Supplement of Atmos. Chem. Phys., 23, 1329–1343, 2023
https://doi.org/10.5194/acp-23-1329-2023-supplement

Atmospheric Chemistry and Physics
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Supplement of

Characteristics of fine particle matter at the top of Shanghai Tower

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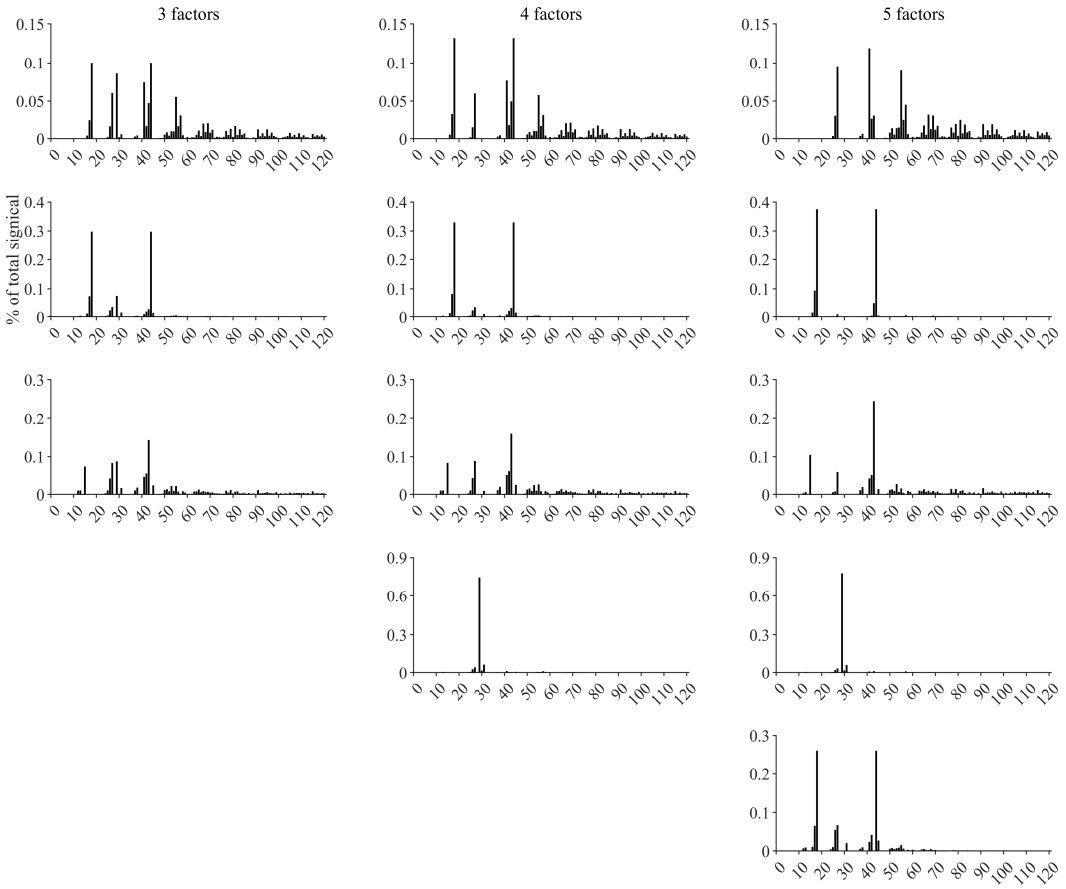

Figure S1: Mass spectra profiles of OA factors for unconstrained three-factor (left), four-factor (middle), and five-factor (right) situations.

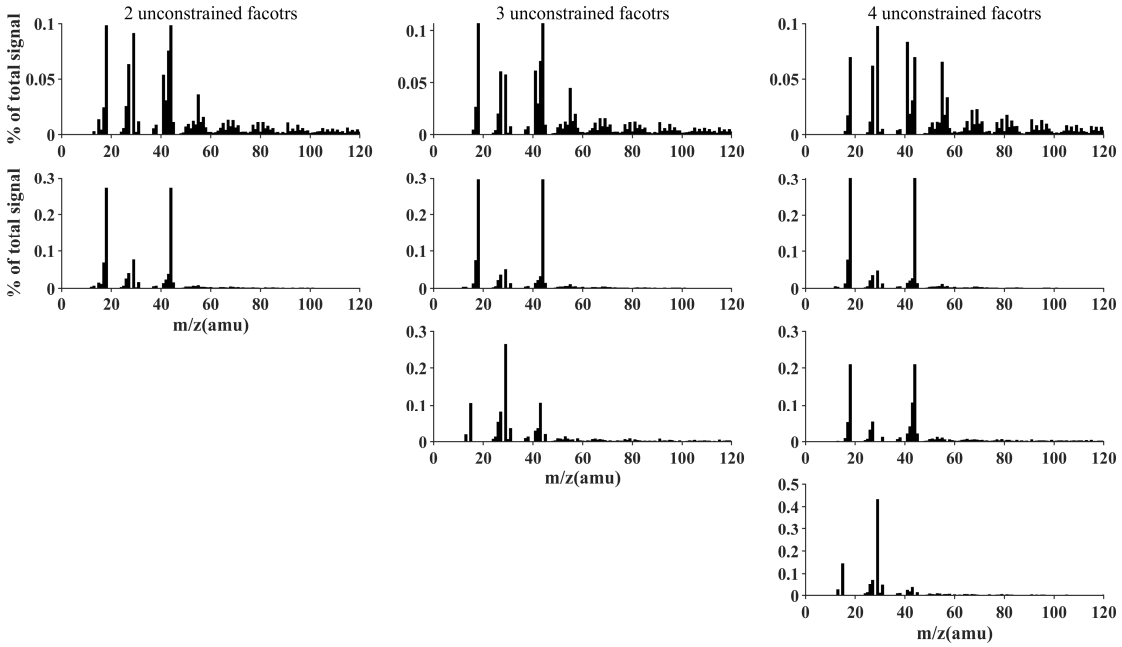

Figure S2: Mass spectra of 2-4 factor solution from unconstrained PMF for spring.

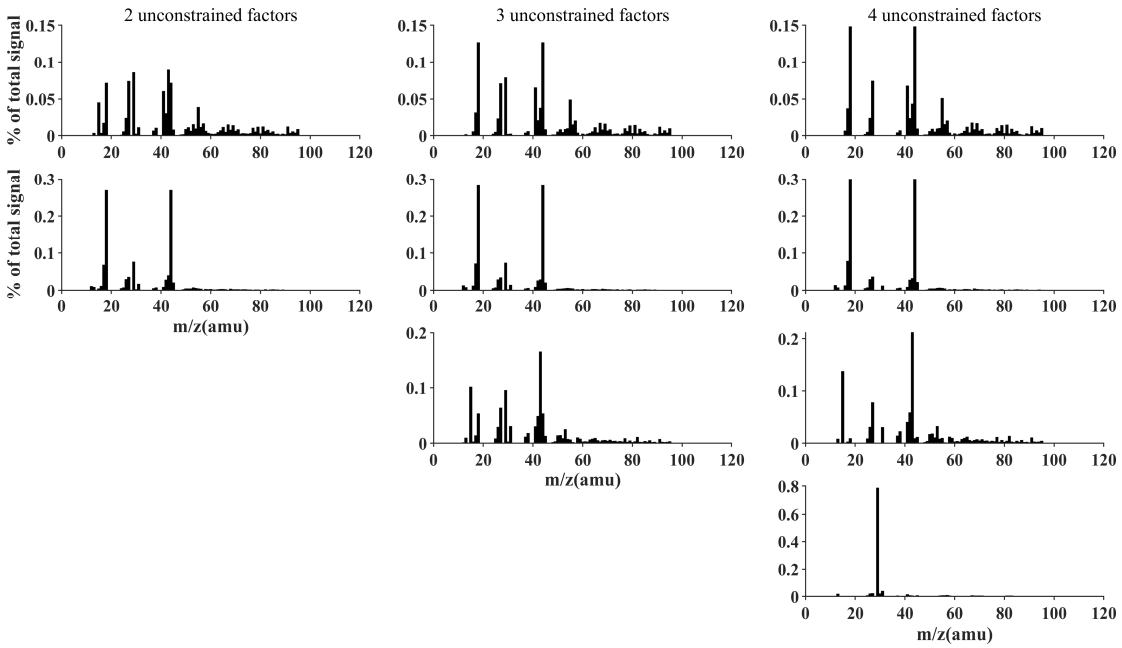

Figure S3: Mass spectra of 2-4 factor solution from unconstrained PMF for summer.

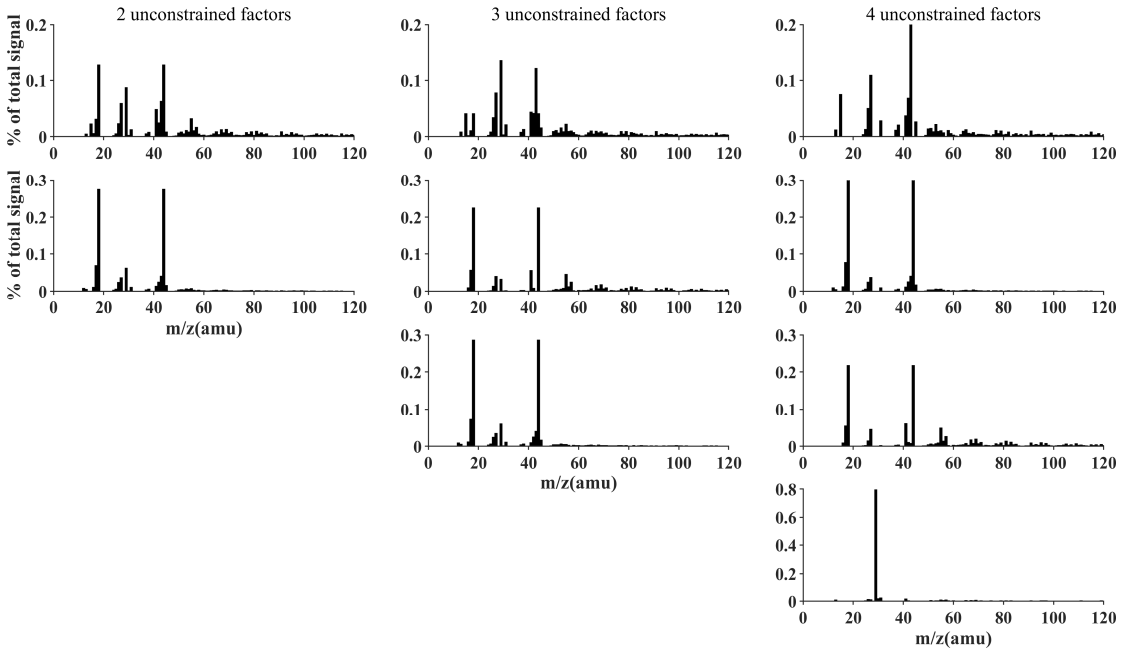

Figure S4: Mass spectra of 2-4 factor solution from unconstrained PMF for autumn.

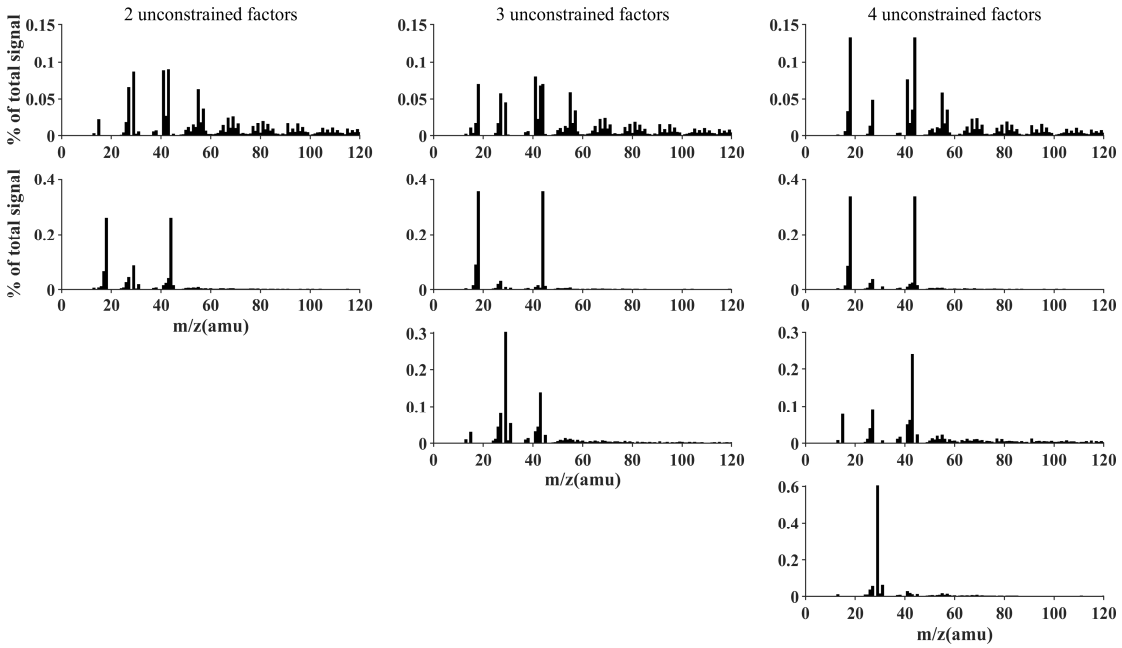

Figure S5: Mass spectra of 2-4 factor solution from unconstrained PMF for winter.

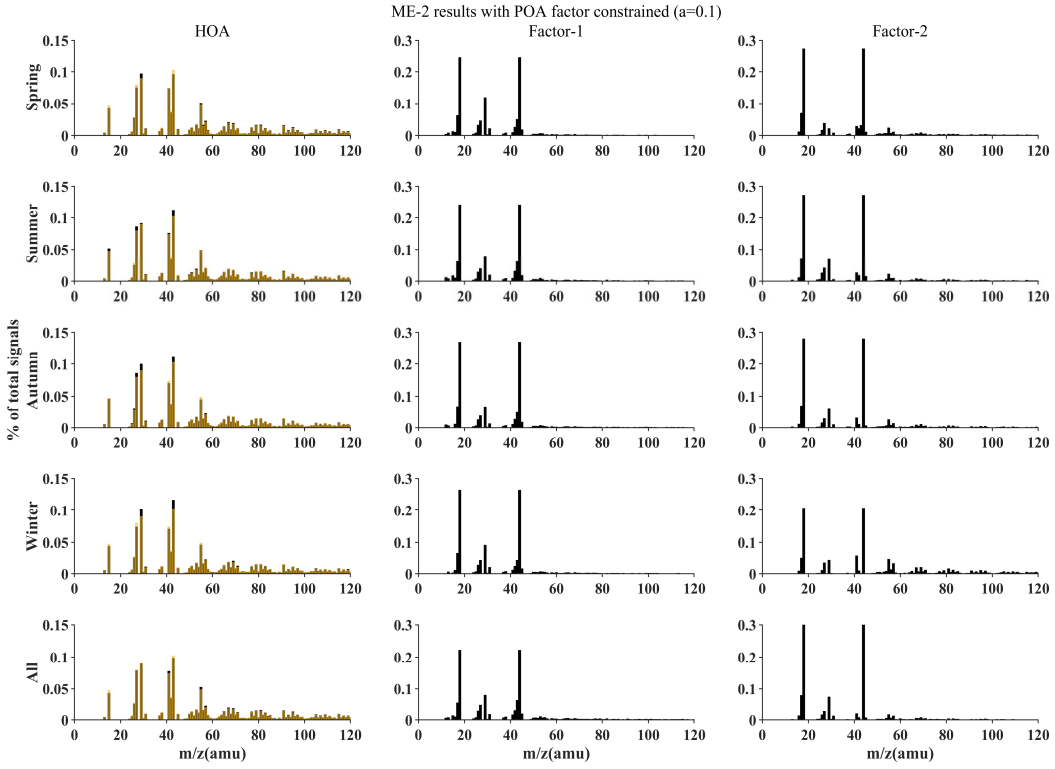

Figure S6: Mass spectra of 3 factor solution from ME-2 analysis (a=0.1) with POA factor constrained for four seasons and the entire study period. Yellow bar stands for priori POA factor mass spectra from unconstrained 2-factor solution.

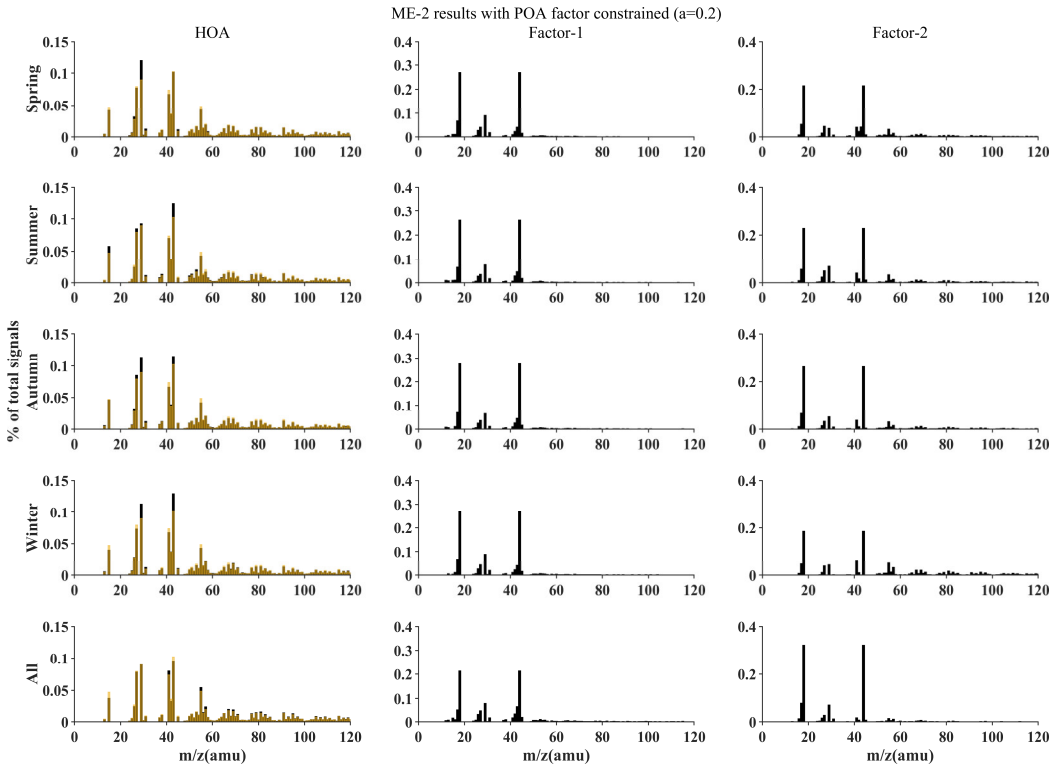

Figure S7: Mass spectra of 3 factor solution from ME-2 analysis (a=0.2) with POA factor constrained for four seasons and the entire study period. Yellow bar stands for priori POA factor mass spectra from unconstrained 2-factor solution.

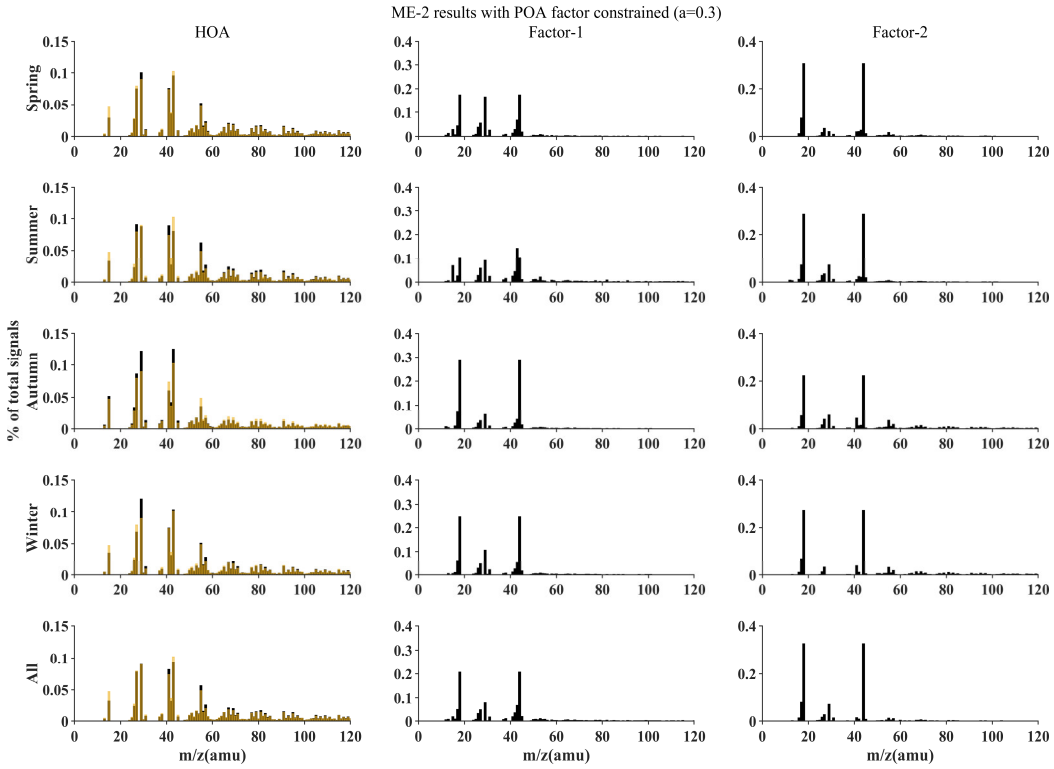

Figure S8: Mass spectra of 3 factor solution from ME-2 analysis (a=0.3) with POA factor

constrained for four seasons and the entire study period. Yellow bar stands for priori POA factor mass spectra from unconstrained 2-factor solution.

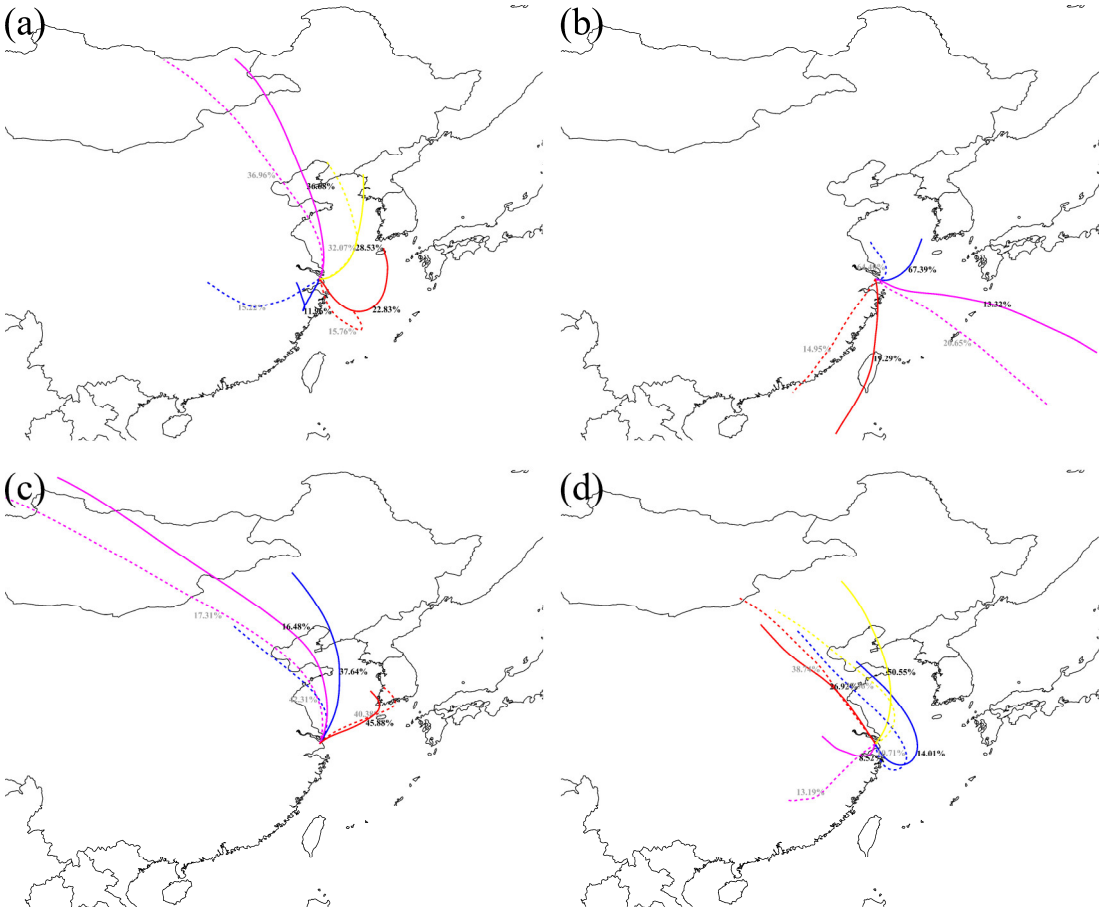

Figure S9: Air transport pathways at the height of 100 m (solid lines) and 600 m (dashed lines) during spring (a), summer (b), autumn (c), and winter (d). The 72h back trajectory was simulated using HYbrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model with the location of Shanghai Tower as central coordinate. Three clusters were determined for summer and autumn, and four clusters for spring and winter. The relative frequency of occurrence of air mass transport belonging to a specific cluster is given in percent for 100m (black) and 600m (gray).

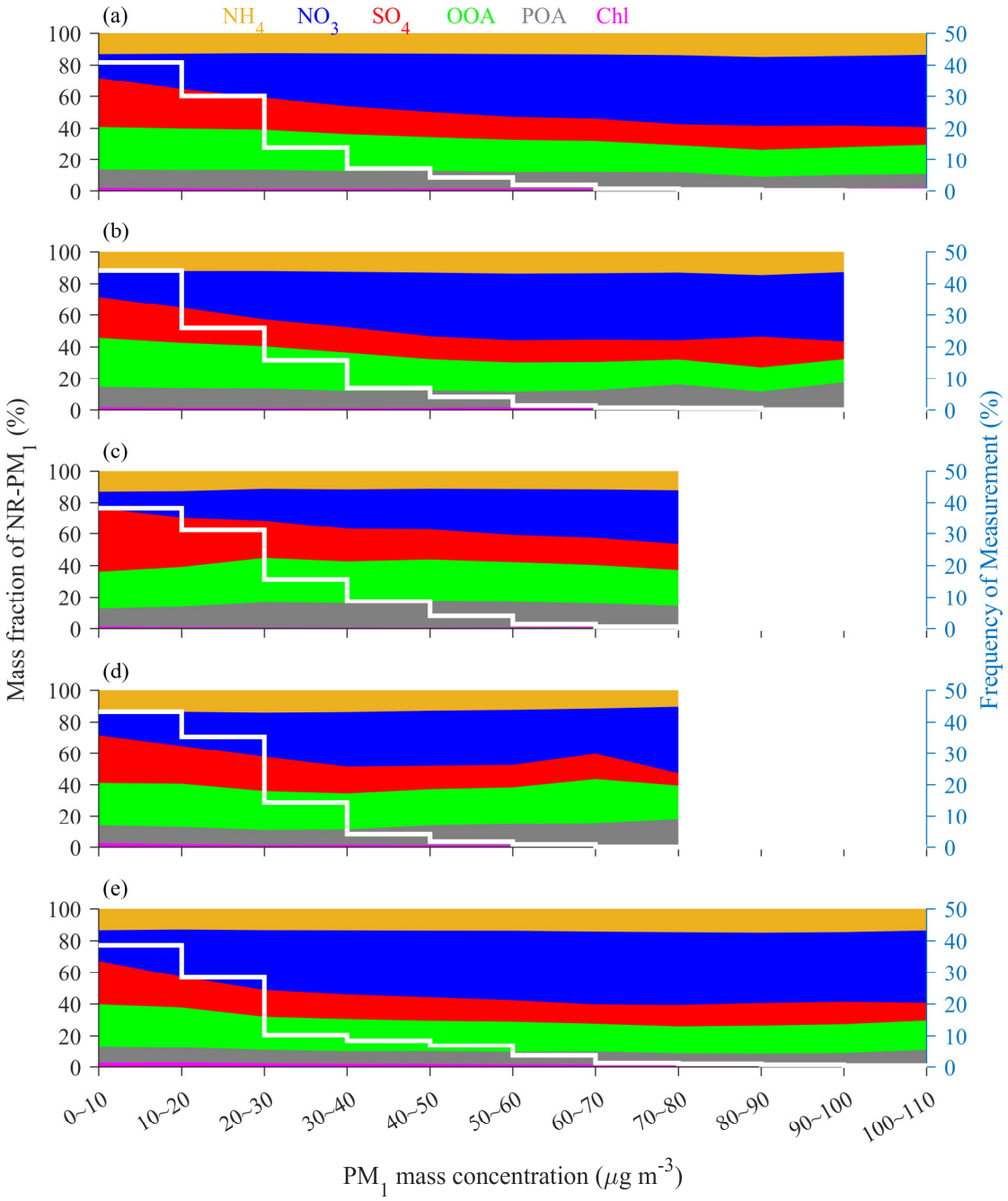

Figure S10: The mass fractions of PM_1 species as a function of PM_1 mass loadings (left), and frequency of measurement (right, with the white lines in the plots) during the entire period (a), spring (b), summer (c), autumn (d) and winter (e).

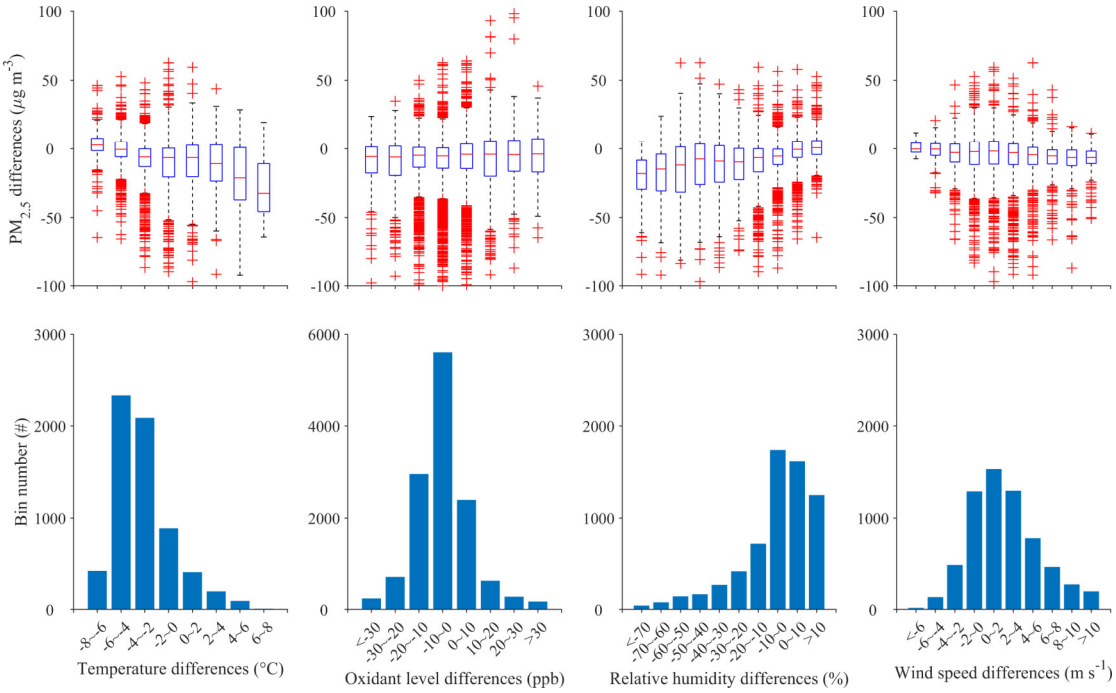

Figure S11: $PM_{2.5}$ differences (μg m^{-3}) bin-counted by temperature differences, oxidant level differences, relative humidity differences, and wind speed differences of SHT and SUR (upper panel). The lower panel shows the corresponding bin number (#). The oxidant level is defined as the sum of O_3 and NO_2, and based on data collected during 2017-2018. The wind speed data are from ERA5 (the fifth generation of ECMWF atmospheric reanalysis) data at nearest grid point (121.50°E, 31.25°N) of SHT. The boxes in the upper panel represent interquartile range of each bin, the red lines represent the median. The upper whiskers depict q3 + 1.5 × (q3 – q1), and the lower whiskers stand for q1 – 1.5 × (q3 – q1), where q1 and q3 are the 25th and 75th percentiles of the bin data. The data outside the range of whiskers are seen as outliers, and plotted using the '+' marker symbol.

Table S1: The NO_3 mass concentrations and mass fractions in Shanghai.

Description of sampling sites	Instruments (Particle nature)	Seasons (Year)	NO_3 mass concentrations (μg m^{-3})	NO_3 mass fractions (%)	References
A residential and business area	HR-ToF-AMS (NR-PM_1)	Spring (2016) Summer (2016) Winter (2017)	3.8±5.7 2.9±4.9 7.3±7.0	15.9% 10.2% 22.9%	Zhu et al. (2021)
A residential and business area	HR-ToF-AMS (NR-PM_1)	Spring-early summer (2010)	~4.8	16.3%	Huang et al. (2012)
A commercial and residential district	MARGA (Water-soluble $PM_{2.5}$)	Late autumn (2018)	12.9±12.8	27.2%	He et al. (2020)
Urban	HR-ToF-AMS	Winter (2016)	7.3±6.9	22.1%	Zhu et al.

	($NR\text{-}PM_1$)				(2018)
Urban	HR-ToF-AMS ($NR\text{-}PM_1$)	Late autumn (2018)	~5.6	26.0%	Cui et al. (2022)
Rural	ACSM ($NR\text{-}PM_1$)	Summer (2015)	~6.5	20.0%	Zhao et al. (2020)
		Autumn (2015)	~9.1	22.0%	
		Winter (2015)	~15.7	26.0%	
		Spring (2016)	~11.2	26.0%	
A central business district	ACSM ($NR\text{-}PM_1$)	Spring (2019)	4.8±4.8	29.9%	This study
		Summer (2019)	3.3±3.2	20.4%	
		Autumn (2019)	3.4±2.9	24.5%	
		Winter (2019)	7.2±7.6	36.8%	
A residential and business area	MARGA (Water-soluble $PM_{2.5}$)	Spring (2019)	7.1	24.5%	This study
		Summer (2019)	4.8	19.6%	
		Autumn (2019)	4.5	18.6%	
		Winter (2019)	12.1	27.7%	

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