6.0 Supplemental Materials - Part A: Tables

Table S1. Lab analytical method for investigations at the Luhe site, Nanjing, China.

Sample Type	Analytical Parameter	Technique/Method Reference	Detection Limit
Soil	VOC	USEPA 8260C	0.05 mg/kg
	SVOC	USEPA 8270D	0.1 mg/kg
Groundwater	VOC	USEPA 8260C	0.5 μg/L
	SVOC	USEPA 8270D	1.0 μg/L

Table S2. Heavy metals in soil samples in garden plot at the Luhe site, Nanjing, China (Unit: mg/kg in dry weight)

Sampling Point	Pb	Cr	Co	Ni	Cu	Cd	As	Se	Hg
Soil-1	30.9	67.9	13.6	31.8	27.4	0.18	12.4	0.13	0.06
Soil-2	31.4	58.9	13.1	25.5	25.4	0.21	11.8	0.32	0.11
Soil-3	32.1	62.1	13.2	28.9	27.2	0.3	12	0.31	0.1
DIV-S	530	380	240	210	190	12	55	100	10
DTV-S	85	100	9	35	36	0.8	29	0.7	0.3

Notes: DIV-S:, Dutch Intervention value for Soil; DTV-S, Dutch Target Value for Soil

Table S3. Calculation of Exposure rate based on non-carcinogenic effects of COCs at the LuHe Site

Exposure Pathways	Oral Soil Ingestion	Soil Dermal Contact	Soil Particle Inhalation	Inhalation of Contaminant Vapor in Outdoor Air			Inhalation of Contaminant Vapor in Indoor Air		Groundwater Consumption
				Surficial Soil	Sub Surficial Soil	Ground water	Surficial Soil	Sub Surficial Soil	
Ethylbenzene	1.21×10^{-6}	6.88×10^{-6}	1.43×10^{-8}	2.50×10^{-7}	1.04×10^{-6}	9.83×10^{-6}	4.80×10^{-4}	1.45×10^{-3}	1.21×10^{-2}
Chlorobenzene	1.21×10^{-6}	6.88×10^{-6}	1.43×10^{-8}	2.50×10^{-7}	8.03×10^{-7}	4.08×10^{-6}	3.70×10^{-4}	6.02×10^{-4}	1.21×10^{-2}
Dichlorobenzene	1.21×10^{-6}	6.88×10^{-6}	1.43×10^{-8}	2.50×10^{-7}	3.07×10^{-7}	2.42×10^{-6}	1.41×10^{-4}	3.56×10^{-4}	1.21×10^{-2}
Benzene	1.21×10^{-6}	6.88×10^{-6}	1.43×10^{-8}	2.50×10^{-7}	2.56×10^{-6}	8.69×10^{-6}	1.18×10^{-3}	1.28×10^{-3}	1.21×10^{-2}
Toluene	1.21×10^{-6}	6.88×10^{-6}	1.43×10^{-8}	2.50×10^{-7}	1.82×10^{-6}	9.40×10^{-6}	8.37×10^{-4}	1.39×10^{-3}	1.21×10^{-2}
Xylenes	1.21×10^{-6}	6.88×10^{-6}	1.43×10^{-8}	2.50×10^{-7}	9.87×10^{-7}	8.01×10^{-6}	4.55×10^{-4}	1.18×10^{-3}	1.21×10^{-2}
1,2.4-Trichlorobenzene	1.21×10^{-6}	6.88×10^{-6}	1.43×10^{-8}	2.50×10^{-7}	2.58×10^{-5}	8.61×10^{-3}	1.19×10^{-6}	1.49×10^{-4}	1.21×10^{-2}

Table S4. Calculation of Exposure rate based on carcinogenic effects of COCs at the LuHe Site

Exposure Pathways	Oral Soil Ingestion	Soil Dermal Contact	Soil Particle Inhalation	Inhalation of Contaminant Vapor in Outdoor Air			Inhalation of Contaminant Vapor in Indoor Air		Groundwater Consumption
				Surficial Soil	Sub Surficial Soil	Ground water	Surficial Soil	Sub Surficial Soil	
Ethylbenzene	4.20×10^{-7}	2.39×10^{-6}	4.97×10^{-9}	8.68×10^{-8}	3.62×10^{-7}	3.41×10^{-6}	1.67×10^{-4}	5.03×10^{-4}	4.20×10^{-3}
Chlorobenzene	4.20×10^{-7}	2.39×10^{-6}	4.97×10^{-9}	8.68×10^{-8}	2.79×10^{-7}	1.42×10^{-6}	1.28×10^{-4}	2.09×10^{-4}	4.20×10^{-3}
Dichlorobenzene	4.20×10^{-7}	2.39×10^{-6}	4.97×10^{-9}	8.68×10^{-8}	1.06×10^{-7}	8.39×10^{-7}	4.91×10^{-5}	1.24×10^{-4}	4.20×10^{-3}
Benzene	4.20×10^{-7}	2.39×10^{-6}	4.97×10^{-9}	8.68×10^{-8}	8.89×10^{-7}	3.02×10^{-6}	4.10×10^{-4}	4.45×10^{-4}	4.20×10^{-3}
Toluene	4.20×10^{-7}	2.39×10^{-6}	4.97×10^{-9}	8.68×10^{-8}	6.30×10^{-7}	3.26×10^{-6}	2.90×10^{-4}	4.81×10^{-4}	4.20×10^{-3}
Xylenes	4.20×10^{-7}	2.39×10^{-6}	4.97×10^{-9}	8.68×10^{-8}	3.43×10^{-7}	2.78×10^{-6}	1.58×10^{-4}	4.10×10^{-4}	4.20×10^{-3}
1,2.4-Trichlorobenzene	4.20×10^{-7}	2.39×10^{-6}	4.97×10^{-9}	8.68×10^{-8}	8.97×10^{-6}	2.99×10^{-3}	4.13×10^{-7}	5.16×10^{-5}	4.20×10^{-3}

Table S5. Toxicity parameters of COCs at the LuHe Site.

Parameters	Ethylbenzene	Chlorobenzene	1,4-Dichlorobenzene
IUR	0.0025	--	0.011
SFi	9.79×10^{-3}	--	4.31×10^{-2}
SFo	0.011	--	0.0054
SFd	0.011	--	0.0054
RfC	1	0.05	0.8
RfDi	2.55×10^{-1}	1.28×10^{-2}	2.04×10^{-1}
RfDo	0.1	0.02	0.07
RfDd	0.1	0.02	0.07
CC*	D	D	NA**

Notes: --: no values in guidelines (HJ25.3-2-14); CC*: Carcinogenic classification; NA**: This substance has not undergone an evaluation through the US EPA's IRIS program for evidence of human carcinogenic potential.

Table S6. Physical and chemical properties, and other relevant parameters for COCs at the LuHe Site.

Parameters	Ethylbenzene	Chlorobenzene	1,4-Dichlorobenzene
H′	3.22×10^{-1}	1.27×10^{-1}	9.85×10^{-2}
Da	6.85×10^{-2}	7.21×10^{-2}	5.50×10^{-2}
Dw	8.46×10^{-6}	9.48×10^{-6}	8.68×10^{-6}
Koc	4.46×10^{2}	2.34×10^{2}	3.75×10^{2}
S	1.69×10^{2}	4.98×10^{2}	8.13×10^{1}
ABSgi	1	1	1
ABSd	0.1	0.1	0.1
ABSo	1	1	1

Supplemental Materials - Part B: Models

Part B1: Models for calculating exposure rate based on non-carcinogenic effects and carcinogenic effects

$$\mathrm{OISER}_{nc} = \frac{\mathrm{OSIR_a} \times ED_a \times EF_a \times ABS_o}{BW_a \times AT_{nc}} \times 10^{-6}$$

$$\mathrm{DCSER}_{nc} = \frac{\mathrm{SAE_a} \times \mathrm{SSAR}_a \times EF_a \times \mathrm{ED}_a \times E_v \times ABS_d}{BW_a \times AT_{nc}} \times 10^{-6}$$

$$SAE_a = 239 \times H_a^{0.417} \times \mathrm{BW}_a^{0.517} \times SER_a$$

$$PISER_{nc} = \frac{PM_{10} \times DAIR_a \times ED_a \times PIAF \times (fspo \times EFO_a + fspi \times EFI_a)}{BW_a \times AT_{nc}} \times 10^{-6}$$

$$IOVER_{nc1} = VF_{suroa} \times \frac{DAIR_\mathrm{a} \times EFO_a \times ED_a}{BW_a \times AT_{nc}}$$

$$IOVER_{nc2} = VF_{suboa} \times \frac{DAIR_\mathrm{a} \times EFO_a \times ED_a}{BW_a \times AT_{nc}}$$

$$IOVER_{nc3} = VF_{gwoa} \times \frac{DAIR_\mathrm{a} \times EFO_a \times ED_a}{BW_a \times AT_{nc}}$$

$$VF_{suroa1} = \frac{\rho_b}{DF_{oa}} \times \sqrt{\frac{4 \times D_s^{eff} \times H'}{\pi \times \tau \times 31536000 \times K_{sw} \times \rho_b}} \times 10^3$$

$$VF_{suroa2} = \frac{d \times \rho_b}{DF_{oa} \times \tau \times 31536000} \times 10^3$$

$$VF_{suroa} = MIN(VF_{suroa1}, VF_{suroa2})$$

$$DF_{oa} = \frac{U_{air} \times W \times \delta_{air}}{A}$$

$$Wdw = A/W$$

$$D_s^{eff} = D_a \times \frac{\theta_{as}^{3.33}}{\theta^2} + D_w \times \frac{\theta_{ws}^{3.33}}{H' \times \theta^2}$$

$$\theta = 1 - \frac{\rho_b}{\rho_s}$$

$$\theta_{ws} = \frac{\rho_b \times P_{ws}}{\rho_w}$$

$$\theta_{as} = \theta - \theta_{ws}$$

$$VF_{suboa1} = \frac{1}{(1 + \frac{DF_{oa} \times L_s}{D_s^{eff}}) \times \frac{K_{sw}}{H'}} \times 10^3$$

$$VF_{suboa2} = \frac{d_s \times \rho_b}{DF_{oa} \times \tau \times 3153600} \times 10^3$$

$$VF_{suboa} = MIN(VF_{suboa1}, VF_{suboa2})$$

$$VF_{gwoa} = \frac{1}{(1 + \frac{DF_{oa} \times L_{gw}}{D_{gws}^{eff}}) \times \frac{1}{H'}} \times 10^3$$

$$D_{gws}^{eff} = \frac{L_{gw}}{\frac{h_{cap}}{D_{cap}^{eff}} + \frac{h_v}{D_s^{eff}}}$$

$$D_{cap}^{eff} = D_a \times \frac{D_{acap}^{3.33}}{\theta^2} + D_w \times \frac{D_{wcap}^{3.33}}{H' \times \theta^2}$$

$$IIVER_{nc1} = VF_{subia} \times \frac{DAIR_a \times EFI_a \times ED_a}{BW_a \times AT_{nc}}$$

$$IIVER_{nc2} = VF_{gwia} \times \frac{DAIR_a \times EFI_a \times ED_a}{BW_a \times AT_{nc}}$$

$$Q_s = 0,$$

$$VF_{subia1} = \frac{1}{\frac{K_{sw}}{H'} + (1 + \frac{D_s^{eff}}{DF_{ia} \times L_s} + \frac{D_s^{eff} \times L_{crack}}{D_{crack}^{eff} \times L_s \times \eta}) \times \frac{DF_{ia}}{D_s^{eff}} \times L_s} \times 10^3$$

$$D_{crack}^{eff} = D_a \times \frac{D_{acrack}^{3.33}}{\theta^2} + D_w \times \frac{D_{wcrack}^{3.33}}{H' \times \theta^2}$$

$$Q_s = 0,$$

$$VF_{gwia1} = \frac{1}{\frac{1}{H'} + (1 + \frac{D_{gws}^{eff}}{DF_{ia} \times Lgw} + \frac{D_{gws}^{eff} \times L_{crack}}{D_{crack}^{eff} \times L_{gw} \times \eta}) \times \frac{DF_{ia}}{D_{gws}^{eff}} \times L_{gw}} \times 10^3$$

$$OISER_{ca} = \frac{OSIR_a \times ED_a \times EF_a \times ABS_o}{BW_a \times AT_{ca}} \times 10^{-6}$$

$$DCSER_{ca} = \frac{SAE_a \times SSAR_a \times EF_a \times ED_a \times E_v \times ABS_d}{BW_a \times AT_{ca}} \times 10^{-6}$$

$$PISER_{ca} = \frac{PM_{10} \times DAIR_a \times ED_a \times PIAF \times (fspo \times EFOa + fspi \times EFI_a)}{BW_a \times AT_{ca}} \times 10^{-6}$$

$$IOVER_{ca1} = VF_{suroa} \times \frac{DAIR_a \times EFO_a \times ED_a}{BW_a \times AT_{ca}}$$

$$IOVER_{ca2} = VF_{suboa} \times \frac{DAIR_a \times EFO_a \times ED_a}{BW_a \times AT_{ca}}$$

$$IOVER_{ca3} = VF_{gwoa} \times \frac{DAIR_a \times EFO_a \times ED_a}{BW_a \times AT_{ca}}$$

$$IIVER_{ca1} = VF_{subia} \times \frac{DAIR_a \times EFI_a \times ED_a}{BW_a \times AT_{ca}}$$

$$IIVER_{ca2} = VF_{gwia} \times \frac{DAIR_a \times EFI_a \times ED_a}{BW_a \times AT_{ca}}$$

$$CGWER_{ca} = \frac{GWCR_a \times EF_a \times ED_a}{BW_a \times AT_{ca}}$$

Part B2: Models for toxicity assessment

$$SF_i = \frac{IUR \times BW_a}{DAIR_a}$$

$$RfD_i = \frac{RfC \times DAIR_a}{BW_a}$$

$$SF_d = \frac{SF_o}{ABS_{gi}}$$

$$RfD_d = RfD_o \times ABS_{gi}$$

Part B3: Models for calculation of hazard quotient and carcinogenic risk

$$HQ_{ois} = \frac{OISER_{nc} \times C_{sur}}{RfD_o \times SAF}$$

$$HQ_{dcs} = \frac{DCSER_{nc} \times C_{sur}}{RfD_d \times SAF}$$

$$HQ_{pis} = \frac{PISER_{nc} \times C_{sur}}{RfD_i \times SAF}$$

$$HQ_{iov1} = \frac{IOVER_{nc1} \times C_{sur}}{RfD_i \times SAF}$$

$$HQ_{iov2} = \frac{IOVER_{nc2} \times C_{sub}}{RfD_i \times SAF}$$

$$HQ_{iiv1} = \frac{IIVER_{nc1} \times C_{sub}}{RfD_i \times SAF}$$

$$HI_n = HQ_{ois} + HQ_{dcs} + HQ_{pis} + HQ_{iov1} + HQ_{iov2} + HQ_{iiv1}$$

$$HQ_{iov3} = \frac{IOVER_{nc3} \times C_{gw}}{RfD_i \times SAF}$$

$$HQ_{iiv2} = \frac{IIVER_{nc2} \times C_{gw}}{RfD_i \times SAF}$$

$$HQ_{cgw} = \frac{CGWER_{nc} \times C_{gw}}{RfD_o \times SAF}$$

$$HI_n = HQ_{iov3} + HQ_{iiv2} + HQ_{cgw}$$

$$CR_{ois} = OISER_{ca} \times C_{sur} \times SF_o$$

$$CR_{dss} = DCSER_{ca} \times C_{sur} \times SF_d$$

$$CR_{pis} = PISER_{ca} \times C_{sur} \times SF_i$$

$$CR_{iov1} = IOVER_{ca1} \times C_{sur} \times SF_i$$

$$CR_{iov2} = IOVER_{ca2} \times C_{sub} \times SF_i$$
$$CR_{iiv1} = IIVER_{ca1} \times C_{sub} \times SF_i$$
$$CR_n = CR_{ois} + CR_{dcs} + CR_{pis} + CR_{iov1} + CR_{iov2} + CR_{iiv1}$$
$$CR_{iov3} = IOVER_{ca3} \times C_{gw} \times SF_i$$
$$CR_{iiv2} = IIVER_{ca2} \times C_{gw} \times SF_i$$
$$CR_{cgw} = CGWER_{ca} \times C_{gw} \times SF_o$$
$$CR_n = CR_{iov3} + CR_{iiv2} + CR_{cgw}$$

Part B4: Models for calculating risk control values based on non-carcinogenic effects and carcinogenic effects

$$HCVS_{ois} = \frac{RfD_o \times SAF \times AHQ}{OISER_{nc}}$$
$$HCVS_{dcs} = \frac{RfD_d \times SAF \times AHQ}{DCSER_{nc}}$$
$$HCVS_{pis} = \frac{RfD_i \times SAF \times AHQ}{PISER_{nc}}$$
$$HCVS_{iov1} = \frac{RfD_i \times SAF \times AHQ}{IOVER_{nc1}}$$
$$HCVS_{iov2} = \frac{RfD_i \times SAF \times AHQ}{IOVER_{nc2}}$$
$$HCVS_{iiv} = \frac{RfD_i \times SAF \times AHQ}{IIVER_{nc1}}$$
$$HCVS_n = \frac{AHQ \times SAF}{\frac{OISER_{nc}}{RfD_o} + \frac{DCSER_{nc}}{RfD_d} + \frac{PISER_{nc} + IOVER_{nc1} + IOVER_{nc2} + IIVER_{nc1}}{RfD_i}}$$
$$HCVG_{iov} = \frac{RfD_i \times WAF \times AHQ}{IOVER_{nc3}}$$
$$HCVG_{cgw} = \frac{RfD_o \times WAF \times AHQ}{CGWER_{nc}}$$
$$HCVG_{iiw} = \frac{RfD_i \times WAF \times AHQ}{IIVER_{nc2}}$$
$$HCVG_n = \frac{AHQ \times WAF}{\frac{IOVER_{nc3} + IIVER_{nc2}}{RfD_i} + \frac{CGWER_{nc}}{RfDo}}$$

$$RCVS_{ois} = \frac{ACR}{OISER_{ca} \times SF_o}$$

$$RCVS_{dcs} = \frac{ACR}{DCSER_{ca} \times SF_d}$$

$$RCVS_{pis} = \frac{ACR}{PISER_{ca} \times SF_i}$$

$$RCVS_{iov1} = \frac{ACR}{IOVER_{ca1} \times SF_i}$$

$$RCVS_{iov2} = \frac{ACR}{IOVER_{ca2} \times SF_i}$$

$$RCVS_{iiv1} = \frac{ACR}{IIVER_{ca1} \times SF_i}$$

$$RCVS_n = \frac{ACR}{OISER_{ca} \times SF_o + DCSER_{ca} \times SF_d + (PISER_{ca} + IOVER_{ca1} + IOVER_{ca2} + IIVER_{ca1}) \times SF_i}$$

$$RCVG_{iov} = \frac{ACR}{IOVER_{ca3} \times SF_i}$$

$$RCVG_{iiv} = \frac{ACR}{IIVER_{ca2} \times SF_i}$$

$$RCVG_{cgw} = \frac{ACR}{CGWER_{ca} \times SF_o}$$

$$RCVG_n = \frac{ACR}{(IOVER_{ca3} + IIVER_{ca2}) \times SF_i + CGWER_{ca} \times SF_o}$$

Part B5: Models for analysis on risk exposure contribution

$$PHQ_i = \frac{HQ_i}{HI_n} \times 100\%$$

$$PCR_i = \frac{CR_i}{CR_n} \times 100\%$$

Supplemental Materials - Part C: Risk-based Parameters and values

Parameter symbol	Parameter name	Unit	
OSIRa	Daily oral ingestion rate of soils of adults	$mg \cdot d^{-1}$	100
EDa	Exposure duration of adults	a	25
EFa	Exposure frequency of adults	$d \cdot a^{-1}$	250
ABSo	Absorption factor of oral ingestion	Dimensionless	1
BWa	Average body weight of adults	kg	56.8
ATnc	Average time for non-carcinogenic effect	d	9125
ATca	Average time for carcinogenic effect	d	26280
Ha	Average height of adults	cm	156.3
SERa	Skin exposure ration of adults	Dimensionless	0.18
SSARa	Adherence rate of soil on skin for adults	$mg \cdot cm^{-2}$	0.2
Ev	Daily exposure frequency of dermal contact event	$1 \cdot d^{-1}$	1
PM10	Content of inhalable particulates in ambient air	$mg \cdot m^{-3}$	0.15
DAIRa	Daily air inhalation rate of adults	$m^3 \cdot d^{-1}$	14.5
PIAF	Retention fraction of inhaled particulates in body	Dimensionless	0.75
EFOa	Outdoor exposure frequency of adults	$d \cdot a^{-1}$	62.5
f_{spi}	Fraction of soil-borne particulates in indoor air	Dimensionless	0.8
EFIa	Indoor exposure frequency of adults	$d \cdot a^{-1}$	187.5
ϱ_b	Soil bulk density	$kg \cdot dm^{-3}$	1.5
Uair	Ambient air velocity in mixing zone	$cm \cdot s^{-1}$	200
Wdw	Length of source zone	cm	1500
δ_{air}	Mixing zone height	cm	200
ϱ_s	Density of soil particulates	$kg \cdot dm^{-3}$	2.65
P_{ws}	Soil water content	$kg \cdot kg^{-1}$	0.1
ϱ_w	Water density	$kg \cdot dm^{-3}$	1
τ	Averaging time for vapor flux	a	25
d	Thickness of surficial soil	cm	80

fom	Organic matter content in soils	$g.kg^{-1}$	10
L_s	Thickness of surficial soil	cm	80
L_{gw}	Depth of groundwater	cm	60
θ_{acap}	Soil air content-capillary fringe zone	Dimensionless	0.038
θ_{wcap}	Soil water content-capillary fringe zone	Dimensionless	0.342
h_{cap}	Capillary zone thickness	cm	5
h_v	Vadose zone thickness	cm	295
L_B	Volume/infiltration area ratio of enclosed space	cm	300
ER	Air exchange rate of enclosed space	$times{\cdot}d^{-1}$	20
X_{crack}	Slab perimeter	cm	3400
A_b	Slab area	cm^2	700000
η	Area fraction of cracks in foundations/walls	Dimensionless	0.01
θ_{acrack}	Soil air content-soil filled foundation cracks	Dimensionless	0.26
θ_{wcarck}	Soil water content-soil filled foundation cracks	Dimensionless	0.12
L_{crack}	Thickness of enclosed-space foundation or wall	cm	15
μ_{air}	Air viscosity	$g.cm^{-1}.s^{-1}$	1.81×10^{-4}
Z_{crack}	Depth to bottom of slab	cm	15
dP	Differential pressure between indoor and outdoor air	$g.cm^{-1}.s^2$	0
Kv	Soil permeability	cm^2	1.00×10^{-8}
π	Constant pi		3.14159
GWCRa	Daily groundwater consumption rate of adults	$L.d^{-1}$	1
SAF	Soil allocation factor	Dimensionless	0.2
WAF	Groundwater allocation factor	Dimensionless	0.2

Supplemental Materials - Part D: List of other Risk-based Parameters

Parameter symbol	Parameter name	Unit
IUR	Inhalation Unit Risk	$(mg.m^{-3})^{-1}$
SFi	Inhalation cancer Slope Factor	$(mg.kg^{-1}.d^{-1})^{-1}$
SFo	Oral ingestion induced cancer Slope Factor	$(mg.kg^{-1}.d^{-1})^{-1}$
SFd	Dermal contact-induced cancer Slope Factor	$(mg.kg^{-1}.d^{-1})^{-1}$
RfC	Inhalation reference Concentration	$mg.m^{-3}$
RfDi	Inhalation reference dose	$mg.kg^{-1}.d^{-1}$
RfDo	Oral ingestion reference dose	$mg.kg^{-1}.d^{-1}$
RfDd	Dermal contact reference dose	$mg.kg^{-1}.d^{-1}$
H′	Dimensionless Henry's constant	Dimensionless
Da	Air diffusion coefficient	$cm^2 \cdot s^{-1}$
Dw	Water diffusion coefficient	$cm^2 \cdot s^{-1}$
Koc	Soil-organic carbon allocation coefficient	$cm^3 \cdot g^{-1}$
S	Water solubility	$mg.L^{-1}$
ABSgi	Digestive tract absorption factor	Dimensionless
ABSd	Skin absorption factor	Dimensionless
ABSo	Absorption factor of oral ingestion	Dimensionless