Supplementary Material (ESI) for Journal of Environmental Monitoring

Supplementary information for

Incidence of organochlorine pesticides in soils of Shenzhen, China

Hong-Gang Ni, Shan-Ping Cao, Hui Zeng

[a] *Shenzhen Key Laboratory of Circular Economy, Shenzhen Graduate School, Peking University, Shenzhen 518055, China.*

[b] *Department of Ecology, College of Urban and Environmental Sciences, Peking University, Beijing 100871, China*

No. of pages: 8

No. of Tables: 6

No. of Figures: 1

Target analytes (21 OCPs):

alpha-hexachlorocyclohexane, blta-hexachlorocyclohexane, gammar-hexachlorocyclohexane, delta- hexachlorocyclohexane, heptachlor, heptachlor epoxide, aldrin, dieldrin, endrin, *o, p′*-DDE, *o, p′*-DDD, *o, p′*-dichlorodiphenyltrichloroethanes, *o,p′*-DDT, *p, p′*-DDE, *p, p′*-DDD, *p,p′*-dichlorodiphenyltrichloroethane, *p, p′*-DDT, *α*-endosulfan , *β*-endosulfan, endrin aldehye, endosulfan sulfate, endrin ketone, methoxychlor were purchased from AccuStandar.

Surrogate standard: PCB67 and PCB191were purchased from Cambridge Isotope Laboratory (Anbe, MA, USA).

Internal standard: PCB82 was purchased from Cambridge Isotope Laboratory (Anbe, MA, USA).

Table S1. Organochlorine pesticides residues (ng/g) and their occurrences in soils in Shenzhen.

Compounds	mean	median	std.dev	min	max	DF%
α-BHC	0.26	0.06	1.21	0.03	9.86	2.4
β-BHC	10.1	3.66	17.4	0.26	114	89
γ-BHC	9.02	0.18	15.6	0.03	90.7	26
δ-BHC	2.63	0.06	9.28	0.03	65.6	9.0
Heptachlor	1.29	0.81	1.26	0.26	5.37	31
Aldrin	1.35	0.64	1.33	0.35	3.90	5.4
Heptachlor epoxide	1.59	0.99	1.70	0.25	10.0	46
DDMU	2.29	2.29		2.29	2.29	0.6
α-Endosulfan	5.09	1.65	8.68	0.26	46.8	58
o,p′-DDE	2.20	1.99	1.20	0.53	3.87	3.6
β-Endosulfan	0.30	0.27	0.06	0.25	0.39	2.4
p,p′-DDE	17.4	13.7	16.4	0.27	50.5	8.4
o,p′-DDD	0.41	0.41		0.41	0.41	0.6
Dieldrin	0.46	0.41	0.22	0.25	0.81	3.6
o,p′-DDT	10.9	7.18	12.8	0.31	25.1	1.8
Endrin sulfate	0.29	0.29		0.29	0.29	0.6
p,p′-DDT	30.0	3.36	48.2	0.41	119	3.6
Methoxychlor	18.4	1.44	47.0	0.33	152	6.0

DF: detection frequency (%)

Table S2. Mean concentrations (ng/g) of organochlorine pesticides in soils from different land use in Shenzhen, China.

Compounds	forest	traffic	industry	greenbelt	commerce	agriculture	orchard	residential
α-BHC	3.2	9.9	ND	ND	0.5	ND	0.3	ND
β-BHC	6.5	18	7.5	8.3	14	5.0	10	9.6
γ-BHC	15	31	9.6	27	35	18	8.8	12
δ-BHC	2.2	29	16	3.2	14	ND	ND	8.6
Heptachlor	0.8	1.8	1.1	0.9	1.8	1.1	1.0	1.3
Aldrin	ND	ND	0.7	3.5	0.4	ND	ND	1.0
Heptachlor epoxide	1.4	2.9	1.6	1.2	1.3	2.6	1.4	0.8
DDMU	ND	2.3	ND	ND	ND	ND	ND	ND
α-Endosulfan	1.2	13	5.2	2.5	5.2	1.8	3.7	4.1
o,p′-DDE	ND	1.1	ND	ND	ND	3.5	ND	2.2
β-Endosulfan	0.4	ND	0.3	ND	0.3	ND	ND	ND
p,p′-DDE	ND	29	18	5.0	ND	14	ND	14
o,p′-DDD	ND	ND	ND	ND	0.4	ND	ND	ND
Dieldrin	0.4	0.8	0.6	0.3	0.4	ND	ND	ND
o,p′-DDT	ND	ND	ND	0.3	ND	7.2	ND	25
Endrin sulfate	ND	0.3	ND	ND	ND	ND	ND	ND
p,p′-DDT	ND	119	53	3.4	ND	1.2	0.4	ND
Methoxychlor	53	ND	ND	ND	0.3	ND	3.6	7.7

ND: not detected.

Table S3. Indexes for OCPs source identification.

	α-/γ-HCH	β-HCH%	*o,p'*-/*p,p'*-DDT	*p,p'*-(DDE+DDD)/DDT
forest	0-0.19	31-100	0	0
traffic	0	27-100	0	0.3
industry	0	28-100	0	0.69
greenbelt	0	37-100	0	0
commerce	0	11-100		
agriculture	0	40-100	0	0-0.35
orchard	0-0.24	36-99	0	0
residential area	0	15-96		
technical HCH	4.64-5.83	5-14		
lindane	0			

Table S4. Mass inventories (kg), yearly loss fluxes by soil erosion (kg) and remnant amount (kg) of OCPs in soil of Shenzhen.

Compounds	inventory	loss flux	remnant
BHCs	5250	22.0	5228
DDTs	3102	60.8	3041
Heptachlor	193	1.29	192
Aldrin	78	1.35	77
Heptachlor epoxide	241	1.59	240
α-Endosulfan	544	5.09	539
β-Endosulfan	19	0.30	19
Dieldrin	23	0.46	22
Endrin sulfate	12	0.29	12
Methoxychlor	2080	18.4	2061

Table S5. Fugacity quotients ($f = f_{soil}/f_{air}$) for the soil-air system at Shenzhen.

chemicals	fugacity quotient				
	mean	median	min	max	std. dev
α-BHC	2.69	1.430	0.195	7.71	3.50
γ-BHC	1.69	1.624	0.022	8.08	1.61
α-endosulfan	0.09	0.030	0.005	0.85	0.16
p,p′-DDE	0.08	0.066	0.001	0.24	0.08
o,p′-DDT	0.10	0.068	0.003	0.24	0.12
p,p′-DDT	0.04	0.005	0.001	0.17	0.07

Table S6. Estimation of human non-dietary exposure to OCPs (pg/kg bw/day) for five sub-groups in residential block of Shenzhen, China.

	children (0-8)			male (9-18)			female (9-18)			male (over 19)			female (over 19)		
	E_{soil}	E_{air}	E	E_{soil}	E_{air}	E	E_{soil}	E_{air}	E	E_{soil}	E_{air}	E	E_{soil}	E_{air}	E
α-BHC	–	21	21	–	16	16	–	14	14	–	11	11	–	10	10
γ-BHC	66	22	88	26	17	43	28	14	43	9	12	21	11	10	21
p,p'-DDE	75	54	128	30	41	70	32	36	68	11	29	39	12	25	38
o,p'-DDT	134	90	224	53	69	121	58	60	118	19	48	67	22	42	65
p,p'-DDT	–	274	274	–	208	208	–	181	181	–	146	146	–	128	128
α-endosulfan	22	48	70	9	37	45	9	32	41	3	26	29	4	23	26

–: No estimated values due to soil concentrations of these chemicals were lower than reporting detected limits. It is notable the symbols **"–"** does not mean no exposure. [a] estimation of exposure via soil ingestion. [b] estimation of exposure via air inhalation. [c] estimation of non-dietary exposure via soil ingestion and air inhalation.

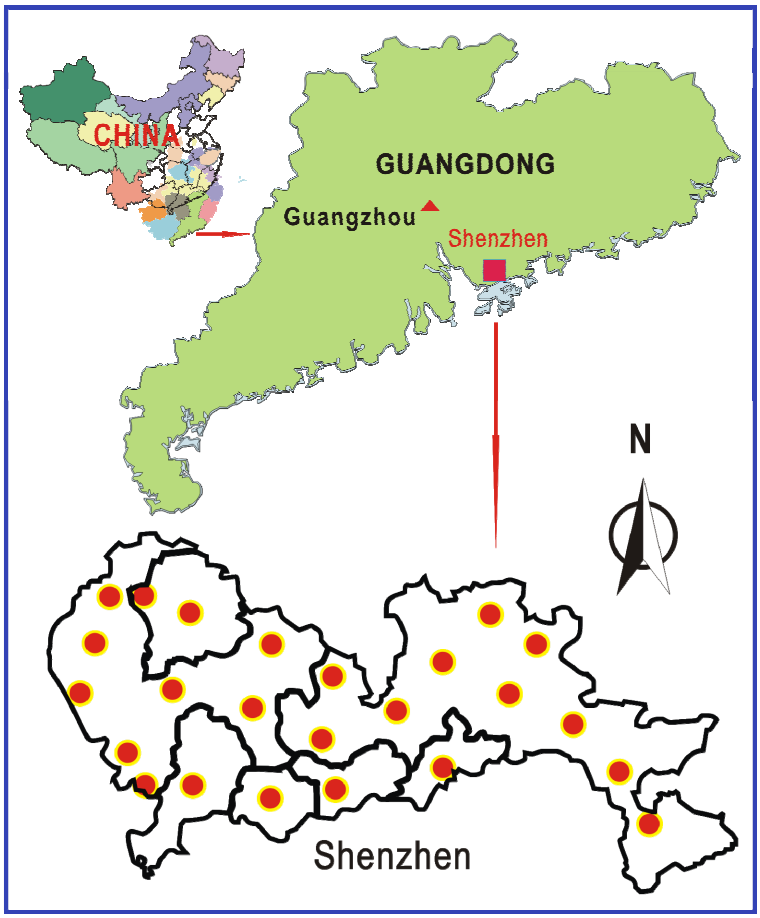

Fig. S1. Map of the general study area and major sampling sites symbolized by dots.