Measurement report: Impact of domestic heating on dust deposition sources in hyper-arid Qaidam Basin, northern Qinghai-Xizang Plateau

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26 pages of Supporting Information

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Supporting Text

PMF Source apportionment initialization

The source apportionment of dust deposition utilized the EPA PMF 5.0 model to analyze 109 samples based on their respective sampling sites. Internal PMF parameters, such as Q_{robust}, Q_{true}, and Q_{expected} were considered to assess performance of PMF. In general, Q is a measure of the fitness of the model; Q_{robust} is calculated using only samples that fit the model well, while all samples are used in calculating Q_{true}. Q_{expected} is equal to the number of samples multiplied by the number of strong species. Multiple iterations of each dataset were processed to identify consistent Q values. Testing for factor peak values across 3 to 6 factors revealed that 4 factors provided the best solution for XZH, LTC, and BLX, while 5 factors were optimal for GEM, NMH, and DLX (Figure S14). High determination coefficients (R² = 0.64~0.98) indicated a strong correlation between calculated and measured element fluxes, with intercepts and slopes nearing unity. The analysis found no need for factor rotation, and the Q_{robust} values closely aligned with the Q_{true}, suggesting a good model fit. Bootstrapping was not used because of the small size of the sample set. High uncertainties were observed in the contribution of certain species to each factor, but each factor contained at least one well-constrained species, highlighting the dominant chemical characteristic of that factor. These high uncertainties stem, in part, from the high and variable values of field blanks that are carried through the model. Rotational swaps, indicating uncertainty in the identified components and their contributions, were not observed during displacement, and the largest change in Q was -0.01%, evidencing the good fit of the solution set.

A theoretical Q-value (also referred to Q_{exp}) may be approximated as a number of points in the data matrix minus the total number of elements in the factor matrices (Paatero and Tapper, 1994)

$$Q_{\exp} = n \cdot m - N \cdot (n+m), \tag{1}$$

where n is the number of samples, m is the number of species and N is the number of obtained factors. Large deviation from the $Q_{\rm exp}$ may indicate that a larger extra modeling uncertainty is needed. The optimal number of factors was determined based on the variation in the $Q_{\rm robust}/Q_{\rm exp}$ ratio and the interpretability of the analytical factor distribution. In our study, the $Q_{\rm true}/Q_{\rm robust}$ ratios for the PMF models at all six monitoring stations were below 1.5, indicating that the simulation results are reasonable. Additionally, the $Q_{\rm robust}/Q_{\rm exp}$ ratio confirms that our simulated results align

with the optimal number of factors.

Error estimates of the base PMF solution are provided through combination of Displacement (DISP) and Bootstrap (BS) tests (DISP-BS). Displacement test explores the rotational ambiguity of the solution by assessing the largest range of source profiles without significant increase in the Q value. DISP%dQ is the parameter displaying in the displacement result matrix. If DISP%dQ is equal to zero that means the displacement analysis result is considered as acceptable. The displacement swap counts (DISP swaps) are a key indicator of the stability of a PMF solution. If it swaps it indicates that there is significant rotational ambiguity and that the solution is not sufficiently robust to be used. Error estimates of the base solution are provided through combination of both Displacement (DISP), and Bootstrap (BS) tests (DISP-BS) (Manousakas et al., 2017).

BS detects disproportionate effects of a small set of observations on the solution and also, to a lesser extent, effects of rotational ambiguity. Mapping of bootstrap factors to base factors is a summary result on factors mapping. Ideally BS factor mapping should be one-to-one with respect to base run factors. Nevertheless, factors with more than 80% mapping are considered acceptable. Base random seed is the seed number corresponding to the result with minimum Q and allows reproducing the same results of PMF solution.

In our study, the decline in DISP%dQ remained consistently within 0.1%, indicating that the global minima of dQ were achieved under the tested configurations. Throughout the four dQmax levels, no factor switching occurred during the DISP run phase, and the factor matching rate during the BS phase exceeded 85%. Additionally, there was no factor switching in the BS-DISP run phase. These findings underscore the stability of the PMF model results (Paatero et al., 2014; Brown et al., 2015; Li, 2020).

Reference

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Supporting Tables

Stations	Latitude (°)	Longitude (°)	Description		
XZH	93.67964745	36.79841344	Lycium berry cultivation base,		
			national climate benchmark station		
GEM	94.90930080	36.42121338	The largest city in the Qaidam Basin,		
			with a high population		
LTC	95.77349782	36.49093842	Desert with camel breeding farms		
NMH	96.42957687	36.44058390	Towns with extensive <i>Lycium</i> berry		
			cultivation in the surrounding areas		
BLX	97.53657818	36.16438395	Pasture with developed agricultural		
			practices		
DLX	98.09684336	36.29662699	County seat with a relatively large		
			population and a thriving mining		
			industry		

Table S1 Geographic coordinates and descriptions of monitoring stations in the study area.

The table lists the latitude and longitude of each site, along with a brief description of the local characteristics and land use. [XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station].

	Rural-HP	Rural-NHP	Urban-HP	Urban-NHP	
Qexp	160	157	111	195	
Qrobust	908.43	813.39	462.26	1429.10	
Qtrue	1131.91	1095.23	463.26	1811.90	
Q_{true}/Q_{robust}	1.25	1.35	1.00	1.27	
$Q_{robust}\!/Q_{exp}$	5.68	5.18	4.16	7.33	
Converged	Yes	Yes	Yes	Yes	
DISP % dQ	<0.1%	<0.1%	<0.1%	<0.1%	
DISP % swaps	0%	0%	0%	0%	
$\mathrm{BS}\mathrm{R}^2$	0.6	0.6	0.6	0.6	
BS mapping	93%	94%	89%	88%	
BS-DISP %swaps	0%	0%	0%	0%	
Extra modeling					
uncertainty	0%	0%	0%	0%	

Table S2 Summary of PMF and error estimate diagnostics

City	Country	Element				P. C	
		Cd	Cr	Cu	Pb	Zn	Reference
Guangzhou	China	1.00-7.44	28.3-121	52.7-261	39.2-123	245-1007	Cai et al., 2013
37:1	China	4.18±1.20	195.92±	125.31±	310.29±	721.20±	Cl 1 2017
Xi'an			48.66	78.80	80.79	237.57	Chen et al., 2017
Suzhou	China	0.25-26.9	11.9-110	13.2-	30.5-	47.6-4290	Ma et al., 2016
				1200	2240		
Changsha	China	9.11	80.7	43.9	66.6	215	Li et al., 2016
Beijing	China	0.130-5.01	32.0-227	5.46-623	16.7- 2450	57.4-908	Wei et al., 2015
Tianjin	China	0.22-1.38	30.9-225	20.7-188	20.6-156	-	Yu et al., 2014
Huainan	China	0.110- 0.449	40.5-129	19.1-87.5	21.2-71.5	_	Tang et al., 2017
C1 1 :	China	0.36-4.72	18.0-	17.0-	28.0-	82-2140	Shi et al., 2008
Shanghai			1325	1175	4443		
I Imama ai	China	0.44-2.40	24.85-	27.13-	4.56-	208.65-	W-: -t -1 2015
Urumqi			102.67	105.54	63.46	2375.97	Wei et al., 2015
Lanzhou	China	0.102-3.21	18.8-135	33.6-151	8.42-61.0	41.5-109	Jiang et al., 2018
Jinan		0.90-3.96	35.17-	27.15-	46.14-	115-1645	Pang et al., 2014
			3126.00	156.60	235.20		
Galicia	Spain	0.08-0.89	35.4-	5.8-58.7	0.87-	30.7-543.3	Franco-Uria et al.,
Gancia			82.92		271.9		2009
Alexandria	Egypt	0.33	24.3	79.7	70.3	169	Dat et al., 2021
Ho Chi Minh City,	Vietnam	0.5	102.4	153.7	49.6	466.4	Jadoon et al., 2021
Cantabria region	Spain	0.1	5.2	11.8	4.5	183	Fernandez-Olmo et al., 2015
Junggar Basin	China	16.65	605.5	100.1	-	5933.9	Yang et al., 2016
Ebinur	China	0.004-0.48	58.15-	15.12-	11.14-	26.25-	Abuduwailil et al.,
Basin			169.25	62.27	124.17	227.51	2015
	China	0.003-5.17	0.04-64.8	0-34.6	0-121.2	0.64-257.7	This study

Table S3 Comparison of dust-fall metal concentrations in this study with those from other regions

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Supporting Figures



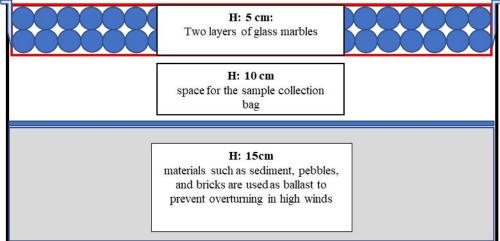


Figure S1. (a) Photo and (b) schematic of dust samples sampling device. The device is a stainless steel box measuring 50 cm in length, 30 cm in width, and 30 cm in height, consisting of three layers. The first layer, 5 cm deep, contains two layers of φ16 mm glass beads with a specific density. The second layer, 10 cm high, contains high-density polyethylene bags for dust collection. The third layer, 15 cm high, is constructed from sand pebble brick material to ensure equipment stability.

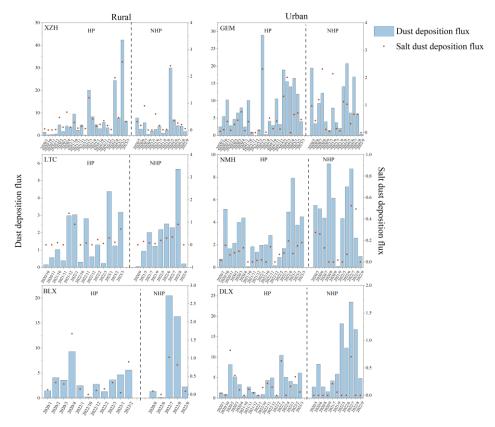


Figure S2 Temporal variation of atmospheric dust (DF) and salt dust deposition flux (SDF) at six stations during heating and non-heating periods. DF represented by blue bars and SDF by red circles. [HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station]

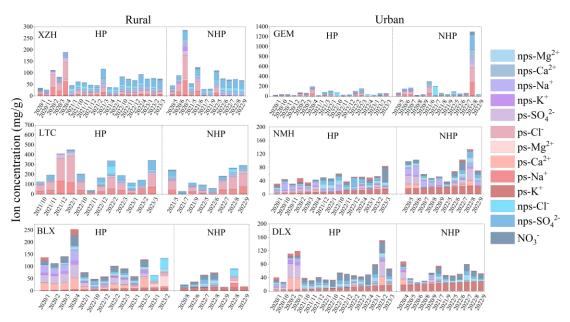
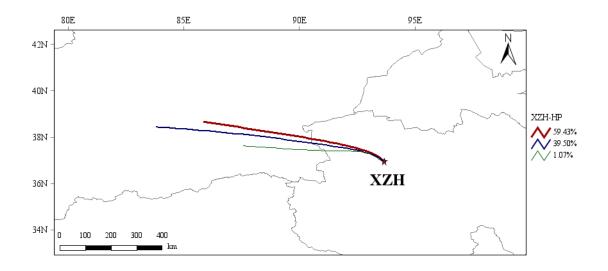
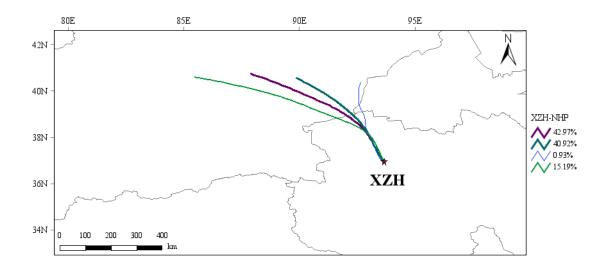
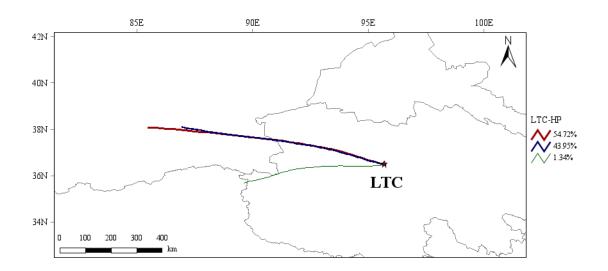


Figure S3 Temporal variations in ion concentrations at six monitoring sites during heating and non-heating periods. HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station







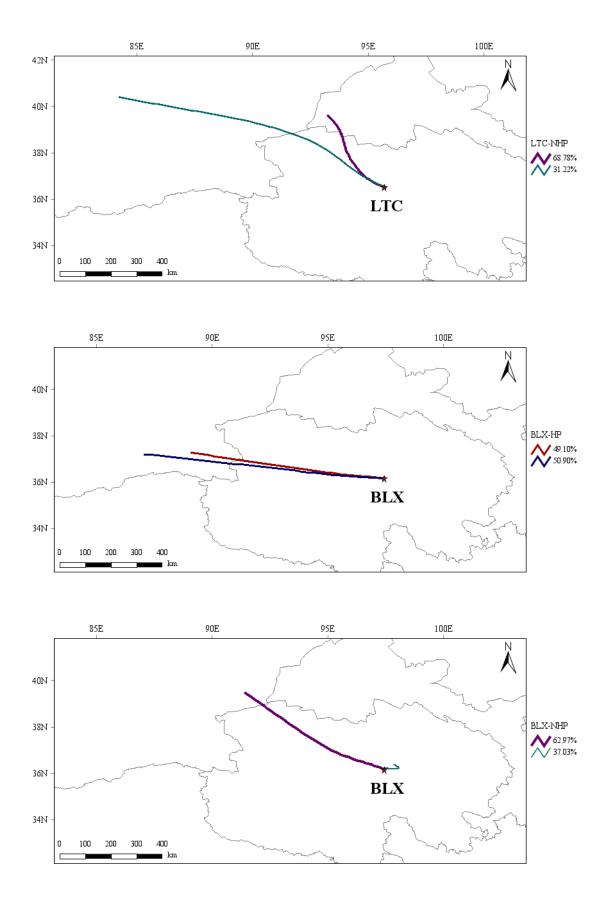
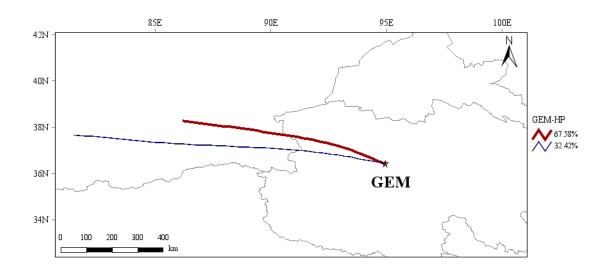
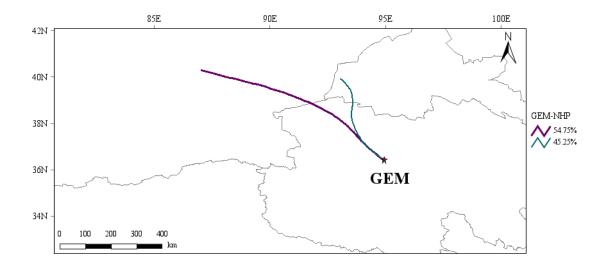
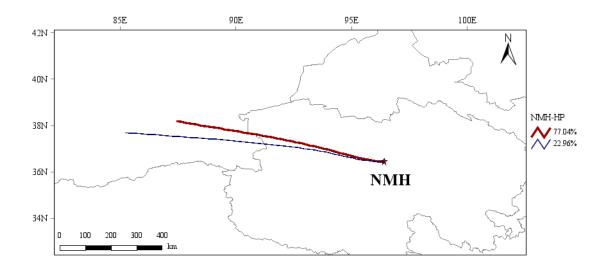


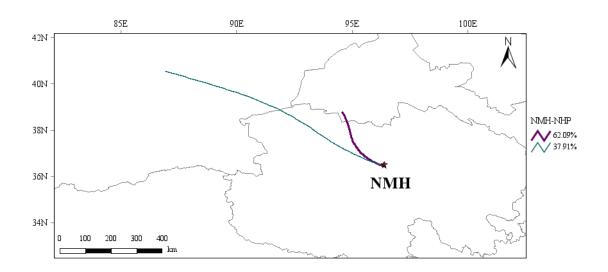
Figure S4 Backward trajectory simulations were conducted at rural monitoring stations during heating and non-heating periods. Different colors denote distinct trajectory paths, while

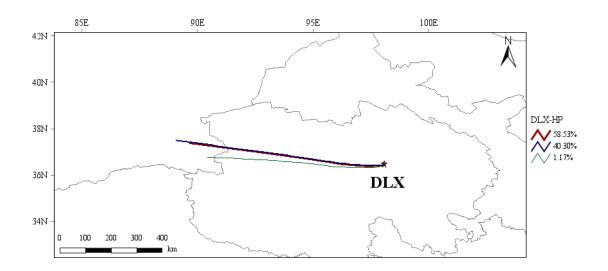
line thickness indicates the degree of contribution from each path. The red star marks the location of the stations. [HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; LTC, Da Gele station; BLX, Balong station].











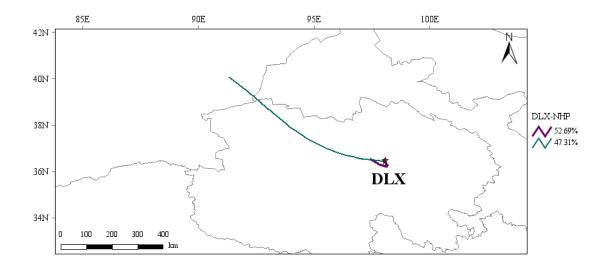


Figure S5 Backward trajectory simulations were conducted at urban monitoring stations during heating and non-heating periods. Different colors denote distinct trajectory paths, while line thickness indicates the degree of contribution from each path. The red star marks the location of the stations. [HP, Heating period; NHP, Non-heating period; GEM, Golmud station; NMH, Nuo Muhong station; DLX, Dulan station].

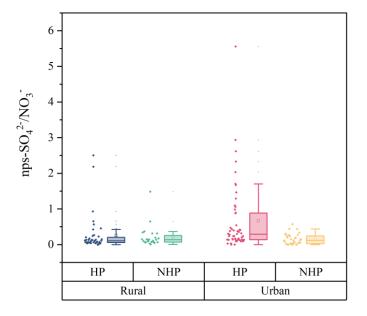


Figure S6 The ratio of nps-SO₄²⁻ to NO₃⁻ in soluble ions during heating and non-heating periods in rural and urban areas. HP: heating period; NHP: non-heating period.

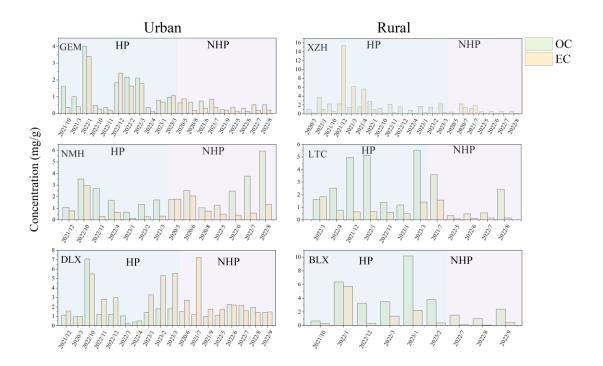


Figure S7 Temporal variations in organic (OC) and element carbon (EC) concentration at six monitoring sites during heating and non-heating periods. HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station

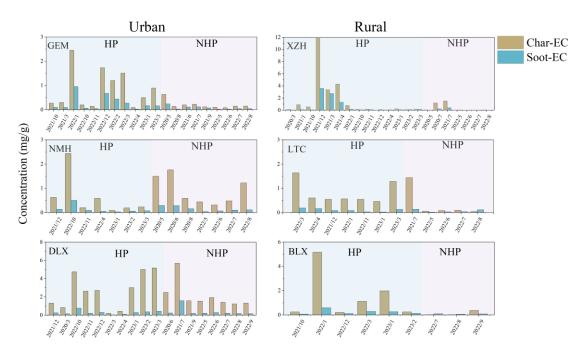


Figure S8 Temporal variations in Char-OC and Soot-EC concentration at six monitoring sites during heating and non-heating periods. HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station

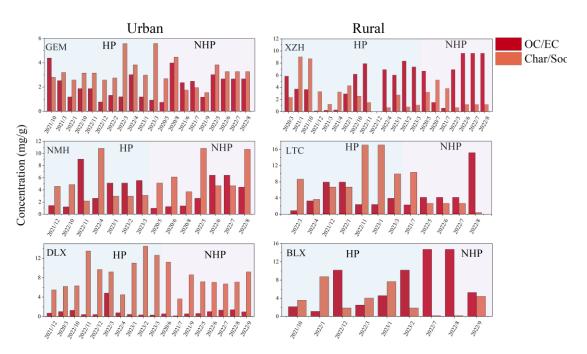


Figure S9 Temporal variations in OC/EC and Char/Soot ratio at six monitoring sites during heating and non-heating periods. HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station

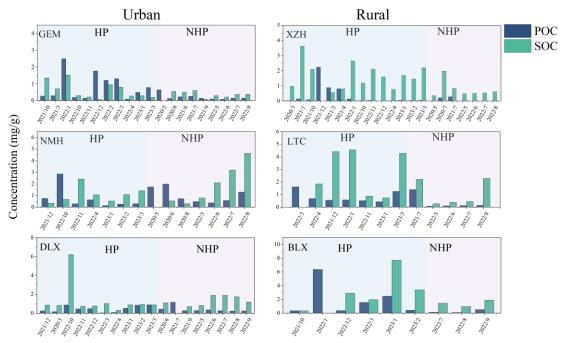


Figure S10 Temporal variations in primary (POC) and secondary organic carbon (SOC) concentration at six monitoring sites during heating and non-heating periods. HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station

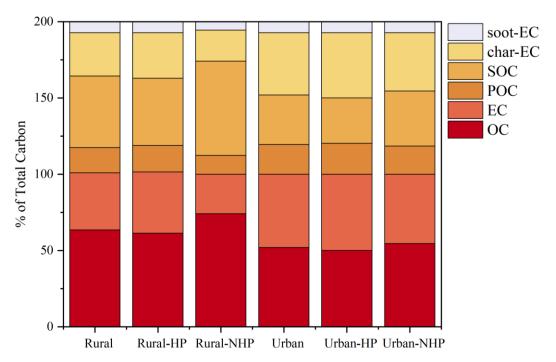


Figure S11 Proportions of various carbon indicators in urban and rural during heating and non-heating periods. HP, Heating period; NHP, Non-heating period.

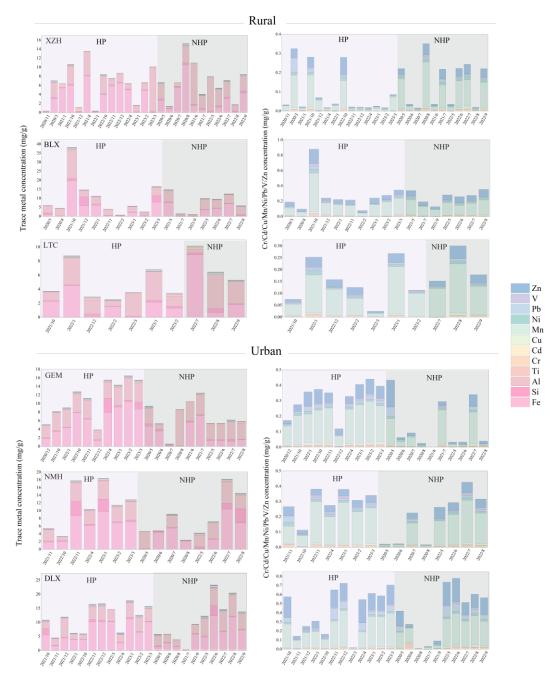
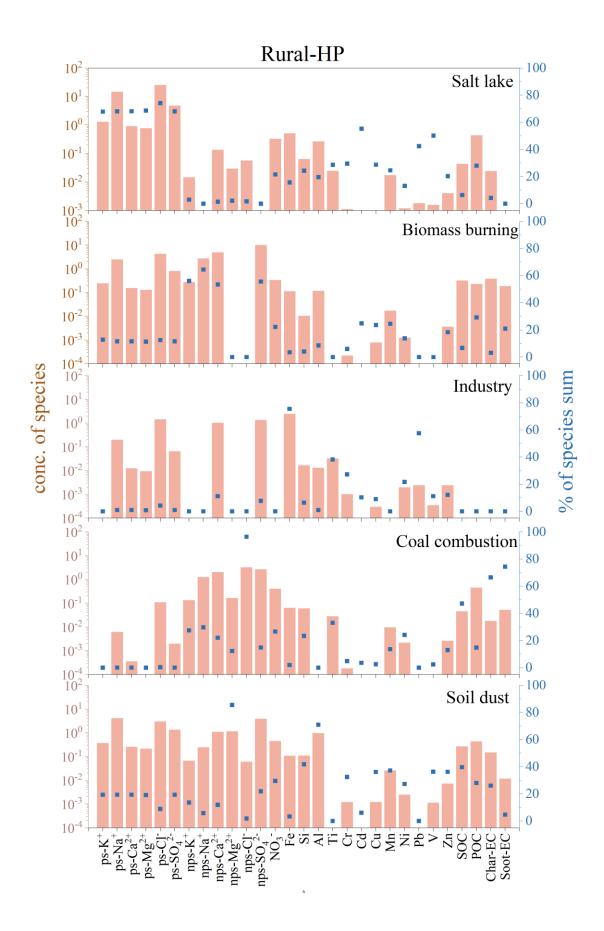
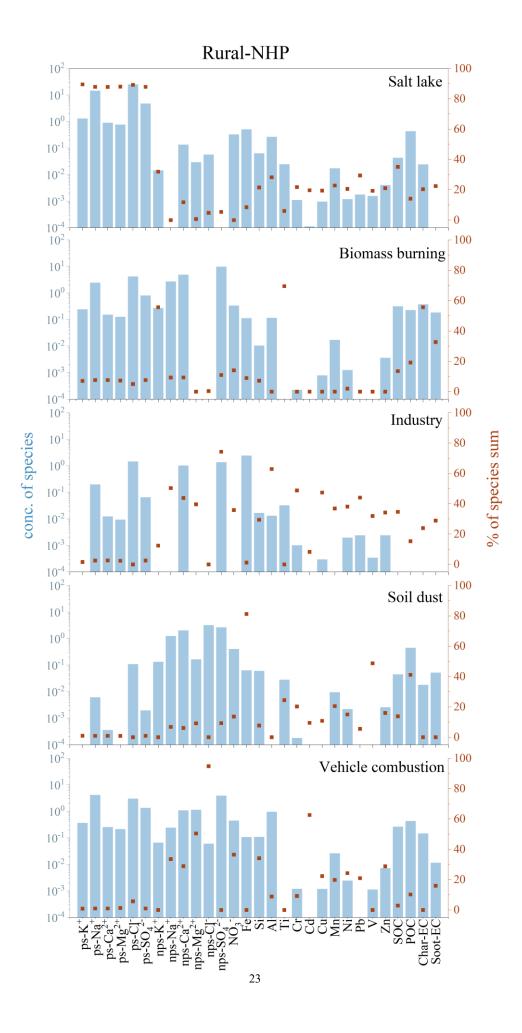
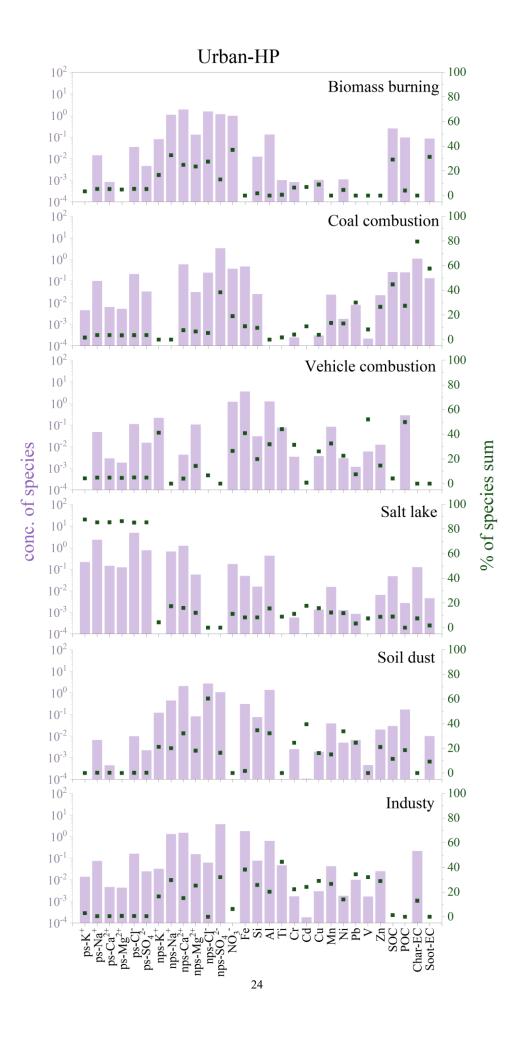


Figure S12 Temporal variations in trace element content at six monitoring sites during heating and non-heating periods. The left panels display trace element concentrations (mg/g) for each site, while the right panels illustrate the smaller concentrations of Cr, Cd, Cu, Mn, Ni, Pb, V, Zn. [HP, Heating period; NHP, Non-heating period; XZH, Xiao Zaohuo station; GEM, Golmud station; LTC, Da Gele station; NMH, Nuo Muhong station; BLX, Balong station; DLX, Dulan station]







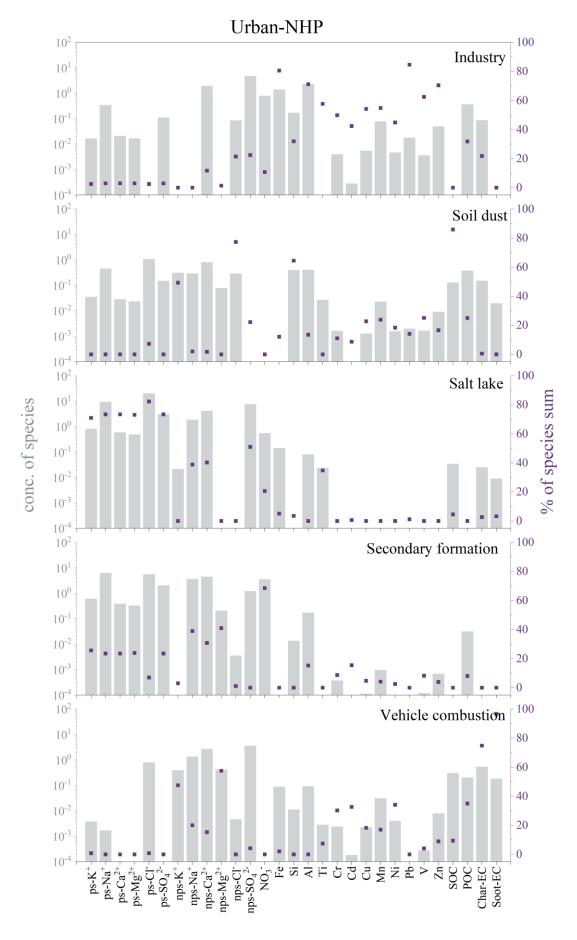


Figure S13 Species profiles and contributions of each resolved source for rural and urban areas during heating and non-heating periods, as determined through PMF dust-fall source apportionment. Contribution of species are presented in a histogram, while the species profile is depicted in a scatter plot. [HP, heating period; NHP non-heating period].