

Supplementary Materials: An Analysis of the Spatial Characteristics and Transport Fluxes of BTEX in Soil and Atmospheric Phases at a Decommissioned Steel Mill Site in China with a Long History

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1. Construction of the Fugacity Model

Table S1. Main physicochemical parameters of the target compounds [35,36].

Name of substance	M(g·mol ⁻¹)	K _{ow}	P _L (Pa)	P _{LS} (Pa)	S(mol·m ⁻³)
Benzene	78.11	134.90	12700	3535	0.022788
Ethylbenzene	106.17	1412.54	1352	147	0.001592
o-Xylene	106.17	1318.26	885	172	0.001677

Note: M is the molecular mass; P_L is the vapor pressure at 25°C; P_{LS} is the vapor pressure of super-cooled liquid at 0°C; S is the solubility at 25°C.

Table S2. Environmental parameters of the study area[37].

Parameters	Atmosphere	Soil
R(Pa·m ³ ·mol ⁻¹ ·K ⁻¹)	8.314	-
T(K)	298	-
V ₁₃	1.04E-10	-
V ₃₁	-	0.2
V ₃₂	-	0.3
V ₃₃	-	0.5
y _{oc} *	-	0.011
q _s *(kg·m ⁻³)	-	2.01

Note: * is the actual test value; R is the gas constant; T is the temperature; V₁₃ is the volume fraction of particulate matter in the air; V₃₁ is the volume fraction of air in the soil; V₃₂ is the volume fraction of moisture in the soil; V₃₃ is the volume fraction of soil particles in the soil; y_{oc} is the mass fraction of organic carbon in the soil; and q_s is the density of the soil.

Table S3. Migration parameters in the study area [37].

Parameters	Notation	Numerical value	Unit
Gas-side mass transfer coefficient at the soil/gas interface	K _{SA}	1.00	m·h ⁻¹
Diffusion path length in soil	Y ₃	0.05	
Molecular diffusion coefficient in air	B _{A3}	0.04	m ² ·h ⁻¹
Molecular diffusion coefficient in water	B _{W3}	0.000004	m ² ·h ⁻¹
Clearance	Q	200000	
Air-soil exchange area *	A ₁₃	Size of the study areas	m ²
Air-water exchange area *	A ₁₂	Size of the study areas	m ²
Precipitation rate *	U _Q	0.00011283	m·h ⁻¹
Dry deposition rate	U _P	10.8	m·h ⁻¹

Note: * are actual test values.

2. Human Health Risk Assessment Methods [39]

2.1. Calculation of exposure by different routes

(1) Oral route of soil ingestion

Carcinogenic risk formula:

$$OISER_{ca} = \frac{(\frac{OSIR_c \times ED_c \times EFC}{BW_c} + \frac{OSIR_a \times ED_a \times EFA}{BW_a}) \times ABS_o}{AT_{ca}} \times 10^{-6}$$

Non-cancer risk formula:

$$OISER_{nc} = \frac{OSIR_c \times ED_c \times EFC \times ABS_o}{BW_c \times AT_{nc}} \times 10^{-6}$$

(2) Dermal route of exposure to soil

Carcinogenic risk formula:

$$DCSER_{ca} = \frac{SAEC \times SSAR_c \times EFC \times ED_c \times Ev \times ABS_d}{BW_c \times AT_{ca}} \times 10^{-6} + \frac{SAEa \times SSAR_a \times EFA \times ED_a \times Ev \times ABS_d}{BW_a \times AT_{ca}} \times 10^{-6}$$

Carcinogenic risk formula:

$$DCSER_{nc} = \frac{SAEC \times SSAR_c \times EFC \times ED_c \times Ev \times ABS_d}{BW_c \times AT_{nc}} \times 10^{-6}$$

(3) Exposure routes for inhaled soil particles

Carcinogenic risk formula:

$$PISER_{ca} = \frac{PM_{10} \times DAIR_c \times ED_c \times PIAF \times (f_{spo} \times EFO_c + f_{spi} \times EFI_c)}{BW_c \times AT_{ca}} \times 10^{-6} + \frac{PM_{10} \times DAIR_a \times ED_a \times PIAF \times (f_{spo} \times EFO_a + f_{spi} \times EFI_a)}{BW_a \times AT_{ca}} \times 10^{-6}$$

Carcinogenic risk formula:

$$PISER_{nc} = \frac{PM_{10} \times DAIR_c \times ED_c \times PIAF \times (f_{spo} \times EFO_c + f_{spi} \times EFI_c)}{BW_c \times AT_{nc}} \times 10^{-6}$$

(4) Exposure pathways for volatile contaminants from inhalation of outdoor surface soils

Carcinogenic risk formula:

$$IOVER_{cal} = VF_{suroa} \times (\frac{DAIR_c \times EFO_c \times ED_c}{BW_c \times AT_{ca}} + \frac{DAIR_a \times EFO_a \times ED_a}{BW_a \times AT_{ca}})$$

Carcinogenic risk formula:

$$IOVER_{nc1} = VF_{suroa} \times \frac{DAIR_c \times EFO_c \times ED_c}{BW_c \times AT_{nc}}$$

Where: the subscript c represents children and a represents adults; $OISER_{ca}$, $DCSER_{ca}$, $PISER_{ca}$ and $IOVER_{cal}$ represent soil exposures from oral ingestion, dermal contact, inhalation of soil particulate matter, and inhalation of volatile contaminants in outdoor surface soil, respectively, $kg\ soil \cdot kg^{-1} \cdot weight \cdot d^{-1}$; ABS_o and ABS_d are absorption efficiency factors for oral and dermal uptake, respectively, dimensionless and taken as 1; CR_{ois} , CR_{dcs} and CR_{pis} represent carcinogenic risks from the oral soil ingestion pathway, dermal soil contact pathway, and inhalation of soil particulate matter pathway, dimensionless; C_{sur} is the contaminant content in topsoil, $\mu g \cdot g^{-1}$; SER is the percentage of exposed skin, dimensionless; $C(PM_{10})$ is the airborne PM mass concentration, $mg \cdot m^{-3}$, taken as the annual average mass concentration in the region in 2021, $0.062\ mg \cdot m^{-3}$.

2.2. Calculation of carcinogenicity risk and hazard quotient

CR= Exposure by exposure route $\times C_{\text{sur}} \times$ Carcinogenic Slope Factors or Factors by Exposure Pathway

HQ= Exposure by exposure route $\times C_{\text{sur}} /$ Reference dose by exposure route \times SAF

Where: CR is the carcinogenic risk of the contaminant; HQ is the hazard quotient of the contaminant; C_{sur} is the concentration of the contaminant in the surface soil, $\text{mg}\cdot\text{kg}^{-1}$; SAF is the reference dose partition coefficient for exposure to soil.

References

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