Electronic Supplementary Material (ESI) for Environmental Science: Processes & Impacts

Supplementary information

Multimedia modeling of the fate of triclosan and triclocarban in the Dongjiang River Basin, South China and comparison with the field data

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1. Sample collection and analysis

Surface water samples were collected in 1 L amber glass bottles from 0.5 to 1 m below the water surface. Then 50 mL methanol and 400 mL 4 M sulfuric acid were added into each bottle to suppress microbial activity. Top 10-cm surface sediments were taken using a stainless steel grab sampler and then one gram sodium azide was added immediately, which was placed in a clean 1 L glass bottle. The samples were kept in 4 °C until extraction. The collected water samples were processed within 48 h using solid phase extraction (SPE), while the sediment samples were freeze-dried and stored at 4 °C for later analysis.

Water samples were first filtered and suspended particulate matters (SPMs) were collected with glass fiber filters. Internal standards of $^{13}C_{12}$-TCS and TCC-d7 were added to the filtered samples, and the target anayltes were enriched into Waters Oasis HLB cartridges (6cc, 500 mg sorbents) using solid phase extraction process. The cartridges were finally eluted with 7 mL methanol and 5 mL dichloromethane in sequence. The combined eluates were combined and dried under gentle nitrogen and prepare for cleanup step. The filtered glass fibers with SPMs were freeze-dried as sediment and then cut into pieces. Each SPM or sediment sample was weighted into a centrifuge tube, and extracted three times with 30 mL ethyl acetate under ultrasonication. Ethyl acetate phase was combined and blew to dry, and ready for cleanup step.

Surface water and sediment extracts were cleaned up with a silica column (0.8 cm inside diameter, 1 g silica gel loaded). Dried elute was dissolved sequentially with 6 mL n-hexane, 6 mL ethyl acetate and 6 mL methanol, and loaded to the silica column in turn. The ethyl acetate phase was collected since the target compounds TCS and TCC as well as their internal standards were in the ethyl acetate phase. After being dried, the elutes were reconstituted in 1 mL of methanol and stored at –18°C for instrumental analysis by liquid chromatography-tandem mass spectrometry (LC-MS/MS).

2. Calculation of total amounts for TCS and TCC

The total amounts of TCS and TCC accumulated in the three media, i.e. water, SPM and sediment, were calculated based on the collected river basin data sets. The following equations are used:

$I_w = C_{22} \times A \times h_2 \times 10^{-9}$, $I_{SPM} = C_{23} \times A \times h_2 \times \rho_{23} \times 10^{-9} \times X_{23}$, $I_s = C_{43} \times A \times h_4 \times \rho_{43} \times 10^{-9}$,

where I_w, I_{SPM} and I_s are the total amounts of a chemical in surface water, suspended particulate matter (SPM) and sediment, respectively, with the unit of kg; C_{22} is the geomean value of a chemical in water with the unit of ng/L; C_{23} and C_{43} are the geomean values of a chemical in suspended particulate matter and sediment with the unit of ng/g, respectively; A is the water area with the unit of m^2; h_2 and h_4 are the average depth of water and sediment, respectively, with the unit of m; ρ_{23} is the SPM density and ρ_{43} is sediment density, and both with the unit of kg/m^3; and X_{23} is the volume fractions of solids in water.

3. Model description and results

3.1 Mass balance equations

For steady-state conditions the total input fluxes from the individual compartment equal to the output flux, and the equation is a simple algebraic expression. The mass balance equations were established in terms of transfer fluxes for the 4 bulk compartments of air, water, soil and sediment, respectively:

$T_{01t} + T_{21d} + T_{31d} = T_{10t} + T_{12d} + T_{12p} + T_{12w} + T_{13d} + T_{13p} + T_{13w} + T_{10m}$,

$T_{02t} + T_{02h} + T_{12d} + T_{12p} + T_{12w} + T_{32e} + T_{32l} + T_{42d} + T_{42r} = T_{20t} + T_{21d} + T_{24d} + T_{24s} + T_{20m} + T_{2f}$,

$T_{13d} + T_{13p} + T_{13w} = T_{30m} + T_{31d} + T_{32e} + T_{32l}$,

$T_{24d} + T_{24s} = T_{40m} + T_{42d} + T_{42r}$,

The parameters used for solving the set of equations and sources of the data are listed in Table S1, which consists of the basic parameters that describe physical-chemical properties of the chemicals (TCS and TCC), dimension and property of the compartments and subcompartments, and thermodynamics and kinetics of both diffusive and non-diffusive processes that are required for modeling the fate of these target chemicals.

3.2 Parameters

1. A nonequilibrium and steady-state model and expressions used in the study are described for emissions, advective flows, degrading reactions, and interphase transport by diffusive and nondiffusive processes. The input parameters to the model consist of a description of the environment (such as area of the water, soil and sediment), the physical-chemical (such as organic carbon normalized partition coefficients, Koc) and reaction properties (such as coefficients of degradation rate in air, water, soil and sediment) of the chemical and emission rates (such as wastewater discharge amount of the target chemicals $T_{02\mathrm{h}}$).

2. The parameters used for solving the equations and the values and sources of the data are tabulated in Table S1. Most of the parameters can be found directly in the published papers or report, including: interface areas between air and water (A_2) and air and soil (A_3); thickness of air, water, soil and sediment (h_1 h_2 h_3 h_4); volume fractions of solids in air, soil and sediment (X_{13} X_{33} X_{43}) and volume fractions of air and water in soil, water in sediment (X_{31} X_{32} X_{42}); densities of solids in water, soil, sediment and fish ($\rho_{23}\rho_{33}\rho_{43}\rho_{\mathrm{f}}$); production of fish ($Y_{\mathrm{f}}$); advection air and water flow in/out of area ($Q_{01\mathrm{t}}$ $Q_{02\mathrm{t}}$ $Q_{20\mathrm{t}}$); the chemical basic parameters (T R H Ps K_{OC} BCF_{f}); the molecular diffusivities in air (B_1); mass transfer coefficients (K_{12} K_{13} K_{21} K_{24}); diffusion path lengths in soil and sediment (L_3 L_4); and some parameters related to the rate (K_{p} K_{w} S_{c} K_{s} K_{l} K_{e} K_{r}). Some parameters need the mathematical methods and data provided in the references, including: molecular diffusivity in water and sediment (B_2 B_4). Other parameters are closely related to the actual environment features, and they are either obtained from laboratory test of the local samples or the literature reported values similar to the model environment. For example, the volume fractions of solid in water (X_{23}) are the measured result of the sample points all from the Dongjiang River. The parameter about the degradation is the half-life (t_1 t_2 t_3 t_4) of each chemical. Coefficient of the degradation rate (K_m) can also describe the degradation and the expression is helpful in getting the t of the chemical: K_m=ln(2)/ t. t and K_m in water is all from the river system in different weather conditions, which will include the comprehensive environmental effects such as biodegradation and photolysis. The half-life in soil is similar to the water phase. Aerobic biodegradation in upper sediment is reasonable for the modeling process.

3. The input transfer fluxes are significant for the model. Advective flows in the area through air (T_{01t}) was extremely low, so we set the value to zero. T_{02h} was the wastewater discharge amount of the target chemicals. Market survey data on the volume of home and personal care (HPC) products sold in south China in 2010 (taken from Euromonitor) (Hodges et al., 2012) was used in this study. Based on data obtained from Mintel's Global New Products Database (GNPD) (www.gnpd.com), which is an online tool that monitors and records product innovation and retail success in the consumer packaged goods market, the data per ingredient in products sold in China from Feb 2011 - Feb 2012 were collected. In addition, under the "worst case" scenario, the inclusion level of TCS and TCC was 0.3% in all HPC products and 1.5% in bar soaps, respectively. Combined with the total population in south China, we got the usage amount per person per day for TCS and TCC to be 0.92 and 1.36 mg in south China, respectively. For the Dongjiang River basin, T_{02h} was calculated using the following equation:

$$T_{02h} = q_{per} \times P_{pop} \times \theta \times f$$

Where, q_{per} is the usage per person per day for TCS or TCC; P_{pop} is the population of the watershed; (We obtained the population data in the total river basin and different sections of the river basin from the sixth China national census data (2010)); θ is the sewage treatment efficiency of the region, which was obtained from Guangdong Statistical Yearbook 2011; f is the removal efficiency of each target compound in sewage treatment plants. The removal efficiency data and detailed description are given in Table S1.

5. The parameters collected used for modeling are listed in Table S1. When there were more than one value available (n > 1), arithmetic or geometric mean and standard deviations were computed. For the log-normal distribution, geometric means were used as input; for the normal distribution, arithmetic mean values were selected. If only a single value was found (n = 1) for a certain parameter, a standard deviation was derived from an artificially assigned coefficient of variation (CV) as follows:

1) For the thicknesses of air, soil, and sediment, 50% was taken, according to the fact that the calculated CV of the thickness of water was 58%;
2) The calculated CV for X_{13} was 23 %, so 20% was adopted for similar parameters of X_{31}, X_{32}, X_{33}, X_{42}, and X_{43};
3) 90% was adopted for CVs of t_1 based on the fact that the calculated CVs of t_2, t_3, t_4 were 79%, 68% and 120%;
4) CV of B_1 and B_4 were both 20%, based on the calculated CV of B_2 (23%). And 20% was adopted for CVs of K_{12}, K_{13}, K_{21} and K_{24};
5) 80% was selected for CVs of K_r and S_c based on the observed CV of K_S (84%);

6) Without relevant information, 100% was used conservatively for L_3, L_4, K_p, K_w, K_l, K_e and C_{02h}.

3.3 Statistical distribution

Fig. S1 showed that the statistical log normal distribution of measured concentrations of TCS and TCC. Statistical distribution of some representative input parameters are displayed in Fig. S2. Raw and log-transformed data are presented as histograms, including organic carbon content in water (O_{23}), organic carbon normalized partition coefficients (K_{OC}), half-lives of the chemicals ($t_{1/2}$) in water (TCS), and temperature (T).

3.4 Model results

Fig. S3 displayed the distribution of the TCS and TCC in the multimedia environment. The modeled transfer fluxes of TCS and TCC in and out of the area as well as each compartment are displayed in Fig. S4. Fig. S5 shows the spatial distribution of the transfer flux along the Dongjiang River. a, b, c, d in the figure refer to four environment media: air, water, soil, sediment, respectively. Numbers 1, 2, 3, 4, 5 in horizontal coordinate refer to the total basin, upstream, midstream, downstream and delta, respectively. Fig. S5-1 is the spatial distribution of the transfer flux for TCS, while Fig. S5-2 is the spatial distribution data for TCC.

The sensitivities of the estimated concentrations to input parameters are shown in Fig. S6. Letter “a” refers to the variable changed by +10% and “b” by -10%. Only TCS was selected to display. As result of 20 000 Monte Carlo simulations, the frequency distributions of TCS and TCC concentrations in each of the environmental media are shown as log-transformed distributions. To qualify the similarity, the overlapping areas of the measured and modeled concentration probability density curves are illustrated in Table S2.

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Figure Captions

Fig. S1 Statistical distribution of the measured concentrations.

Fig. S2 Statistical distribution of some representative input parameters. Raw and log-transformed data are presented as histograms.

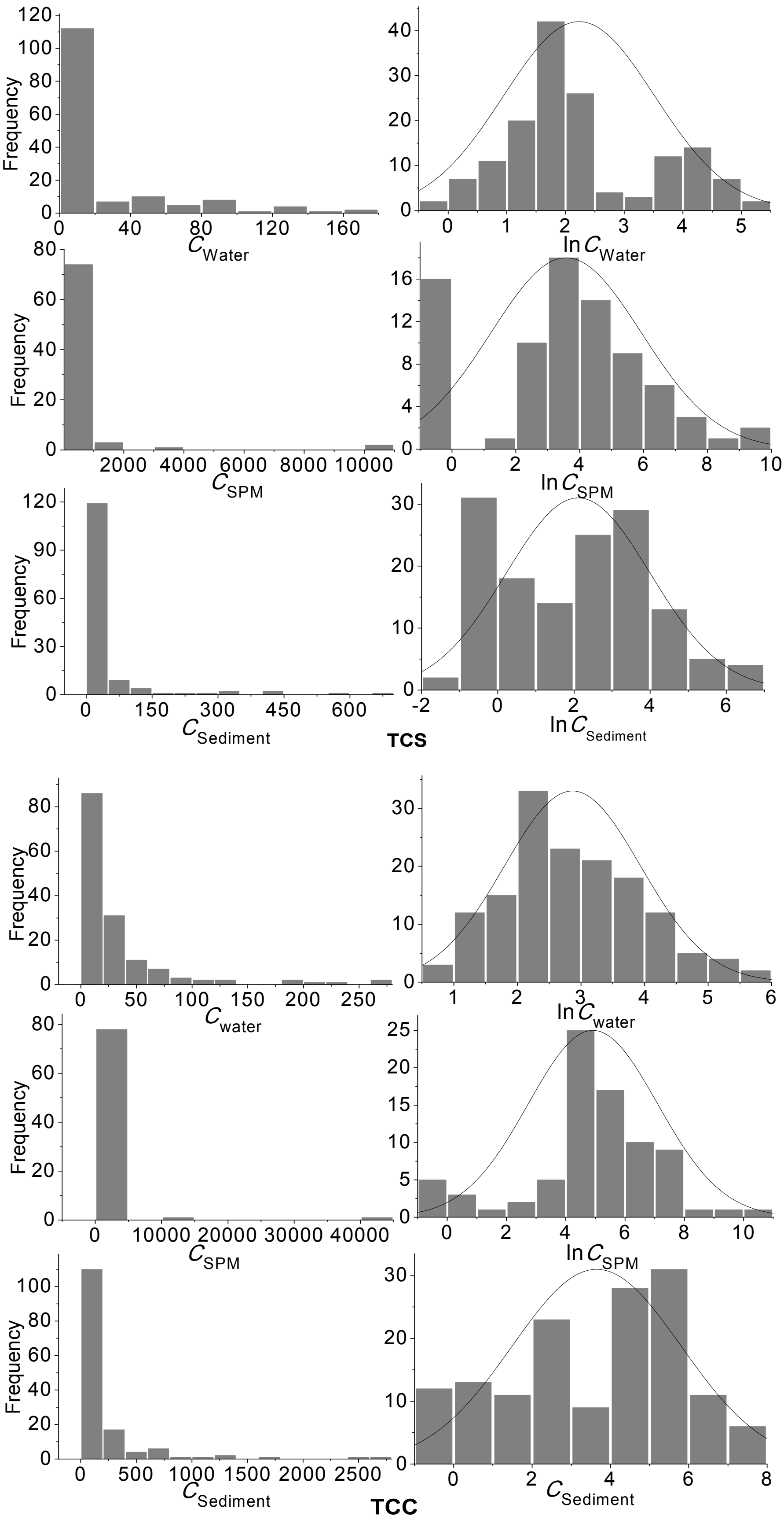
Fig. S3 Distribution of the TCS and TCC in the multimedia environment.

Fig. S4 The modeled transfer fluxes of TCS and TCC in and out of the area as well as each compartment.

Fig. S5 Spatial distribution of the transfer flux along the Dongjiang River. a, b, c, d refer to four environment media: Air, Water, Soil and Sediment, respectively. 1, 2, 3, 4, 5 in horizontal coordinate refer to the total basin, upstream, midstream, downstream and delta, respectively. Fig. S5-1 is the spatial distribution of the transfer flux for TCS and Fig. S5-2 is for TCC.

Fig. S6 Sensitivities of the estimated concentrations to input parameters. a refers to the variable changed by +10% and b is by -10%. Only TCS was selected to display.

Fig .S1


Frequency
C_{Water}
$\ln C_{Water}$
C_{SPM}
$\ln C_{SPM}$
$C_{Sediment}$
$\ln C_{Sediment}$
TCS
C_{water}
$\ln C_{water}$
C_{SPM}
$\ln C_{SPM}$
$C_{Sediment}$
$C_{Sediment}$
TCC
0 40 80 120 160
0 20 40 60 80 100 120
0 1 2 3 4 5
0 10 20 30 40
2000 4000 6000 8000 10000
0 20 40 60 80
0 2 4 6 8 10
0 4 8 12 16
0 150 300 450 600
0 30 60 90 120
-2 0 2 4 6
0 10 20 30
0 50 100 150 200 250
0 20 40 60 80
1 2 3 4 5 6
0 10 20 30
0 10000 20000 30000 40000
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0 5 10 15 20 25
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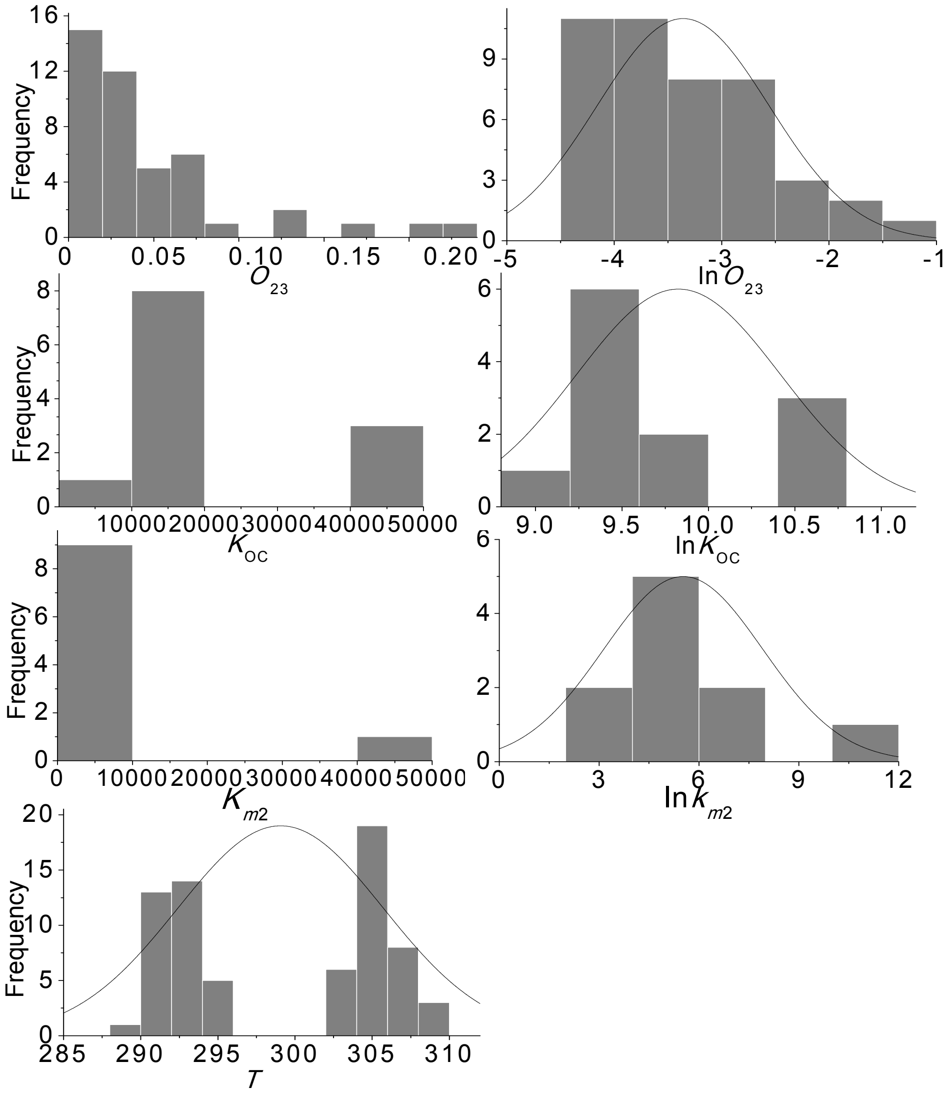
0 2 4 6 8
0 10 20 30

Fig. S2


Frequency
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4
8
12
16
0
0.05
0.10
0.15
0.20
O_{23}
0
3
6
9
-5
-4
-3
-2
-1
$\ln O_{23}$
Frequency
0
2
4
6
8
10000
20000
30000
40000
50000
K_{OC}
0
2
4
6
9.0
9.5
10.0
10.5
11.0
$\ln K_{OC}$
Frequency
0
2
4
6
8
0
10000
20000
30000
40000
50000
K_{m2}
0
2
4
6
0
3
6
9
12
$\ln k_{m2}$
Frequency
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5
10
15
20
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290
295
300
305
310
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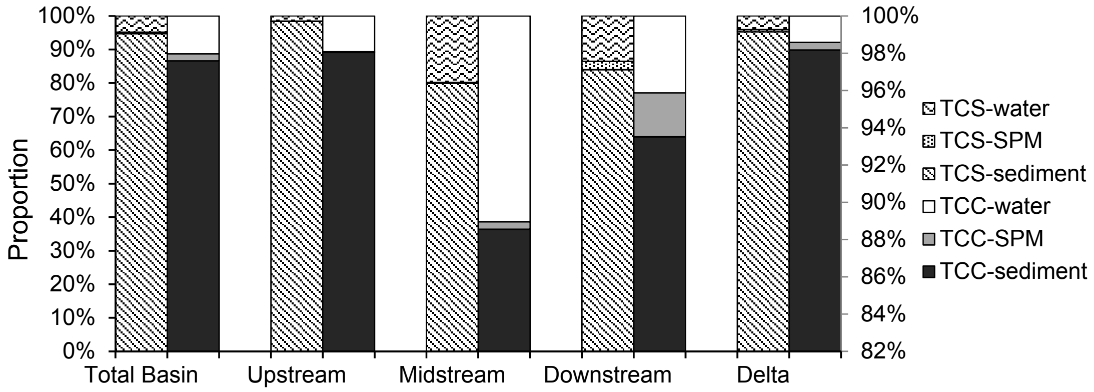
Fig. S3


Proportion
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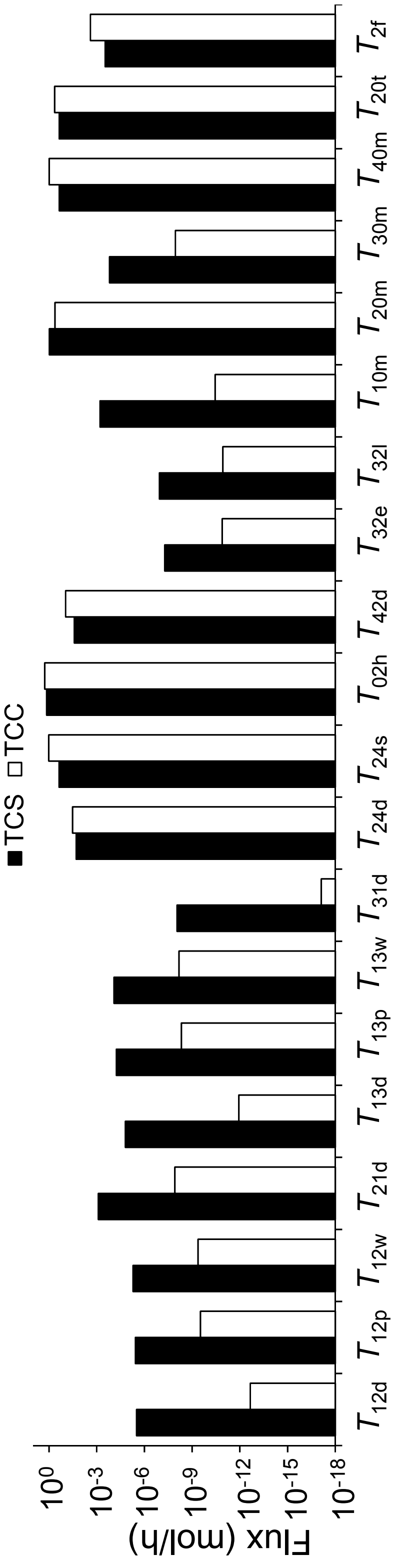
80%
70%
60%
50%
40%
30%
20%
10%
0%
100%
98%
96%
94%
92%
90%
88%
86%
84%
82%
Total Basin
Upstream
Midstream
Downstream
Delta
TCS-water
TCS-SPM
TCS-sediment
TCC-water
TCC-SPM
TCC-sediment


■TCS □TCC
Flux (mol/h)
10^0
10^-3
10^-6
10^-9
10^-12
10^-15
10^-18
T_{12d}
T_{12p}
T_{12w}
T_{21d}
T_{13d}
T_{13p}
T_{13w}
T_{31d}
T_{24d}
T_{24s}
T_{02h}
T_{42d}
T_{32e}
T_{32l}
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T_{20t}
T_{2f}

Fig. S4

Fig. S5

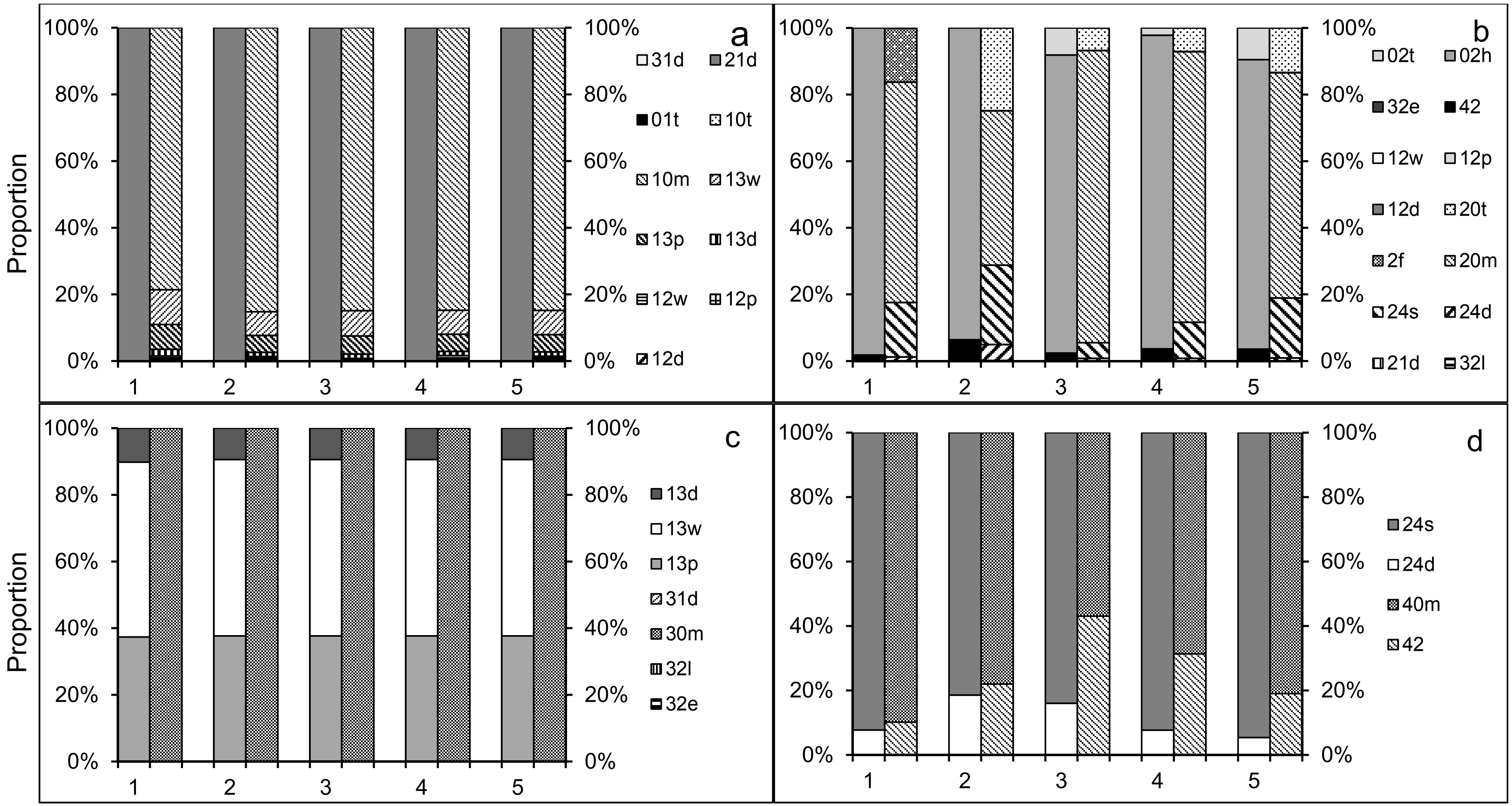


Fig. S5-1 Spatial distribution of the transfer flux for TCS

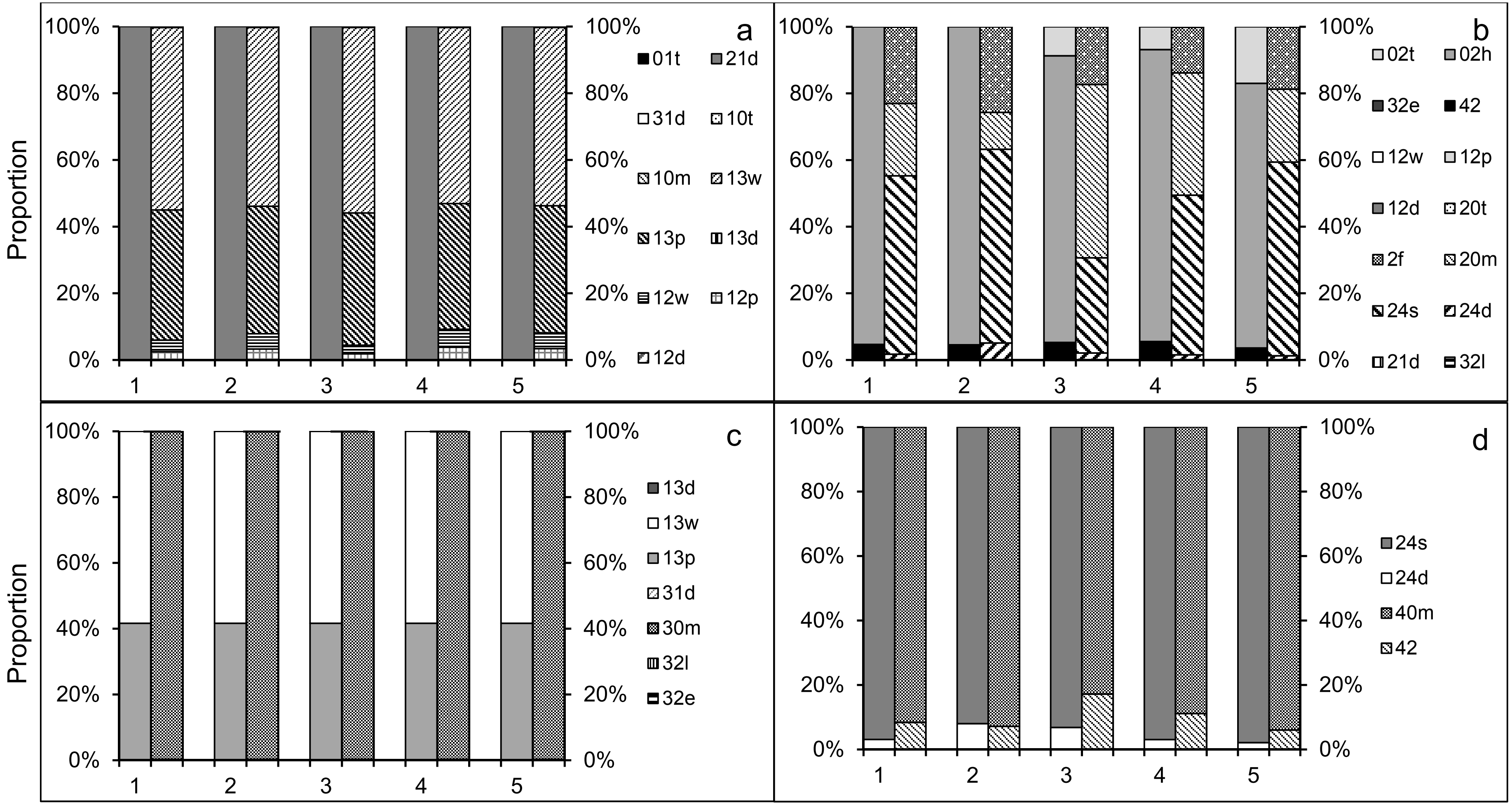
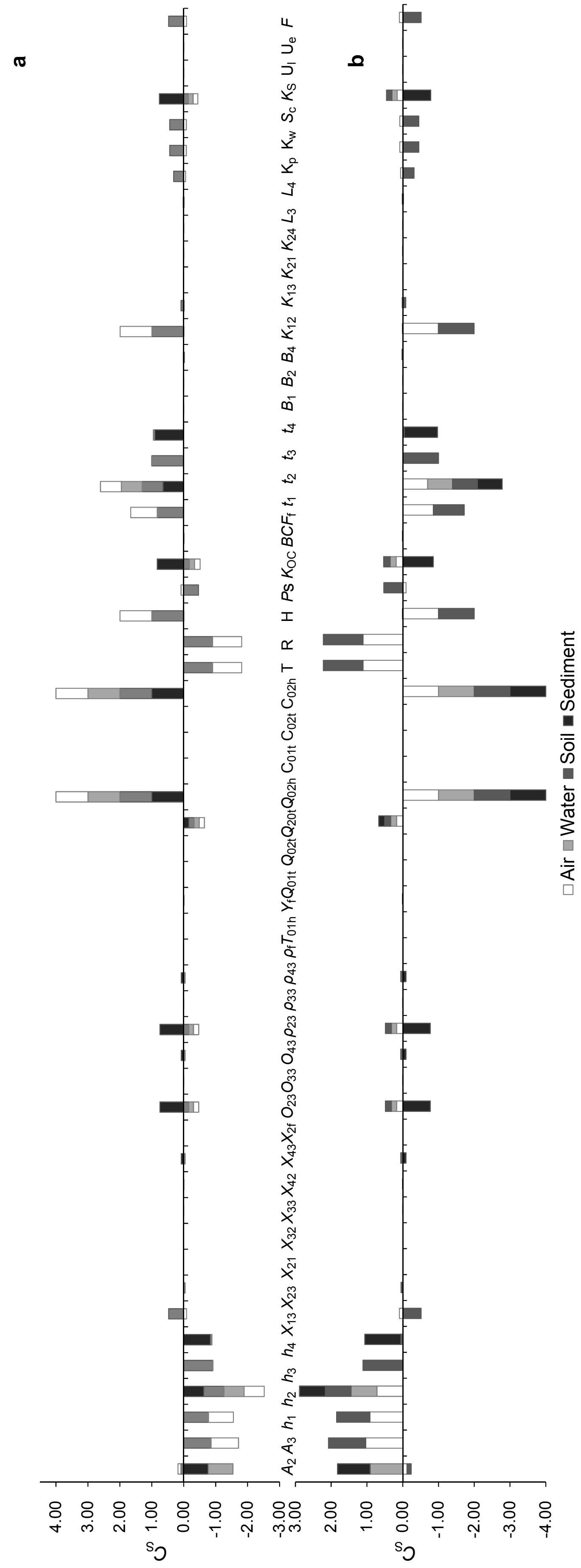


Fig. S5-2 Spatial distribution of the transfer flux for TCC


a
b
S_c
4.00
3.00
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1.00
0.00
-1.00
-2.00
-3.00
-4.00
A_2 A_3 h_1 h_2 h_3 h_4 X_{13} X_{23} X_{21} X_{32} X_{33} X_{42} X_{43} X_{2f} O_{23} O_{33} O_{43} ρ_{23} ρ_{33} ρ_{43} ρ_f T_{01h} Y_f Q_{01t} Q_{02t} Q_{20t} Q_{02h} C_{01t} C_{02t} C_{02h} T R H Ps K_{OC} BCF_f t_1 t_2 t_3 t_4 B_1 B_2 B_4 K_{12} K_{13} K_{21} K_{24} L_3 L_4 K_p K_w S_c K_S U_l U_e F
□ Air ▨ Water ■ Soil ■ Sediment

Fig.S6

Table S1-1 Collected parameters used in the multimedia model-Total Basin.

Symbol	Unit	Definition	Mean[a]	Standard deviation[a,c]	N[b]	Ref[θ].
A_2	m^2	Area of water phase	2.083×10^{9}	1.072×10^{0}	2	11,33
A_3	m^2	Area of soil phase	3.273×10^{10}	1.024×10^{0}	2	11,33
h_1	m	Thickness of air	5.984×10^{2}	1.604×10^{0}	1	25
h_2	m	Depth of water	4.801×10^{0}	2.433×10^{0}	3	23,46,53
h_3	m	Thickness of soil	1.485×10^{-1}	1.604×10^{0}	1	53
h_4	m	Thickness of sediment	4.470×10^{-2}	1.604×10^{0}	1	7,53
X_{13}	v/v	Volume fractions of solids in air	7.878×10^{-11}	1.219×10^{0}	1	25
X_{23}	v/v	Volume fractions of solids in water	9.504×10^{-6}	2.814×10^{0}	72	-[g]
X_{31}	v/v	Volume fractions of air in soil	1.960×10^{-1}	1.219×10^{0}	1	4
X_{32}	v/v	Volume fractions of water in soil	2.449×10^{-1}	1.219×10^{0}	1	4
X_{33}	v/v	Volume fractions of solids in soil	5.389×10^{-1}	1.219×10^{0}	1	4
X_{42}	v/v	Volume fractions of water in sediment	6.859×10^{-1}	1.219×10^{0}	1	25
X_{43}	v/v	Volume fractions of solids in sediment	2.939×10^{-1}	1.219×10^{0}	1	25
X_{2f}	v/v	Volume fractions of fish in water	5.500×10^{-9}	2.243×10^{0}	4	24,37
O_{23}	w/w	Contents of organic carbon in solids in water	3.480×10^{-2}	2.231×10^{0}	45	50, -[g]
O_{33}	w/w	Contents of organic carbon in solids in soil	1.828×10^{-2}	1.219×10^{0}	3	14
O_{43}	w/w	Contents of organic carbon in solids in sediment	9.800×10^{-3}	2.635×10^{0}	72	23, -[g]
ρ_{23}	kg/L	Densities of solids in water	2.397×10^{0}	1.604×10^{0}	36[g]	47, -[g]
ρ_{33}	kg/L	Densities of solids in soil	1.821×10^{0}	1.628×10^{0}	2	4,14
ρ_{43}	kg/L	Densities of solids in sediment	2.397×10^{0}	1.604×10^{0}	36[g]	23, -[g]
ρ_f	kg/L	Densities of fish	1.234×10^{0}	1.256×10^{0}	2	4,24
Y_f	t/h	Production of fish	5.768×10^{1}	1.639×10^{0}	3	37
Q_{01t}	m^3/h	Advection air flow in area	0	-	-	-
Q_{02t}	m^3/h	Advection water flow in area	7.718×10^{5}	3.495×10^{0}	4	38,-[g]
Q_{20t}	m^3/h	Advection water flow out of area	3.943×10^{6}	3.305×10^{0}	5	10,12,46,-[g]
Q_{02h}	m^3/h	Wastewater discharge rate	2.882×10^{5}	1.056×10^{0}	3	37
C_{02t}	m^3/h	Concentration in flowing water	0(TCS)	-	-	-[i]
			0(TCC)	-	-	-[i]
C_{02h}	mol/m^3	Wastewater concentration	4.824×10^{-6}(TCS)	2.299×10^{0}(TCS)	1	-[h], 37
			6.408×10^{-6}(TCC)	2.299×10^{0}(TCC)	1	-[h], 37
T	K	Local absolute temperature	2.964×10^{2}	1.007×10^{0}	71	37,-[g]
R	$Pa\cdot m^3/mol\cdot K$	Universal gas constant	8.314×10^{0}	1.000×10^{0}	-	-
H	$Pa\cdot m^3/mol$	Henry's constant	5.500×10^{-3}(TCS)	7.670×10^{0}(TCS)	4	3,20,26,41

			4.557×10^{-8}(TCC)	1.105×10^{0}(TCC)	2	52, -[k]
Ps	Pa	Vapor pressure	4.972×10^{-4}(TCS)	1.745×10^{0}(TCS)	5	3, 32,49,50
			4.705×10^{-9}(TCC)	6.956×10^{2}(TCC)	2	42,49
K_{OC}	L/kg	Organic carbon normalized partition coefficients	2.357×10^{4}(TCS)	1.973×10^{0}(TCS)	12	5,20,27,29,32,35,44, 49
			5.596×10^{4}(TCC)	1.415×10^{0}(TCC)	9	6,15,27,42,44,52
t_1[d]	h	Half-life of the chemical in air	1.182×10^{1}(TCS)	2.160×10^{0}(TCS)	1	-[k]
			1.476×10^{1}(TCC)	1.324×10^{0}(TCC)	1	-[k]
t_2	h	Half-life of the chemical in water	4.304×10^{2}(TCS)	2.630×10^{0}(TCS)	11	20,28,32,36,39,-[k]
			1.859×10^{3}(TCC)	1.435×10^{0}(TCC)	2	42,-[k]
t_3	h	Half-life of the chemical in soil	1.155×10^{3}(TCS)	2.076×10^{0}(TCS)	9	32,34,43,44,49, -[k]
			3.802×10^{3}(TCC)	1.678×10^{0}(TCC)	7	40,44,49, -[k]
t_4	h	Half-life of the chemical in sediment	3.524×10^{3}(TCS)	6.336×10^{0}(TCS)	3	49,-[k]
			7.395×10^{3}(TCC)	2.650×10^{0}(TCC)	3	34,40,49,-[k]
BCF_f		Bioconcentration factors for fish in water	9.000×10^{1}(TCS)	4.725×10^{0}(TCS)	3	29,41,49
			4.031×10^{2}(TCC)	4.601×10^{0}(TCC)	2	40,49
B_1	m^2/h	Molecular diffusivity in air	3.920×10^{-2}	1.219×10^{0}	1	25
B_2	m^2/h	Molecular diffusivity in water	4.746×10^{-6}(TCS)	1.274×10^{0}(TCS)	2	25,45
			4.510×10^{-6}(TCC)	1.185×10^{0}(TCC)	2	25,45
B_4	m^2/h	Molecular diffusivity in sediment	5.869×10^{-7}(TCS)	1.219×10^{0}(TCS)	1	45
			5.351×10^{-7}(TCC)	1.219×10^{0}(TCC)	1	45
K_{12}	m/h	Air-side mass transfer coefficient over water	2.942×10^{0}	1.219×10^{0}	1	25
K_{13}	m/h	Air-side mass transfer coefficient over soil	9.860×10^{-1}	1.219×10^{0}	1	25
K_{21}	m/h	Water-side mass transfer coefficient over air	2.942×10^{-2}	1.219×10^{0}	1	25
K_{24}	m/h	Water-side mass transfer coefficient over sediment	9.800×10^{-3}	1.219×10^{0}	1	25
L_3	m	Diffusion path lengths in soil	3.540×10^{-2}	2.299×10^{0}	1	25
L_4	m	Diffusion path lengths in sediment	3.540×10^{-3}	2.299×10^{0}	1	24
K_p	m/h	Dry deposition velocity	7.637×10^{0}	2.299×10^{0}	1	25
K_w	m/h	Rain rate	6.859×10^{-5}	2.299×10^{0}	1	25
S_c	m/h	Rain scavenging rate	1.562×10^{5}	2.021×10^{0}	1	25
K_s	m/h	Sedimentation rate in water	9.900×10^{-7}	1.670×10^{0}	8	8,17,19,21,23,31
K_l	m/h	Runoff rates of dissolved components	2.758×10^{-5}	2.299×10^{0}	1	25
K_e	m/h	Runoff rates of solid in soil	1.626×10^{-8}	2.299×10^{0}	1	25
K_r[e]	m/h	Resuspension rate in sedimentation	0	-	-	-
f'[f]		Removal efficiency of target compounds in STP	9.453×10^{-1}(TCS)	-	4	2,18,36,48
			9.715×10^{-1}(TCC)	-	6	1,13,15,40

Table S1-2 Collected parameters used in the multimedia model-Upstream

Symbol	Unit	Definition	Mean^{a}	Standard deviation ^{a,c}	N^{b}	Ref$^{\theta}$.
A_2	m^2	Area of water phase	4.727×10^{8}	3.939×10^{0}	2	33,54
A_3	m^2	Area of soil phase	5.510×10^{9}	1.645×10^{0}	2	33,54
h_1	m	Thickness of air	5.984×10^{2}	1.604×10^{0}	1	25
h_2	m	Depth of water	8.615×10^{-1}	1.384×10^{0}	3	38
h_3	m	Thickness of soil	1.485×10^{-1}	1.604×10^{0}	1	53
h_4	m	Thickness of sediment	4.470×10^{-2}	1.604×10^{0}	1	53
X_{13}	v/v	Volume fractions of solids in air	7.878×10^{-11}	1.219×10^{0}	1	25
X_{23}	v/v	Volume fractions of solids in water	4.142×10^{-6}	2.465×10^{0}	9	-^{g}
X_{31}	v/v	Volume fractions of air in soil	1.960×10^{-1}	1.219×10^{0}	1	4
X_{32}	v/v	Volume fractions of water in soil	2.449×10^{-1}	1.219×10^{0}	1	4
X_{33}	v/v	Volume fractions of solids in soil	5.389×10^{-1}	1.219×10^{0}	1	4
X_{42}	v/v	Volume fractions of water in sediment	6.859×10^{-1}	1.219×10^{0}	1	25
X_{43}	v/v	Volume fractions of solids in sediment	2.939×10^{-1}	1.219×10^{0}	1	25
X_{2f}	v/v	Volume fractions of fish in water	3.162×10^{-9}	2.071×10^{0}	4	24,37
O_{23}	w/w	Contents of organic carbon in solids in water	1.800×10^{-2}	1.312×10^{0}	45	-^{g}
O_{33}	w/w	Contents of organic carbon in solids in soil	1.828×10^{-2}	1.219×10^{0}	3	14
O_{43}	w/w	Contents of organic carbon in solids in sediment	1.147×10^{-2}	1.667×10^{0}	8	23, -^{g}
ρ_{23}	kg/L	Densities of solids in water	2.434×10^{0}	1.017×10^{0}	36	47, -^{g}
ρ_{33}	kg/L	Densities of solids in soil	1.821×10^{0}	1.628×10^{0}	2	4,14
ρ_{43}	kg/L	Densities of solids in sediment	2.434×10^{0}	1.017×10^{0}	36	23, -^{g}
ρ_f	kg/L	Densities of fish	1.234×10^{0}	1.256×10^{0}	2	4,24
Y_f	t/h	Production of fish	9.853×10^{-1}	1.067×10^{0}	3	37
Q_{01t}	m^3/h	Advection air flow in area	0	-	-	-
Q_{02t}	m^3/h	Advection water flow in area	2.517×10^{5}	1.383×10^{0}	4	38,-^{g}
Q_{20t}	m^3/h	Advection water flow out of area	3.513×10^{5}	1.949×10^{0}	5	38
Q_{02h}	m^3/h	Wastewater discharge rate	2.375×10^{3}	1.000×10^{0}	3	37
C_{02t}	m^3/h	Concentration in flowing water	0(TCS)	-	-	-^{i}
			0(TCC)	-	-	-^{i}
C_{02h}	mol/m^3	Wastewater concentration	2.144×10^{-5}(TCS)	2.299×10^{0}(TCS)	1	-^{h}, 37
			2.636×10^{-5}(TCC)	2.299×10^{0}(TCC)	1	-^{h}, 37
T	K	Local absolute temperature	2.964×10^{2}	7.071×10^{-2}	11	37,-^{g}
R	$Pa\cdot m^3/mol\cdot K$	Universal gas constant	8.314×10^{0}	1.000×10^{0}	-	-
H	$Pa\cdot m^3/mol$	Henry's constant	5.500×10^{-3}(TCS)	7.670×10^{0}(TCS)	4	3,20,26,41

Ps	Pa	Vapor pressure	4.557×10^{-8}(TCC)	1.105×10^{0}(TCC)	2	52, -[k]
			4.972×10^{-4}(TCS)	1.745×10^{0}(TCS)	5	3, 32,49,50
			4.705×10^{-9}(TCC)	6.956×10^{2}(TCC)	2	42,49
K_{OC}	L/kg	Organic carbon normalized partition coefficients	2.357×10^{4}(TCS)	1.973×10^{0}(TCS)	12	5,20,27,29,32,35,44, 49
			5.596×10^{4}(TCC)	1.415×10^{0}(TCC)	9	6,15,27,42,44,52
$t_1{}^{d}$	h	Half-life of the chemical in air	1.182×10^{1}(TCS)	2.160×10^{0}(TCS)	1	-[k]
			1.476×10^{1}(TCC)	1.324×10^{0}(TCC)	1	-[k]
t_2	h	Half-life of the chemical in water	4.304×10^{2}(TCS)	2.630×10^{0}(TCS)	11	20,28,32,36,39,-[k]
			1.859×10^{3}(TCC)	1.435×10^{0}(TCC)	2	42,-[k]
t_3	h	Half-life of the chemical in soil	1.155×10^{3}(TCS)	2.076×10^{0}(TCS)	9	32,34,43,44,49, -[k]
			3.802×10^{3}(TCC)	1.678×10^{0}(TCC)	7	40,44,49, -[k]
t_4	h	Half-life of the chemical in sediment	3.524×10^{3}(TCS)	6.336×10^{0}(TCS)	3	49,-[k]
			7.395×10^{3}(TCC)	2.650×10^{0}(TCC)	3	34,40,49,-[k]
BCF_f		Bioconcentration factors for fish in water	9.000×10^{1}(TCS)	4.725×10^{0}(TCS)	3	29,41,49
			4.031×10^{2}(TCC)	4.601×10^{0}(TCC)	2	40,49
B_1	m^2/h	Molecular diffusivity in air	3.920×10^{-2}	1.219×10^{0}	1	25
B_2	m^2/h	Molecular diffusivity in water	4.746×10^{-6}(TCS)	1.274×10^{0}(TCS)	2	25,45
			4.510×10^{-6}(TCC)	1.185×10^{0}(TCC)	2	25,45
B_4	m^2/h	Molecular diffusivity in sediment	5.869×10^{-7}(TCS)	1.219×10^{0}(TCS)	1	45
			5.351×10^{-7}(TCC)	1.219×10^{0}(TCC)	1	45
K_{12}	m/h	Air-side mass transfer coefficient over water	2.942×10^{0}	1.219×10^{0}	1	25
K_{13}	m/h	Air-side mass transfer coefficient over soil	9.860×10^{-1}	1.219×10^{0}	1	25
K_{21}	m/h	Water-side mass transfer coefficient over air	2.942×10^{-2}	1.219×10^{0}	1	25
K_{24}	m/h	Water-side mass transfer coefficient over sediment	9.800×10^{-3}	1.219×10^{0}	1	25
L_3	m	Diffusion path lengths in soil	3.540×10^{-2}	2.299×10^{0}	1	25
L_4	m	Diffusion path lengths in sediment	3.540×10^{-3}	2.299×10^{0}	1	24
K_p	m/h	Dry deposition velocity	7.637×10^{0}	2.299×10^{0}	1	25
K_w	m/h	Rain rate	6.859×10^{-5}	2.299×10^{0}	1	25
S_c	m/h	Rain scavenging rate	1.562×10^{5}	2.021×10^{0}	1	25
K_s	m/h	Sedimentation rate in water	6.936×10^{-7}	1.187×10^{0}	3	8, 19, 31
K_l	m/h	Runoff rates of dissolved components	2.758×10^{-5}	2.299×10^{0}	1	25
K_e	m/h	Runoff rates of solid in soil	1.626×10^{-8}	2.299×10^{0}	1	25
$K_r{}^{e}$	m/h	Resuspension rate in sedimentation	0	-	-	-
f^{f}		Removal efficiency of target compounds in STP	9.453×10^{-1}(TCS)	-	4	2,18,36,48
			9.715×10^{-1}(TCC)	-	6	1,13,15,40

Table S1-3 Collected parameters used in the multimedia model-Midstream

Symbol	Unit	Definition	Mean[a]	Standard deviation [a,c]	N[b]	Ref[θ].
A_2	m^2	Area of water phase	6.156×10^{8}	1.553×10^{0}	2	33,54
A_3	m^2	Area of soil phase	1.325×10^{10}	1.064×10^{0}	2	33,54
h_1	m	Thickness of air	5.984×10^{2}	1.604×10^{0}	1	25
h_2	m	Depth of water	9.823×10^{0}	1.350×10^{0}	5	46
h_3	m	Thickness of soil	1.485×10^{-1}	1.604×10^{0}	1	53
h_4	m	Thickness of sediment	4.470×10^{-2}	1.604×10^{0}	1	53
X_{13}	v/v	Volume fractions of solids in air	7.878×10^{-11}	1.219×10^{0}	1	25
X_{23}	v/v	Volume fractions of solids in water	3.248×10^{-6}	1.707×10^{0}	10	-[g]
X_{31}	v/v	Volume fractions of air in soil	1.960×10^{-1}	1.219×10^{0}	1	4
X_{32}	v/v	Volume fractions of water in soil	2.449×10^{-1}	1.219×10^{0}	1	4
X_{33}	v/v	Volume fractions of solids in soil	5.389×10^{-1}	1.219×10^{0}	1	4
X_{42}	v/v	Volume fractions of water in sediment	6.859×10^{-1}	1.219×10^{0}	1	25
X_{43}	v/v	Volume fractions of solids in sediment	2.939×10^{-1}	1.219×10^{0}	1	25
X_{2f}	v/v	Volume fractions of fish in water	3.162×10^{-9}	2.071×10^{0}	4	24,37
O_{23}	w/w	Contents of organic carbon in solids in water	2.161×10^{-2}	2.440×10^{0}	10	-[g]
O_{33}	w/w	Contents of organic carbon in solids in soil	1.828×10^{-2}	1.219×10^{0}	3	14
O_{43}	w/w	Contents of organic carbon in solids in sediment	4.279×10^{-3}	2.464×10^{0}	10	-[g]
ρ_{23}	kg/L	Densities of solids in water	2.420×10^{0}	1.016×10^{0}	36 [g]	47, -[g]
ρ_{33}	kg/L	Densities of solids in soil	1.821×10^{0}	1.628×10^{0}	2	4,14
ρ_{43}	kg/L	Densities of solids in sediment	2.420×10^{0}	1.016×10^{0}	36[g]	23, -[g]
ρ_f	kg/L	Densities of fish	4.238×10^{0}	1.256×10^{0}	2	4,24
Y_f	t/h	Production of fish	5.768×10^{1}	1.035×10^{0}	3	37
Q_{01t}	m^3/h	Advection air flow in area	0	-	-	-
Q_{02t}	m^3/h	Advection water flow in area	3.513×10^{5}	1.949×10^{0}	4	38
Q_{20t}	m^3/h	Advection water flow out of area	7.487×10^{5}	1.883×10^{0}	5	11
Q_{02h}	m^3/h	Wastewater discharge rate	1.399×10^{5}	1.158×10^{0}	3	37
C_{02t}	m^3/h	Concentration in flowing water	5.805×10^{-8}(TCS)	1.196×10^{0}(TCS)	1	-[i]
			1.122×10^{-7}(TCC)	1.196×10^{0}(TCC)	1	-[i]
C_{02h}	mol/m^3	Wastewater concentration	1.608×10^{-5}(TCS)	2.299×10^{0}(TCS)	1	-[h], 37
			2.778×10^{-5}(TCC)	2.299×10^{0}(TCC)	1	-[h], 37
T	K	Local absolute temperature	2.959×10^{2}	1.007×10^{0}	11	37,-[g]
R	$Pa\cdot m^3/mol\cdot K$	Universal gas constant	8.314×10^{0}	1.000×10^{0}	-	-
H	$Pa\cdot m^3/mol$	Henry's constant	5.500×10^{-3}(TCS)	7.670×10^{0}(TCS)	4	3,20,26,41

			4.557×10^{-8}(TCC)	1.105×10^{0}(TCC)	2	52, -[k]
Ps	Pa	Vapor pressure	4.972×10^{-4}(TCS)	1.745×10^{0}(TCS)	5	3, 32,49,50
			4.705×10^{-9}(TCC)	6.956×10^{2}(TCC)	2	42,49
K_{OC}	L/kg	Organic carbon normalized partition coefficients	2.357×10^{4}(TCS)	1.973×10^{0}(TCS)	12	5,20,27,29,32,35,44, 49
			5.596×10^{4}(TCC)	1.415×10^{0}(TCC)	9	6,15,27,42,44,52
t_1^{d}	h	Half-life of the chemical in air	1.182×10^{1}(TCS)	2.160×10^{0}(TCS)	1	-[k]
			1.476×10^{1}(TCC)	1.324×10^{0}(TCC)	1	-[k]
t_2	h	Half-life of the chemical in water	4.304×10^{2}(TCS)	2.630×10^{0}(TCS)	11	20,28,32,36,39,-[k]
			1.859×10^{3}(TCC)	1.435×10^{0}(TCC)	2	42,-[k]
t_3	h	Half-life of the chemical in soil	1.155×10^{3}(TCS)	2.076×10^{0}(TCS)	9	32,34,43,44,49, -[k]
			3.802×10^{3}(TCC)	1.678×10^{0}(TCC)	7	40,44,49, -[k]
t_4	h	Half-life of the chemical in sediment	3.524×10^{3}(TCS)	6.336×10^{0}(TCS)	3	49,-[k]
			7.395×10^{3}(TCC)	2.650×10^{0}(TCC)	3	34,40,49,-[k]
BCF_f		Bioconcentration factors for fish in water	9.000×10^{1}(TCS)	4.725×10^{0}(TCS)	3	29,41,49
			4.031×10^{2}(TCC)	4.601×10^{0}(TCC)	2	40,49
B_1	m^2/h	Molecular diffusivity in air	3.920×10^{-2}	1.219×10^{0}	1	25
B_2	m^2/h	Molecular diffusivity in water	4.746×10^{-6}(TCS)	1.274×10^{0}(TCS)	2	25,45
			4.510×10^{-6}(TCC)	1.185×10^{0}(TCC)	2	25,45
B_4	m^2/h	Molecular diffusivity in sediment	5.869×10^{-7}(TCS)	1.219×10^{0}(TCS)	1	45
			5.351×10^{-7}(TCC)	1.219×10^{0}(TCC)	1	45
K_{12}	m/h	Air-side mass transfer coefficient over water	2.942×10^{0}	1.219×10^{0}	1	25
K_{13}	m/h	Air-side mass transfer coefficient over soil	9.860×10^{-1}	1.219×10^{0}	1	25
K_{21}	m/h	Water-side mass transfer coefficient over air	2.942×10^{-2}	1.219×10^{0}	1	25
K_{24}	m/h	Water-side mass transfer coefficient over sediment	9.800×10^{-3}	1.219×10^{0}	1	25
L_3	m	Diffusion path lengths in soil	3.540×10^{-2}	2.299×10^{0}	1	25
L_4	m	Diffusion path lengths in sediment	3.540×10^{-3}	2.299×10^{0}	1	24
K_p	m/h	Dry deposition velocity	7.637×10^{0}	2.299×10^{0}	1	25
K_w	m/h	Rain rate	6.859×10^{-5}	2.299×10^{0}	1	25
S_c	m/h	Rain scavenging rate	1.562×10^{5}	2.021×10^{0}	1	25
K_s	m/h	Sedimentation rate in water	6.936×10^{-7}	1.187×10^{0}	3	8, 19, 31
K_l	m/h	runoff rates of dissolved components	2.758×10^{-5}	2.299×10^{0}	1	25
K_e	m/h	runoff rates of solid in soil	1.626×10^{-8}	2.299×10^{0}	1	25
K_r^{e}	m/h	Resuspension rate in sedimentation	0	-	-	-
f^{f}		Removal efficiency of target compounds in STP	9.453×10^{-1}(TCS)	-	4	2,18,36,48
			9.715×10^{-1}(TCC)	-	6	1,13,15,40

Table S1-4 Collected parameters used in the multimedia model-Downstream

Symbol	Unit	Definition	Mean[a]	Standard deviation [a,c]	N[b]	Ref[θ].
A_2	m^2	Area of water phase	7.296×10^{8}	1.219×10^{0}	1	33
A_3	m^2	Area of soil phase	7.168×10^{9}	1.219×10^{0}	1	33
h_1	m	Thickness of air	5.984×10^{2}	1.604×10^{0}	1	25
h_2	m	Depth of water	8.812×10^{0}	1.593×10^{0}	4	12,46
h_3	m	Thickness of soil	1.485×10^{-1}	1.604×10^{0}	1	53
h_4	m	Thickness of sediment	4.470×10^{-2}	1.604×10^{0}	1	53
X_{13}	v/v	Volume fractions of solids in air	7.878×10^{-11}	1.219×10^{0}	1	25
X_{23}	v/v	Volume fractions of solids in water	1.287×10^{-5}	3.035×10^{0}	20	-[g]
X_{31}	v/v	Volume fractions of air in soil	1.960×10^{-1}	1.219×10^{0}	1	4
X_{32}	v/v	Volume fractions of water in soil	2.449×10^{-1}	1.219×10^{0}	1	4
X_{33}	v/v	Volume fractions of solids in soil	5.389×10^{-1}	1.219×10^{0}	1	4
X_{42}	v/v	Volume fractions of water in sediment	6.859×10^{-1}	1.219×10^{0}	1	25
X_{43}	v/v	Volume fractions of solids in sediment	2.939×10^{-1}	1.219×10^{0}	1	25
X_{2f}	v/v	Volume fractions of fish in water	3.162×10^{-9}	2.071×10^{0}	4	24,37
O_{23}	w/w	Contents of organic carbon in solids in water	4.968×10^{-2}	2.705×10^{0}	18	-[g]
O_{33}	w/w	Contents of organic carbon in solids in soil	1.828×10^{-2}	1.219×10^{0}	3	14
O_{43}	w/w	Contents of organic carbon in solids in sediment	7.086×10^{-3}	3.112×10^{0}	19	-[g]
ρ_{23}	kg/L	Densities of solids in water	2.420×10^{0}	1.016×10^{0}	20[g]	47, -[g]
ρ_{33}	kg/L	Densities of solids in soil	1.821×10^{0}	1.628×10^{0}	2	4,14
ρ_{43}	kg/L	Densities of solids in sediment	2.424×10^{0}	1.015×10^{0}	20[g]	23, -[g]
ρ_f	kg/L	Densities of fish	1.234×10^{0}	1.256×10^{0}	2	4,24
Y_f	t/h	Production of fish	2.446×10^{1}	1.028×10^{0}	3	37
Q_{01t}	m^3/h	Advection air flow in area	0	-	-	-
Q_{02t}	m^3/h	Advection water flow in area	7.487×10^{5}	1.883×10^{0}	4	11
Q_{20t}	m^3/h	Advection water flow out of area	8.956×10^{5}	2.706×10^{0}	5	11
Q_{02h}	m^3/h	Wastewater discharge rate	1.925×10^{5}	1.037×10^{0}	3	37
C_{02t}	m^3/h	Concentration in flowing water	2.259×10^{-8}(TCS)	1.196×10^{0}(TCS)	1	-[i]
			1.047×10^{-7}(TCC)	1.196×10^{0}(TCC)	1	-[i]
C_{02h}	mol/m^3	Wastewater concentration	3.812×10^{-6}(TCS)	2.299×10^{0}(TCS)	1	-[h], 37
			5.190×10^{-6}(TCC)	2.299×10^{0}(TCC)	1	-[h], 37
T	K	Local absolute temperature	2.972×10^{2}	6.585×10^{0}	20	37,-[g]
R	$Pa\cdot m^3/mol\cdot K$	Universal gas constant	8.314×10^{0}	1.000×10^{0}	-	-
H	$Pa\cdot m^3/mol$	Henry's constant	5.500×10^{-3}(TCS)	7.670×10^{0}(TCS)	4	3,20,26,41

			4.557×10^{-8}(TCC)	1.105×10^{0}(TCC)	2	52, -[k]
Ps	Pa	Vapor pressure	4.972×10^{-4}(TCS)	1.745×10^{0}(TCS)	5	3, 32,49,50
			4.705×10^{-9}(TCC)	6.956×10^{2}(TCC)	2	42,49
K_{OC}	L/kg	Organic carbon normalized partition coefficients	2.357×10^{4}(TCS)	1.973×10^{0}(TCS)	12	5,20,27,29,32,35,44, 49
			5.596×10^{4}(TCC)	1.415×10^{0}(TCC)	9	6,15,27,42,44,52
t_1[d]	h	Half-life of the chemical in air	1.182×10^{1}(TCS)	2.160×10^{0}(TCS)	1	-[k]
			1.476×10^{1}(TCC)	1.324×10^{0}(TCC)	1	-[k]
t_2	h	Half-life of the chemical in water	4.304×10^{2}(TCS)	2.630×10^{0}(TCS)	11	20,28,32,36,39,-[k]
			1.859×10^{3}(TCC)	1.435×10^{0}(TCC)	2	42,-[k]
t_3	h	Half-life of the chemical in soil	1.155×10^{3}(TCS)	2.076×10^{0}(TCS)	9	32,34,43,44,49, -[k]
			3.802×10^{3}(TCC)	1.678×10^{0}(TCC)	7	40,44,49, -[k]
t_4	h	Half-life of the chemical in sediment	3.524×10^{3}(TCS)	6.336×10^{0}(TCS)	3	49,-[k]
			5.436×10^{3}(TCC)	2.7343×10^{0}(TCC)	3	34,40,49,-[k]
BCF_f		Bioconcentration factors for fish in water	9.000×10^{1}(TCS)	4.725×10^{0}(TCS)	3	29,41,49
			4.031×10^{2}(TCC)	4.601×10^{0}(TCC)	2	40,49
B_1	m^2/h	Molecular diffusivity in air	3.920×10^{-2}	1.219×10^{0}	1	25
B_2	m^2/h	Molecular diffusivity in water	4.746×10^{-6}(TCS)	1.274×10^{0}(TCS)	2	25,45
			4.510×10^{-6}(TCC)	1.185×10^{0}(TCC)	2	25,45
B_4	m^2/h	Molecular diffusivity in sediment	5.869×10^{-7}(TCS)	1.219×10^{0}(TCS)	1	45
			5.351×10^{-7}(TCC)	1.219×10^{0}(TCC)	1	45
K_{12}	m/h	Air-side mass transfer coefficient over water	2.942×10^{0}	1.219×10^{0}	1	25
K_{13}	m/h	Air-side mass transfer coefficient over soil	9.860×10^{-1}	1.219×10^{0}	1	25
K_{21}	m/h	Water-side mass transfer coefficient over air	2.942×10^{-2}	1.219×10^{0}	1	25
K_{24}	m/h	Water-side mass transfer coefficient over sediment	9.800×10^{-3}	1.219×10^{0}	1	25
L_3	m	Diffusion path lengths in soil	3.540×10^{-2}	2.299×10^{0}	1	25
L_4	m	Diffusion path lengths in sediment	3.540×10^{-3}	2.299×10^{0}	1	24
K_p	m/h	Dry deposition velocity	7.637×10^{0}	2.299×10^{0}	1	25
K_w	m/h	Rain rate	6.859×10^{-5}	2.299×10^{0}	1	25
S_c	m/h	Rain scavenging rate	1.562×10^{5}	2.021×10^{0}	1	25
K_s	m/h	Sedimentation rate in water	6.936×10^{-7}	1.187×10^{0}	3	8, 19, 31
K_l	m/h	runoff rates of dissolved components	2.758×10^{-5}	2.299×10^{0}	1	25
K_e	m/h	runoff rates of solid in soil	1.626×10^{-8}	2.299×10^{0}	1	25
K_r[e]	m/h	Resuspension rate in sedimentation	0	-	-	-
f[f]		Removal efficiency of target compounds in STP	9.453×10^{-1}(TCS)	-	4	2,18,36,48
			9.715×10^{-1}(TCC)	-	6	1,13,15,40

Table S1-5 Collected parameters used in the multimedia model-Delta

Symbol	Unit	Definition	Mean[a]	Standard deviation [a,c]	N[b]	Ref[θ].
A_2	m^2	Area of water phase	3.701×10^{8}	1.219×10^{0}	2	33,55
A_3	m^2	Area of soil phase	4.168×10^{9}	1.219×10^{0}	2	33,55
h_1	m	Thickness of air	5.984×10^{2}	1.604×10^{0}	1	25
h_2	m	Depth of water	6.574×10^{0}	1.448×10^{0}	8	12,23
h_3	m	Thickness of soil	1.485×10^{-1}	1.604×10^{0}	1	53
h_4	m	Thickness of sediment	4.470×10^{-2}	1.604×10^{0}	1	53
X_{13}	v/v	Volume fractions of solids in air	7.878×10^{-11}	1.219×10^{0}	1	25
X_{23}	v/v	Volume fractions of solids in water	1.112×10^{-5}	2.382×10^{0}	36	-[g]
X_{31}	v/v	Volume fractions of air in soil	1.960×10^{-1}	1.219×10^{0}	1	4
X_{32}	v/v	Volume fractions of water in soil	2.449×10^{-1}	1.219×10^{0}	1	4
X_{33}	v/v	Volume fractions of solids in soil	5.389×10^{-1}	1.219×10^{0}	1	4
X_{42}	v/v	Volume fractions of water in sediment	6.859×10^{-1}	1.219×10^{0}	1	25
X_{43}	v/v	Volume fractions of solids in sediment	2.939×10^{-1}	1.219×10^{0}	1	25
X_{2f}	v/v	Volume fractions of fish in water	3.162×10^{-9}	2.071×10^{0}	4	24,37
O_{23}	w/w	Contents of organic carbon in solids in water	3.098×10^{-2}	1.737×10^{0}	20	-[g]
O_{33}	w/w	Contents of organic carbon in solids in soil	1.828×10^{-2}	1.219×10^{0}	3	14
O_{43}	w/w	Contents of organic carbon in solids in sediment	1.383×10^{-2}	2.346×10^{0}	33	-[g]
ρ_{23}	kg/L	Densities of solids in water	2.428×10^{0}	1.013×10^{0}	35[g]	47, -[g]
ρ_{33}	kg/L	Densities of solids in soil	1.821×10^{0}	1.628×10^{0}	2	4,14
ρ_{43}	kg/L	Densities of solids in sediment	2.428×10^{0}	1.013×10^{0}	35[g]	23, -[g]
ρ_f	kg/L	Densities of fish	1.234×10^{0}	1.256×10^{0}	2	4,24
Y_f	t/h	Production of fish	8.287×10^{1}	1.070×10^{0}	3	37
Q_{01t}	m^3/h	Advection air flow in area	0	-	-	-
Q_{02t}	m^3/h	Advection water flow in area	6.579×10^{5}	3.872×10^{0}	4	11
Q_{20t}	m^3/h	Advection water flow out of area	7.724×10^{5}	3.623×10^{0}	5	11
Q_{02h}	m^3/h	Wastewater discharge rate	7.914×10^{4}	1.141×10^{0}	3	37
C_{02t}	m^3/h	Concentration in flowing water	6.093×10^{-8}(TCS)	1.196×10^{0}(TCS)	1	-[i]
			1.736×10^{-7}(TCC)	1.196×10^{0}(TCC)	1	-[i]
C_{02h}	mol/m^3	Wastewater concentration	4.636×10^{-6}(TCS)	2.299×10^{0}(TCS)	1	-[h], 37
			6.774×10^{-6}(TCC)	2.299×10^{0}(TCC)	1	-[h], 37
T	K	Local absolute temperature	2.969×10^{2}	6.771×10^{0}	36	37,-[g]
R	Pa·m^3/mol·K	Universal gas constant	8.314×10^{0}	1.000×10^{0}	-	-
H	Pa·m^3/mol	Henry's constant	5.500×10^{-3}(TCS)	7.670×10^{0}(TCS)	4	3,20,26,41

			4.557×10^{-8}(TCC)	1.105×10^{0}(TCC)	2	52, -[k]
Ps	Pa	Vapor pressure	4.972×10^{-4}(TCS)	1.745×10^{0}(TCS)	5	3, 32,49,50
			4.705×10^{-9}(TCC)	6.956×10^{2}(TCC)	2	42,49
K_{OC}	L/kg	Organic carbon normalized partition coefficients	2.357×10^{4}(TCS)	1.973×10^{0}(TCS)	12	5,20,27,29,32,35,44, 49
			5.596×10^{4}(TCC)	1.415×10^{0}(TCC)	9	6,15,27,42,44,52
t_1^d	h	Half-life of the chemical in air	1.182×10^{1}(TCS)	2.160×10^{0}(TCS)	1	-[k]
			1.476×10^{1}(TCC)	1.324×10^{0}(TCC)	1	-[k]
t_2	h	Half-life of the chemical in water	4.304×10^{2}(TCS)	2.630×10^{0}(TCS)	11	20,28,32,36,39,-[k]
			1.859×10^{3}(TCC)	1.435×10^{0}(TCC)	2	42,-[k]
t_3	h	Half-life of the chemical in soil	1.155×10^{3}(TCS)	2.076×10^{0}(TCS)	9	32,34,43,44,49, -[k]
			3.802×10^{3}(TCC)	1.678×10^{0}(TCC)	7	40,44,49, -[k]
t_4	h	Half-life of the chemical in sediment	3.524×10^{3}(TCS)	6.336×10^{0}(TCS)	3	49,-[k]
			7.395×10^{3}(TCC)	2.650×10^{0}(TCC)	3	34,40,49,-[k]
BCF_f		Bioconcentration factors for fish in water	9.000×10^{1}(TCS)	4.725×10^{0}(TCS)	3	29,41,49
			4.031×10^{2}(TCC)	4.601×10^{0}(TCC)	2	40,49
B_1	m^2/h	Molecular diffusivity in air	3.920×10^{-2}	1.219×10^{0}	1	25
B_2	m^2/h	Molecular diffusivity in water	4.746×10^{-6}(TCS)	1.274×10^{0}(TCS)	2	25,45
			4.510×10^{-6}(TCC)	1.185×10^{0}(TCC)	2	25,45
B_4	m^2/h	Molecular diffusivity in sediment	5.869×10^{-7}(TCS)	1.219×10^{0}(TCS)	1	45
			5.351×10^{-7}(TCC)	1.219×10^{0}(TCC)	1	45
K_{12}	m/h	Air-side mass transfer coefficient over water	2.942×10^{0}	1.219×10^{0}	1	25
K_{13}	m/h	Air-side mass transfer coefficient over soil	9.860×10^{-1}	1.219×10^{0}	1	25
K_{21}	m/h	Water-side mass transfer coefficient over air	2.942×10^{-2}	1.219×10^{0}	1	25
K_{24}	m/h	Water-side mass transfer coefficient over sediment	9.800×10^{-3}	1.219×10^{0}	1	25
L_3	m	Diffusion path lengths in soil	3.540×10^{-2}	2.299×10^{0}	1	25
L_4	m	Diffusion path lengths in sediment	3.540×10^{-3}	2.299×10^{0}	1	24
K_p	m/h	Dry deposition velocity	7.637×10^{0}	2.299×10^{0}	1	25
K_w	m/h	Rain rate	6.859×10^{-5}	2.299×10^{0}	1	25
S_c	m/h	Rain scavenging rate	1.562×10^{5}	2.021×10^{0}	1	25
K_s	m/h	Sedimentation rate in water	1.620×10^{-7}	3.025×10^{0}	4	7, 17, 23,31
K_l	m/h	runoff rates of dissolved components	2.758×10^{-5}	2.299×10^{0}	1	25
K_e	m/h	runoff rates of solid in soil	1.626×10^{-8}	2.299×10^{0}	1	25
K_r^e	m/h	Resuspension rate in sedimentation	0	-	-	-
f^f		Removal efficiency of target compounds in STP	9.453×10^{-1}(TCS)	-	4	2,18,36,48
			9.715×10^{-1}(TCC)	-	6	1,13,15,40

[a] For the log-normal distribution, the geomean and geo standard deviation was selected as the statistical variable. Except one normal distribution: the parameter T (f' with no distribution for later), the remaining parameters were all defined as the log-normal distribution.

[b] N refers to the total number of parameters collected from literature or measured in the laboratory.

[c] For parameters each with only single value available, an artificially assigned coefficient of variation (CV) was adopted, and through the relationship between the standard deviations of a log normal distribution, we can get the geometric means and geometric standard deviations.

[θ] Ref. refers to the sources of the data. The numbers in this column are the order number of the reference.

[d] t refers to the half-life ($t_{1/2}$) of each chemical in different environment media.

[e] To better understand the exchange process between water and sediment, we describe both sedimentation and resuspension rate. While the value of latter is set to zero since sedimentation rate is calculated from reported sedimentary cores which is the actual value that ruled out the resuspension caused by water flow and various biological disturbances.

[f] With no distribution, the average values were selected for the calculation of T_{02h}, not for the simulation.

[g] The sampling data are determined in our laboratory.

[h] It is from T_{02h}.

[i] The corresponding upstream output is the source of the chemical input in flowing water. Due to the water source protection in local government, the article assumes that there are no chemical input for the total basin and upstream.

[k] No article is available, so we simulate the parameter from EPISUIT 4.1.

Table S2 The overlapping areas of the measured and modeled concentration probability density curve.

Compounds	Symbol	S-Cover	S-Measured	% [a]
TCS	$\log C_{\mathrm{water}}$	0.804	1.000	80.4%
	$\log C_{\mathrm{SPM}}$	0.686	1.000	68.7%
	$\log C_{\mathrm{sediment}}$	0.723	1.000	72.3%
TCC	$\log C_{\mathrm{water}}$	0.863	1.000	86.3%
	$\log C_{\mathrm{SPM}}$	0.631	1.000	63.1%
	$\log C_{\mathrm{sediment}}$	0.823	1.000	82.3%

[a] % means the percentage of overlapping area of the corresponding measured concentration probability density curves area.