

Intra-urban levels, spatial variability, possible sources and health risks of PM_{2.5} bound phthalate esters in Xi'an

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Meteorological condition

The temperature (T) and relative humidity (H) were received from the National Oceanic and Atmospheric Administration (NOAA); the data of wind speed (U) was obtained from the National Meteorological Information Center (<http://data.cma.gov.cn>). And the boundary layer height (MLH) was got from the European Centre for Medium-Range Weather Forecasts (<http://apps.ecmwf.int/datasets/>).

Spatial distributions and possible sources of PAEs

In addition, the coefficient of diversity (CD) was used to identify the similarities between PAEs concentrations and profiles at different site. The CD was determined as follows:

$$CD_{jk} = \sqrt{\frac{1}{p} \sum_{i=1}^p \left(\frac{X_{ij} - X_{ik}}{X_{ij} + X_{ik}} \right)^2} \quad (1)$$

where j and k stand for the two different sampling sites, p is the number of investigated components, x_{ij} and x_{ik} represent the average concentrations of chemical component i for j and k (Wongphatarakul et al., 1998; Xu et al., 2016).

References

Wongphatarakul, V., Friedlander, S.K., Pinto, J.P., 1998. A comparative study of PM_{2.5} ambient aerosol chemical databases. *Environ. Sci. Technol.* 32, 3926-3934.

Xu, H.M., Ho, S.S.H., Gao, M.L., Cao, J.J., Guinot, B., Ho, K.F., Long, X., Wang, J.Z., Shen, Z.X., Liu, S.X., Zheng, C.L., Zhang, Q., 2016. Microscale spatial distribution and health assessment of PM_{2.5}-bound polycyclic aromatic hydrocarbons (PAHs) at nine communities in Xi'an, China. *Environ. Pollut.* 218, 1065-1073.

Table S1. Environments of the sampling sites in Xi'an.

Sites	Environment	Sampling height(m)
A1	Medium-rise housing within old city walls	Ground
A2	Medium-rise housing within old city walls, tree-lined roads	10
A3	Public library, heavy traffic area	10
A4	Quiet, tree-lined campus	13
A5	Quiet, residential high rises, old city wall-2 nd ring road	~1
A6	Mix of office buildings	10
A7	Quiet, tree-lined campus	7
A8	Quiet, residential high rises, old city wall-2 nd ring road	4
A9	Quiet, tree-lined campus	3
A10	residential high rises, 2 nd -3 rd ring road	Ground
A11	Medium-rise housing, family member courtyard	~5
A12	Urban-rural fringe zone, village	3
A13	Urban-rural fringe zone, village	3
A14	Quiet residential, near 3 rd ring road	18
A15	residential high rises, 2 nd -3 rd ring road	Ground
A16	residential high rises, 2 nd -3 rd ring road	10
A17	Near a road, and a restaurant	8
A18	Medium-rise housing, family member courtyard	5
A19	Near a power station, and a highway	13

Table S2. Summary of the PAEs concentrations (ng/m³) in PM_{2.5} at sampling sites in Xi'an.

	DMP	DEP	DBP	BBZP	DEHP	DNOP	DEHA	ΣPAEs
A1	73.8 ± 16.9	70.9 ± 23.1	108.8 ± 29.5	85.8 ± 27.6	797.3 ± 419.8	71.4 ± 24.0	55.7 ± 19.7	1264 ± 530
A2	80.9 ± 15.9	79.8 ± 18.3	119.4 ± 30.0	93.6 ± 22.2	678.8 ± 324.9	76.3 ± 18.5	60.4 ± 15.9	1189 ± 416.8
A3	98.4 ± 37.4	93.6 ± 33.9	148.8 ± 44.6	109.4 ± 37.8	791.7 ± 282.1	89.9 ± 28.8	67.5 ± 16.4	1399 ± 309.6
A4	80.6 ± 12.7	80.8 ± 15.6	167.2 ± 28.5	96.6 ± 19.5	875.8 ± 308.7	80.5 ± 16.4	65.1 ± 13.5	1447 ± 390.5
A5	77.1 ± 16.5	78.4 ± 15.5	102.5 ± 19.6	101.1 ± 27.8	610.3 ± 302.8	79.5 ± 16.6	63.4 ± 18.6	1112 ± 362.6
A6	80.8 ± 29.0	82.2 ± 23.0	97.6 ± 31.5	116.1 ± 31.7	494.5 ± 320.5	85.2 ± 17.6	73.4 ± 16.4	1030 ± 345.2
A7	74.6 ± 22.5	79.1 ± 11.2	107.4 ± 26.6	128.4 ± 34.5	368.3 ± 140.1	88.9 ± 7.8	83.4 ± 14.7	930.2 ± 144.4
A8	74.4 ± 24.1	78.8 ± 10.5	95.6 ± 25.4	128.2 ± 35.2	406.8 ± 184.6	88.6 ± 8.1	86.4 ± 14.2	958.8 ± 187.2
A9	57.2 ± 21.7	74.1 ± 10.1	81.2 ± 21.8	153.6 ± 32.0	386.0 ± 245.8	95.0 ± 7.1	95.6 ± 11.7	942.9 ± 250.2
A10	49.6 ± 17.1	69.0 ± 7.8	110.5 ± 21.7	164.3 ± 26.4	297.6 ± 92.6	96.8 ± 7.0	96.7 ± 17.3	884.5 ± 85.4
A11	52.7 ± 19.7	77.6 ± 27.5	66.8 ± 13.5	207.8 ± 73.8	267.6 ± 64.4	118.3 ± 41.4	122.1 ± 41.9	912.8 ± 257.4
A12	44.0 ± 5.1	65.0 ± 6.0	66.9 ± 11.9	175.2 ± 16.2	313.7 ± 80.1	100.6 ± 9.1	103.5 ± 9.7	868.9 ± 102.1
A13	41.4 ± 1.6	65.3 ± 1.9	45.6 ± 7.8	177.2 ± 6.7	275.1 ± 127.9	100.8 ± 2.8	102.7 ± 3.0	808.1 ± 135.4
A14	41.7 ± 1.8	64.2 ± 0.9	57.5 ± 16.2	174.2 ± 2.4	179.6 ± 31.1	99.0 ± 1.6	100.0 ± 1.5	716.2 ± 40.2
A15	48.0 ± 4.0	63.8 ± 1.4	28.5 ± 3.1	174.0 ± 3.8	147.9 ± 19.3	98.3 ± 2.1	98.7 ± 2.2	659.3 ± 25.1
A16	43.2 ± 4.2	64.3 ± 1.4	36.0 ± 19.3	173.7 ± 2.4	158.6 ± 55.4	98.2 ± 1.5	100.1 ± 3.4	674.0 ± 82.7
A17	50.4 ± 4.2	65.4 ± 0.3	55.2 ± 14.5	174.0 ± 0.1	203.1 ± 59.5	98.8 ± 0.8	104.5 ± 1.4	751.4 ± 73.5
A18	47.7 ± 2.2	65.1 ± 0.1	49.2 ± 8.6	173.9 ± 0.1	183.2 ± 24.9	98.5 ± 0.4	104.4 ± 1.0	722.0 ± 31.5
A19	48.0 ± 10.8	68.8 ± 14.7	104.2 ± 129.0	184.6 ± 39.0	192.4 ± 47.6	104.5 ± 22.0	106.2 ± 21.6	808.6 ± 209.5

ΣPAEs is sum of dimethylphthalate (DMP), diethylphthalate (DEP), di-n-butyl phthalate (DBP), benzyl butyl phthalate (BBZP), bis (2-ethyl(hexyl))phthalate (DEHP), di-n-octyl phthalate (DNOP), and bis(2-ethylhexyl)adipate (DEHA).

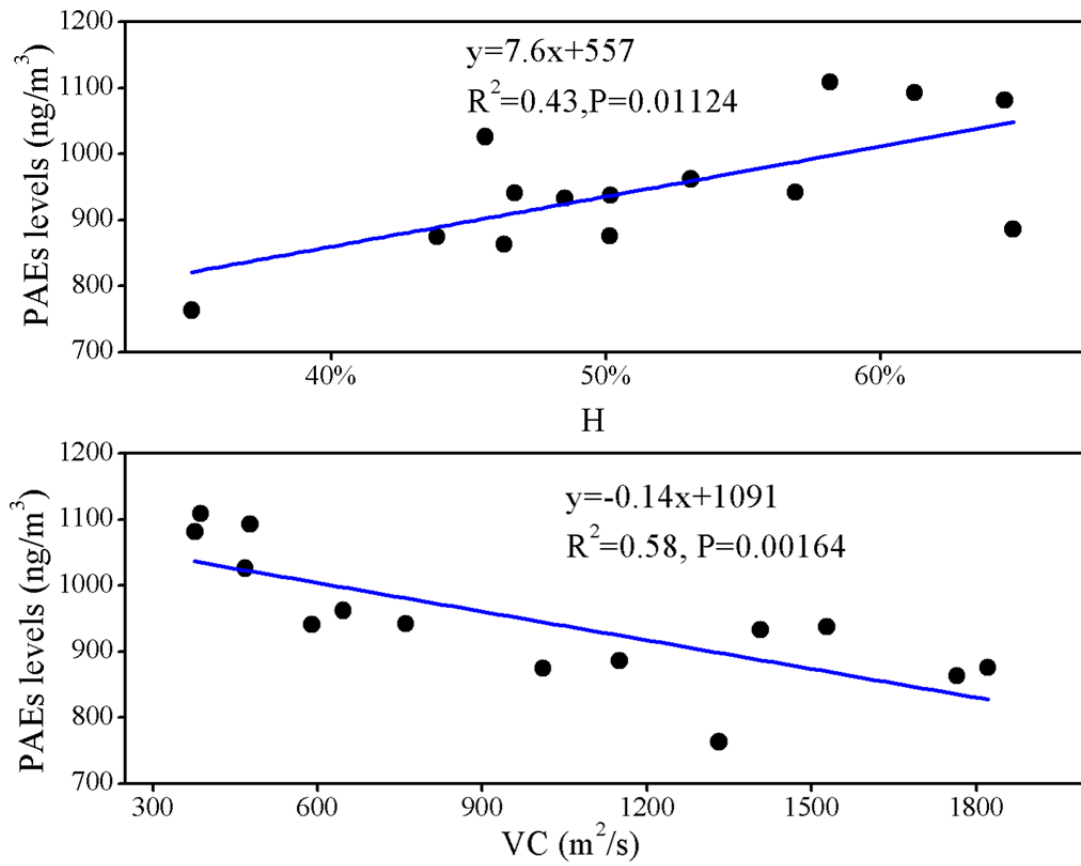


Figure S1. The correlations of weather conditions and PAEs in this study.

Table S3. The coefficients of divergence between communities for PAEs in Xi'an.

	A1	A2	A3	A4	A5	A6	A7	A8	A9	A10	A11	A12	A13	A14	A15	A16	A17	A18	A19
A1		0.052	0.120	0.097	0.071	0.128	0.181	0.173	0.217	0.250	0.318	0.280	0.321	0.338	0.393	0.376	0.323	0.341	0.313
A2			0.084	0.081	0.041	0.091	0.146	0.140	0.194	0.226	0.297	0.265	0.31-	0.326	0.384	0.367	0.309	0.329	0.291
A3				0.064	0.106	0.127	0.170	0.168	0.223	0.248	0.313	0.295	0.341	0.355	0.409	0.395	0.337	0.357	0.308
A4					0.114	0.151	0.190	0.189	0.238	0.257	0.332	0.305	0.351	0.364	0.417	0.403	0.349	0.368	0.318
A5						0.059	0.118	0.108	0.160	0.200	0.265	0.231	0.276	0.295	0.355	0.337	0.276	0.297	0.266
A6							0.068	0.055	0.117	0.162	0.220	0.194	0.242	0.259	0.325	0.305	0.237	0.261	0.228
A7								0.030	0.086	0.106	0.178	0.159	0.212	0.219	0.295	0.273	0.197	0.222	0.171
A8									0.073	0.116	0.173	0.151	0.203	0.218	0.292	0.270	0.194	0.220	0.182
A9										0.083	0.116	0.083	0.143	0.168	0.253	0.224	0.145	0.171	0.146
A10											0.122	0.099	0.163	0.156	0.257	0.226	0.146	0.172	0.088
A11												0.078	0.105	0.115	0.201	0.169	0.090	0.114	0.115
A12													0.076	0.107	0.205	0.168	0.092	0.116	0.125
A13														0.091	0.146	0.112	0.077	0.082	0.165
A14															0.135	0.090	0.044	0.040	0.115
A15																0.050	0.135	0.109	0.223
A16																	0.097	0.068	0.190
A17																		0.031	0.118
A18																			0.137

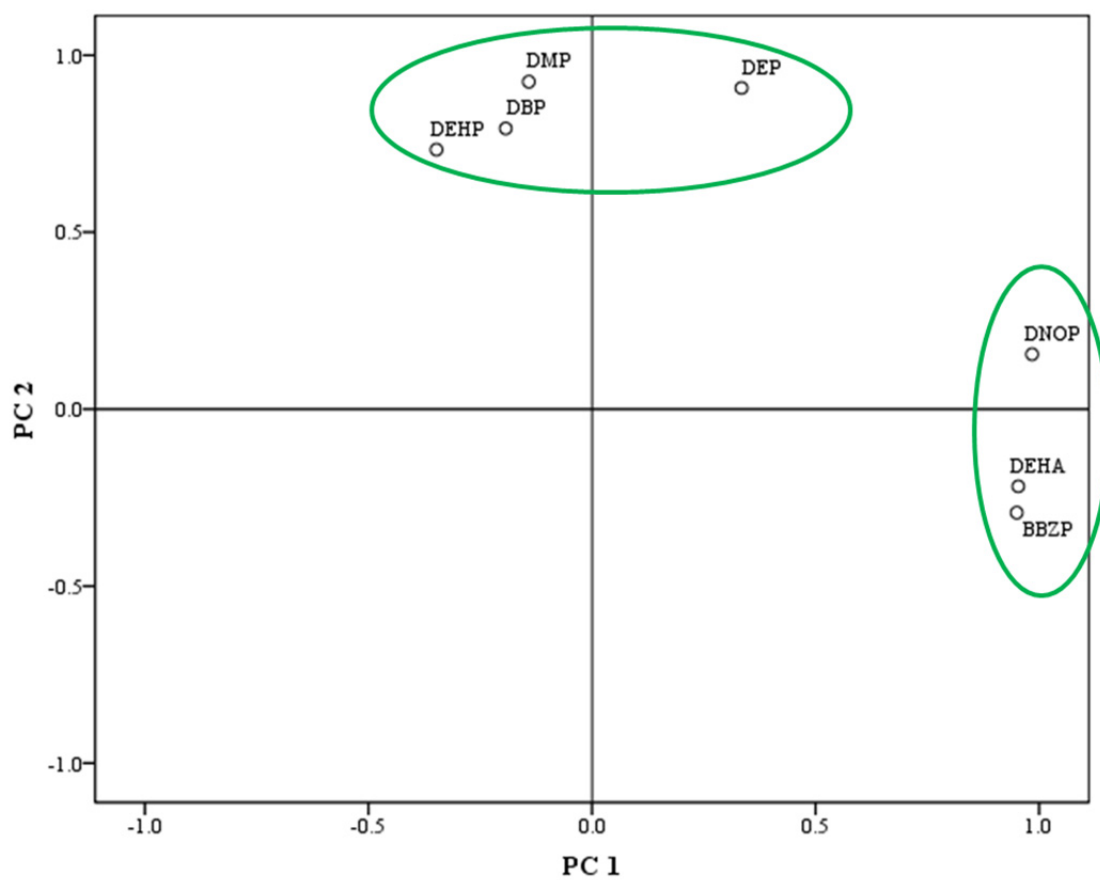


Figure S2. Principal Component Analysis results for PAEs in PM_{2.5} in this study.

Table S4. The average daily inhalations of PAEs (ng/kg/day) for various age groups in Xi'an.

EI	DMP	DEP	DBP	BBZP	DEHP	DNOP	DEHA	ΣPAEs	Carcinogenic risk by DEHP
Infants	49.7	59.1	70.5	118.9	326.0	75.4	72.0	771.6	4.56×10^{-6}
Toddlers	22.1	26.3	31.3	52.9	144.9	33.5	32.0	342.9	2.03×10^{-6}
Children	20.7	24.7	29.4	49.7	136.1	31.5	30.1	322.2	1.91×10^{-6}
Teenagers	14.6	17.4	20.7	34.9	95.7	22.1	21.1	226.5	1.34×10^{-6}
Adults	11.6	13.9	16.5	27.9	76.5	17.7	16.9	181.0	1.07×10^{-6}
TDI ^a (μg/kg/d)	-	750	100	200	37	-	-		
RfD ^a (μg/kg/d)	-	800	100	200	20	400	-		

^aTDI Value from EU CSTE, and RfD from US EPA.