Electronic Supplementary Information

Vertical records of sedimentary PAHs and their freely dissolved fraction in porewater profiles from the northern bays of Taihu Lake, Eastern China

Pei Lei[a,b], Hong Zhang[a,*], Baoqing Shan[a]

[a] *State Key Laboratory of Environmental Aquatic Chemistry, Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, Beijing 100085, China*

[b] *University of Chinese Academy of Sciences, Beijing 100049, China*

*Corresponding author at: Research Center for Eco-Environmental Sciences, Chinese Academy of Sciences, 18th Shuangqing Road, Haidian District, Beijing 100085, China. Tel.: +86 10 6284 9307; Fax: +86 10 6292 9307.
E-mail address: hongzhang@rcees.ac.cn (H. Zhang)

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Table S1 Sampling sites of sediment cores in the northern bays and central lake of Taihu Lake

Lake area	Sampling sites	Longitude(E)	Latitude(N)	Sediment depth(cm)
Zhushan Bay (ZS)	ZS1[a]	120° 2'14.4"E	31°27'04.2"N	34
	ZS2	120° 2'29.96"E	31°25'10.12"N	12
	ZS3	120° 1'46.32"E	31°22'51.10"N	36
Meiliang Bay (ML)	ML1[a]	120°11'15.12"E	31°30'14.27"N	18
	ML2	120°10'23.09"E	31°27'57.61"N	4
	ML3	120°10'36.57"E	31°24'51.84"N	6
Gonghu Bay (GH)	GH1	120°21'48.78"E	31°25'40.92"N	10
	GH2[a]	120°19'11.92"E	31°24'3.22"N	28
	GH3	120°16'25.22"E	31°22'4.10"N	36
Central lake (CL)	CL1	120° 9'45.18"E	31°15'29.74"N	6
	CL2	120°10'53.82"E	31°19'44.38"N	24
	CL3	120° 6'34.98"E	31°18'52.73"N	6
	CL4	120° 3'58.88"E	31°15'50.75"N	8
	CL5	120° 9'24.19"E	31°11'42.15"N	16
	CL6	120°14'26.15"E	31°12'13.40"N	4
	CL7[a]	120°14'58.76E	31°14'51.77"N	10
	CL8	120°13'46.2"E	31°18'02.3"N	16

[a] The four sediment cores were chosen to analyze the temporal trends of PAHs, a duplicate sediment core was also taken to acquire porewater and corresponding overlying water.

Table S2 Profiles of ΣPAHs accumulation fluxs versus depth in the sediment cores from the Taihu Lake

1. Sediment core taken from the northern bay								
Depth (cm)	Net dry weight (g)	Dry bulk density (g cm^{-3}) [a]	Linear sedimentation rate (cm a^{-1})	Sediment accumulation rate (g cm^2 a^{-1})	Zhushan Bay (ZS)		Gonghu Bay (GH)	
					Concentration of ΣPAHs (ng g^{-1})	Accumulation flux ofΣPAHs (ng cm^{-2} a^{-1}) [b]	Concentration of ΣPAHs (ng g^{-1})	Accumulation flux ofΣPAHs (ng cm^{-2} a^{-1})
2	34.499	0.610	0.832	0.508	723	368	642	326
4	34.194	0.605	0.681	0.412	1133	467	571	235
6	43.106	0.763	0.594	0.453	801	363	683	310
8	39.258	0.695	0.847	0.588	630	371	692	407
10	44.588	0.789	0.780	0.615	1179	725	782	481
12	41.898	0.741	0.750	0.556	1330	739	698	388
14	50.500	0.893	0.532	0.476	1026	488	817	389
16	52.246	0.924	0.409	0.378	1050	399	546	206
18	48.902	0.865	0.324	0.280	722	202	469	131
20	49.640	0.878	0.221	0.194	611	119	466	90.5
22	55.070	0.974	0.113	0.110	683	75.1	462	50.8
24	55.767	0.987	0.161	0.159	494	78.5	373	59.2

26	57.106	1.010	0.118	0.119	424	50.4	390	46.5
28	54.264	0.960	0.082	0.079	392	31.0	544	43.0
2. Sediment core taken from the central part of the Lake								
Depth (cm)	Net dry weight (g)	Dry bulk density (g cm^{-3})	Linear sedimentation rate (cm a^{-1})	Accumulation sedimentation rate (g cm^2 a^{-1})	the central part of the Lake (CL)			
					Concentration of ΣPAHs (ng g^{-1})	Accumulation flux ofΣPAHs (ng cm^{-2} a^{-1})		
2	28.985	0.513	0.414	0.213	570	121		
4	33.625	0.595	0.468	0.278	456	127		
6	38.065	0.673	0.250	0.168	585	98.5		
8	45.744	0.809	0.166	0.134	634	85.2		
10	44.955	0.795	0.122	0.097	520	50.3		

[a] Sediment density as dry bulk density (*BD*):

BD = *m*/*v* (S1)

where *BD* is the bulk density, in grams per cubic centimeter (g cm^{-3}),

m is the mass (net dry weight) of the sample, in grams (g), and

v is the volume of the sample, in cubic centimeters (cm^3).

Sediment cores were taken by a core sampler (Corer 60, Uwitec, Austria) with length of 60 cm and inner diameter of 6 cm. The details about the composition and usage of this sediment core sampler were shown on the website (http://www.uwitec.at/html/frame.html). The sediment cores were carefully pulled out from the cylindrical tubes after the overlying water sucked out

and then cut into sections with identical length by a supporting cutting device of the gravity corer.

Volume for a cylindrical core sample:

$$v = h\,[\pi d^2/4] \qquad \text{(S2)}$$

where v is the volume of the sample (cm^3),

h is the height of the cylinder, in centimeters (cm),

d is the inside diameter of the cylinder (cm), and

π is the ratio of the circumference of a circle to its diameter (non-dimensional parameter).

Every slice was assumed to a cylindrical core with the same height and area, here $h = 2$, $d = 6$ and $\pi = 3.14$, then, the volume of the sample (v) for each slice was 56.52 cm^3 and this value were used to estimate the dry bulk density.

[b] The sediment accumulation rate (*SAR*) and Linear sedimentation rate (*LSR*) were calculated from ^{210}Pb profiles and physical properties. Based on the results of ^{210}Pb dating, the ΣPAHs accumulation flux (*AF*) were estimated according to

$$AF = LSR \times BD \times CN \qquad \text{(S3)}$$

where AF is the accumulation flux of ΣPAHs in ng cm^{-2} a^{-1},

LSR is the linear sedimentation rate in cm a^{-1},

BD is bulk dry density in g cm^{-3}, and

CN is the concentration of sedimentary ΣPAHs in ng g^{-1}.

Table S3 Statistics of sediment accumulation rate (SAR) or linear sedimentation rate (LSR) in the sediment cores from Taihu Lake and other lakes in the lower Yangtze River Basin

Lake	Location	Description	Sampling year	Methods of dating	Range of dating	Sediment accumulation rate (g cm^2 a^{-1})		Linear sedimentation rate (cm a^{-1})		References
						Range	Average	Range	Average	
Taihu Lake	near the northern bays	receiving discharges from input rivers	2014	the CRS model [a]	1900~2014	0.079~ 0.615	0.334	0.082~0.847	0.435	This study
Taihu Lake	Zhushan Bay, the northern bays	receiving discharges from input rivers	*NA*	the CIC model [b]	1910~2007	0.13~ 0.76	*NA* [c]	*NA*	*NA*	Shu *et al*. 2008
Taihu Lake	Meiliang Bay, the northern bays	receiving discharges from input rivers	2012	the CRS model	1865~2011	0.09~0.810	0.290	*NA*	*NA*	Mi *et al*. 2014
Taihu Lake	the central part of the Lake	open water	2014	the CRS model	1978~2014	0.097~0.278	0.178	0.122~0.468	0.284	This study
Taihu Lake	East Taihu Lake	open water	2009	the CRS model	1965~2008	0.188~0.392	0.240	*NA*	*NA*	Yao *et al*. 2012
Taihu Lake	Southern Taihu Lake	open water	*NA*	the CIC model	1910~2007	0.10~0.56	*NA*	*NA*	*NA*	Xue *et al*. 2011
Chaohu Lake	the central lake	a shallow, eutrophic lake	*NA*	the CIC model	1950~2005	0.106~0.241	*NA*	*NA*	0.240	Xue *et al*. 2011
Shijiuhu Lake	the central lake	river-communicating lakes	*NA*	the CRS model	1910~2007	0.054~0.410	*NA*	*NA*	*NA*	Xue *et al*. 2011
Nanyihu Lake	the eastern lake	the largest lakes in southern Anhui	*NA*	the CIC model	1965~2007	*NA*	0.250	*NA*	*NA*	Xue *et al*. 2011

		Province								

[a] the CIC (constant initial concentration) model is

$t_x = \lambda^{-1}\ln(C_0/C_x)$ (S4)

where t is the age in years,

λ is the decay constant for ^{210}Pb (0.03114 a^{-1}),

x is the depth in core (cm^{-1} or g cm^{-2}),

C_0 is the $^{210}Pb_{ex}$ (unsupported ^{210}Pb) activity at the sediment water interface (Bq kg^{-1}), and

C_x is the $^{210}Pb_{ex}$ at depth x in the sedimentary section.

[b] the CRS (constant initial concentration) model is:

$t_x = \lambda^{-1}\ln(A_0/A_x)$ (S5)

where A_0 is the inventory of $^{210}Pb_{ex}$ in the core (Bq cm^{-2}),

A_x is the inventory of $^{210}Pb_{ex}$ below depth x.

[c] *NA*, not available.

Table S4 Physical & chemical properties of the16 priority PAHs

Compounds	Rings	logK_{ow}[a]	logK_{OC}[b]	Chronic toxicity[c] (μg L^{-1})
Naphthalene (Nap)	2	3.37	3.08	970
Acenaphthylene (Acy)	2	4.03	3.70	180
Acenaphthene (Ace)	2	3.92	3.68	270
Fluorene (Fluo)	2	4.18	3.93	150
Phenanthrene (Phe)	3	4.57	4.21	60
Anthracene (Ant)	3	4.54	4.20	55
Fluoranthene (Flua)	3	5.18	4.68	11
Pyrene (Pyr)	4	5.22	4.61	12
Benz[*a*]anthracene (BaA)	4	5.91	5.37	2
Chrysene (Chry)	4	5.91	5.37	2.2
Benzo[*b*]fluoranthene (BbF)	4	5.8	5.82	2.9
Benzo[*k*]fluoranthene (BkF)	4	6.0	5.82	1.7
Benzo[*a*]pyrene (BaP)	5	5.91	5.67	1.5
Indeno[1,2,3-*c*,*d*]pyrene (IncdP)	5	6.75	6.26	0.13
Dibenz[*a*,*h*]anthracene (DBA)	5	6.5	6.19	0.25
Benzo[*g*,*h*,*i*]perylene (BghiP)	6	6.52	6.26	0.49

[a] Data were adopted from (Mackay *et al.* 1992).

[b] Data were adopted from (Hawthorne *et al.* 2006).

[c] A search of the U.S. EPA Toxicity Information Retrieval (USEPA 1997) database identified more than 300 values for the acute toxicity (median lethal concentration, LC50) of aromatic hydrocarbons to freshwater and marine invertebrates and fish. And the chronic toxicity of each PAH was estimated by dividing the acute value by an acute/chronic ratio. Acute/chronic ratios for aromatic hydrocarbons calculated from their data are between 2 and 4 (Suter and Rosen 1988). The specific value of chronic toxicity for individual PAH were adopted from (Neff *et al.* 2005).

Table S5 Volumes of overlying water and porewater (mL) and concentrations of dissolved organic carbon (DOC, mg L^{-1}) at different depths (cm) of four sampling locations

Sampling site	Type	Depth	Volume	DOC
ZS	Overlying water	/	329	7.736
	Porewater	0-5	57.0	15.03
	Porewater	5-10	47.0	9.080
	Porewater	10-15	42.3	11.08
	Porewater	15-20	40.5	11.35
	Porewater	20-25	34.8	11.67
	Porewater	25-30	46.5	12.96
ML	Overlying water	/	1120	6.098
	Porewater	0-5	49.5	18.05
GH	Overlying water	/	815	9.504
	Porewater	0-5	56.0	10.41
	Porewater	5-10	48.8	6.809
	Porewater	10-15	30.8	8.424
	Porewater	15-20	31.0	7.644
	Porewater	20-25	39.0	6.059
CL	Overlying water	/	1010	4.933
	Porewater	0-5	49	7.932
	Porewater	5-10	36.5	7.552
	Porewater	10-15	40.5	7.610
	Porewater	15-20	26.0	6.840

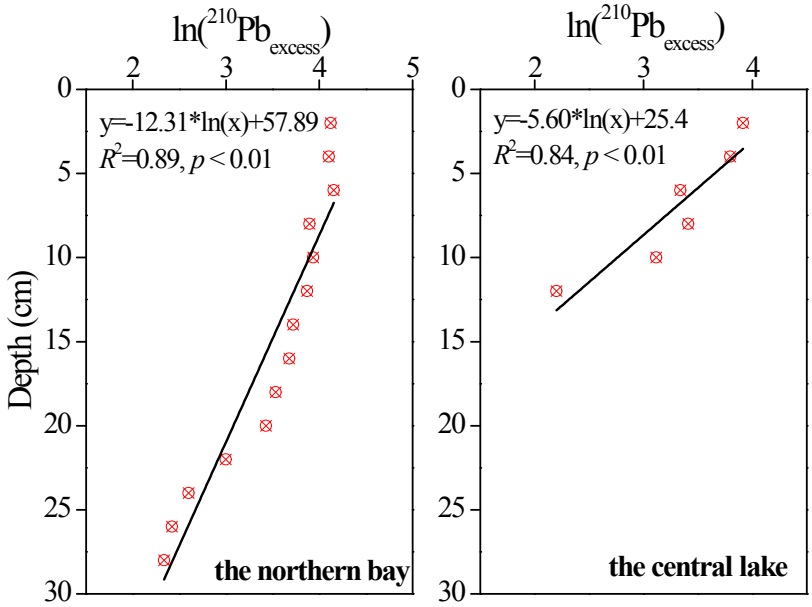

Fig. S1 ^{210}Pb age dating of sediment cores from the northern bay and the central part of Taihu Lake.

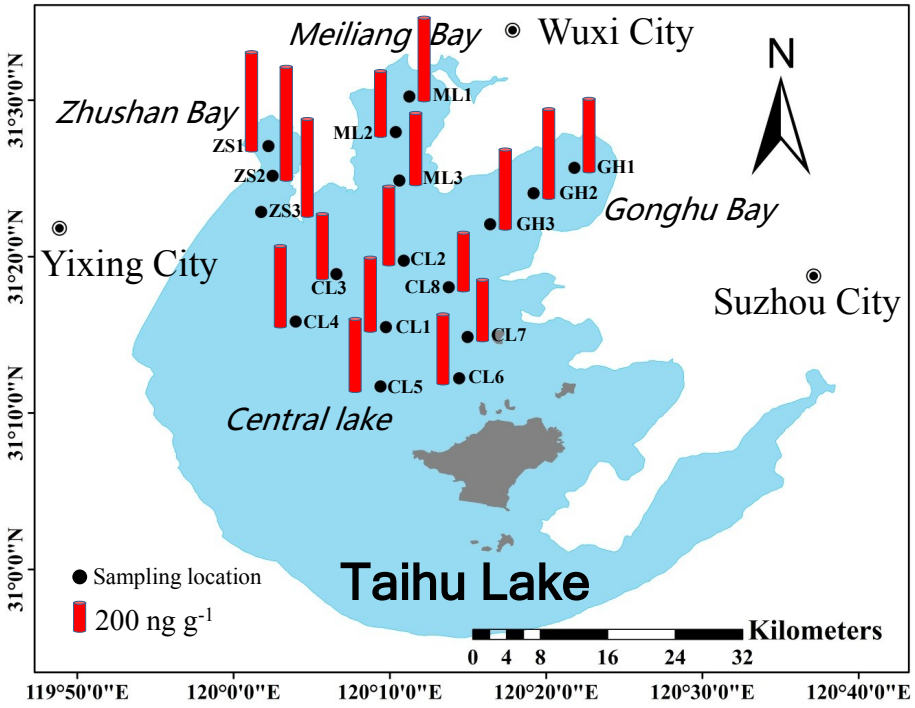

Fig.S2 Spatial concentrations of ΣPAHs in surface sediments

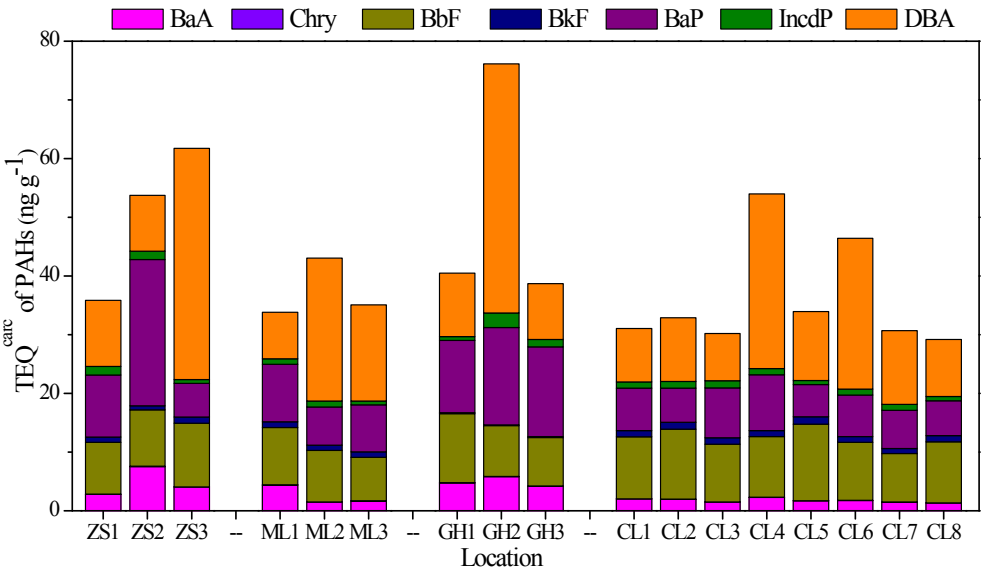

Fig. S3 Toxic benzo[a]pyrene equivalent (TEQ^{carc}) of the seven carcinogenic PAHs in surface sediments

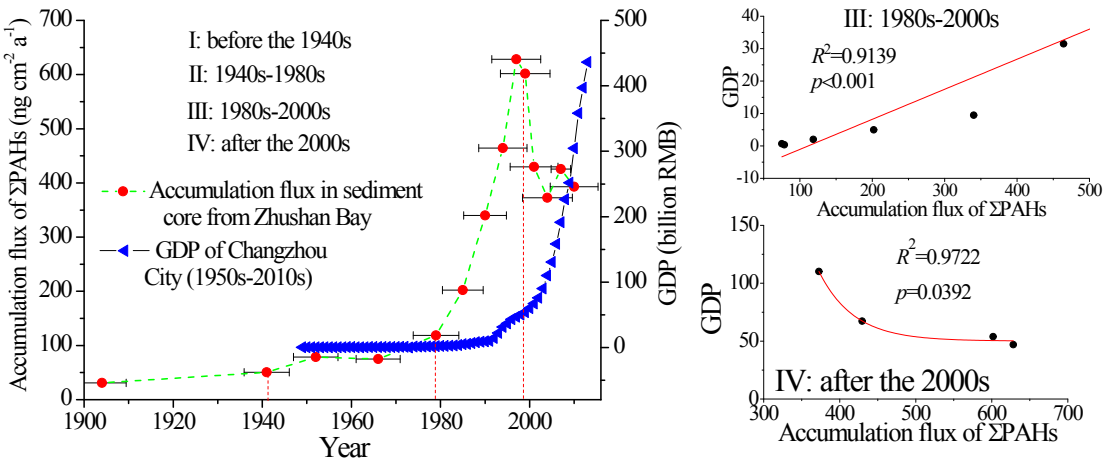

Fig. S4 Correlation between accumulation fluxes of ΣPAHs in the sediment core from Zhushan Bay with the economic indicators in the Changzhou City

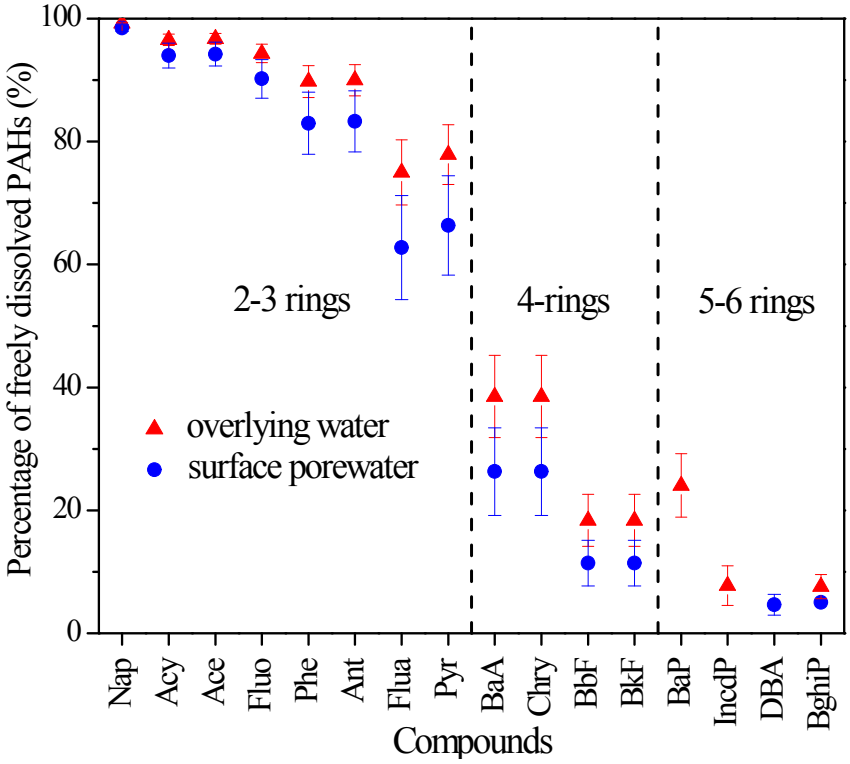

Fig. S5 The percentage of freely dissolved PAHs in overlying water and surface porewater

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