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Source apportionment of fine organic carbon at an urban site of Beijing using a chemical mass balance model

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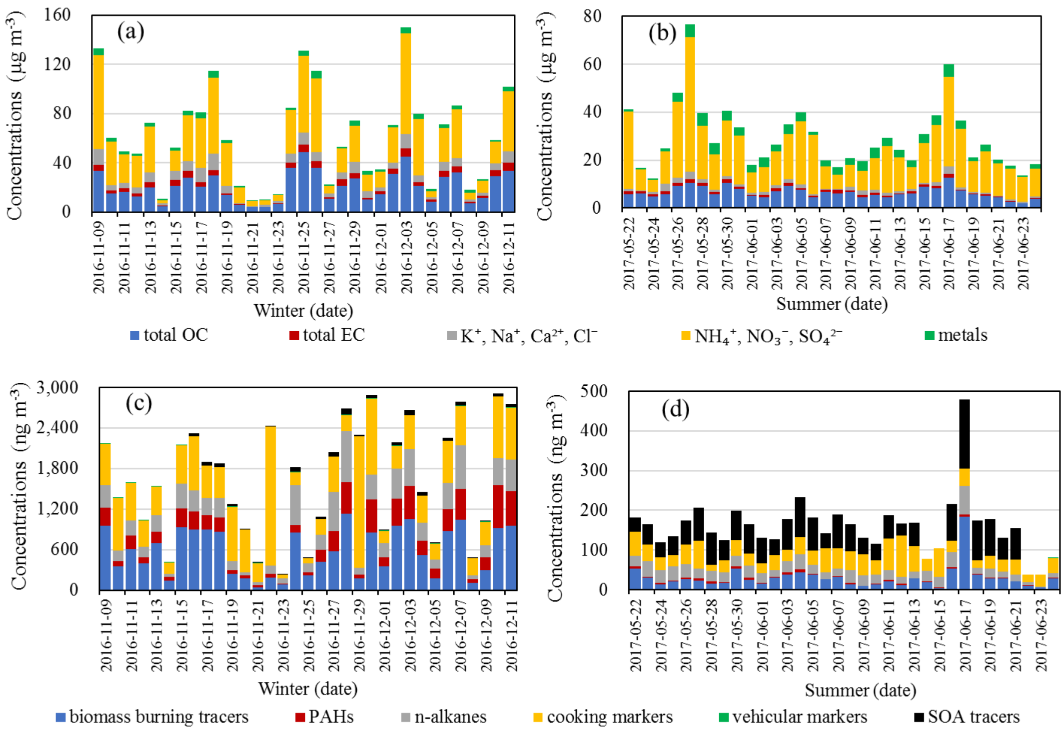

Figure S1. Stacked bar plots of the concentrations of $PM_{2.5}$ components. **Abbreviations:** OC: organic carbon; EC: elemental carbon; PAH: polycyclic aromatic hydrocarbon; SOA: secondary organic aerosol. “Metals” is the summed concentrations of Al, Ti, V, Cr, Mn, Fe, Co, Ni, Cu, Zn, Cd, Sr, Sb, Sn, Ba, Pb; “PAH” is the summed concentrations of phenanthrene, anthracene, fluoranthene, acenaphthylne, acenaphthene, fluorene, pyrene, benzo(a)anthracene, chrysene, benzo(b)fluorene, benzo(b)fluoranthene, benzo(k)fluoranthene, benzo(a)pyrene, benzo(e)pyrene, perylene, indeno(1,2,3-cd)pyrene, dibenzo(a,h)anthracene, benzo(ghi)perylene, coronene, picence and retene; “n-alkane” is the summed concentrations of C24, C25, C26, C27, C28, C29, C30, C31, C32, C33, C34; “cooking markers” is the summed concentrations of palmitic acid, stearic acid, cholesterol; “vehicle markers” is the summed concentrations of 17a(H)-22,29,30-trisnorhopane and 17b(H),21a(H)-norhopane; “SOA” is the summed concentrations of 2-methylthreitol, 2-methylerythritol, 2-methylglyceric acid, cis-2-methyl-1,3,4-trihydroxy-1-butene, 3-methyl-2,3,4-trihydroxy-1-butene, trans-2-methyl-1,3,4-trihydroxy-1-butene, 3-hydroxyglutaric acid(3-HGA), Pinic acid, Pinonic acid, C5-alkene triols, 2-methyltetrols, 3- MBTCA (3-Methyl-1,2,3-butanetricarboxylic Acid), beta-caryophyllinic acid, 3-acetylpentanedioic acid, 3-acetylhexanedioic acid, 3-isopropylpentanedioic acid, DHOPA (2,3-dihydroxy-4-oxopentanoic acid) and 3-Hydroxy-4,4-dimethylglutaric acid.

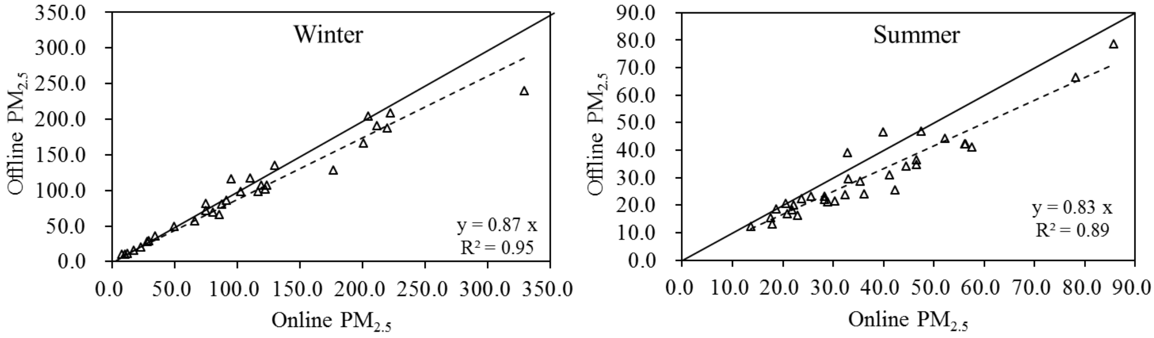

Figure S2. Regression analysis of gravimetrically measured $PM_{2.5}$ (offline $PM_{2.5}$) and online $PM_{2.5}$ in winter and summer at IAP, Beijing

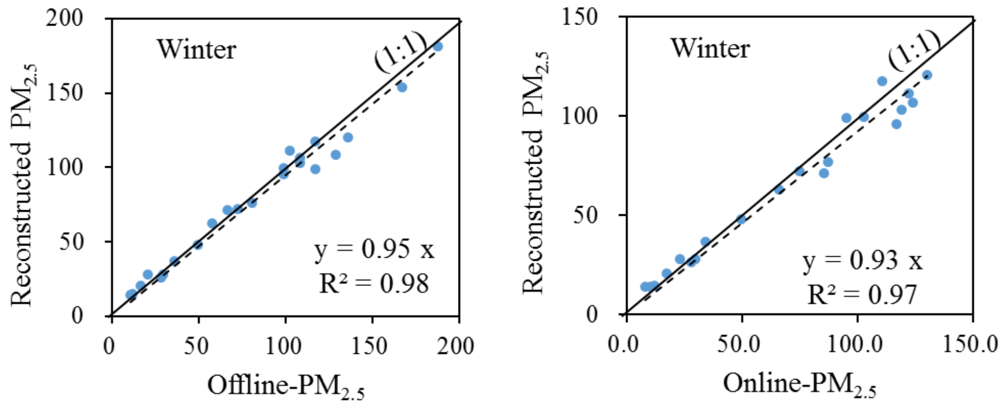

Figure S3. Regression results between reconstructed $PM_{2.5}$ and offline/online $PM_{2.5}$ by chemical mass closure method in winter excluding outliers.

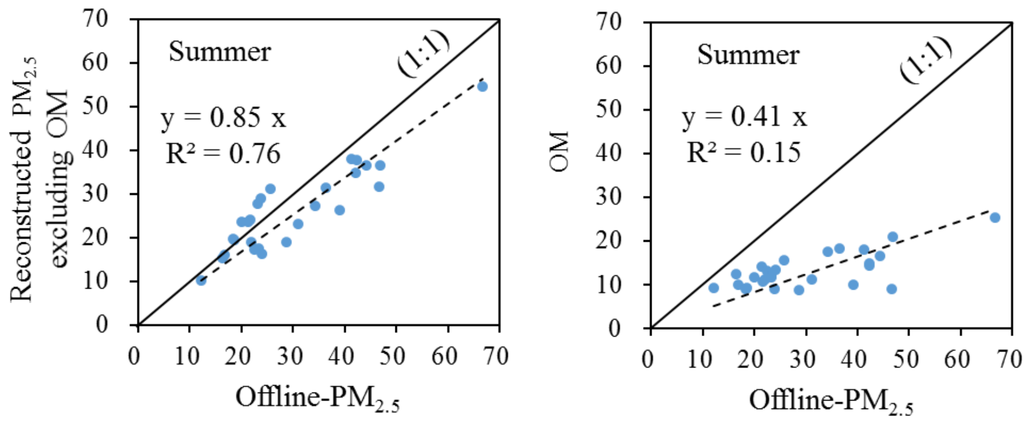

Figure S4. Regression results between inorganics (reconstructed $PM_{2.5}$ excluding OM) and OM with offline-$PM_{2.5}$ by chemical mass closure method in winter excluding outliers.

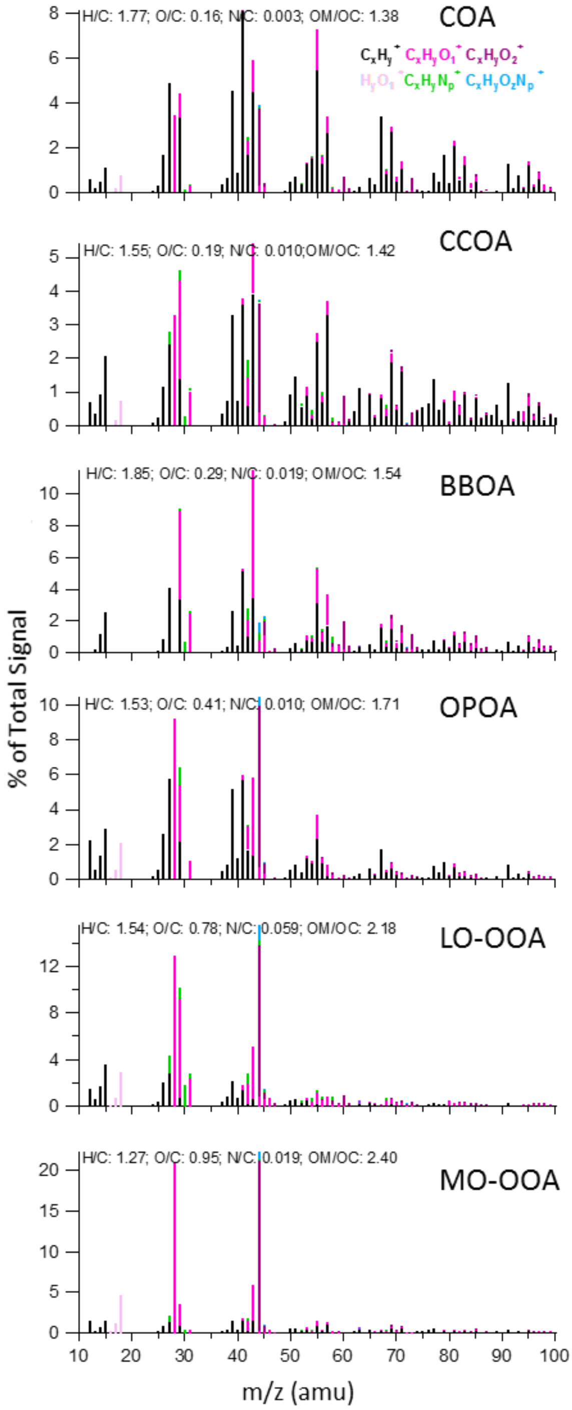

Figure S5. Source profiles of AMS-PMF factors in winter

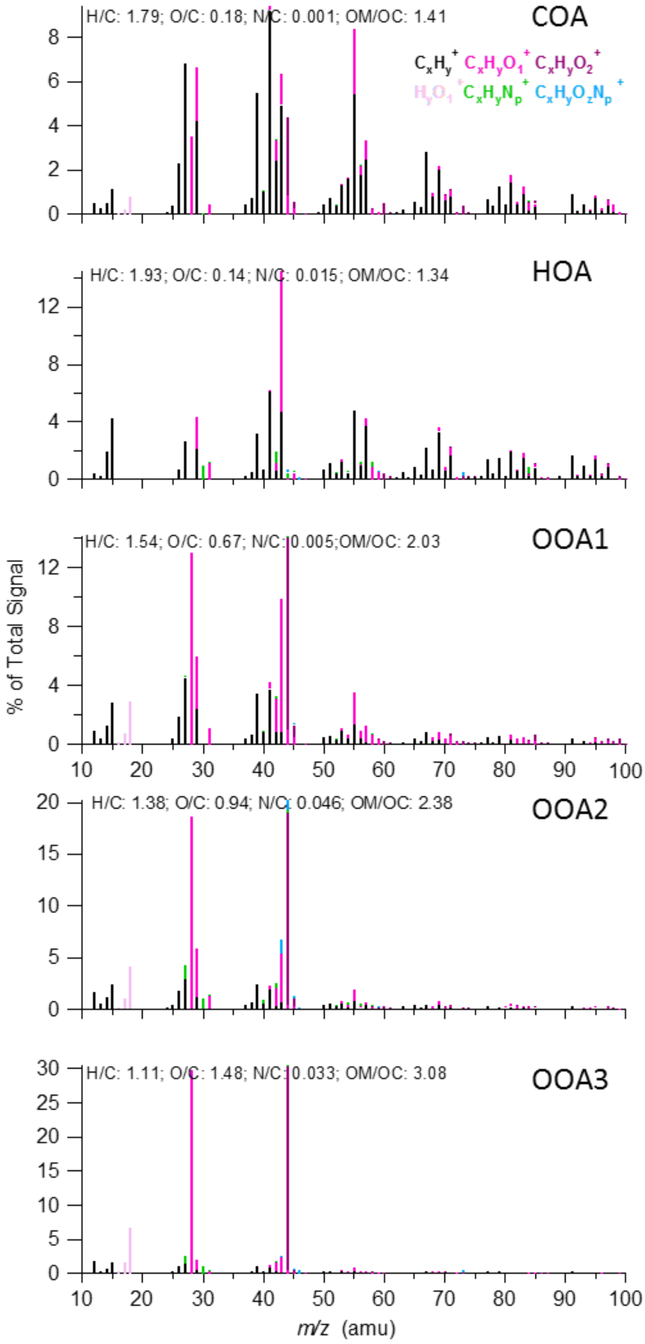

Figure S6. Source profiles of AMS-PMF factors in summer

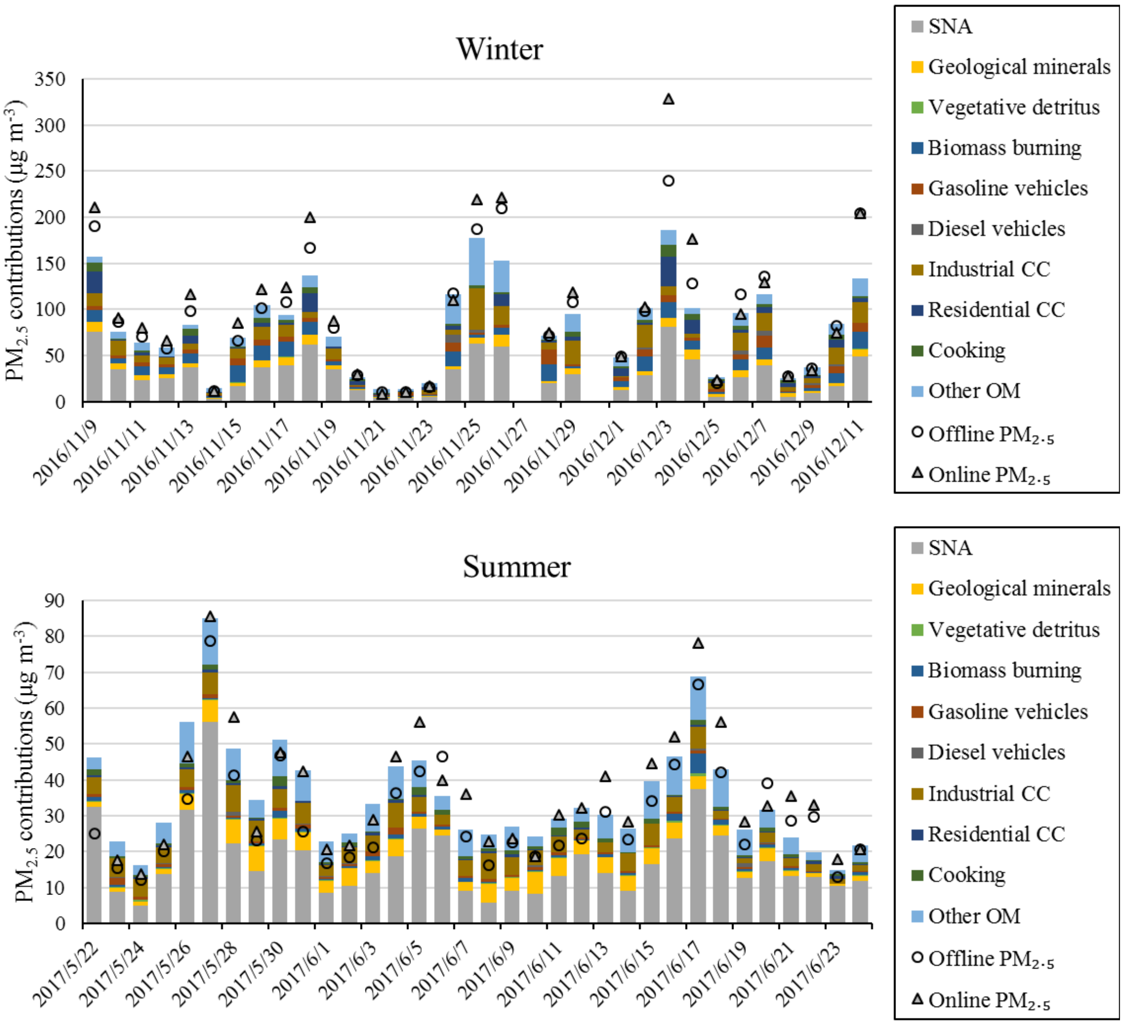

Figure S7. Daily $PM_{2.5}$ source contribution estimates from the CMB model

Table S1. Concentrations (mean±SD (min-max), μg m^{-3}) of chemical components in $PM_{2.5}$ by applying chemical mass closure method

Component	Winter	Summer
NO_3^-	12.49±9.38 (0.87-34.63)	7.16±4.94 (1.53-26.12)
SO_4^{2-}	8.53±7.05 (1.27-24.21)	6.87±3.96 (1.96-19.48)
NH_4^+	8.24±5.63 (0.50-22.62)	3.62±3.14 (0.08-14.83)
Cl^-	3.80±2.32 (0.00-8.73)	0.47±0.42 (0.12-1.96)
K^+	1.30±1.01 (0.15-3.80)	0.37±0.35 (0.11-2.05)
Na^+	0.42±0.24 (0.09-0.93)	0.20±0.16 (0.03-0.73)
Geological minerals	5.33±3.25 (1.03-12.72)	3.52±1.79 (0.65-6.99)
Total other elements	0.53±0.35 (0.12-1.29)	0.35±0.20 (0.07-1.00)
EC	3.5±2.0 (0.3-6.6)	0.9±0.4 (0.2-1.7)
OM	37.7±21.5 (6.9-85.4)	12.9±4.7 (3.6-25.4)
Bound water-Offline	4.0±3.7 (0.2-13.4)	2.8±1.4 (0.8-7.3)
Reconstructed $PM_{2.5}$-Offline	83.4±53.6 (14.0-202.1)	39.4±13.0 (19.6-80.0)
Offline $PM_{2.5}$	88.6±63.6 (10.3-239.9)	30.0±12.7 (12.2-66.7)
Bound water-Online	4.5±4.1 (0.3-14.9)	3.5±1.8 (0.9-9.1)
Reconstructed $PM_{2.5}$-Online	83.8±53.9 (14.0-203.7)	40.1±13.4 (19.8-81.8)
Online $PM_{2.5}$	99.7±79.1 (8.1-328.7)	36.4±14.9 (13.7-78.1)

Note: 5 samples in winter and 7 samples in summer were not included for the calculation of bound water and reconstructed $PM_{2.5}$ due to insufficient ions and NH_3 data. These samples were excluded for the calculation of average online and offline $PM_{2.5}$ in this table as well for better comparison.

Table S2. Annual average primary OC emissions (Unit: tonne) in Beijing from the 2016 and 2017 Multi-resolution Emission Inventory for China (MEIC)

Sector	Fuel	2016	2017
Power	Coal	0	0
Power	Oil	0	0
Power	Natural Gas	0	0
Industry	Coal	0	0
Industry	Oil	538	583
Industry	Natural Gas	0	0
Industry	Process	1161	1083
Residential	Coal	6687	4312
Residential	Oil	24	23
Residential	Natural Gas	0	0
Residential	Biofuel	5548	4993
Transportation	Oil	1059	1026
Total		15017	12020

Table S3. Comparison of the source contribution estimates (SCE in μg m^{-3} (%OC)) at IAP with those at a rural site in Beijing- Pinggu

	IAP (Urban) (This study)		Pinggu (Rural)	
	Winter (31 days)	Summer (34 days)	Winter (14 days)	Summer (6 days)
OC	21.5±12.3	6.4±2.3	36.5±29.3	10.7±4.9
OC explained	75.7±11.0%	56.1±11.3%	69.1±7.1%	63.4±12.6%
Vegetative detritus	0.1±0.1 (0.5±0.4%)	0.1±0.1 (1.7±0.8%)	1.5±3.0 (2.8±3.4%)	0.3±0.3 (2.1±1.4%)
Biomass burning	3.8±2.6 (17.4±8.7%)	0.3±0.4 (4.8±3.4%)	6.8±5.6 (18.1±3.4%)	1.1±0.6 (10.7±2.6%)
Gasoline	2.0±1.6 (10.2±6.6%)	0.3±0.2 (4.9±2.2%)	1.0±0.9 (3.4±1.6%)	0.1±0.0 (1.3±0.6%)
Diesel	0.5±1.2 (1.9±3.7%)	0.1±0.2 (1.2±2.5%)	6.2±6.0 (13.7±6.0%)	0.6±0.3 (6.2±4.8%)
Industrial CC	4.9±4.1 (22.0±11.2%)	1.8±0.7 (29.0±9.0%)	3.2±2.6 (10.2±5.7%)	3.8±2.5 (34.1±11.0%)
Residential CC	2.6±3.1 (12.5±10.2%)	0.2±0.1 (3.3±3.5%)	5.7±4.3 (19.0±12.4%)	0.4±0.2 (4.2±1.8%)
Cooking	2.2±2.1 (10.6±7.3%)	0.7±0.4 (11.1±7.1%)	0.5±0.5 (2.0±2.3%)	0.5±0.4 (4.9±3.9%)
Other OC	5.3±4.9 (24.8±12.1%)	2.9±1.5 (43.9±11.4%)	11.7±10.4 (30.9±7.1%)	3.9±2.3 (36.6±12.6%)

Table S4. The ratios of OC/$PM_{2.5}$ (or OM/OC) for different sources

	OC/$PM_{2.5}$	Reference
Straw burning	0.546	(Zhang et al., 2007)
Wood burning	0.3	(Wang et al., 2009)
Cooking	1.4 (OM/OC)	(Zhao et al., 2007)
Light-duty gasoline cars	0.317	
Heavy-duty gasoline cars	0.549	(Cai et al., 2017)
Diesel cars	0.569	
Vegetative detritus	2.1 (OM/OC)	(Bae et al., 2006b)
Anthracite	0.446	
Bituminite	0.403	(Zhang et al., 2008)
Coal briquette	0.432	
Secondary organic aerosol	2.17 (OM/OC)	(Bae et al., 2006a)
Oxygenated OA	2.2 (OM/OC)	(Zhang et al., 2005)
Oxygenated OA	1.85 ~ 2.3 (OM/OC)	(Aiken et al., 2008)

Table S5. Reconstructed source contributions (mean±SD of the daily values) and their relative abundance (mean±SD of the daily values) in reconstructed $PM_{2.5}$ mass in urban Beijing

	Mass concentrations (μg m^{-3})			Mass concentrations/ Reconstructed mass (%)	
	Winter	Summer		Winter	Summer
SNA	30.5±21.8	17.7±10.5	SNA/ RM	34.1±9.7	48.5±11.9
Geological minerals	5.3±3.2	3.5±1.8	Geological minerals/ RM	7.0±3.0	10.4±5.5
Vegetative detritus	0.2±0.2	0.2±0.2	Vegetative detritus/ RM	0.3±0.2	0.7±0.4
Biomass burning	8.9±6.2	0.8±0.9	Biomass burning/ RM	11.0±5.9	2.1±1.5
Gasoline vehicles	4.7±3.6	0.7±0.4	Gasoline vehicles/ RM	6.5±4.8	2.2±1.4
Diesel vehicles	0.9±2.0	0.1±0.3	Diesel vehicles/ RM	1.0±2.0	0.4±0.9
Industrial CC	11.6±9.7	4.3±1.7	Industrial CC/ RM	13.8±7.3	13.2±6.1
Residential CC	6.1±7.3	0.4±0.3	Residential CC/ RM	7.6±5.7	1.4±1.1
Cooking	3.1±3.0	0.9±0.6	Cooking/ RM	3.9±2.5	2.8±1.6
Other OM	11.7±10.8	6.5±3.2	Other OM/ RM	14.8±7.9	18.3±5.9
Reconstructed mass (RM)	83.1±49.0	35.1±15.0			
Offline $PM_{2.5}$ mass	105.0±77.4	36.5±17.0	Reconstructed mass/ Offline $PM_{2.5}$ mass	96.6±17.6	121.7±26.6
Online $PM_{2.5}$ mass	94.8±64.4	30.2±14.8	Reconstructed mass/ Offline $PM_{2.5}$ mass	91.9±24.1	99.0±19.1

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