Supplementary Information (SI) for Environmental Science: Advances.

Utilizing PMF and Monte Carlo-based models to evaluate toxic metals enrichment pathways, sources, and public health risks in an unplanned urbanized dumpsite soil

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Supplementary Materials

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Table S1 Formulation and value-wise classification of soil enrichment and pollution indicators used in this study.

Pollution & Risk Indicators	Parameter Descriptions	Interpretation of Class Criteria
Geoaccumulation Index (I_{geo}) $I_{geo} = \log_2\left[\frac{C_n}{1.5 \text{ x } B_n}\right]$	C_n = Target HM concentration B_n = Corresponding Background value	Unpolluted ($I_{geo} \leq 0$) Unpolluted to moderately polluted ($0 < I_{geo} \leq 1$) Moderately polluted ($1 < I_{geo} \leq 2$) Moderately to heavily polluted ($2 < I_{geo} \leq 3$) Heavily polluted ($3 < I_{geo} \leq 4$) Heavily to extremely polluted ($4 < I_{geo} \leq 5$) Extremely polluted ($I_{geo} > 5$)
Enrichment Factor (EF) $EF = \frac{[C_n/C_{ref}]_{sample}}{[C_n/C_{ref}]_{background}}$	C_n = Target HM concentration C_{ref} = Reference HM concentration	Minimal enrichment (EF < 2) Moderate enrichment ($2 \leq EF < 5$) Significant enrichment ($5 \leq EF < 20$) Very high enrichment ($20 \leq EF < 40$) Extremely high enrichment ($EF \geq 40$)
Contamination Factor (CF) $CF = \frac{C_n}{B_n}$	C_n = Target HM concentration B_n = Corresponding Background value	Low contamination (CF < 1) Moderate contamination ($1 \leq CF < 3$) Considerable contamination ($3 \leq CF < 6$) Very high contamination ($CF \geq 6$)
Modified Degree of Contamination (mCd) $mC_d = \frac{\sum_{i=1}^{n} CF_i}{n}$	CF = Contamination Factor n = Number of HMs	Uncontaminated ($mC_d \leq 1.5$) Low contamination ($1.5 < mC_d \leq 2$) Moderate contamination ($2 < mC_d \leq 4$) High contamination ($4 < mC_d \leq 8$) Very high contamination ($8 < mC_d \leq 16$) Extremely high contamination ($16 < mC_d \leq 32$) Ultra-high contamination ($mC_d > 32$)
Pollution Load Index (PLI)	CF = Contamination Factor	No contamination (PLI < 1)

$PLI = \sqrt[n]{CF_1 \times CF_2 \times \ldots\ldots \times CF_n}$		Possible contamination ($PLI \geq 1$)
Nemerow Integrated Pollution Index (NIPI) $PI_i = \frac{C_i}{S_i}$ $NIPI = \sqrt{\frac{PI_{max}^2 + PI_{ave}^2}{2}}$	C_n = Target HM concentration S_i = Corresponding Background value	Uncontaminated ($NIPI < 0.5$) Uncontaminated to moderately contaminated ($0.5 \leq NIPI < 1$) Moderately contaminated ($1 \leq NIPI < 2$) Moderately to heavily contaminated ($2 \leq NIPI < 3$) Heavily contaminated ($3 \leq NIPI < 4$) Heavily to extremely contaminated ($4 \leq NIPI < 5$) Extremely contaminated ($NIPI \geq 5$)
Individual Ecological Risk (E_i) $E_i = \frac{T_i \times C_i}{B_i}$	T_i = Toxic-response factor for i-th HM (Cd=30, Cr=2, Cu=5, Mn=1, Ni=5, Pb=5, and Zn=1) C_i = Target HM concentration B_i = Corresponding Background value	Low risk ($E_i < 40$) Moderate risk ($40 \leq E_i < 80$) Considerable risk ($80 \leq E_i < 160$) High risk ($160 \leq E_i < 320$) Extremely high risk ($E_i \geq 320$)
Total Ecological Risk (ERI) $ERI = \sum E_i = \sum \left[\frac{T_i \times C_i}{B_i}\right]$	T_i = Toxic-response factor for i-th HM (Cd=30, Cr=2, Cu=5, Mn=1, Ni=5, Pb=5, and Zn=1) C_i = Target HM concentration B_i = Corresponding Background value	Low risk ($ERI < 150$) Moderate risk ($150 \leq ERI < 300$) Considerable risk ($300 \leq ERI < 600$) High risk ($600 \leq ERI < 1200$) Extremely high risk ($ERI \geq 1200$)

Table S2 Values of exposure parameters used in the carcinogenic and non-carcinogenic health risk assessment in the recent studies (Ferreira-Baptista & De Miguel, 2005; Huang et al., 2020; Karimian et al., 2021; Obiri-Nyarko et al., 2021; USEPA, 1989a, 2001; Wijngaarde et al., 2020).

Parameters	**Symbol**	**Units**	**Children**	**Adults**	**Distribution**
HM Concentration	HMC	mg/kg	-	-	Log-normal
Ingestion Rate	IGR	mg/day	200 ± 4.0	100 ± 1.7	Log-normal
Inhalation Rate	INR	m^3/day	10 ± 2.39	20 ± 1.27	Log-normal
Exposure Frequency	EF	day/year	250 (180, 365)	250 (180, 365)	Triangular
Exposure Duration	ED	year	6 ± 2.39	25 ± 2.74	Log-normal
Skin Adherence Factor	SAF	mg/cm^2/day	0.2	0.2	Point
Dermal Absorption Factor	ABS	unitless	0.001	0.001	Point
Exposed Skin Area	ESA	cm^2	2800 ± 1171	3300 ± 440	Log-normal
Particle Emission Factor	PEF	m^3/kg	$1.316x10^{-9}$	$1.316x10^{-9}$	Point
Average Body Weight	ABW	kg	15 ± 1.5	70 ± 10.71	Log-normal
Average Time (Non-Cancer)	AT_{nc}	day	ED x 365	ED x 365	Point
Average Time (Cancer)	AT_c	day	70 x 365	70 x 365	Point

Table S3 Values of reference dose (RfD) in mg/kg/day and cancer slope factor (CSF) in kg-day/mg used during health risk evaluation through different exposure routes. (Karimian et al., 2021; Li & Zhang, 2010; USEPA, 1989b)

HM	**RfD_{ing}**	**RfD_{der}**	**RfD_{inh}**	**CSF_{ing}**	**CSF_{der}**	**CSF_{inh}**
Cd	1.00E-03	1.00E-05	5.70E-05	3.80E-01	3.80E-01	6.30E+00
Co	2.00E-02	1.60E-02	5.71E-02	-	-	-
Cr	3.00E-03	6.00E-05	2.86E-05	5.00E-01	2.00E+00	4.20E+01
Cu	4.00E-02	1.20E-02	4.02E-02	-	-	-
Fe	7.00E-01	4.50E-02	2.20E-04	-	-	-
Mn	4.60E-02	1.84E-03	1.43E-05	-	-	-
Ni	2.00E-02	5.40E-03	2.06E-02	1.70E+00	4.25E+01	9.00E-01
Pb	1.40E-03	5.25E-05	3.52E-03	8.50E-03	8.50E-03	4.20E-02
Zn	3.00E-01	6.00E-02	3.00E-01	-	-	-

Table S4 Estimated ecological risk indices (E_i and ERI) for the studied HMs.

E_i							**ERI**
Cd	**Cr**	**Cu**	**Mn**	**Ni**	**Pb**	**Zn**	
421.1		21.4			12.8		460.9
4	0.64	5	0.44	1.71	8	2.66	4

Table S5 Summarized average daily dose (ADD) of HMs from the dumpsite soils for children and adults.

HM	Children			Adults		
	ADD_{ing}	**ADD_{der}**	**ADD_{inh}**	**ADD_{ing}**	**ADD_{der}**	**ADD_{inh}**
Cd	3.85E-05	1.46E-09	1.08E-07	4.12E-06	6.26E-10	2.72E-08
Co	5.73E-05	2.18E-09	1.61E-07	6.14E-06	9.33E-10	4.05E-08
Cr	2.66E-04	1.01E-08	7.44E-07	2.85E-05	4.32E-09	1.88E-07
Cu	1.76E-03	6.70E-08	4.94E-06	1.89E-04	2.87E-08	1.25E-06
Fe	9.43E-02	3.58E-06	2.64E-04	1.01E-02	1.54E-06	6.67E-05
Mn	3.38E-03	1.28E-07	9.47E-06	3.62E-04	5.50E-08	2.39E-06
Ni	2.13E-04	8.08E-09	5.96E-07	2.28E-05	3.46E-09	1.50E-07
Pb	4.71E-04	1.79E-08	1.32E-06	5.04E-05	7.66E-09	3.33E-07
Zn	2.31E-03	8.78E-08	6.47E-06	2.48E-04	3.76E-08	1.63E-06

Table S6 Summary of hazard quotients (HQ) caused by each HMs through three exposure pathways (ingestion, dermal contact, and inhalation) for dumpsite soils for both children and adults.

HM	Children			Adults		
	HQ_{ing}	HQ_{der}	HQ_{inh}	HQ_{ing}	HQ_{der}	HQ_{inh}
Cd	3.85E-02	1.46E-04	1.89E-03	4.12E-03	6.26E-05	4.77E-04
Co	2.87E-03	1.36E-07	2.81E-06	3.07E-04	5.83E-08	7.10E-07
Cr	8.85E-02	1.68E-04	2.60E-02	9.49E-03	7.21E-05	6.57E-03
Cu	4.41E-02	5.58E-06	1.23E-04	4.72E-03	2.39E-06	3.10E-05
Fe	1.35E-01	7.97E-05	1.20E+00	1.44E-02	3.41E-05	3.03E-01
Mn	7.35E-02	6.98E-05	6.62E-01	7.87E-03	2.99E-05	1.67E-01
Ni	1.06E-02	1.50E-06	2.89E-05	1.14E-03	6.41E-07	7.30E-06
Pb	3.36E-01	3.41E-04	3.74E-04	3.60E-02	1.46E-04	9.45E-05
Zn	7.71E-03	1.46E-06	2.16E-05	8.26E-04	6.27E-07	5.45E-06
$(\text{Children/Adult Ratio})_{\text{Ingestion}}$	9.34					
$(\text{Children/Adult Ratio})_{\text{Dermal}}$	2.33					
$(\text{Children/Adult Ration})_{\text{Inhalation}}$	1.54					

Table S7 Summary of cancer risk (CR) caused by each HMs through three exposure pathways (ingestion, dermal contact, and inhalation) for dumpsite soils for both children and adults.

HM	**Children**			**Adults**		
	CR_{ing}	**CR_{der}**	**CR_{inh}**	**CR_{ing}**	**CR_{der}**	**CR_{inh}**
Cd	1.25E-06	4.76E-11	5.82E-08	5.59E-07	8.50E-11	6.12E-08
Cr	1.14E-05	1.73E-09	2.68E-06	5.08E-06	3.09E-09	2.82E-06
Ni	3.10E-05	2.94E-08	4.59E-08	1.38E-05	5.26E-08	4.83E-08
Pb	3.43E-07	1.30E-11	4.74E-09	1.53E-07	2.33E-11	4.99E-09
$(\text{Children/Adult Ratio})_{\text{Ingestion}}$	2.25					
$(\text{Children/Adult Ratio})_{\text{Dermal}}$	0.56					
$(\text{Children/Adult Ration})_{\text{Inhalation}}$	0.95					

Table S8 Summary of sensitivity analysis indicating the contribution of each variable in the non-carcinogenic and carcinogenic risk from the Monte Carlo Simulation for both children and adults.

Explored	Non-carcinogenic Risk		Carcinogenic Risk	
Variables	Child	Adult	Child	Adult
ABW	-5.60%	-15.60%	-3.30%	-14.70%
ESA	41.30%	9.80%	0.20%	0.10%
ED	0.00%	0.00%	53.10%	8.40%
EF	13.00%	14.40%	7.30%	13.00%
IGR	0.00%	0.00%	0.00%	0.20%
INR	0.00%	0.00%	0.00%	0.00%
Cd	0.10%	0.10%	0.40%	0.60%
Co	0.00%	0.00%	-	-
Cr	4.00%	4.00%	8.00%	18.10%
Cu	0.10%	0.00%	-	-
Fe	23.80%	39.70%	-	-
Mn	12.00%	18.90%	-	-
Ni	0.00%	0.00%	27.70%	44.70%
Pb	3.80%	1.10%	0.00%	0.00%
Zn	0.00%	0.00%	-	-

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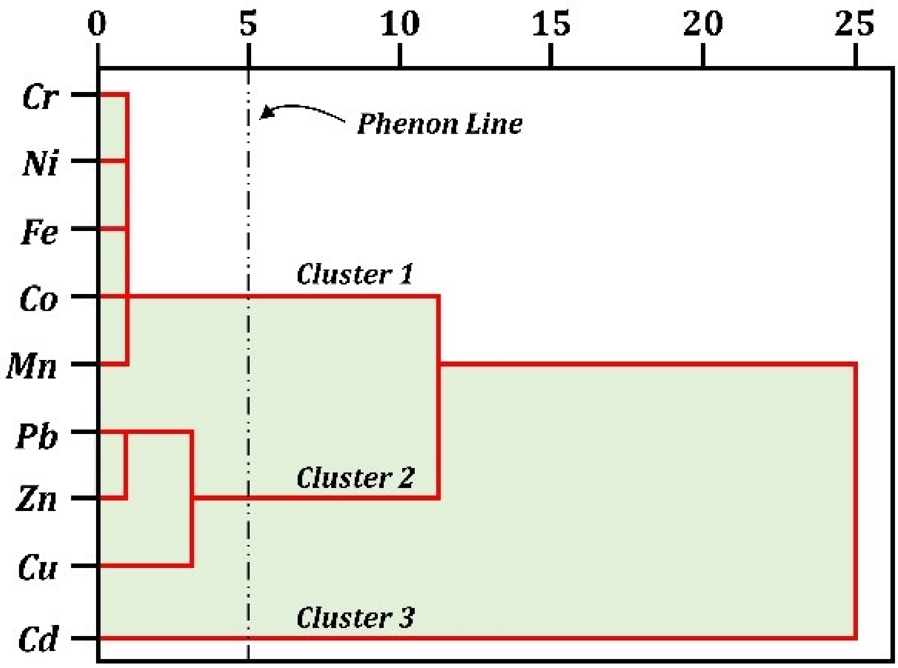

Fig. S1 Dendrogram illustrating hierarchical clustering of heavy metal concentrations in soils from the Dewanganj Dumpsite.

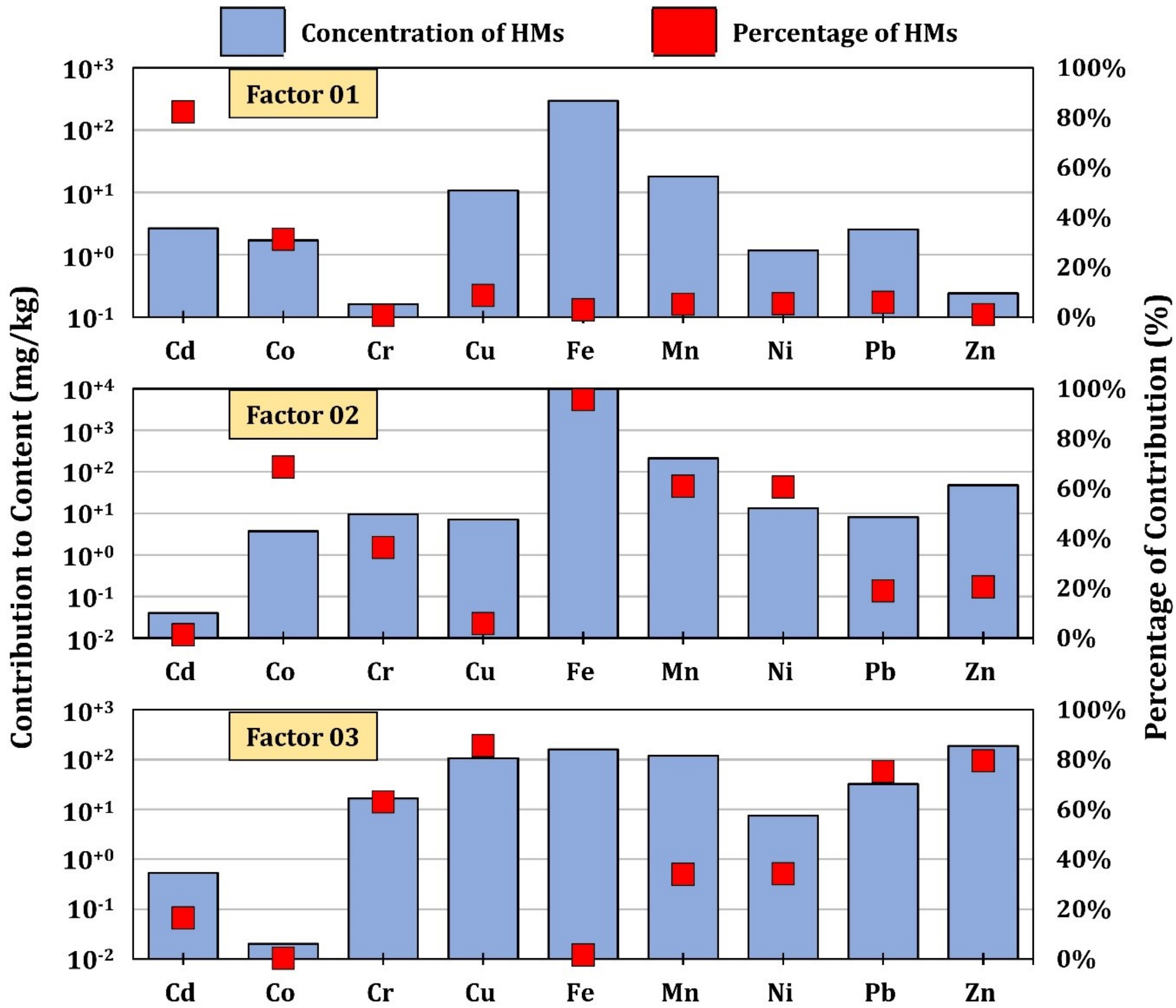

Fig. S2 Source profiles and contribution percentages of identified sources to heavy metal (HM) concentrations in dumpsite soil from the Positive Matrix Factorization (PMF) analysis.

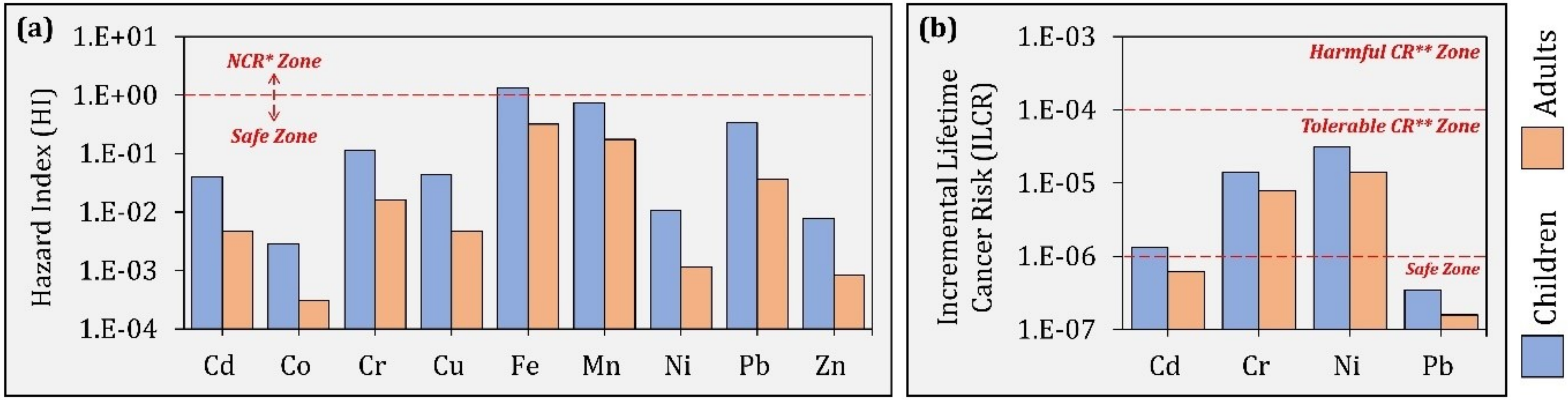

Fig. S3 Health risk assessment at Dewanganj dumpsite: (a) Hazard Index (HI) representing non-carcinogenic risk*, and (b) Incremental Lifetime Cancer Risk (ILCR) representing carcinogenic risk** due to heavy metal exposure.

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