A Multimedia Model for PAHs and Nitro-PAHs in Lake Michigan

Lei Huang and Stuart A. Batterman*

Supporting Information

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1. Modeling methods

1.1 Fugacity-based multimedia model

The steady-state (level III) model equations

The mass balance equations for each compartment are as follows. They are the same for PAHs and NPAHs.

Air (subscript 1)

$$0 = (E_1 + G_{A1}C_{B1} + D_{21}f_2 + D_{31}f_3) - f_1 (D_{12} + D_{13} + D_{R1} + D_{A1}) \quad \text{(S1)}$$

Water (subscript 2)

$$0 = (E_2 + G_{A2}C_{B2} + D_{12}f_1 + D_{42}f_4) - f_2 (D_{21} + D_{24} + D_{R2} + D_{A2}) \quad \text{(S2)}$$

Soil (subscript 3)

$$0 = (E_3 + D_{13}f_1) - f_3 (D_{31} + D_{32} + D_{R3}) \quad \text{(S3)}$$

Sediment (subscript 4)

$$0 = (E_4 + D_{24}f_2) - f_4 (D_{42} + D_{R4} + D_{A4}) \quad \text{(S4)}$$

Biota (the i^{th} organism)

$$0 = D_W(f_2 \cdot XW + f_4 \cdot XS) + \sum_{i=1}^{8} Feed_{ij} \cdot D_{ij} - f_F(D_W + D_M + D_E + D_G) \quad \text{(S5)}$$

f: fugacity (Pa)

E: emission rate (mol/h)

G_A: advection flow rate (m^3/h)

C_B: background concentration (mol/m^3)

D: D value (mol/Pa-h). D values are parameters that describe the transport rate of a chemical in a process [1].

D_{12} represents the transport D value from compartment 1 to compartment 2, others in the same way.

Subscript *R:* reaction.

Subscript *F:* the organism *i*.

Subscript *W:* gill respiration.

Subscript *M:* metabolism.

Subscript *E:* egestion.

Subscript *G*: growth.

XW: fraction of respiration from water

XS: fraction of respiration from sediment

$Feed_{ij}$: fraction of species i in the diet of species j

D_{ij}: effective D value of food consumption when species *i* is consumed by species *j*

The dynamic (level IV) model equations

Air (subscript 1)

$$V_1Z_1(df_1/dt) = (E_1 + G_{A1}C_{B1} + D_{21}f_2 + D_{31}f_3) - f_1 (D_{12} + D_{13} + D_{R1} + D_{A1}) \quad \text{(S6)}$$

Water (subscript 2)

$$V_2Z_2(df_2/dt) = (E_2 + G_{A2}C_{B2} + D_{12}f_1 + D_{42}f_4) - f_2 (D_{21} + D_{24} + D_{R2} + D_{A2}) \quad \text{(S7)}$$

Soil (subscript 3)

$$V_3Z_3(df_3/dt) = (E_3 + D_{13}f_1) - f_3 (D_{31} + D_{32} + D_{R3}) \quad \text{(S8)}$$

Sediment (subscript 4)

$$V_4Z_4(df_4/dt) = (E_4 + D_{24}f_2) - f_4 (D_{42} + D_{R4} + D_{A4}) \quad \text{(S9)}$$

Biota (the i^{th} organism)

$$V_FZ_F(\frac{df_F}{dt}) = D_W(f_2 \cdot XW + f_4 \cdot XS) + \sum_{i=1}^{8} Feed_{ij} \cdot D_{ij} - f_F(D_W + D_M + D_E + D_G) \quad \text{(S10)}$$

V: compartment volume (m^3)

Z: fugacity capacity (mol/m^3-Pa)

1.2 Model inputs for environmental properties

Parameters for air, water, soil and sediment compartments, including transport velocities between compartments, are presented below. Transport velocities are estimated using data for Lake Huron [32], which shares a similar climate.

Figure S1. The study area includes Lake Michigan (blue area) and its drainage basin (green area). The wind rose plot at the bottom left corner indicates the prevailing wind directions from 1961 to 1990 at Chicago [2]. This figure is adapted from the Michigan Sea Grant [3].

Table S1. Environmental properties and transport velocities.

Compartment	Parameter	Lake Michigan	Reference
	Mean temperature (°C)	11.6	*a*
Air	Area (m^2)	1.76E+11	*b*
	Height (m)	1000	*c*
	Aerosol volume fraction	5.22E-12	*c*
	Aerosol density (kg/m^3)	1800	*d*
	Wind speed at 5m (m/s)	5.35	*a*
	Residence time (h)	20.96	*d*
Water	Area (m^2)	5.78E+10	*b*
	Depth (m)	85	*b*
	Suspended particles fraction	5.00E-06	*d*
	Suspended density (kg/m^3)	2400	*d*
	Suspended OC fraction	0.2	*d*
	Biota fraction	1.00E-06	*d*
	Biota density (kg/m^3)	1000	*d*
	Biota lipid fraction	0.05	*d*
	Residence time (h)	8.67E+05	*b*
Soil	Depth (m)	0.25	*c*
	Air fraction	0.2	*d*
	Water fraction	0.3	*d*
	Solid density (kg/m^3)	2400	*d*
	Soil OC fraction	0.02	*d*
Sediment	Depth (m)	0.01	*c*
	Water fraction	0.7	*d*
	Solid fraction	0.3	*d*
	Solid density (kg/m^3)	2400	*d*
	Sediment OC fraction	0.04	*d*
	Residence time (h)	2.92E+04	*e*
Transfer rate (m/h)	Rain rate	9.30E-05	*d*
	Dry deposition	18.04	*d*
	Air side air-water MTC	41.85	*c*
	Water side air-water MTC	0.0801	*c*
	Soil-air phase diffusion MTC	0.04	*c*
	Soil-water phase diffusion MTC	1.00E-05	*c*
	Soil-air boundary layer MTC	1	*c*
	Sediment-water diffusion MTC	1.00E-04	*c*
	Sediment deposition	4.57E-07	*d*
	Sediment resuspension	1.14E-07	*d*
	Soil-water runoff rate	3.72E-05	*d*
	Soil-soid runoff rate	2.28E-08	*d*

a Reference [4]; *b* Reference [5]; *c* Reference [6]; *d* Reference [7]; *e* Reference [1].

MTC: mass transfer coefficient.

1.3 Model inputs for physiochemical properties

Physiochemical properties of the chemicals, e.g., vapor pressure, melting point, water solubility and logKow at 25 °C, were obtained from the EPISuite [41] experimental database, if available, otherwise estimated using EPIWIN. Vapor pressure, water solubility and logKow at the Lake Michigan's mean temperature (11.7 °C) were recalculated using the van't Hoff equation and phase-change enthalpies [42-46]. Degradation half-lives in air, water, soil, sediment and top trophic-level fish (lake trout) were obtained from EPISuite. Physiochemical parameters are provided in Table S2.

Table S2. Physiochemical properties and degradation half-lives of modeled compounds

Group	Chemical	Abbrev.	CAS#	MW	Melting point	Data temperature: 11.7 °C				Degradation half-lives				
						Water solubility	Vapor pressure	LogKow	Henry's law constant	Air	Water	Soil	Sediment	Fish (fat)
				(g/mol)	(°C)	(g/m^3)	(Pa)		($Pa \cdot m^3/mol$)	(h)	(h)	(h)	(h)	(h)
PAHs	Naphthalene	NAP	91-20-3	128.2	80	2.65E+01	7.94E+00	3.36	3.84E+01	11.9	900	1800	8100	108.7
	Acenaphthylene	ACY	208-96-8	152.2	93	1.47E+01	5.90E-01	4.01	6.10E+00	1	360	720	3240	89.5
	Acenaphthene	ACE	83-32-9	154.2	93	3.30E+00	1.89E-01	3.99	8.92E+00	4.4	900	1800	8100	6.0
	Fluorene	FLU	86-73-7	166.2	115	1.44E+00	4.97E-02	4.11	5.74E+00	19.7	360	720	3240	33.0
	Phenanthrene	PHE	85-01-8	178.2	99	1.00E+00	1.05E-02	4.53	1.86E+00	20	1440	2880	13000	61.3
	Anthracene	ANT	120-12-7	178.2	215	3.43E-02	5.68E-04	4.52	2.95E+00	6	1440	2880	13000	60.8
	Fluoranthene	FLA	206-44-0	202.3	108	2.23E-01	7.14E-04	5.23	6.48E-01	23.3	1440	2880	13000	61.6
	Pyrene	PYR	129-00-0	202.3	151	1.17E-01	3.50E-04	4.95	6.04E-01	5	1440	2880	13000	13.4
	Benz[a]anthracene	BAA	56-55-3	228.3	84	7.89E-03	1.64E-05	5.86	4.74E-01	5.1	1440	2880	13000	72.8
	Chrysene	CHR	218-01-9	228.3	258	1.61E-03	4.71E-07	5.89	6.65E-02	5	1440	2880	13000	75.4
	Benzo[b]fluoranthene	BBF	205-99-2	252.3	168	1.22E-03	3.77E-05	5.88	7.77E+00	14	1440	2880	13000	64.1
	Benzo[k]fluoranthene	BKF	207-08-9	252.3	217	6.38E-04	7.28E-08	6.21	2.88E-02	4.8	1440	2880	13000	80.9
	Benzo[a]pyrene	B[a]P	50-32-8	252.1	175	1.41E-03	4.09E-07	6.22	7.31E-02	5	1440	2880	13000	21.7
	Indeno[1,2,3-cd]pyrene	IcdP	193-39-5	276.3	164	1.47E-04	9.13E-09	6.80	1.71E-02	4.0	1440	2880	13000	28.1
	Dibenzo[a,h]anthracene	DBA	53-70-3	278.4	270	7.98E-04	6.87E-08	6.64	2.39E-02	5.1	1440	2880	13000	84.8
	Benzo[g,h,i]perylene	BghiP	191-24-2	276.3	278	2.26E-04	7.16E-09	6.73	8.77E-03	3.0	1440	2880	13000	7.1
NPAHs	1-Nitronaphthalene	1-NNAP	86-57-7	173.2	61	7.90E+00	3.70E-02	3.19	8.11E-01	47.5	900	1800	8100	31.5
	2-Nitronaphthalene	2-NNAP	581-89-5	173.2	79	8.07E+00	2.18E-02	3.24	4.67E-01	45.8	900	1800	8100	32.7
	2-Nitrofluorene	2-NFLU	607-57-8	211.2	157	1.74E-01	2.95E-04	3.37	3.57E-01	61.7	900	1800	8100	7.3
	1-Nitropyrene	1-NPYR	5522-43-0	247.3	155	9.80E-03	4.76E-06	5.06	1.20E-01	41.1	4320	8640	38900	6.0
	6-Nitrochrysene	6-NCHR	7496-02-8	273.3	187	1.25E-02	4.13E-07	5.34	9.06E-03	41.1	4320	8640	38900	21.3

All values are from EPISuite [8]

1.4 Model inputs for food web parameters

The eight species in the food web were selected because they have been reported as dominant species in Lake Michigan [9-11]. A diagram of this food web is shown in Figure S2. This food web includes benthic (*Diporeia*) and pelagic (plankton, mysid, fish) organisms. Dietary preferences were based on previous Lake Michigan studies [12-14]. The species' physiological parameters, and the feeding matrix are listed in Tables S3 and S4.

For many chemicals and aquatic organisms, experimental data regarding metabolic half-lives are limited. Metabolism in aquatic organisms is important for PAHs (unlike the more persistent PCBs and PBDEs), and rates differ by trophic level [15, 16]. Compared to the top tropic species (lake trout), we assumed that metabolic half-lives were three times longer for prey fish (alewife, bloater, sculpin, smelt), 30 times longer for Diporeia and mysid, and 300 times longer in plankton (food web base). While these ratios are uncertain, they are designed to reflect the presence of the Ah receptor and sufficient cytochrome P450 in fish (but not invertebrates) to metabolize PAHs [15, 17], as well as biodilution observed in marine and freshwater organisms [16, 18, 19]. Metabolic half-lives are listed in Table S5.

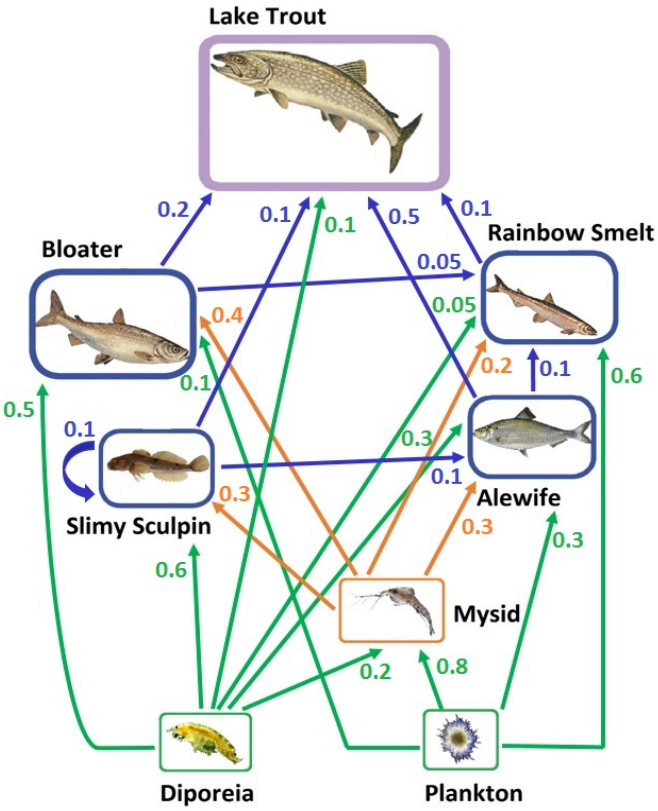

Figure S2. Schematic diagram of the Lake Michigan food web. Colors indicate trophic levels. Dietary preferences are expressed as fractions of the total diet. For example, the diet of lake trout consists of 50% alewife, 20% bloater, 10% rainbow smelt, 10% slimy sculpin and 10% *Diporeia*.

Table S3. Aquatic organisms and their physiological properties in the food web of Lake Michigan

No.	Species	Volume (cm3)	LF	QD	GR (g/g-day)	FR (% per day)	XW	XS	GAW	GAO
1	Plankton	0.0005	0.015	3	0.025	0	1	0	5.3E-08	4
2	Mysid	0.1	0.04	3	0.02	20	1	0	5.3E-08	3.5
3	Diporeia	0.002	0.03	3	0.02	0	0	1	5.3E-08	4
4	Sculpin	5.4	0.08	3	0.005	4	1	0	5.3E-08	1.5
5	Rainbow Smelt	16	0.04	3	0.005	4	1	0	5.3E-08	1.5
6	Bloater	62[a]	0.1[b]	3	0.004	3.5	1	0	5.3E-08	1.5
7	Alewife	32	0.07	3	0.004	3.5	1	0	5.3E-08	1.5
8	Lake trout	2962[c]	0.15	3	0.002	2	1	0	5.3E-08	1.2

LF: lipid volume fraction.

QD: digestion factor.

GR: growth rate (fraction of volume/body mass per day).

FR: feeding rate (percent of body mass per day).

XW: fraction of respiration from water.

XS: fraction of respiration from sediment.

GAO: gut absorption efficiency parameter (organic).

GAW: gut absorption efficiency parameter (water).

[a] Reference [14]; [b] Reference [20]; [c] Our measurements in Lake Michigan lake trout [18].

All other values were obtained from the FoodWeb model software [21].

Table S4. Feeding matrix of the Lake Michigan food web

		Predator							
		Plankton	Mysid	Diporeia	Sculpin	Rainbow Smelt	Bloater	Alewife	Lake trout
Prey	Plankton	0	0.8	0	0	0.6	0.1	0.3	0
	Mysid	0	0	0	0.3	0.2	0.4	0.3	0
	Diporeia	0	0.2	0	0.6	0.05	0.5	0.3	0.1
	Sculpin	0	0	0	0.1	0	0	0.1	0.1
	Rainbow Smelt	0	0	0	0	0	0	0	0.1
	Bloater	0	0	0	0	0.05	0	0	0.2
	Alewife	0	0	0	0	0.1	0	0	0.5
	Lake trout	0	0	0	0	0	0	0	0

Table S5. Metabolic half-lives in aquatic organisms used in the food web model

Group	Chemical	Metabolic half-lives (h)							
		Plankton	Mysid	Diporeia	Sculpin	Rainbow Smelt	Bloater	Alewife	Lake trout
PAHs	Naphthalene	32610	3261	3261	326	326	326	326	109
	Acenaphthylene	26850	2685	2685	269	269	269	269	90
	Acenaphthene	1800	180	180	18	18	18	18	6
	Fluorene	9900	990	990	99	99	99	99	33
	Phenanthrene	18390	1839	1839	184	184	184	184	61
	Anthracene	18252	1825	1825	183	183	183	183	61
	Fluoranthene	18480	1848	1848	185	185	185	185	62
	Pyrene	4020	402	402	40	40	40	40	13
	Benz[a]anthracene	21840	2184	2184	218	218	218	218	73
	Chrysene	22620	2262	2262	226	226	226	226	75
	Benzo[b]fluoranthene	19230	1923	1923	192	192	192	192	64
	Benzo[k]fluoranthene	24270	2427	2427	243	243	243	243	81
	Benzo[a]pyrene	6504	650	650	65	65	65	65	22
	Indeno[1,2,3-cd]pyrene	8430	843	843	84	84	84	84	28
	Dibenzo[a,h]anthracene	25440	2544	2544	254	254	254	254	85
	Benzo[g,h,i]perylene	2130	213	213	21	21	21	21	7

1.5 Emissions and background concentrations

The PAH air emission rates used in the level III model were derived from annual emission estimates reported in the 2008 Great Lakes Regional Air Toxic Emissions Inventory [22], which include point, area and mobile sources in the Great Lakes region. Emissions in the Lake Michigan basin were assumed to be 24% of this total [7]. Annual rates were converted to kg/h, and water discharges were calculated as 1/9 of the air emission rate. Emission data are listed in Table S6.

Air concentrations of 13 target PAHs (excluding NAP, ACY and ACE) have been monitored in the IADN at urban (Chicago) and rural (Sleeping Bear Dunes) sites near Lake Michigan since 1990. The most recent report [23] provides average particulate and vapor phase concentrations from 1996 to 2003 (vapor phase since 1992 at the rural site). A lake-wide background concentration was estimated by summing the two phases and weighting totals by 0.75 and 0.25 for urban and rural sites, respectively, based on the prevailing southwestern winds [24]. ACY and ACE concentrations were estimated using ratios of their airborne concentrations to B[a]P obtained from Chicago and off-shore measurements [25]. For NAP, air monitoring data are scarce. The background level was estimated by determining the NAP/B[a]P ratio for U.S. air emissions [26], which was multiplied by the B[a]P background concentration discussed above.

Airborne measurements of NPAHs in the region are unavailable. Using data from Maryland, California, Europe, Japan and Brazil [27-32], we determined the average ratio of each NPAH relative to B[a]P, which was then multiplied by the estimated B[a]P background concentration to estimate NPAH background levels. Background concentrations of PAHs and NPAHs are listed in Table S6.

Table S6. Emission rates and background concentrations used in the level III model

Group	Chemical	Emission rate				Background concentration	
		To air (kg/h)	To water (kg/h)	To soil (kg/h)	To sediment (kg/h)	In air (ng/m^3)	In water (ng/L)
PAHs	Naphthalene	98.5	10.9	0	0	158.5	0
	Acenaphthylene	15.7	1.74			1.22	
	Acenaphthene	1.46	0.16			2.44	
	Fluorene	3.27	0.36			12.2	
	Phenanthrene	9.90	1.10			30.2	
	Anthracene	2.04	0.23			1.23	
	Fluoranthene	3.27	0.36			8.90	
	Pyrene	4.19	0.47			4.15	
	Benz[a]anthracene	1.91	0.21			0.56	
	Chrysene	1.36	0.15			0.85	
	Benzo[b]fluoranthene	0.55	0.06			1.16	
	Benzo[k]fluoranthene	0.41	0.05			0.38	
	Benzo[a]pyrene	0.81	0.09			0.61	
	Indeno[1,2,3-cd]pyrene	0.72	0.08			0.80	
	Dibenzo[a,h]anthracene	0.10	0.01			0.13	
	Benzo[g,h,i]perylene	0.98	0.11			0.62	
NPAHs	1-Nitronaphthalene	TBD	0	0	0	2.51	0
	2-Nitronaphthalene					2.51	
	2-Nitrofluorene					0.38	
	1-Nitropyrene					0.13	
	6-Nitrochrysene					0.063	

TBD: to be estimated by the model; results are presented in the main article, Table 2.

2. Results

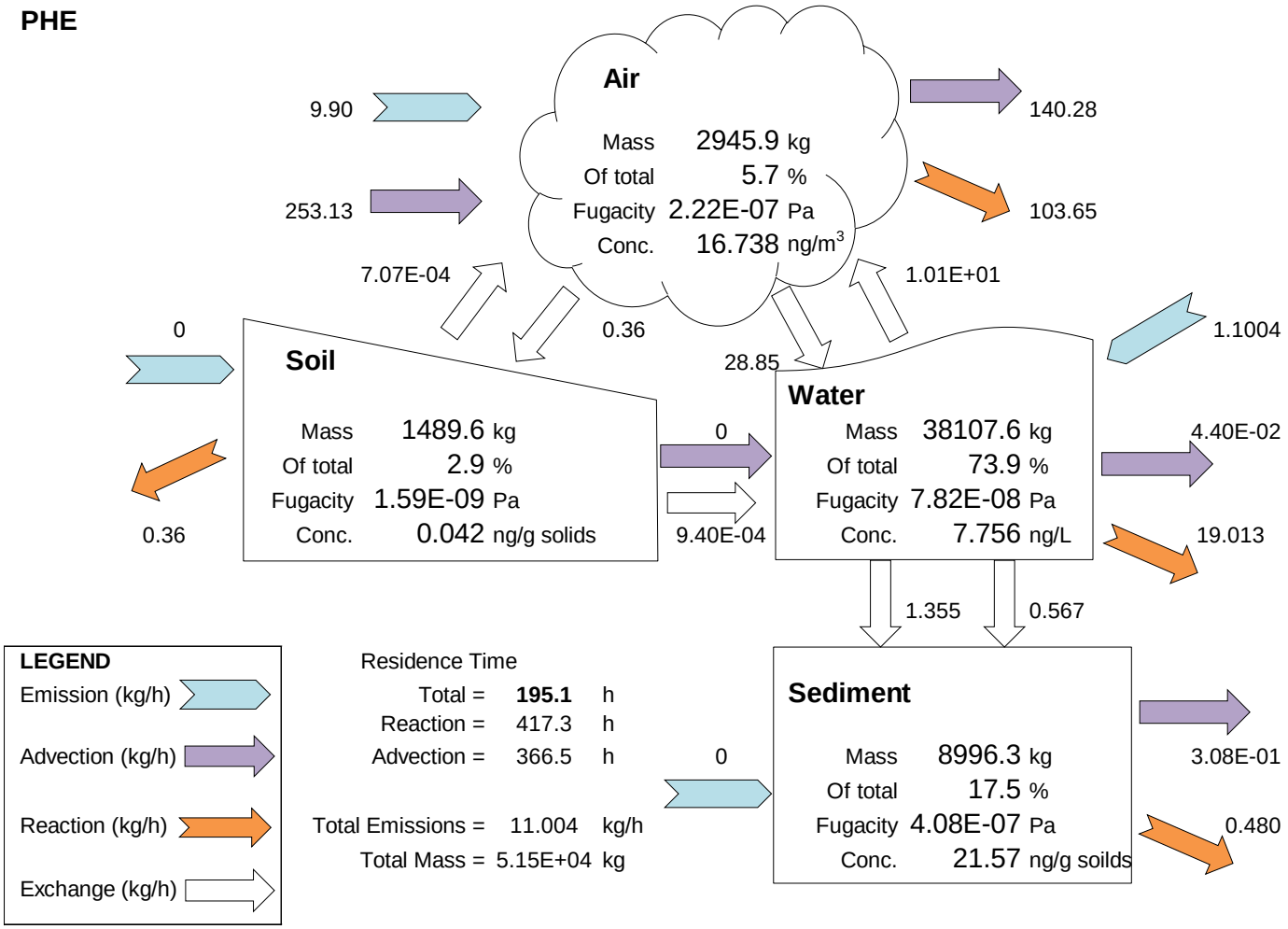

Figure S3. Level III mass balance diagram showing fluxes (kg/h) of phenanthrene in Lake Michigan. Adapted from 61. The size of the arrows is NOT proportional to the magnitude of the fluxes.

Table S7. Comparison between PAH concentrations predicted using the level III model and observed concentrations.

Compound	Air (ng/m^3)		Water (ng/L)		Soil (ng/g dry)		Sediment (ng/g dry)	
	Predicted[e]	Observed	Predicted[e]	Observed	Predicted[e]	Observed	Predicted[e]	Observed[f]
Naphthalene	76.36 (40.4%)	n/a	3.84 (56.8%)	n/a	2.20E-02 (2.4%)	n/a	0.30 (0.4%)	6.2 (2.5-12.7) [c]
Acenaphthylene	0.15 (3.3%)	0.3 [a]	0.16 (93.6%)	0.7 [b]	4.08E-05 (0.2%)	n/a	0.06 (3.0%)	1.4 (0.7-3.9) [c]
Acenaphthene	0.60 (18%)	0.8 [a]	0.09 (76.4%)	1.2 [b]	3.39E-04 (2.0%)	n/a	0.05 (3.6%)	0.01 (0.01-0.03) [c]
Fluorene	6.86 (26.7%)	5.4 [a]	0.64 (68.9%)	2.1 [b]	1.95E-03 (1.5%)	n/a	0.31 (2.9%)	17.3 (5.9-30.3) [d]
Phenanthrene	16.74 (5.7%)	11.0 [a]	7.76 (73.9%)	3.0 [b]	4.20E-02 (2.9%)	n/a	21.57 (17.5%)	70.4 (29.1-179.1) [c]
Anthracene	0.44 (5.8%)	0.3 [a]	0.20 (74.6%)	0.1 [b]	8.27E-04 (2.2%)	n/a	0.55 (17.3%)	9.1 (3.8-18.7) [c]
Fluoranthene	5.01 (2.6%)	3.0 [a]	2.95 (42.6%)	1.5 [b]	3.96E-02 (4.1%)	n/a	41.33 (50.6%)	134.1 (47.3-385.2) [c]
Pyrene	1.14 (3.2%)	1.6 [a]	0.70 (55.8%)	0.8 [b]	8.76E-03 (5.0%)	n/a	5.35 (36%)	110.3 (25.3-236.3) [c]
Benz[a]anthracene	0.19 (0.9%)	0.2 [a]	0.12 (16.7%)	0.2 [b]	2.53E-02 (24.6%)	n/a	5.07 (57.8%)	55.8 (12-167.4) [c]
Chrysene	0.24 (0.9%)	0.5 [a]	0.15 (16.6%)	0.4 [b]	2.89E-02 (22.6%)	n/a	6.51 (59.8%)	75.9 (19.3-175.3) [c]
Benzo[b]fluoranthene	0.57 (4.4%)	0.5 [a]	0.09 (19%)	0.4 [b]	6.20E-03 (9.6%)	n/a	3.68 (67%)	28.5 (13.2-71.9) [c]
Benzo[k]fluoranthene	0.09 (0.6%)	0.0 [a]	0.04 (8.1%)	0.3 [b]	3.76E-02 (50.1%)	n/a	2.64 (41.2%)	22.5 (10.4-44.2) [c]
Benzo[a]pyrene	0.16 (0.8%)	0.2 [a]	0.05 (7.2%)	0.4 [b]	5.19E-02 (55.2%)	n/a	2.94 (36.8%)	2.7 (1.0-10.2) [c]
Indeno[1,2,3-cd]pyrene	0.16 (0.6%)	0.2 [a]	0.04 (4.4%)	0.4 [b]	8.25E-02 (63.7%)	n/a	3.44 (31.2%)	24.9 (7.8-95.4) [c]
Dibenzo[a,h]anthracene	0.03 (0.6%)	0.0 [a]	0.01 (7.6%)	0.3 [b]	9.91E-03 (40.9%)	n/a	1.05 (50.9%)	18.2 (5.9-74.1) [c]
Benzo[g,h,i]perylene	0.11 (0.8%)	0.2 [a]	0.02 (2.9%)	0.3 [b]	5.39E-02 (76.5%)	n/a	1.19 (19.9%)	6.7 (2.3-27.5) [c]

[a] Reference [25]

[b] Reference [33]

[c] Reference [34]

[d] Reference [35]

[e] Percentage of total mass in that compartment in parentheses. The predicted concentrations were point estimates without MC analysis. They were not means.

[f] Mean (range).

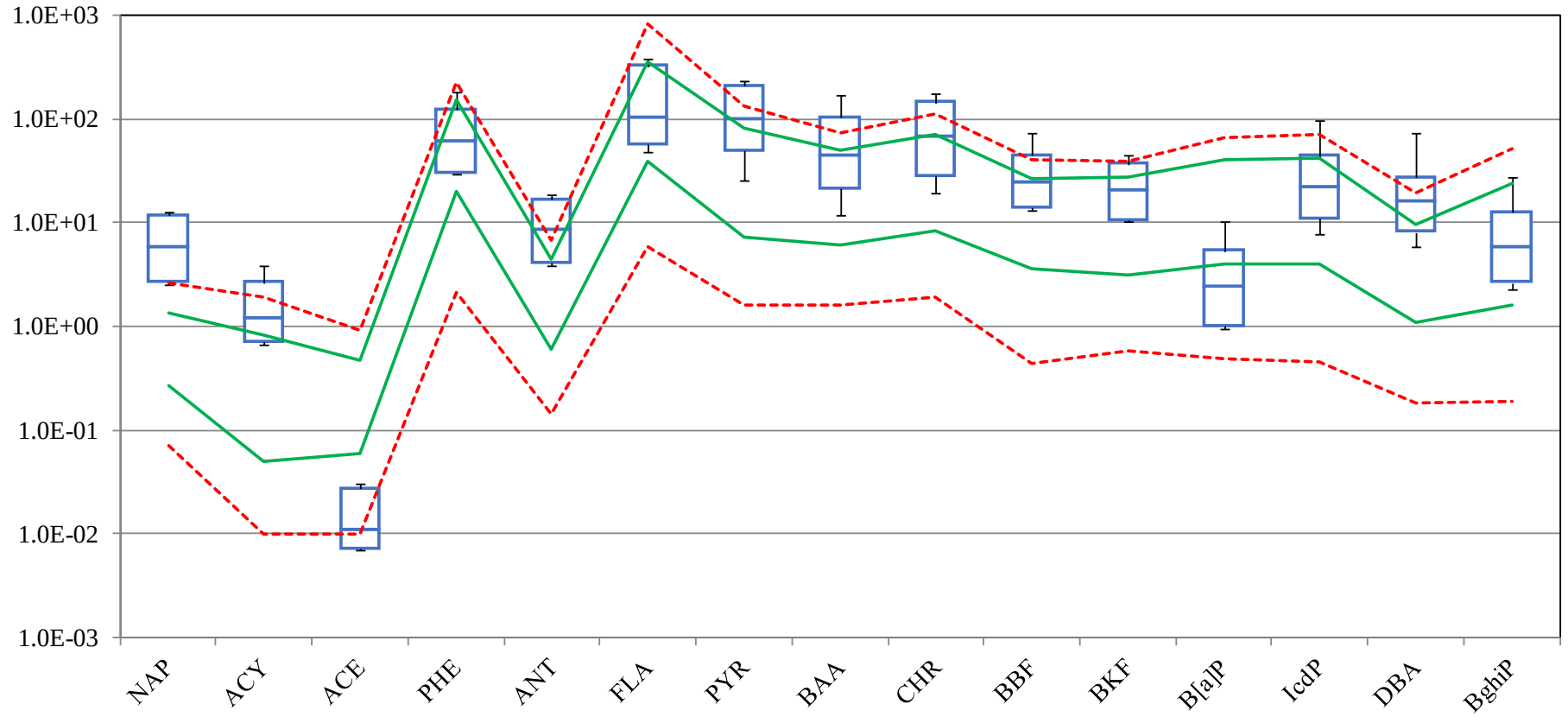

Figure S4. Comparison of measured and predicted PAH concentrations in Lake Michigan sediments. Boxplots show measured levels (including maximum, 95th, 50th and 5th percentiles, and minimum). Monte-Carlo results shown as solid lines for 95th and 5th percentiles, and as dashed lines for maximum and minimum.

Table S8. Concentrations in aquatic organisms predicted by the steady-state food web model

Group	Compound	Model predictions (pg/g wet)								Measurement[a] (pg/g wet)
		Plankton	Mysid	Diporeia	Slimy Sculpin	Rainbow Smelt	Bloater	Alewife	Lake trout	Lake trout
PAHs	Naphthalene	132	351	549	692	347	832	598	596	74.8 (3.0-172.6)
	Acenaphthylene	24	63	110	119	60	129	99	44	125.6 (21.2-483.1)
	Acenaphthene	13	35	91	35	19	20	21	2	64.4 (6.5-478.2)
	Phenanthrene	3813	10268	39386	16765	8280	14494	12274	2351	163.3 (16.8-849.9)
	Anthracene	98	263	1004	430	212	372	315	61	22.3 (4.5-178.4)
	Fluoranthene	6469	18203	74935	21073	8955	15398	12780	1711	28.7 (8.7-284.7)
	Pyrene	860	2285	9691	1210	607	683	662	51	25.1 (4.8-141.1)
	Benz[a]anthracene	779	2482	8955	2217	728	1687	1254	167	7.4 (4.9-23.8)
	Chrysene	1001	3222	11473	2901	943	2217	1642	222	8.8 (6.9-43.5)
	Benzo[b]fluoranthene	564	1795	6482	1440	470	1086	806	100	22.5 (12.1-70.1)
	Benzo[k]fluoranthene	402	1422	4484	1127	339	882	635	85	17.5 (12.6-97.7)
	Benzo[a]pyrene	453	1295	4738	354	105	264	188	15	18.4 (5.6-43.4)
	Indeno[1,2,3-cd]pyrene	495	1400	4356	343	99	269	188	14	45.6 (34.4-146.9)
	Dibenzo[a,h]anthracene	152	588	1594	379	110	303	214	27	53.4 (47.2-92.8)
	Benzo[g,h,i]perylene	176	227	1124	23	7	18	13	1	23.5 (1.9-149.4)

[a] Mean (range).

Table S9. Degradation half-lives of phenanthrene (PHE) used in level IV models

	Half-life (h)	Reference
Air	19.7	*a*
Water	1440	*a*
Soil	17000	*b*
Sediment	55000	*b*
Plankton	3000	*c*
Mysid	300	*c*
Diporeia	300	*c*
Slimy Sculpin	30	*c*
Rainbow Smelt	30	*c*
Bloater	30	*c*
Alewife	30	*c*
Lake trout	10	*c*

a Reference [8]; *b* Reference [36].

c Values are reduced by 5 times (compared to Table S5) based on level III model results.

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