

Supplementary Materials:

Impact of COVID-19 Lockdown on Inhaled Toxic Elements in PM_{2.5} in Beijing: Composition Characterization and Source-Specific Health Risks Assessment

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Table S1. Detailed descriptions of the sampling sites.

Sites	Longitude	Latitude	Functional zone	Descriptions
Beijing	116.41°E	40.04°N	Commercial, educational, and traffic areas	There are major arterial roads within 1000 meters, with a large traffic volume and serious vehicle exhaust emissions. There are schools, institutions, residents, etc. nearby.

Sample processing: Before sampling, the quartz filter was placed in a muffle furnace and fired at 600 °C for 2 h to remove residual carbon components and other impurities. The filters were equilibrated in a desiccator in a balance chamber for 48 h and then weighed using a one-per-million electronic balance (CP225D, Sartorius, Germany). The membranes were equilibrated in a constant temperature and humidity chamber at a temperature of (20 ± 2.5) °C and a relative humidity of (50 ± 5) % for 48 h before and after sampling, and the mass of the membranes was weighed using a one hundred thousandth analytical balance (Sartorius, Germany). Half of the membrane sample was cut out and placed in a 30 mL washed PTFE digestion jar, and the digestion solution (0.2 mL HF, 2 mL H₂O₂ and 6 mL HNO₃) was added, and the sample was pre-digested for 45 min at room temperature, and then microwaved according to the programmed temperature increase (the low temperature was increased to 120 °C for 3 min, and then the temperature was continuously increased to 170 °C for 10 min, and then increased to 190 °C for 50 min. The digest was transferred to a PET bottle, and the volume of ultrapure water was fixed to 100 ml. The samples were kept stationary and protected from light, to be measured.

Element analysis: Inductively coupled plasma mass spectrometry (ICP-MS, Agilent 7800, America) was used to determine the contents of 17 elements (Na, Mg, Al, K, Ca, Fe, V, Cr, Mn, Ni, Cu, Zn, As, Se, Cd, Ba, and Pb) in the samples. For analysis the elements, a blank film, parallel samples and standard samples were analyzed every 10 samples. The analysis of parallel samples needs to ensure that the relative error is less than 20%, and the recovery of standard samples is controlled between 80% and 120% to reduce the impact of errors on the experiment.

The OC and EC analysis: The NIOSH 5040 method is recommended by the National Institute of Occupational Safety and Health (NIOSH), a division of the U.S. Environmental Protection Agency (US EPA). A 1.5 cm² circular quartz filter was heated stepwise to temperatures of 140°C, 280°C, 480°C, and 580°C in a non-oxidizing helium (He) oven to analyze OC1, OC2, OC3, and OC4, respectively. Then, the oven was added to an oxidizing atmosphere of 2% oxygen (O₂) and 98% He, and the quartz filter membrane was gradually heated to 580°C, 740°C, and 840°C to analyze EC1, EC2, and EC3, respectively. The POC is defined as the carbon combusted after the initial introduction of oxygen and before the laser reflectance signal achieves its original value and the POC is specified as the fraction of OC. According to the

IMPROVE A protocol, OC is defined as OC1+OC2+OC3+OC4+POC, and EC is defined as EC1+EC2+EC3+POC. The method detection limits (MDLs) of OC and EC are 0.82 and 0.19 $\mu\text{g C}/\text{cm}^2$, respectively. For QA/QC, we carried out the measurements with the field blank filter membranes, standard sucrose solutions, and repeated analyses in the study. In order to ensure the precision of instrument, a replicate sample was analyzed for every ten samples, and the standard deviation $< \pm 5\%$ was accepted.

Table S2. Input data treatment from PMF analysis.

Table S2. Parameters summary for calculating average daily dose.

Parameter	Notation	Unit	Children	Adults
Exposure time	ET	$\text{h}\cdot\text{day}^{-1}$	24	24
Exposure frequency	EF	$\text{days}\cdot\text{year}^{-1}$	180	180
Exposure duration	ED	year	6	24
Average lifetime	ATn	hours	$\text{ED} \times 365 \times 24$	$\text{ED} \times 365 \times 24$
			(For non-carcinogens)	(For non-carcinogens)
			$70 \times 365 \times 24$	$70 \times 365 \times 24$
			(For carcinogens)	(For carcinogens)

There were 19 species in total resolved in PMF analysis, including 17 elements of Na, Mg, Al, K, Ca, Fe, V, Cr, Mn, Ni, Cu, Zn, As, Se, Cd, Ba, and Pb and 2 carbon components of OC and EC. The $\text{PM}_{2.5}$ concentration was also included as a fitting species.

The rationale is to decompose the sample composition dataset (X) into two matrices, namely source profile (F) and source contribution (G), expressed as follows:

$$X_{ij} = \sum_{k=1}^p g_{ik} f_{kj} + e_{ij}$$

where X_{ij} is the species concentration ($\mu\text{g}\cdot\text{m}^{-3}$) for the j th species in the i th sample; g_{ik} is the contribution from the k th source to the i th sample ($\mu\text{g}\cdot\text{m}^{-3}$); f_{kj} is a source section for the j th species from the k th source; e_{ij} is the residue level for the j th species in the i th sample; and p represents the number of sources.

The target feature Q was used to examine the distribution of each species and assess the stability of the solution, expressed as follows:

$$Q = \sum_{i=1}^n \sum_{j=1}^m \left[\frac{X_{ij} - \sum_{k=1}^p g_{ik} f_{kj}}{\mu_{ij}} \right]^2$$

where μ_{ij} denotes the uncertainty associated with the j th species in the i th sample.

To reduce impact of the inclusion of PM_{2.5} concentration on modelling, it was classified as the total variable with uncertainties set as 4 times of the concentration. In order to obtain the optimal result, signal-to-noise ratio (S/N) is applied to address weak and bad species when running PMF model. According to the EPA PMF v5.0 fundamentals and user guide, species are categorized as “Bad” if the S/N ratio is less than 0.5 and “Weak” if the S/N ratio is greater than 0.5 but less than 1.

The error fraction for elemental concentrations was set to 10 for uncertainty calculations.

Table S3. The RfC_i and IUR of inhaled health risks for eight selected toxic elements [1].

Parameter	RfC _i /(mg·m ⁻³)	IUR/((μg·m ⁻³) ⁻¹)
Pb	3.52E-03	1.20E-05
As	1.50E-05	4.30E-03
Cr	1.00E-04	8.40E-02
Ni	9.00E-05	2.60E-04
Cd	1.50E-05	1.80E-03
Se	2.00E-02	
Zn	3.01E-01	
Cu	4.02E-02	

Table S4. The method detection limits (MDLs) of chemical species resolved in PMF analysis.

Species	MDLs (μg·m ⁻³)	Species	MDLs (μg·m ⁻³)
OC	0.2985	Mn	5.56E-05
EC	0.0728	Ni	1.08E-04
Na	6.32E-03	Cu	1.35E-04
Mg	6.17E-04	Zn	2.65E-04
Al	1.35E-03	As	1.42E-03
K	5.92E-03	Se	1.54E-03
Ca	6.16E-02	Mo	2.53E-05
Fe	2.17E-03	Cd	2.53E-05
V	1.14E-03	Ba	7.25E-05
Cr	1.35E-04	Pb	1.52E-05

Table S5. The concentrations of selected toxic elements in PM_{2.5} at different cities worldwide.

City	Period	Toxic Elements (ng·m ⁻³)							
		Cr	Se	Ni	Cu	Zn	As	Cd	Pb
Tehran [2]	Dec 2016 to Feb 2017	70.0		32.0	340.0	190.0	60.0	34.0	190.0
Beijing [3]	14 Nov to 31 Dec 2016	8.2		4.2	40.6	407.0	8.3	1.4	71.0
Taiwan [4]	Dec 2013 to Feb 2014	2.8	1.5	2.6	7.1	42.6	9.1	0.3	19.0
Baoding [5]	Jan to Dec 2015	33.5	12.2	6.2			33.3	5.9	262.2
Nanjing [6]	2 to 10 Dec 2013	37.0		26.0	129.0	798.0	26.0	8.9	407.0
Gwangju [7]	1 to 8 Feb 2011	9.0	8.0	6.0	23.0	130.0	17.0	6.0	130.0
Agra [8]	7 Dec 2015 to 29 Jan 2016	354.0		67.0	210.0	758.0	35.0	26.0	670.0
Taiyuan [9]	26 Nov to 31 Dec 2016	100.1		36.4	90.1	467.4	4.1	9.2	457.7

Shijiazhuang [10]	15 Oct 2018 to 31 Jan 2019	10.9	8.7	51.9	213.5	17.7	1.8	60.9	
Linfen [11]	29 October 2019 to 30 March 2020	3.3	5.7	49.8	194.7	56.4	1.8	74.5	
This study (Beijing)	2 Jan 2020 to 28 Feb 2020	7.2	6.9	2.2	53.8	150.2	6.6	0.7	48.7

Table S6. The materials used for producing fireworks [12].

Name	Chemical formula	Role	Characteristic
Potassium nitrate	KNO ₃	to produce purple sparks	Melting point: 334 °C Boiling Point: 400 °C
Potassium	KClO ₄	oxidant	Melting point: 610 °C Solubility in 20°C water: 1.5 g/100 mL
Potassium chlorate	KClO ₃	oxidant	Melting point: 356 °C Solubility in 20°C water: 1 g/16.5 mL
Barium nitrate	Ba(NO ₃) ₂	to produce green sparks	Melting point: 590 °C Solubility in 20°C water: 9.02g/100mL
Potassium dichromate	K ₂ Cr ₂ O ₇	oxidant	Melting point: 398°C Boiling Point: 500°C
Potassium Permanganate	KMnO ₄	oxidant	Melting point: 240°C SW: 6.38 g/100 mL
Copper (II) oxide	CuO	to produce blue sparks, or serve as oxidant	Melting point: 1326°C
Copper carbonate basic	Cu ₂ (OH) ₂ CO ₃	to produce blue sparks	Melting point: 220°C
Aluminum	Al	serve as luminescence agent or deoxidizer, or to produce tracer bullets	Melting point: 660°C
magnesium powder	Mg	to produce white sparks, or serve as luminescence agent and deoxidizer	
Aluminium-magnesium alloy powder	Mg ₄ Al ₃	luminescence agent and deoxidizer	

Table S7. The non-carcinogenic (HQ) and carcinogenic risks (CR) in adults and children during the whole sampling period. (The adult non-carcinogenic risk was consistent with that of children.).

Toxic elements	HQ in Beijing	CR in Beijing	
	Adults (Children)	Adults	Children
	During the whole sampling period		
As	2.18E-01	4.81E-06	1.20E-06
Cd	2.41E-02	2.23E-07	5.57E-08
Pb	6.82E-03	9.87E-08	2.47E-08
Cr (VI)	5.09E-03	1.47E-05	3.67E-06
Ni	1.19E-02	9.53E-08	2.38E-08
Se	1.69E-04		
Zn	2.46E-04		
Cu	5.99E-04		

Total	2.70E-01	1.99E-05	4.98E-06
During the pre-lockdown			
As	1.75E-01	3.86E-06	9.66E-07
Cd	2.30E-02	2.13E-07	5.33E-08
Pb	7.27E-03	1.05E-07	2.63E-08
Cr (VI)	3.43E-03	9.89E-06	2.47E-06
Ni	1.32E-02	1.06E-07	2.66E-08
Se	1.55E-04		
Zn	2.76E-04		
Cu	3.01E-04		
Total	2.20E-01	1.42E-05	3.54E-06
During the full lockdown			
As	1.98E-01	4.39E-06	1.10E-06
Cd	2.15E-02	1.99E-07	4.98E-08
Pb	6.30E-03	9.12E-08	2.28E-08
Cr (VI)	8.46E-03	2.44E-05	6.09E-06
Ni	1.06E-02	8.50E-08	2.12E-08
Se	2.01E-04		
Zn	2.29E-04		
Cu	1.35E-03		
Total	2.50E-01	2.91E-05	7.28E-06
During the partial lockdown			
As	3.29E-01	7.28E-06	1.82E-06
Cd	2.96E-02	2.74E-07	6.86E-08
Pb	6.62E-03	9.58E-08	2.40E-08
Cr (VI)	3.83E-03	1.10E-05	2.76E-06
Ni	1.09E-02	8.77E-08	2.19E-08
Se	1.55E-04		
Zn	2.11E-04		
Cu	1.78E-04		
Total	3.80E-01	1.88E-05	4.69E-06

Table S8. The non-carcinogenic risk of toxic elements from emission sources for children and adults during the sampling period and different COVID-19 lockdown periods in Beijing (the adult non-carcinogenic risk was consistent with that of children). (BB & FB: biomass burning and fireworks; DE: dust emissions; CC: coal combustion; IE: industrial emissions; TE: traffic emissions).

Periods	Sources	Se	Cd	Pb	Zn	As	Cu	Ni	Cr (VI)	Total
Sampling period	BB & FB	0.00E+00	5.68E-05	0.00E+00	3.83E-06	1.87E-03	1.70E-04	3.88E-04	4.74E-04	2.96E-03
	DE	0.00E+00	1.31E-03	5.47E-04	1.91E-05	2.14E-02	1.77E-05	2.68E-03	7.91E-04	2.68E-02
	CC	6.45E-05	3.10E-03	1.70E-03	5.05E-05	6.18E-02	4.27E-05	1.34E-03	2.86E-04	6.84E-02
	IE	5.27E-05	7.95E-03	1.84E-03	3.73E-05	2.02E-02	3.45E-05	1.98E-03	1.95E-03	3.40E-02
	TE	1.70E-05	5.84E-03	2.27E-03	9.91E-05	1.84E-02	3.97E-05	1.25E-03	2.28E-04	2.82E-02
Pre-lockdown	BB & FB	0.00E+00	6.12E-06	0.00E+00	4.13E-07	2.01E-04	1.84E-05	4.18E-05	5.11E-05	3.19E-04
	DE	0.00E+00	1.36E-03	5.68E-04	1.98E-05	2.23E-02	1.84E-05	2.78E-03	8.22E-04	2.78E-02

	CC	6.68E-05	3.21E-03	1.76E-03	5.23E-05	6.40E-02	4.42E-05	1.39E-03	2.96E-04	7.08E-02
	IE	4.61E-05	6.96E-03	1.61E-03	3.27E-05	1.77E-02	3.02E-05	1.73E-03	1.71E-03	2.98E-02
	TE	2.04E-05	7.01E-03	2.73E-03	1.19E-04	2.21E-02	4.77E-05	1.51E-03	2.74E-04	3.38E-02
Full lockdown	BB & FB	0.00E+00	1.86E-04	0.00E+00	1.25E-05	6.10E-03	5.56E-04	1.27E-03	1.55E-03	9.67E-03
	DE	0.00E+00	1.60E-03	6.67E-04	2.33E-05	2.62E-02	2.16E-05	3.27E-03	9.65E-04	3.27E-02
	CC	8.18E-05	3.93E-03	2.15E-03	6.40E-05	7.83E-02	5.41E-05	1.70E-03	3.62E-04	8.67E-02
	IE	4.15E-05	6.26E-03	1.45E-03	2.94E-05	1.59E-02	2.71E-05	1.56E-03	1.54E-03	2.68E-02
	TE	1.34E-05	4.60E-03	1.79E-03	7.81E-05	1.45E-02	3.13E-05	9.88E-04	1.80E-04	2.22E-02
Partial lockdown	BB & FB	0.00E+00	1.03E-06	0.00E+00	6.95E-08	3.39E-05	3.09E-06	7.04E-06	8.60E-06	5.37E-05
	DE	0.00E+00	1.00E-03	4.18E-04	1.46E-05	1.64E-02	1.35E-05	2.05E-03	6.05E-04	2.05E-02
	CC	4.72E-05	2.27E-03	1.24E-03	3.69E-05	4.52E-02	3.12E-05	9.81E-04	2.09E-04	5.00E-02
	IE	6.36E-05	9.60E-03	2.22E-03	4.51E-05	2.43E-02	4.16E-05	2.39E-03	2.36E-03	4.11E-02
	TE	1.61E-05	5.55E-03	2.16E-03	9.41E-05	1.75E-02	3.77E-05	1.19E-03	2.17E-04	2.68E-02

Table S9. The carcinogenic risk of toxic elements from emission sources for children during the sampling period and different COVID-19 lockdown periods in Beijing. (BB & FB: biomass burning and fireworks; DE: dust emissions; CC: coal combustion; IE: industrial emissions; TE: traffic emissions).

Periods	Sources	Cd	Pb	As	Ni	Cr (VI)	Total
Sampling period	BB & FB	1.32E-10	0.00E+00	1.03E-08	7.78E-10	3.41E-07	3.52E-07
	DE	3.03E-09	1.98E-09	1.19E-07	5.37E-09	5.70E-07	6.98E-07
	CC	7.17E-09	6.14E-09	3.42E-07	2.69E-09	2.06E-07	5.63E-07
	IE	1.84E-08	6.65E-09	1.11E-07	3.97E-09	1.41E-06	1.55E-06
	TE	1.35E-08	8.23E-09	1.02E-07	2.51E-09	1.64E-07	2.91E-07
Pre-lockdown	BB & FB	1.42E-11	0.00E+00	1.11E-09	8.39E-11	3.68E-08	3.80E-08
	DE	3.15E-09	2.06E-09	1.23E-07	5.58E-09	5.92E-07	7.26E-07
	CC	7.43E-09	6.36E-09	3.54E-07	2.79E-09	2.13E-07	5.84E-07
	IE	1.61E-08	5.82E-09	9.76E-08	3.48E-09	1.23E-06	1.36E-06
	TE	1.62E-08	9.88E-09	1.22E-07	3.02E-09	1.97E-07	3.49E-07
Full lockdown	BB & FB	4.30E-10	0.00E+00	3.37E-08	2.54E-09	1.11E-06	1.15E-06
	DE	3.69E-09	2.41E-09	1.45E-07	6.55E-09	6.95E-07	8.52E-07
	CC	9.09E-09	7.78E-09	4.33E-07	3.41E-09	2.61E-07	7.14E-07
	IE	1.45E-08	5.24E-09	8.78E-08	3.13E-09	1.11E-06	1.22E-06
	TE	1.06E-08	6.49E-09	8.03E-08	1.98E-09	1.29E-07	2.29E-07
Partial lockdown	BB & FB	2.39E-12	0.00E+00	1.87E-10	1.41E-11	6.19E-09	6.40E-09
	DE	2.31E-09	1.51E-09	9.06E-08	4.11E-09	4.35E-07	5.34E-07
	CC	5.25E-09	4.49E-09	2.50E-07	1.97E-09	1.51E-07	4.12E-07
	IE	2.22E-08	8.03E-09	1.35E-07	4.80E-09	1.70E-06	1.87E-06
	TE	1.28E-08	7.82E-09	9.68E-08	2.39E-09	1.56E-07	2.76E-07

Table S10. The carcinogenic risk of toxic elements from emission sources for adults during the sampling period and different COVID-19 lockdown periods in Beijing. (BB & FB: biomass burning and fireworks; DE: dust emissions; CC: coal combustion; IE: industrial emissions; TE: traffic emissions).

Periods	Sources	Cd	Pb	As	Ni	Cr (VI)	Total
Sampling period	BB & FB	5.26E-10	0.00E+00	4.13E-08	3.11E-09	1.36E-06	1.41E-06
	DE	1.21E-08	7.92E-09	4.74E-07	2.15E-08	2.28E-06	2.79E-06
	CC	2.87E-08	2.46E-08	1.37E-06	1.08E-08	8.23E-07	2.25E-06
	IE	7.36E-08	2.66E-08	4.46E-07	1.59E-08	5.63E-06	6.19E-06
	TE	5.41E-08	3.29E-08	4.08E-07	1.01E-08	6.57E-07	1.16E-06
Pre-lockdown	BB & FB	5.67E-11	0.00E+00	4.45E-09	3.35E-10	1.47E-07	1.52E-07
	DE	1.26E-08	8.22E-09	4.92E-07	2.23E-08	2.37E-06	2.90E-06
	CC	2.97E-08	2.54E-08	1.42E-06	1.11E-08	8.53E-07	2.33E-06
	IE	6.44E-08	2.33E-08	3.90E-07	1.39E-08	4.93E-06	5.42E-06
	TE	6.49E-08	3.95E-08	4.90E-07	1.21E-08	7.89E-07	1.40E-06
Full lockdown	BB & FB	1.72E-09	0.00E+00	1.35E-07	1.02E-08	4.46E-06	4.61E-06
	DE	1.48E-08	9.66E-09	5.78E-07	2.62E-08	2.78E-06	3.41E-06
	CC	3.64E-08	3.11E-08	1.73E-06	1.36E-08	1.04E-06	2.86E-06
	IE	5.80E-08	2.09E-08	3.51E-07	1.25E-08	4.43E-06	4.88E-06
	TE	4.26E-08	2.59E-08	3.21E-07	7.92E-09	5.18E-07	9.15E-07
Partial lockdown	BB & FB	9.55E-12	0.00E+00	7.49E-10	5.65E-11	2.48E-08	2.56E-08
	DE	9.26E-09	6.05E-09	3.62E-07	1.64E-08	1.74E-06	2.14E-06
	CC	2.10E-08	1.80E-08	1.00E-06	7.87E-09	6.02E-07	1.65E-06
	IE	8.89E-08	3.21E-08	5.38E-07	1.92E-08	6.80E-06	7.47E-06
	TE	5.13E-08	3.13E-08	3.87E-07	9.55E-09	6.24E-07	1.10E-06

Figures



Figure S1. Map of the sampling site in Beijing.

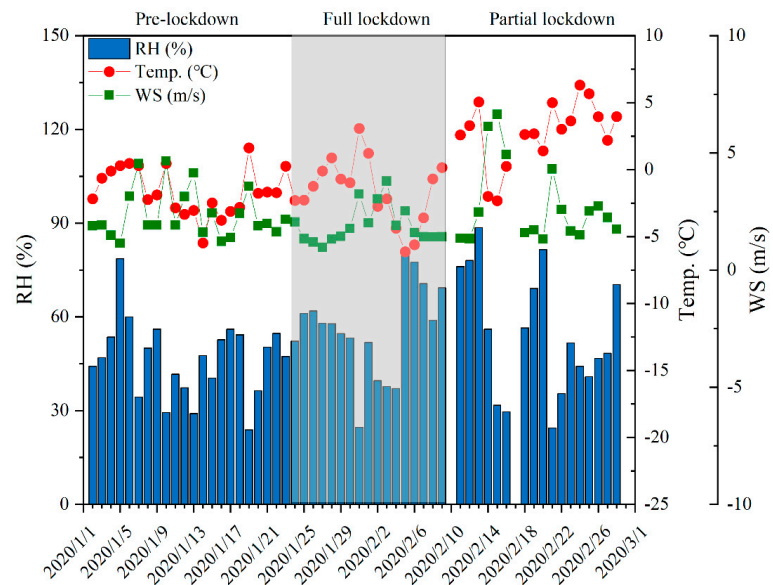


Figure S2. Time series of wind speed (WS), temperature and relatively humidity (RH) during sampling period in Beijing.

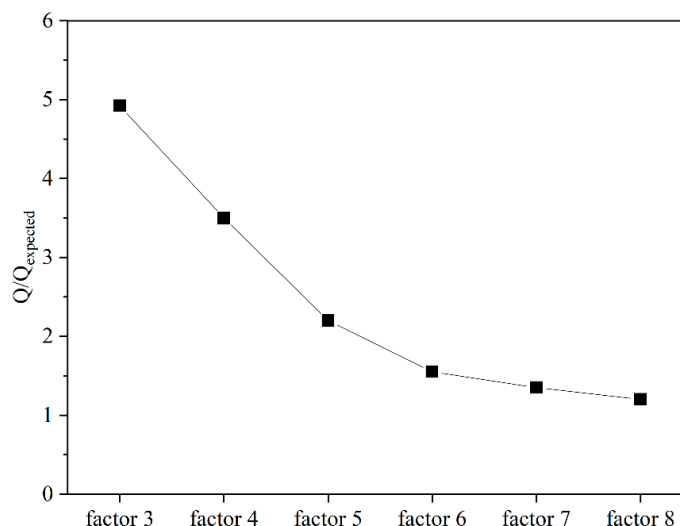


Figure S3. The Q/Q_{expected} values and relative contribution of emission sources to $\text{PM}_{2.5}$ -bound element mass resolved by PMF model under the different factor numbers

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