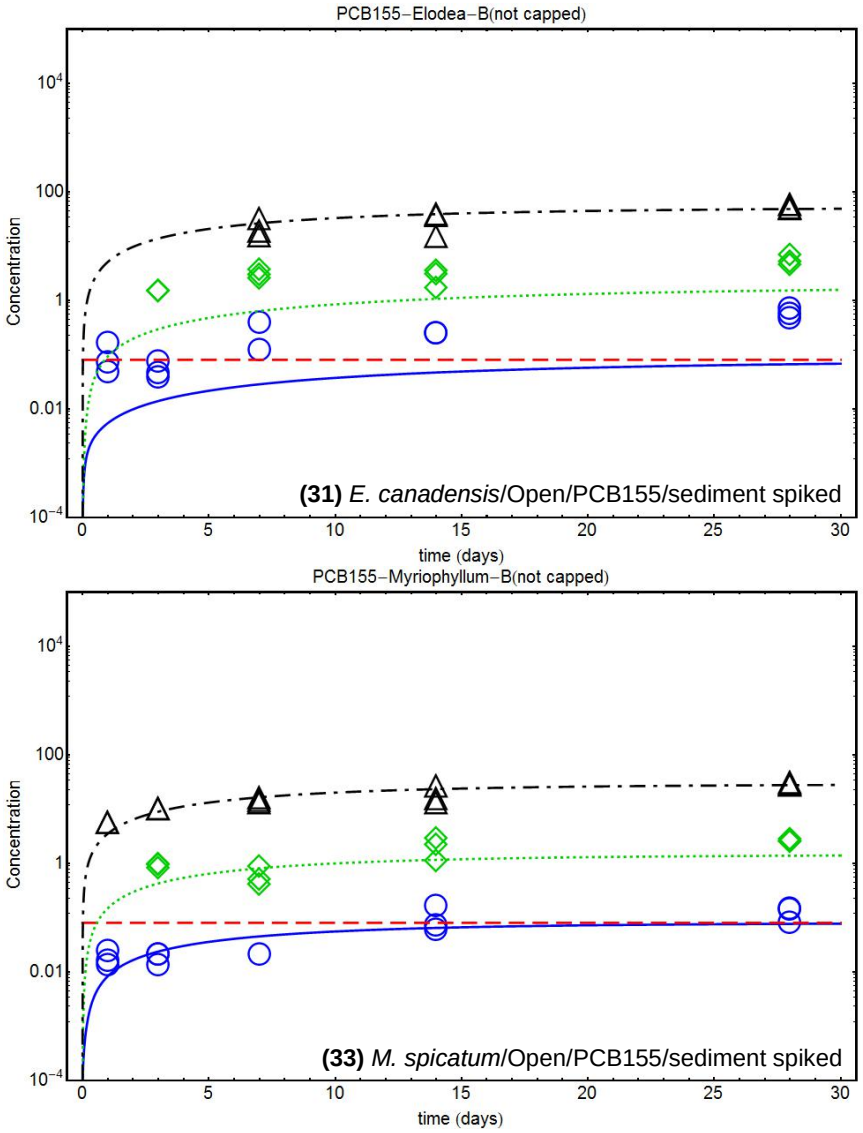


Figure S2 (Continued). Panels 30-33.

Parameter Estimates.

Table S24. Parameters and their confidence intervals obtained from fitting with data from the separate experiments for *Elodea canadensis* (E) and *Myriophyllum spicatum* (M) in capped and open systems. * not estimated, parameter fixed at zero, - confidence limit not within two orders of magnitude above or below estimated value, L90= lower boundary of the 90% Confidence Interval, H90= higher boundary of the 90% Confidence Interval.

		CPF				PCB 2				PCB 3			
	CI	**E capped**	**E open**	**M capped**	**M open**	**E capped**	**E open**	**M capped**	**M open**	**E capped**	**E open**	**M capped**	**M open**
	L90					0.05	0.08	0.03	0.01				
k_{LOSS} (m^3/kg)		*	*	*	*	0.11	0.13	0.12	0.12	1.53E-09	0.01	3.05E-09	2.43E-03
	H90					0.19	0.18	0.29	0.29		0.04		0.02
	L90	-	2.56E-03	-	-	0.95	0.49	-	-	-	5.12E-05	-	-
P_S (m/d)		615.37	0.01	0.17	2.14E-03	1.53	0.68	104.75	102.71	3.34E-04	4.76E-04	22.56	26.98
	H90	-	0.11	-	0.18	2.85	0.90	-	-	-	0.01	-	-
	L90	-	-	-	-	63.62	65.63	7.18	-	0.00	0.00	0.01	-
P_R (m/d)		1297.47	2818.15	619.17	135.08	841.77	186.39	17.49	30.45	0.04	0.02	0.60	0.31
	H90	-	-	-	-	-	-	48.11	-	-	-	-	-
	L90	-	-	1756	-	236498	387833	31268	-	-	-	-	-
P_{TR} (m/d)		17	9E-02	17081	1673	327560	510307	65280	20286	738342	8E-04	2604081	1093457
	H90	-	-	246801	18039	433362	642987	90684	43717	-	-	-	-
K_S (m^3/kg)[a]		37	37	37	37	3	4	2	1	3	4	2	1
K_R (m^3/kg)[a]		5.5	6.4	3.6	4.8	2.7	2.7	5.3	4.8	2.7	2.7	5.3	4.8
K_L (m^3/kg)[a]		0	0.025	0	0.025	0	0.025	0	0.025	0.025	0.025	0	0.025
N of experimental data points		22	30	22	34	37	33	35	36	4	12	9	16
F-ratio value		1.259	1.179	1.259	1.155	1.199	1.228	1.212	1.205	161.780	1.938	2.644	1.591

[a] Independently measured value after 28 d.

Table S24 (continued).

		PCB 28				PCB 29			
	Cl	**E capped**	**E open**	**M capped**	**M open**	**E capped**	**E open**	**M capped**	**M open**
k_{LOSS} (m^3/kg)	*L90*	*	*	*	*	*	*	*	*
	H90								
P_S (m/d)	*L90*	0.85	0.47	0.15	0.18	-	0.11	-	-
		1.51	0.75	0.24	0.26	1.51	0.35	0.02	5.86E+13
	H90	-	-	0.86	-	-	-	-	-
P_R (m/d)	*L90*	9.50	8.12	0.82	0.55	0.48	0.18	-	-
		19.83	13.80	1.32	0.81	0.96	0.23	224.46	436.99
	H90	49.47	23.30	2.34	1.18	2.07	0.33	-	-
P_{TR} (m/d)	*L90*	31646	17113	107461	53504	20701	-	-	-
		41640	26263	224349	86432	247208	646	5314	5761
	H90	49968	36484	-	205356	-	15973	-	-
K_S (m^3/kg)[a]		37	22	22	16	37	22	22	16
K_R (m^3/kg)[a]		34.8	71.0	4.0	5.9	34.8	71.0	4.0	5.9
K_L (m^3/kg)[a]		0	0.025	0	0.025	0	0.025	0	0.025
N of experimental data points		45	42	39	41	24	37	17	35
F-ratio value		1.113	1.122	1.133	1.129	1.233	1.141	1.359	1.150

[a] Independently measured value after 28 d.

Table S24 (continued).

		PCB 149				PCB 155			
	Cl	**E capped**	**E open**	**M capped**	**M open**	**E capped**	**E open**	**M capped**	**M open**
k_{LOSS} (m^3/kg)	*L90*	*	*	*	*	*	*	*	*
	H90								
P_S (m/d)	*L90*	0.51	0.21	0.20	0.06	-	-	4.96E-03	-
		0.74	0.30	0.31	0.20	269.18	2.82	0.24	6.61
	H90	1.19	0.43	0.89	-	-	-	-	-
P_R (m/d)	*L90*	53.28	64.52	55.47	4.61	0.84	1.43	1.33	1.19
		90.60	109.71	94.33	11.81	1.43	2.70	1.94	1.65
	H90	160.63	185.26	159.28	1155.49	3.13	-	2.98	2.29
P_{TR} (m/d)	*L90*	25906	10400	59826	1621	-	-	220717	161369
		32383	15162	74782	3750	40428891	18082	6889427	2028466
	H90	38859	20060	89738	73264	-	-	-	-
K_S (m^3/kg)[a]		58	23	36	18	58	23	36	18
K_R (m^3/kg)[a]		375.8	649.8	278.6	360.3	375.8	649.8	278.6	360.3
K_L (m^3/kg)[a]		0	0.025	0	0.025	0	0.025	0	0.025
N of experimental data points		45	42	39	41	14	31	14	36
F-ratio value		1.113	1.122	1.133	1.125	1.468	1.172	1.468	1.145

[a] Independently measured value after 28 d.

Table S25. Parameters estimated using combined data sets of open and capped systems, per chemical, for *Elodea canadensis* (E) and *Myriophyllum spicatum* (M). * not estimated, parameter fixed at zero, - confidence limit not within two orders of magnitude above or below estimated value

		LIN		CPF			PCB 2			
	CI	M	E		M		E		M	
k_{LOSS} (m^3/kg)	*L90*	*	*		*		0.08		0.03	
							0.12		0.09	
	H90						0.17		0.19	
P_S (m/d)	*L90*	0.02	0.00		0.00		0.83		-	
		0.90	0.03		0.02		1.10		182.77	
	H90	-	-		-		1.45		-	
P_R (m/d)	*L90*	4.92E-03	-		-		109.04		7.63	
		0.02	1170.20		1126.66		909.35		18.57	
	H90	0.04	-		-		-		48.64	
P_{TR} (m/d)	*L90*	8670	668		2110		294428		25553	
		82000	6843		5407		368035		45739	
	H90	-	-		28043		463724		60512	
K_S (m^3/kg)[a]		0.8	37	37	37	37	3	4	2	1
K_R (m^3/kg)[a]		0.14	5.5	6.4	3.6	4.7	2.7	0.5	0.5	0.5
K_L (m^3/kg)[a]		0.00073	0	0.025	0	0.025	0	0.025	0	0.025
N of experimental data points		90	52		56		70		71	
F-ratio value		1.054	1.096		1.089		1.070		1.069	

[a] Independently measured value after 28 d.

Table S25 (continued).

		PCB 3				PCB 28				PCB 29			
	Cl	**E**		**M**		**E**		**M**		**E**		**M**	
	L90		-		-								
k_{LOSS} (m^3/kg)			0.02		0.02		*		*		*		*
	H90		0.05		0.05								
	L90		-		-		0.75		0.17		0.19		-
P_S (m/d)			3.5E-04		3.5E-04		1.22		0.25		16.06		1.1E-03
	H90		-		-		-		0.52		-		-
	L90		0.02		0.02		11.59		0.69		0.17		-
P_R (m/d)			0.10		0.10		17.79		0.96		0.23		1217.26
	H90		-		-		27.25		1.47		0.36		-
	L90		-		-		28197		89576		495		115
P_{TR} (m/d)			478627		478627		35247		168777		2117		5484
	H90		-		-		42296		919101		8605		-
K_S (m^3/kg)[a]		3	3	3	3	37	22	22	16	37	22	22	16
K_R (m^3/kg)[a]		2.7	2.7	2.7	2.7	34.8	71.0	4.0	5.9	34.8	71.0	4.0	5.9
K_L (m^3/kg)[a]		0.025	0.025	0.025	0.025	0	0.025	0	0.025	0	0.025	0	0.025
N of experimental			16		16								
data points							87		79		61		52
F-ratio value			1.390		1.390		1.056		1.062		1.081		1.096

[a] Independently measured value after 28 d.

Table S25 (continued).

		PCB 149				PCB 155			
	Cl	**E**		**M**		**E**		**M**	
k_{LOSS} (m^3/kg)	*L90*		*		*		*		*
	H90								
P_S (m/d)	*L90*		0.37		0.21		0.02		0.01
			0.51		0.35		0.77		0.45
	H90		0.74		-		-		-
P_R (m/d)	*L90*		77.57		54.45		1.98		1.41
			119.05		83.57		3.03		1.77
	H90		191.45		127.99		5.38		2.22
P_{TR} (m/d)	*L90*		16897		39866		-		301408
			21121		49833		11488102		1429720
	H90		26613		59799		-		-
K_S (m^3/kg)[a]		58	23	36	18	58	23	36	18
K_R (m^3/kg)[a]		375.8	649.8	278.6	360.3	375.8	649.8	278.6	360.3
K_L (m^3/kg)[a]		0	0.025	0	0.025	0	0.025	0	0.025
N of experimental data points			87		80		45		50
F-ratio value			1.056		1.061		1.113		1.101

[a] Independently measured value after 28 d.

Definition of equations used to calculate fluxes across the interfaces between pore water, overlying water roots and shoots.

Fluxes (ø; µg/d) were calculated between the four compartments: sediment, overlying water, shoots, and roots (see also schematic representation in Figure 2):

Flux from pore water to overlying water:

$$ø_{pw-w} = K_L A_{SED}(C_{PW} - C_{OW}) \quad \text{(S13)}$$

Flux from overlying water to shoots:

$$ø_{ow-s} = P_S A_{S,t}\left(C_{OW} - \frac{C_S}{K_S}\right) \quad \text{(S14)}$$

Flux from pore water to roots:

$$ø_{pw-r} = P_R A_{R,t}\left(C_{PW} - \frac{C_R}{K_R}\right) \quad \text{(S15)}$$

Flux from roots to shoots (translocation):

$$ø_{r-s} = P_{TR} A_{TR,t}\left(\frac{C_R}{K_R} - \frac{C_S}{K_S}\right) \quad \text{(S16)}$$

Fluxes were calculated using the parameters from single experiment data (Table S25).

Note that fluxes in Figure 6 and Figure S3 are reported as positive if they occur in the direction as indicated in eqs S13-S16.

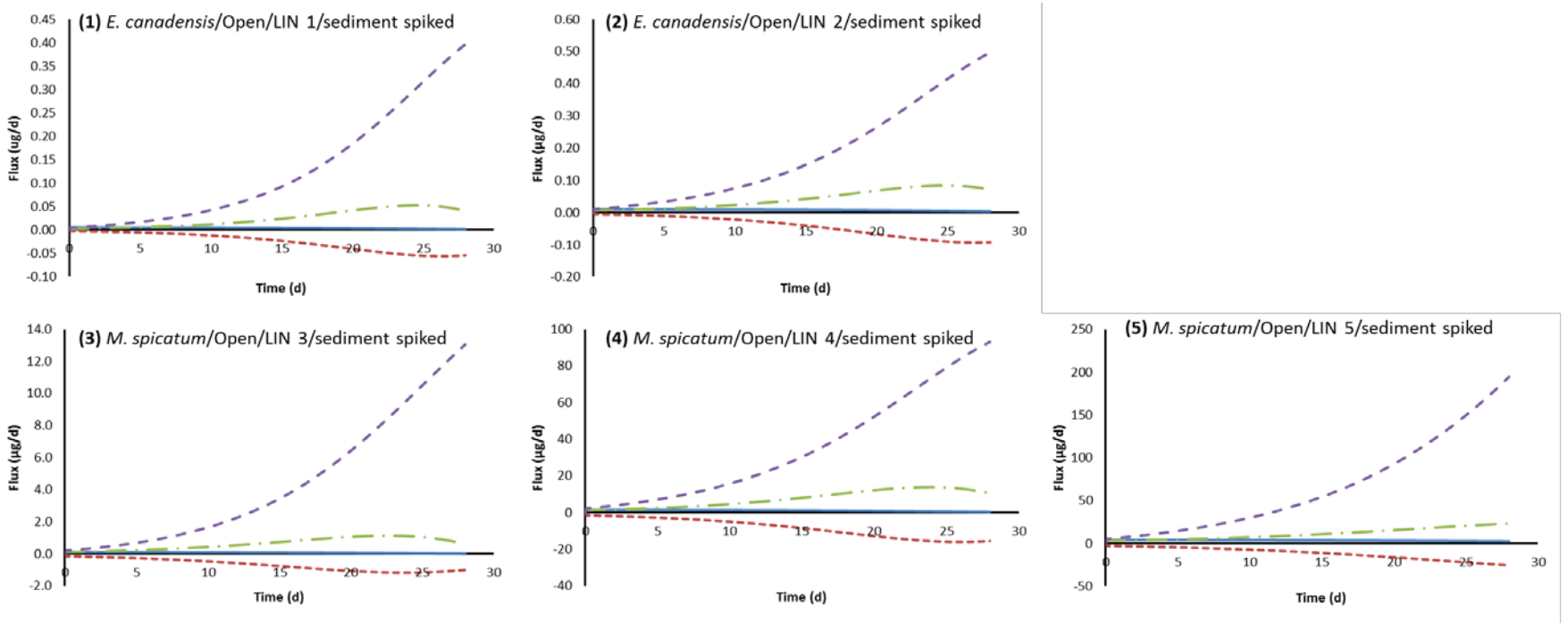


Figure S3. Chemical fluxes (µg/d) from pore water to overlying water (Eq. S7; blue solid line), from overlying water to shoots (Eq. S8; red dotted line), from pore water to roots (Eq. S9; green dash dot line), and from roots to shoots (Eq. S10; purple dash line) for water spiked and sediment spiked PCB, CPF and LIN for *Elodea canadenis,* and *Myriophyllum spicatum* in capped and open systems, as indicated. LIN was only spiked in the sediment. Panels 1-5 Linuron (LIN) data.

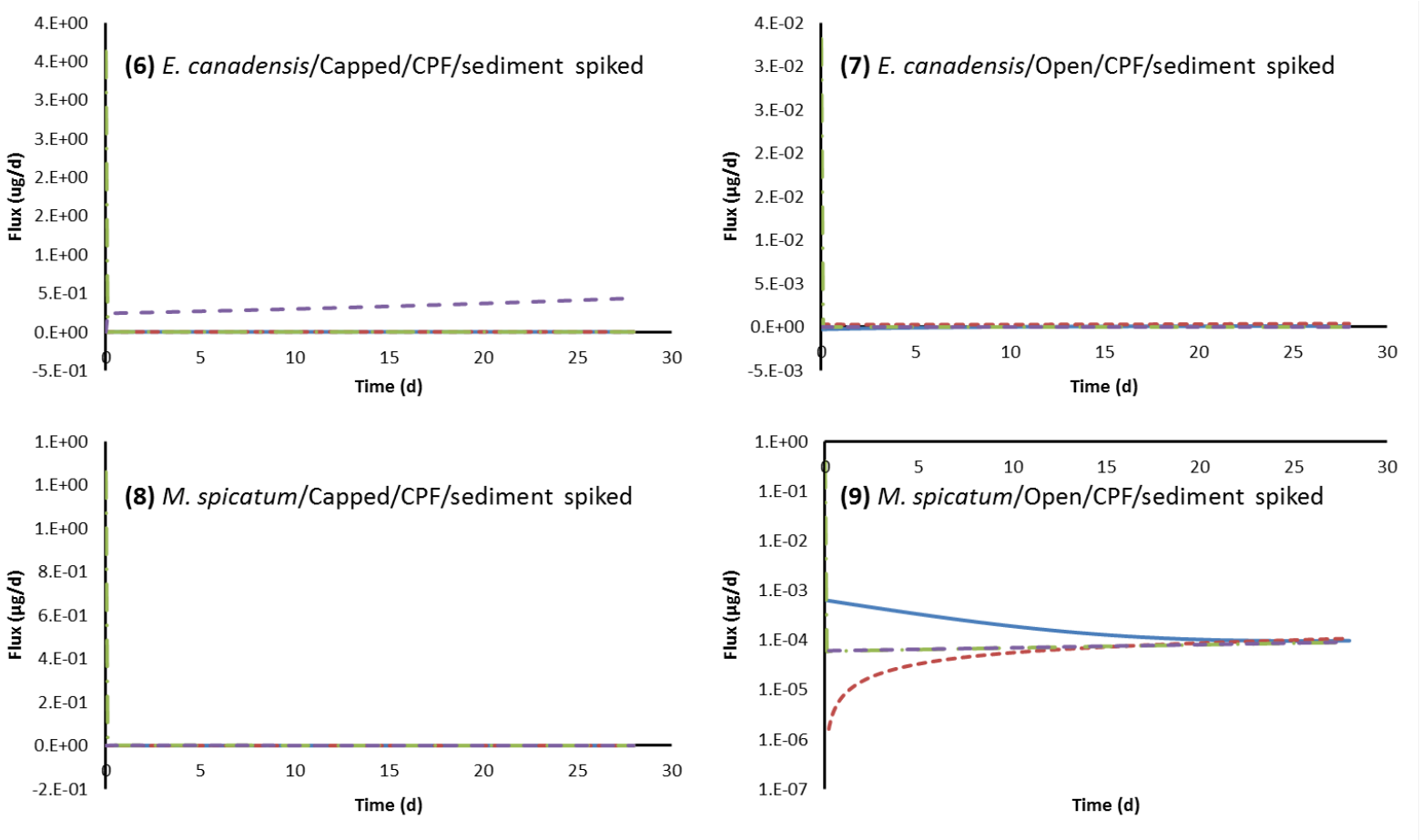


Figure S3 (continued). Panels 6-9, CPF data.

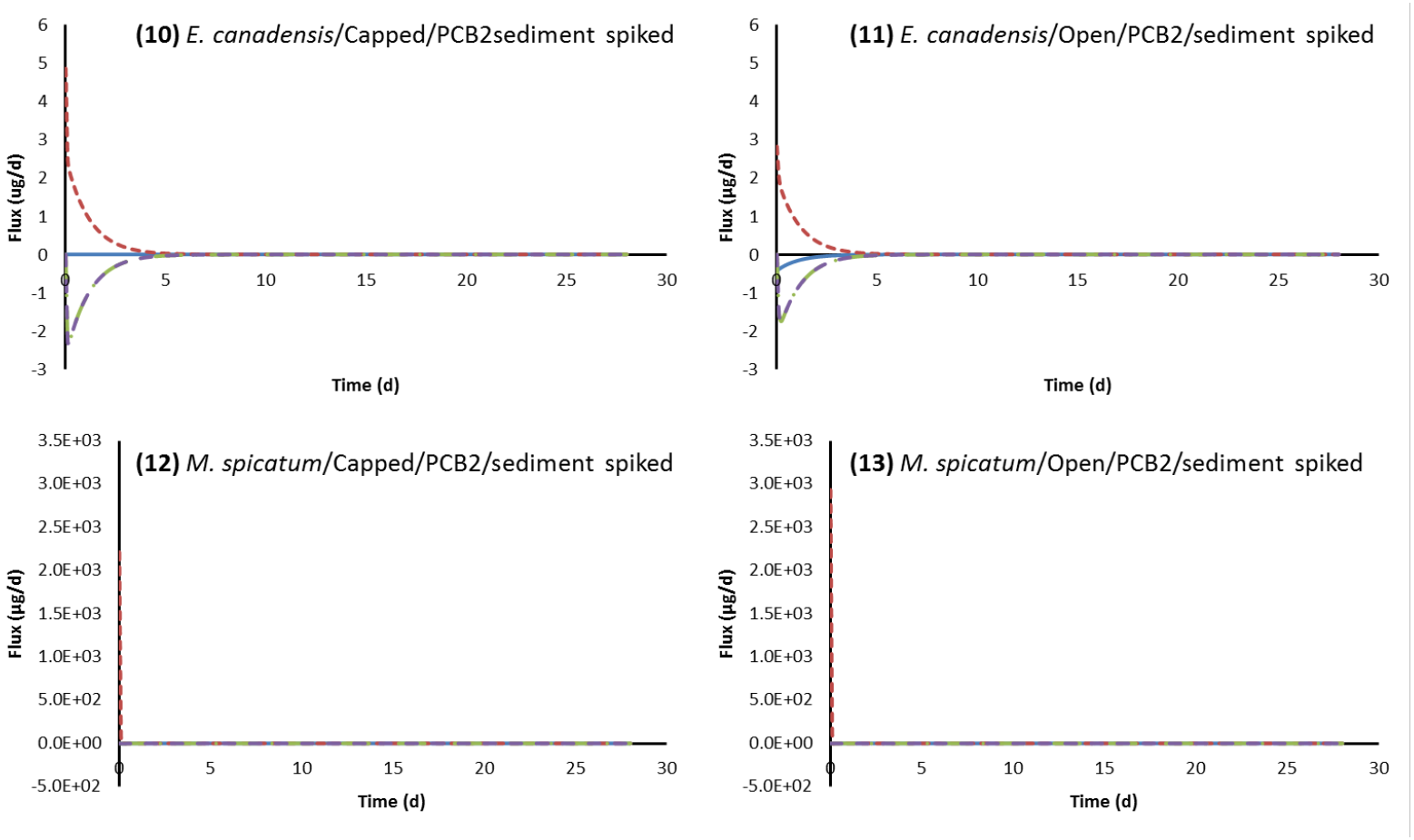


Figure S3 (continued). Panels 10-13, PCB 2 data.

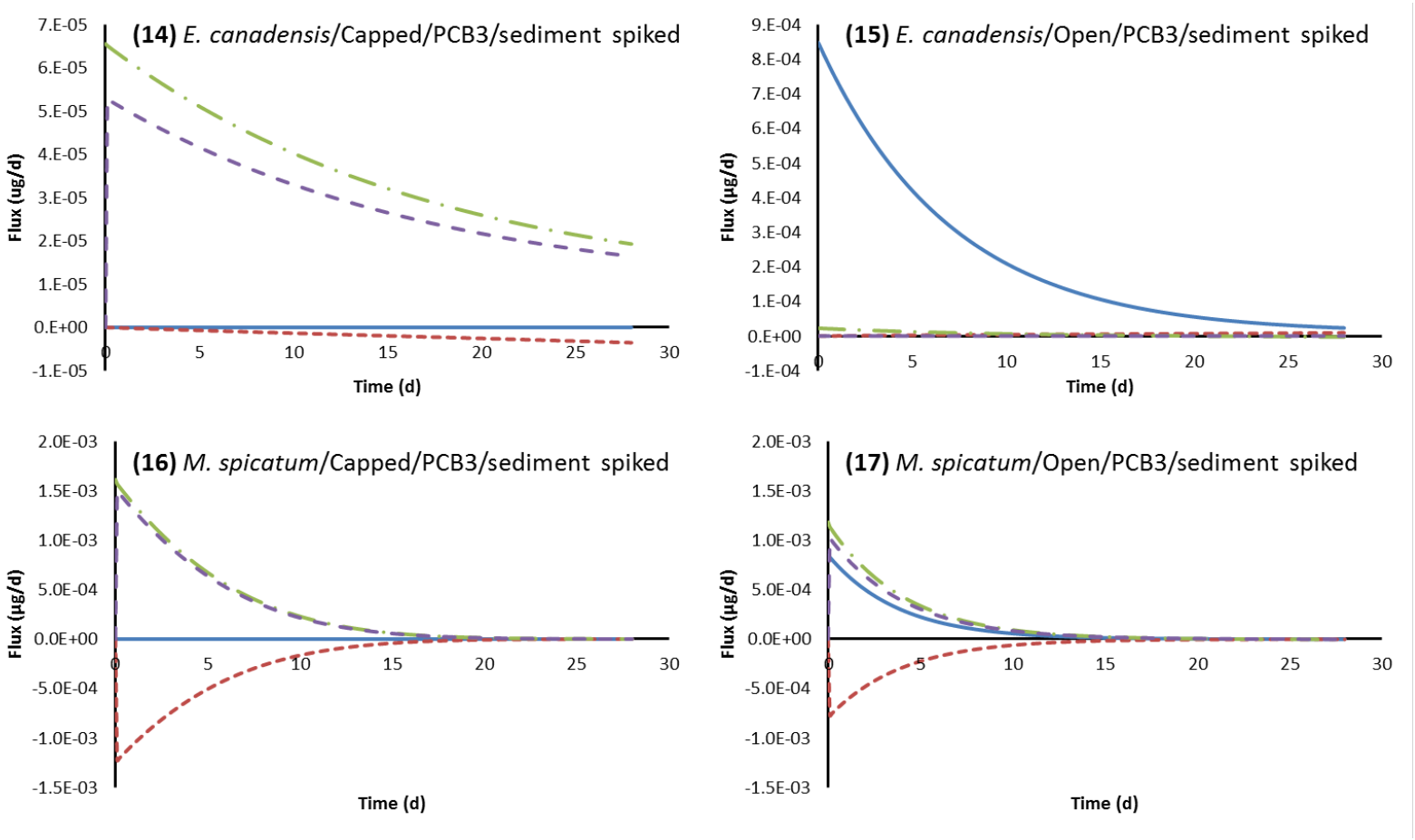


Figure S3 (continued). Panels 14-17, PCB 3 data.

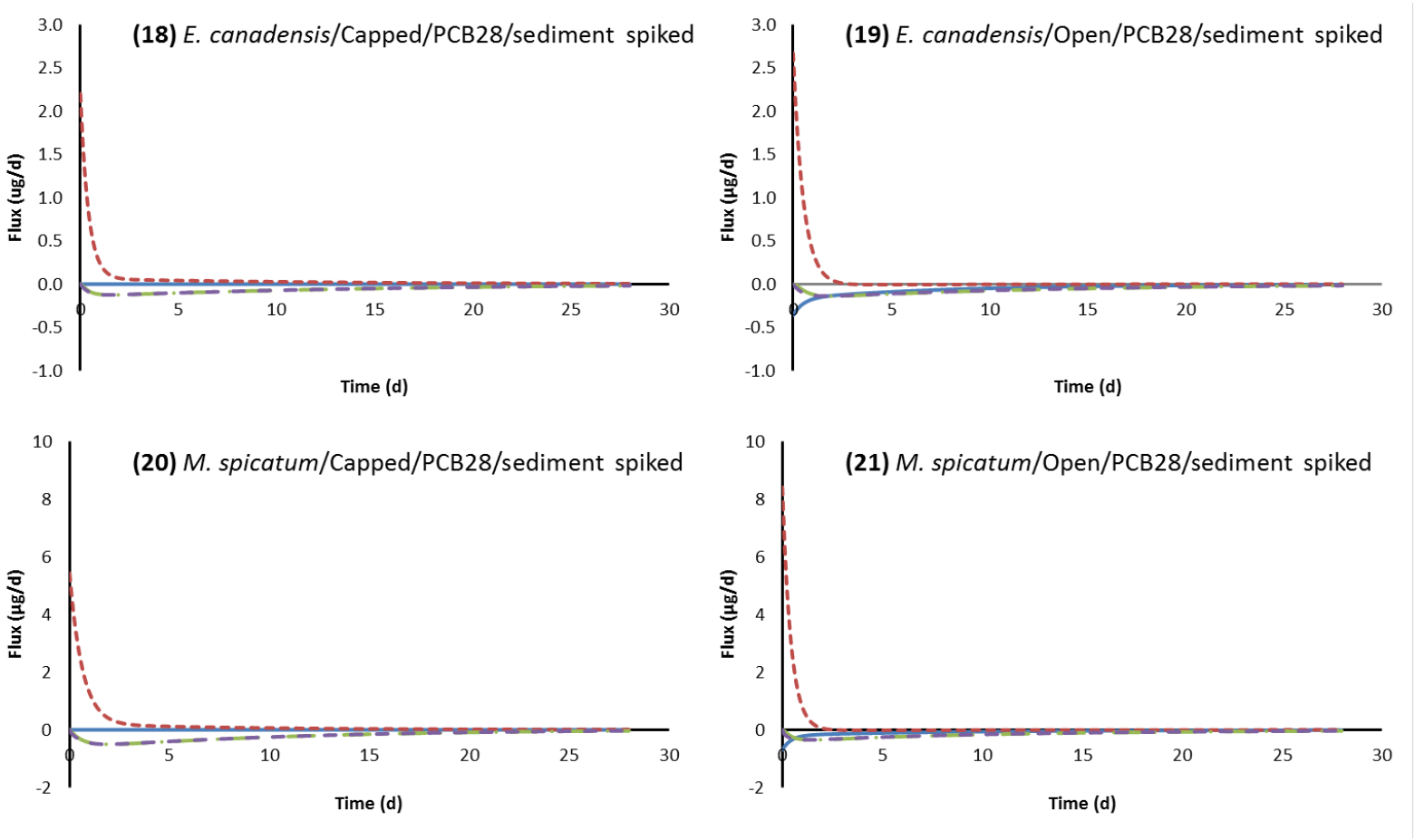


Figure S3 (continued). Panels 18-21, PCB 28 data.

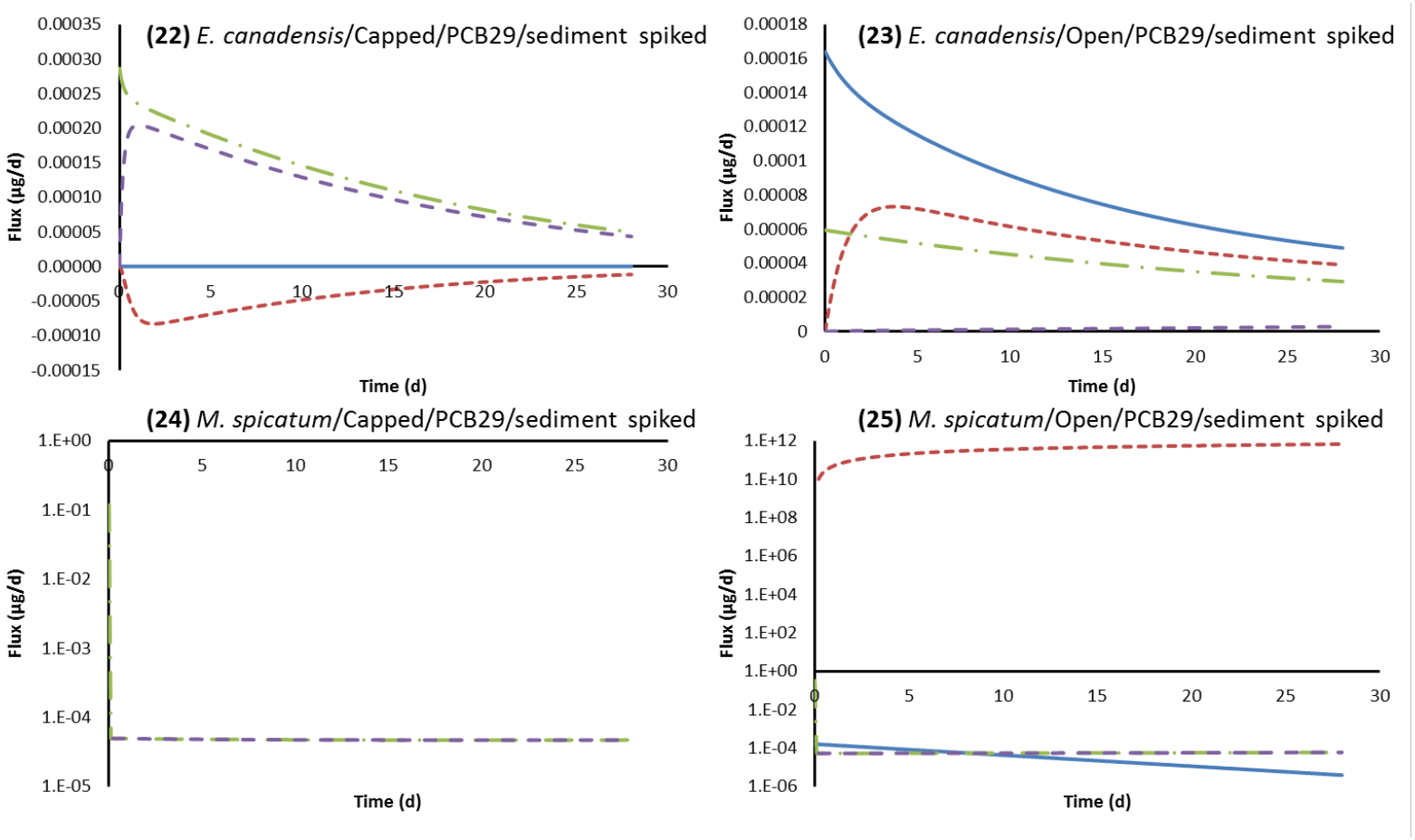


Figure S3 (continued). Panels 22-25, PCB 29 data.

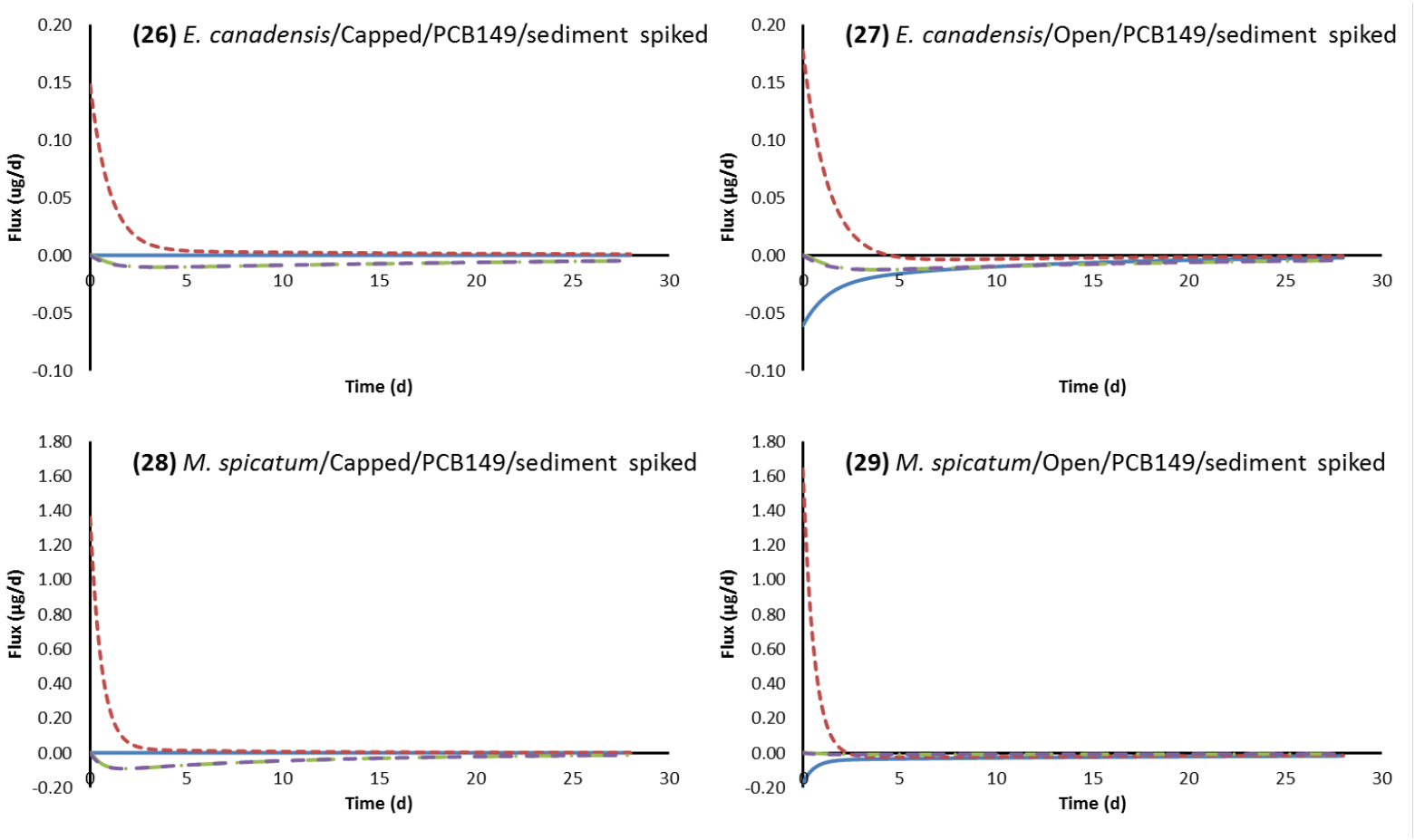


Figure S3 (continued). Panels 26-29, PCB 149 data.

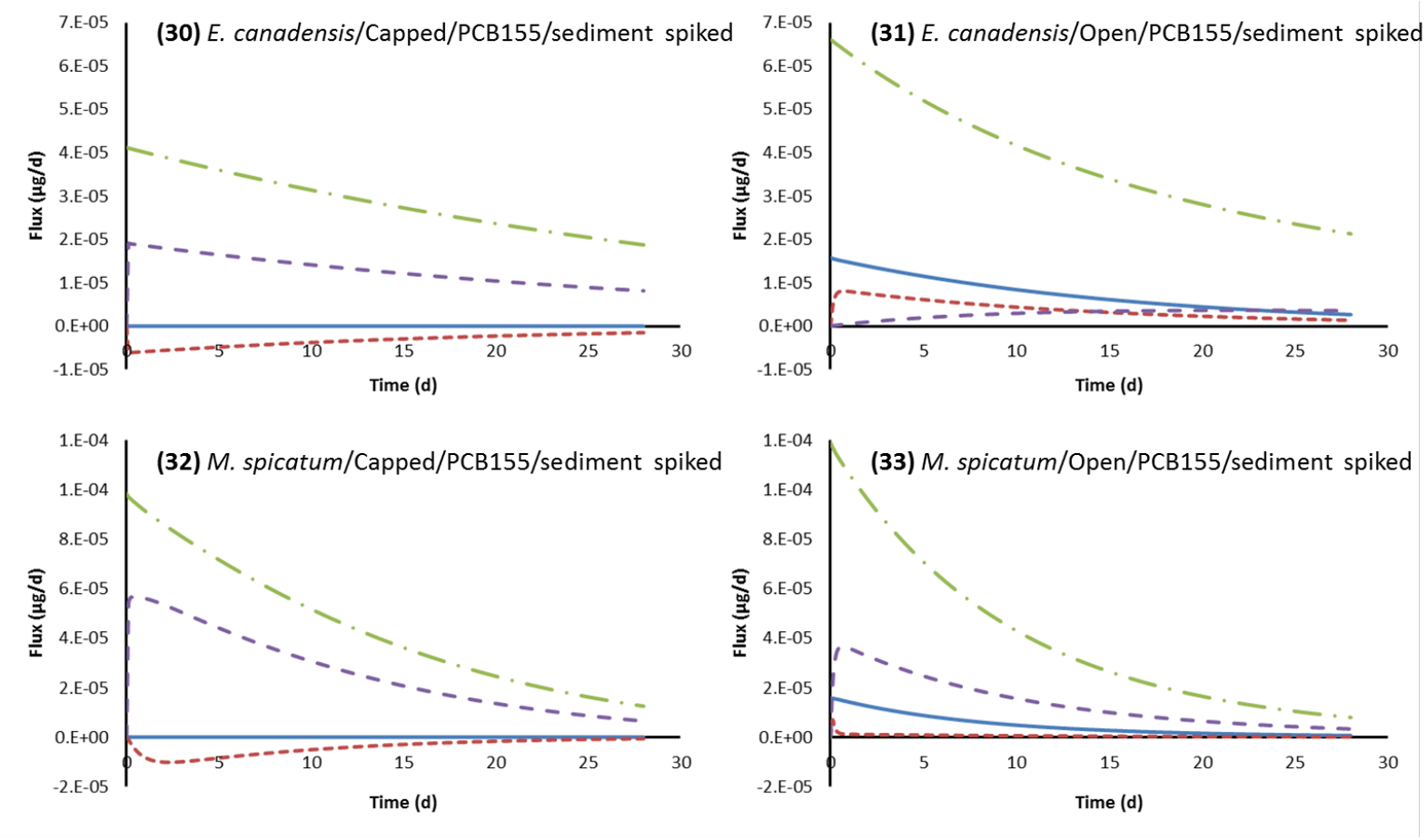


Figure S3 (continued). Panels 30-33, PCB 155 data.

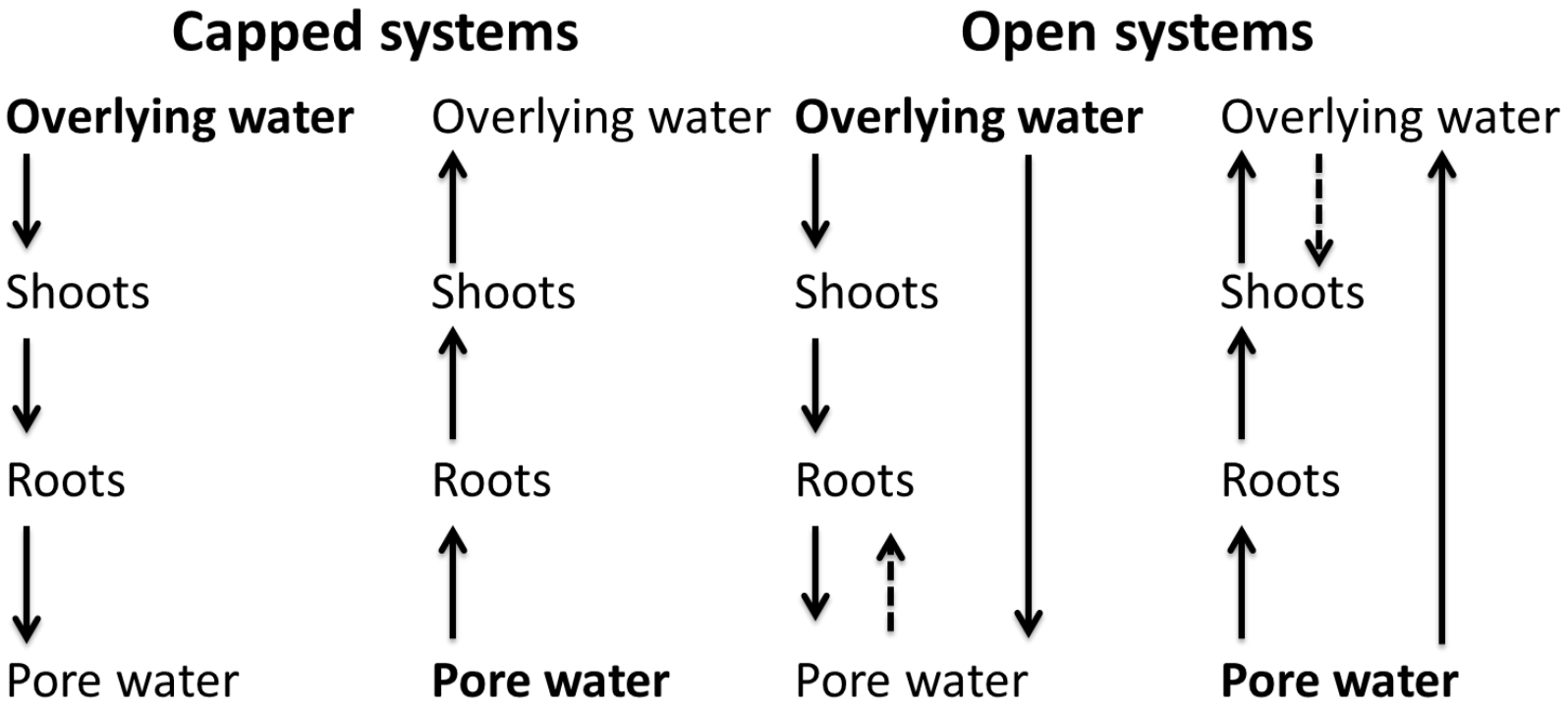


Figure S4. General patterns in the modelled fluxes between pore water and overlying water, overlying water and shoots, pore water and roots, and roots and shoots for water spiked and sediment spiked capped and open systems. Spiked compartments indicated **in bold**.

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