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Characteristics and sources of nonmethane volatile organic compounds (NMVOCs) and O_3–NO_x–NMVOC relationships in Zhengzhou, China

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Supplementary Materials

Table list:

Figure list:

Table S1. Results of NMVOCs observed: concentrations with statistical analysis, ppbv.

Groups	Species	Mean ± SD	Median	25%	75%	MCM v3.3.1 name
Alkanes						
	Ethane	3.52 ± 1.58	3.07	2.28	4.41	C2H6
	Propane	1.68 ± 0.9	1.44	1.03	2.12	C3H8
	Isobutane	0.9 ± 0.59	0.73	0.5	1.13	IC4H10
	n-butane	1.1 ± 0.75	0.9	0.59	1.34	NC4H10
	Isopentane	1.01 ± 0.64	0.84	0.6	1.23	IC5H12
	n-Pentane	0.48 ± 0.39	0.38	0.26	0.55	NC5H12
	2,2-Dimethylbutane	0.02 ± 0.02	0.02	0.01	0.03	M22C4
	Cyclopentane	0.08 ± 0.04	0.07	0.05	0.09	
	2,3-Dimethylbutane	0.03 ± 0.02	0.03		0.04	M23C4
	2-Methylpentane	0.17 ± 0.11	0.14	0.1	0.2	M2PE
	3-Methylpentane	0.1 ± 0.09	0.08	0.06	0.12	M3PE
	n-Hexane	0.62 ± 0.36	0.56	0.38	0.77	NC6H14
	Methylcyclopentane	0.04 ± 0.03	0.03	0.02	0.04	
	2,4-Dimethylpentane	0.01 ± 0.01	0.01	0.01	0.01	
	Cyclohexane	0.03 ± 0.02	0.02	0.01	0.03	CHEX
	2-Methylhexane	0.01 ± 0.01	0.01	0.01	0.02	M2HEX
	2,3-Dimethylpentane	0.01 ± 0.01	0.01	0.01	0.01	
	3-Methylhexane	0.01 ± 0.01	0.01	0.01	0.02	M3HEX
	2,2,4-Trimethylpentane	0.02 ± 0.02	0.02	0.01	0.02	
	n-Heptane	0.01 ± 0.01	0.01	0.01	0.02	NC7H16
	Methylcyclohexane	0.02 ± 0.02	0.02	0.01	0.03	
	2,3,4-Trimethylpentane	0.01 ± 0.01	0.01	0.01	0.01	
	2-Methylheptane	0.01 ± 0	0	0	0.01	
	3-Methylheptane	0.01 ± 0	0.01	0	0.01	
	Octane	0.02 ± 0.02	0.01	0.01	0.02	NC8H18
	n-Nonane	0.01 ± 0.01	0.01	0.01	0.01	NC9H20
	n-Decane	0.01 ± 0	0.01	0.01	0.01	NC10H22
	Undecane	0.01 ± 0	0.01	0.01	0.01	NC11H24
	Dodecane	0.01 ± 0	0.01	0.01	0.01	NC12H26
Alkenes						
	1-Hexene	0.13 ± 0.3	0.04	0.03	0.06	HEX1ENE
	Ethylene	0.89 ± 0.52	0.82	0.49	1.14	C2H4
	Propylene	0.45 ± 0.57	0.22	0.12	0.66	C3H6
	trans-2-Butene	0.03 ± 0.02	0.02	0.02	0.03	TBUT2ENE
	1-Butene	0.05 ± 0.03	0.04	0.04	0.06	BUT1ENE
	cis-2-Butene	0.02 ± 0.01	0.02	0.01	0.03	CBUT2ENE
	trans-2-Pentene	0 ± 0.01	0	0	0	TPENT2ENE
	1-Pentene	0.01 ± 0.01	0.01	0	0.01	PENT1ENE
	cis-2-Pentene	0.01 ± 0.01	0	0	0.01	CPENT2ENE
	Isoprene	0.38 ± 0.54	0.14	0.02	0.52	C5H8
	1,3-Butadiene	0.01 ± 0.01	0.01	0.01	0.02	C4H6
Alkynes						
	Ethyne	1.07 ± 0.58	0.95	0.63	1.42	C2H2
Aromatics						
	Benzene	0.29 ± 0.14	0.25	0.19	0.36	BENZENE

	Toluene	0.47 ± 0.33	0.36	0.25	0.57	TOLUENE
	Ethylbenzene	0.07 ± 0.05	0.05	0.03	0.08	EBENZ
	m/p-Xylene	0.14 ± 0.11	0.11	0.07	0.18	MXYL
	Styrene	0.01 ± 0.01	0.01	0	0.01	STYRENE
	o-Xylene	0.07 ± 0.06	0.05	0.03	0.09	OXYL
	Isopropyl benzene	0 ± 0	0	0	0	IPBENZ
	n-Propyl benzene	0.01 ± 0	0.01	0	0.01	PBENZ
	3-Ethyltoluene	0.01 ± 0.01	0.01	0.01	0.02	METHTOL
	4-Ethyltoluene	0.01 ± 0.01	0.01	0	0.01	PETHTOL
	1,3,5-Trimethylbenzene	0.01 ± 0	0.01	0	0.01	TM135B
	2-Ethyltoluene	0.01 ± 0	0.01	0	0.01	OETHTOL
	1,2,4-Trimethylbenzene	0.02 ± 0.02	0.02	0.01	0.03	TM124B
	1,2,3-Trimethylbenzene	0.01 ± 0.01	0.01	0	0.01	TM123B
	1,3-Diethylbenzene	0 ± 0	0	0	0	
	1,4-Diethylbenzene	0 ± 0	0	0	0.01	
	Naphthalene	0.01 ± 0.01	0.01	0.01	0.02	
Halohydrocarbons						
	Freon12	0.13 ± 0.02	0.13	0.12	0.13	
	Freon114	0.12 ± 0.02	0.12	0.1	0.14	
	Chloromethane	0.64 ± 0.17	0.61	0.52	0.73	CH3CL
	Vinyl chloride	0.02 ± 0.04	0.01	0.01	0.02	VINCL
	Bromomethane	0.01 ± 0	0.01	0.01	0.01	CH3BR
	Chloroethane	0.02 ± 0.01	0.02	0.02	0.03	CH3CH2CL
	Freon11	0.21 ± 0.02	0.21	0.21	0.22	
	1,1-Dichloroethylene	0 ± 0	0	0	0	CCL2CH2
	Freon113	0.07 ± 0.01	0.07	0.07	0.08	
	Dichloromethane	1.06 ± 1.2	0.89	0.67	1.23	CH2CL2
	1,1-Dichloroethane	0.08 ± 0.08	0.06	0.04	0.09	CHCL2CH3
	cis-1,2-Dichloroethylene	0 ± 0	0	0	0	CDICLETH
	Chloroform	0.74 ± 0.55	0.58	0.35	0.95	CHCL3
	1,1,1-Trichloroethane	0 ± 0	0	0	0	CH3CCL3
	Tetrachloromethane	0.09 ± 0.01	0.09	0.09	0.1	
	1,2-Dichloroethane	0.51 ± 0.33	0.42	0.31	0.62	CH2CLCH2CL
	Trichloroethylene	0.01 ± 0	0.01	0	0.01	TRICLETH
	1,2-Dichloropropane	0.19 ± 0.16	0.15	0.11	0.22	CL12PROP
	Bromodichloromethane	0 ± 0	0	0	0	
	trans-1,3-Dichloropropene	0.01 ± 0.01	0.01	0	0.01	
	cis-1,3-Dichloropropene	0 ± 0	0	0	0	
	1,1,2-Trichloroethane	0.03 ± 0.03	0.03	0.02	0.04	CH2CLCHCL2
	Tetrachloroethylene	0.32 ± 0.36	0.21	0.1	0.41	TCE
	1,2-Dibromoethane	0 ± 0	0	0	0	DIBRET
	Chlorobenzene	0.01 ± 0	0.01	0.01	0.01	
	Bromoform	0 ± 0	0	0	0	
	1,1,2,2-Tetrachloroethane	0 ± 0	0	0	0	CHCL2CHCL2
	1,3-Dichlorobenzene	0 ± 0	0	0	0	
	1,2-Dichlorobenzene	0 ± 0	0	0	0	

	trans-1,2-Dichloroethylene	0.01 ± 0	0	0	0.01	
	Dibromochloromethane	0 ± 0	0	0	0	
	1,4-Dichlorobenzene	0.02 ± 0.01	0.02	0.01	0.02	
	Benzyl chloride	0 ± 0	0	0	0	
	1,2,4-Trichlorobenzene	0 ± 0	0	0	0	
	Hexachloro-1,3-butadiene	0.01 ± 0	0.01	0.01	0.01	
OVOCs						
	acetaldehyde	0.2 ± 0.15	0.16	0.1	0.24	CH3CHO
	n-butyraldehyde	0.07 ± 0.1	0.05	0.04	0.06	
	1,4-Dioxane	0.01 ± 0	0.01	0	0.01	
	Acrolein	0.14 ± 0.07	0.12	0.09	0.16	ACR
	propanal	0.33 ± 0.1	0.33	0.26	0.4	C2H5CHO
	Acetone	2.74 ± 0.7	2.78	2.25	3.2	CH3COCH3
	MTBE	0.04 ± 0.04	0.03	0.02	0.04	MTBE
	methylacrolein	0.1 ± 0.09	0.08	0.06	0.12	MACR
	valeraldehyde	0.05 ± 0.02	0.05	0.04	0.06	C4H9CHO
	caproaldehyde	0.08 ± 0.06	0.07	0.02	0.11	
	Isopropanol	0.02 ± 0.02	0.02	0.01	0.03	IPROPOL
	Vinyl acetate	0 ± 0	0	0	0.01	
	Ethyl acetate	0.24 ± 0.2	0.19	0.13	0.3	ETHACET
	2-Butanone	0.24 ± 0.1	0.21	0.17	0.29	MEK
	Tetrahydrofuran	0.03 ± 0.02	0.02	0.01	0.03	
	Methyl methacrylate	0.01 ± 0	0.01	0	0.01	
	4-Methyl-2-pentanone	0.01 ± 0.01	0.01	0.01	0.02	MIBK
	2-Hexanone	0.22 ± 0.22	0.19	0.03	0.32	HEX2ONE
	Crotonaldehyde	0.02 ± 0.02	0.02	0.01	0.03	
	benzaldehyde	0.01 ± 0	0.01	0.01	0.01	
	m-methylbenzaldehyde	0 ± 0	0	0	0	
Sulfide						
	Carbon disulfide	0.13 ± 0.22	0.06	0.03	0.12	

Table S2. The setup and parameters of the OBM model.

Parameters	Value	Method
Latitude	34.748°	
Longitude	113.603°	
Output time step interval	1 hour	
Integration time step	<100 seconds	Adapetive
chemical_mechanism		MCM v3.3.1
Chemistry solver		SMV-GEAR
Output species	NO SO2 NO2 CO O3 C2H6 C3H8 IC4H10 NC4H10 NC5H12 M22C4 M23C4 M2PE M3PE NC6H14 CHEX M2HEX M3HEX NC7H16 NC8H18 NC9H20 NC10H22 NC11H24 NC12H26 HEX1ENE C2H4 C3H6 TBUT2ENE BUT1ENE CBUT2ENE TPENT2ENE PENT1ENE CPENT2ENE C5H8 C4H6 C2H2 BENZENE TOLUENE EBENZ MXYL OH HONO NO3 H2O2 PAN HCHO HO2 STYRENE OXYL IPBENZ PBENZ METHTOL PETHTOL TM135B OETHTOL TM124B TM123B CH3CL VINCL CH3BR CH3CH2CL CCL2CH2 CH2CL2 CHCL2CH3 CDICLETH CHCL3 CH3CCL3 CH2CLCH2CL TRICLETH CL12PROP CH2CLCHCL2 TCE DIBRET CHCL2CHCL2 ACR C2H5CHO CH3COCH3 MTBE MACR C4H9CHO IPROPOL ETHACET MEK MIBK HEX2ONE CH3CHO	
Gas initial concentration (ppmv)	O3: 0.04, NO2: 0.01, HONO: 0.01	
Aerosol Initial concentration ($\mu g/m^3$)	ASO4J: 5.0, ANH4J: 2.0, ASO4I: 0.1, ANH4I: 0.05, ANO3J: 1.0, AECJ: 1.0	
Meteorological parameters		Observation interpolated
Photolysis rate		Inline

Table S3. Source apportionment results of NMVOCs in different cities.

Obervation sites	Time	sources	Contribution (%)	References
Qingdao	March-May	vehicular exhaust	17-22	Wu et al. (2023)
		solvent usage	14-23	
		industrial production	12-14	
Xuchang	May-September	vehicular exhaust	16	Qin et al. (2021)
		solvent usage	15	
		industrial production	16	
Guangzhou	September-November	vehicular exhaust	21	Meng et al. (2022)
		solvent usage	29	
		industrial production	13	
Nanjing	July-August	vehicular exhaust	23	Fan et al. (2021)
		solvent usage	12	
		industrial production	18	
Shijiazhuang	April-August	vehicular exhaust	12	Guan et al. (2020)
		solvent usage	12	
		industrial production	41	
Weinan	July-September	vehicular exhaust	18-21	Hui et al. (2020)
		solvent usage	12	
		industrial production	13-16	
Changzhou	August-October	vehicular exhaust	39	Liu et al. (2023)
		solvent usage	14-19	
		industrial production	5-6	
Beijing	July	vehicular exhaust	28	Liu et al. (2020)
		solvent usage	7.6	
		industrial production	-	

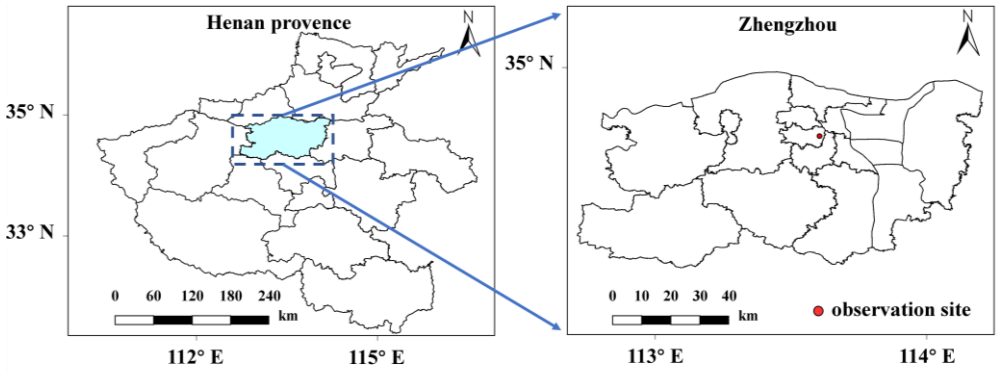


Fig. S1. The location of the observation site.

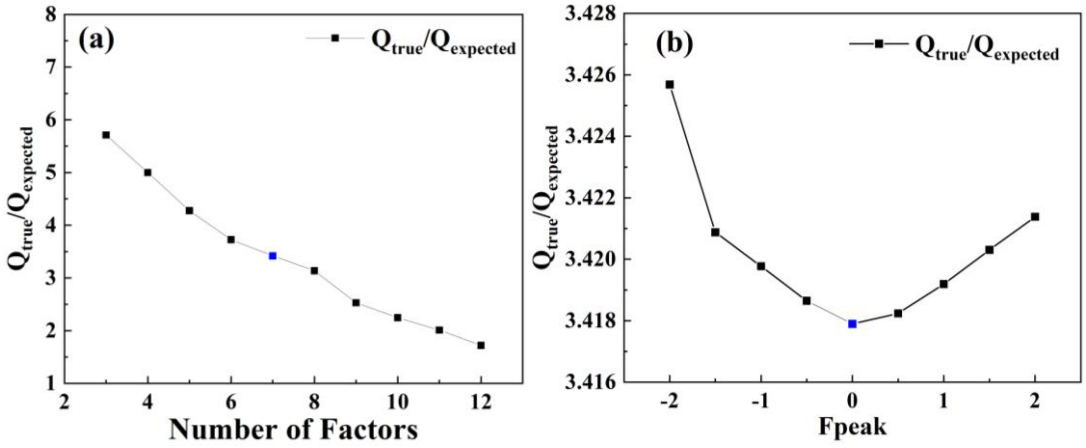


Fig. S2. (a) The $Q_{true}/Q_{expected}$ ratios in different solutions; (b) the $Q_{true}/Q_{expected}$ ratio for different Fpeak value solutions.

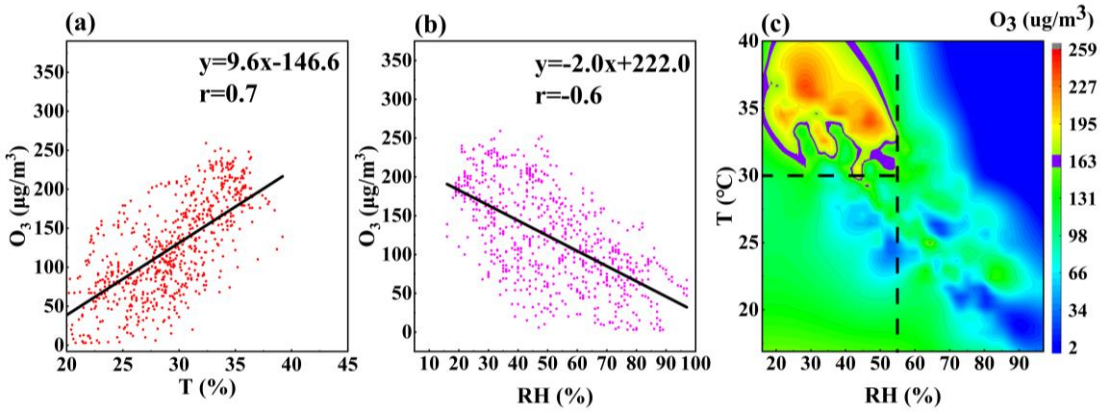


Fig. S3. Correlation analysis of O_3, T, and RH.

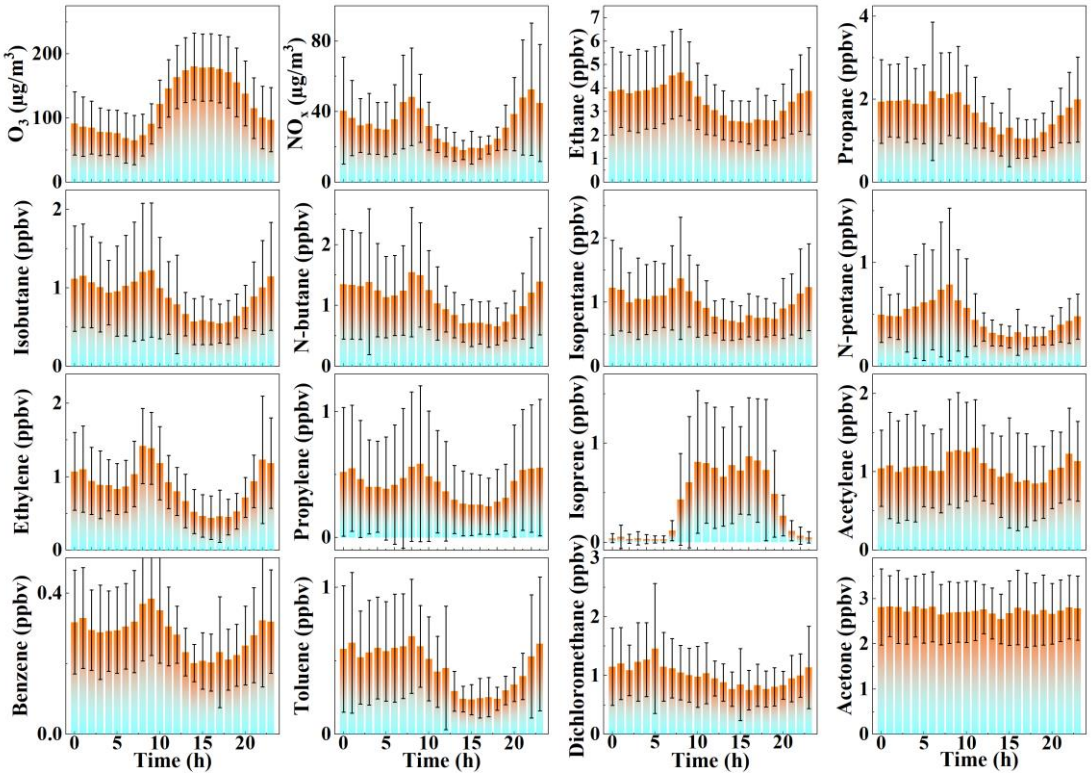


Fig. S4. Diurnal variations of O_3, NO_x, and NMVOCs during the observation period.

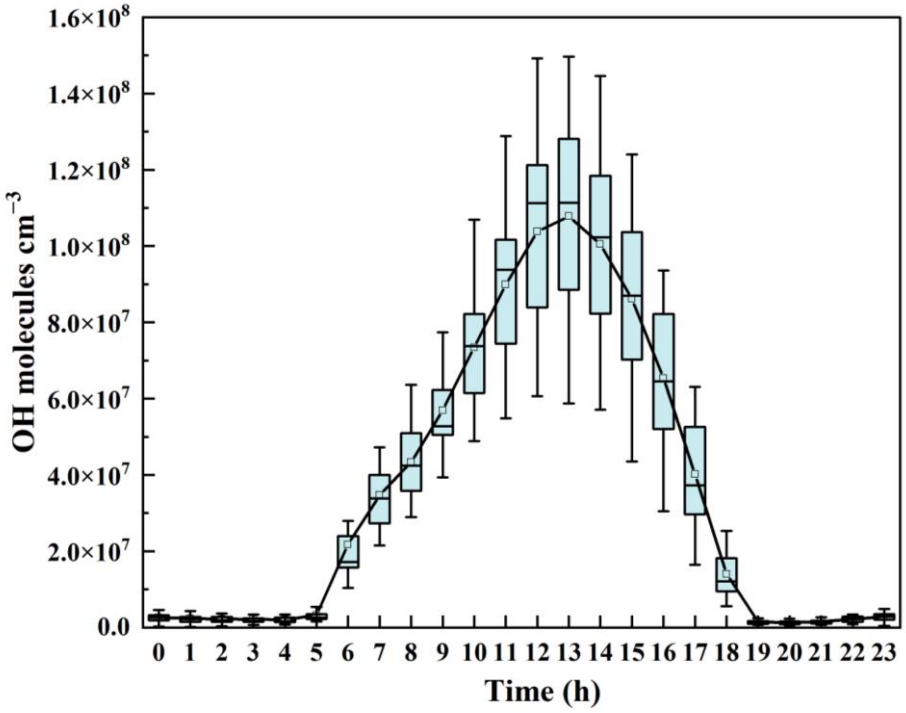


Fig. S5. Model-simulated average diurnal variations in OH concentrations.

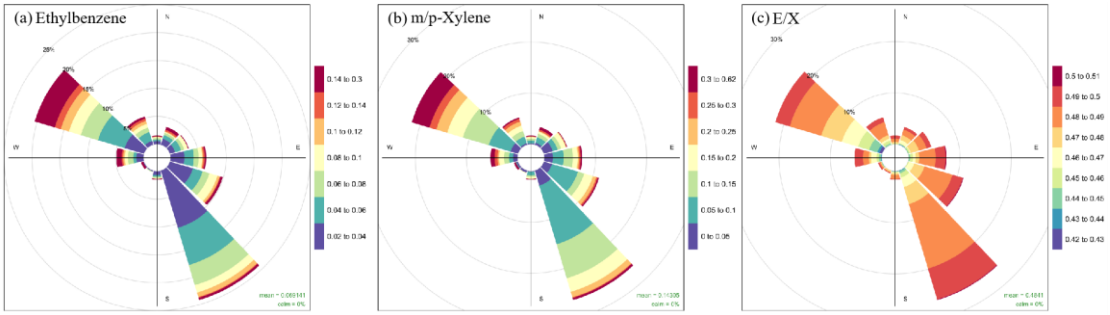


Fig. S6. Wind rose diagrams for ethylbenzene, m/p-Xylene, and E/X.

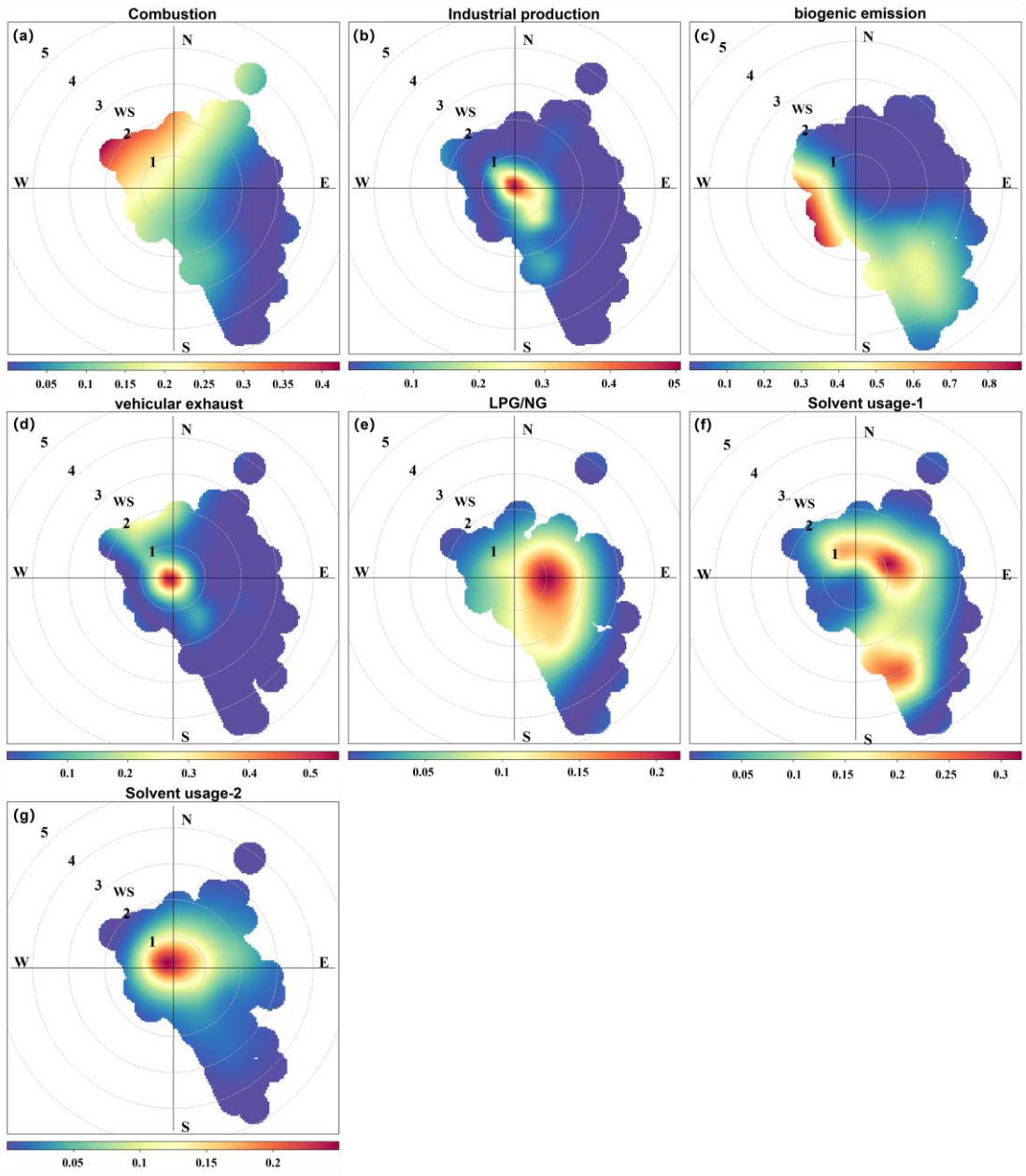


Fig. S7. CPF plots for the seven factors resolved by the multiple PMF methods.

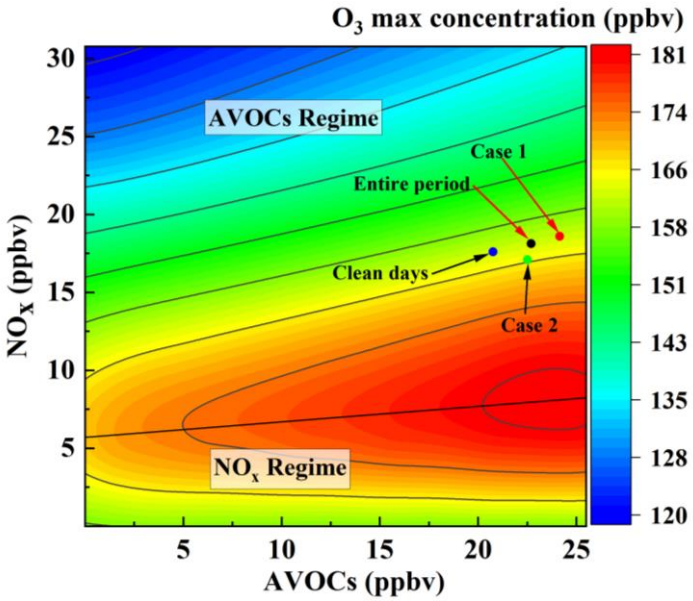
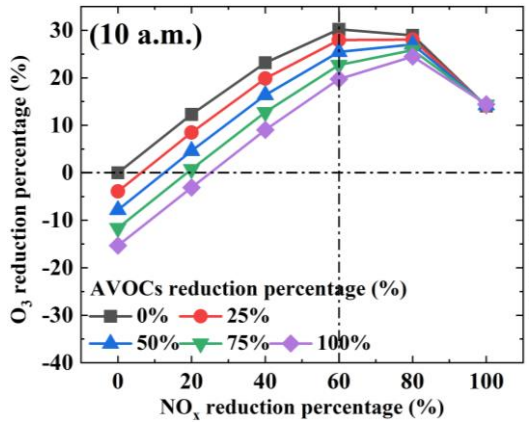
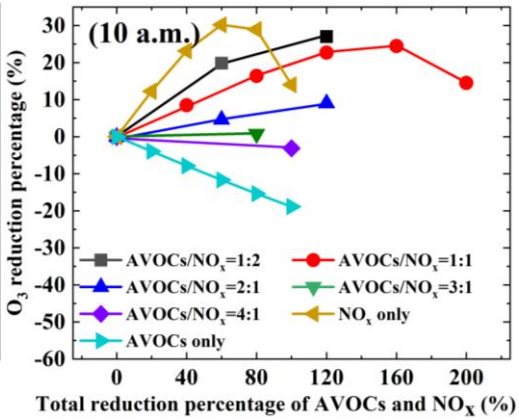
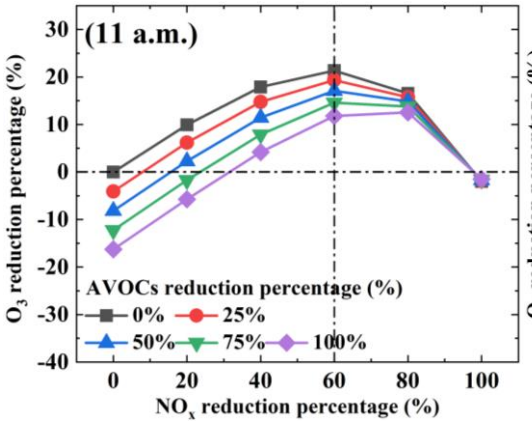
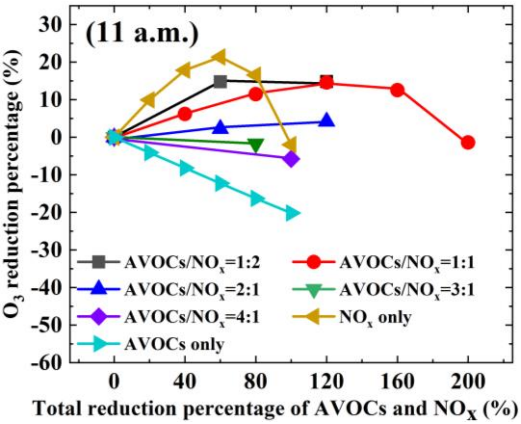


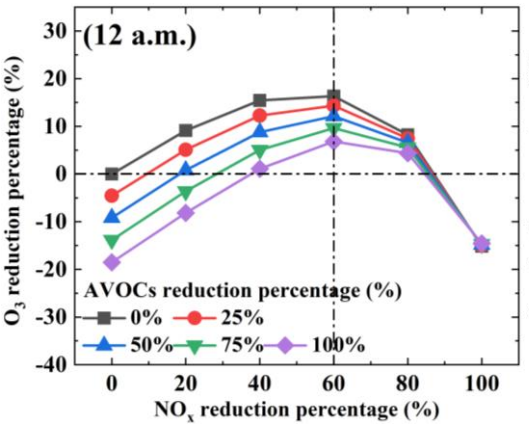
Fig. S8. EKMA curves of the O_3 max concentration.

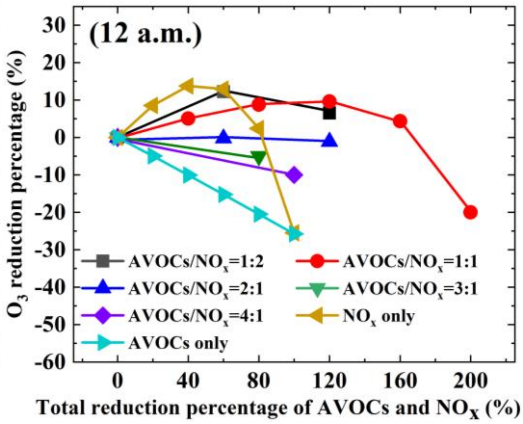

(10 a.m.)
O3 reduction percentage (%)
NOx reduction percentage (%)
AVOCs reduction percentage (%)
0%
25%
50%
75%
100%

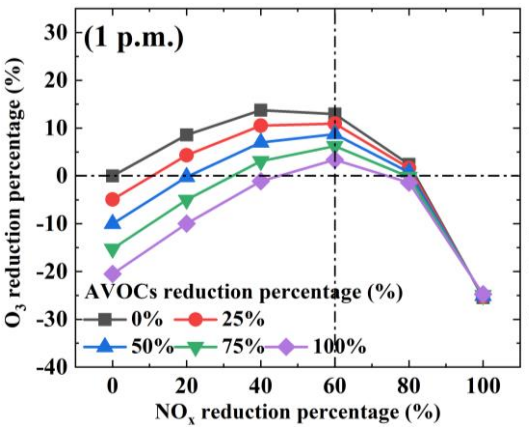

(10 a.m.)
O3 reduction percentage (%)
Total reduction percentage of AVOCs and NOX (%)
AVOCs/NOx=1:2
AVOCs/NOx=1:1
AVOCs/NOx=2:1
AVOCs/NOx=3:1
AVOCs/NOx=4:1
NOx only
AVOCs only


(11 a.m.)
O3 reduction percentage (%)
NOx reduction percentage (%)
AVOCs reduction percentage (%)
0%
25%
50%
75%
100%


(11 a.m.)
O3 reduction percentage (%)
Total reduction percentage of AVOCs and NOX (%)
AVOCs/NOx=1:2
AVOCs/NOx=1:1
AVOCs/NOx=2:1
AVOCs/NOx=3:1
AVOCs/NOx=4:1
NOx only
AVOCs only


(12 a.m.)
O3 reduction percentage (%)
NOx reduction percentage (%)
AVOCs reduction percentage (%)
0%
25%
50%
75%
100%


(12 a.m.)
O3 reduction percentage (%)
Total reduction percentage of AVOCs and NOX (%)
AVOCs/NOx=1:2
AVOCs/NOx=1:1
AVOCs/NOx=2:1
AVOCs/NOx=3:1
AVOCs/NOx=4:1
NOx only
AVOCs only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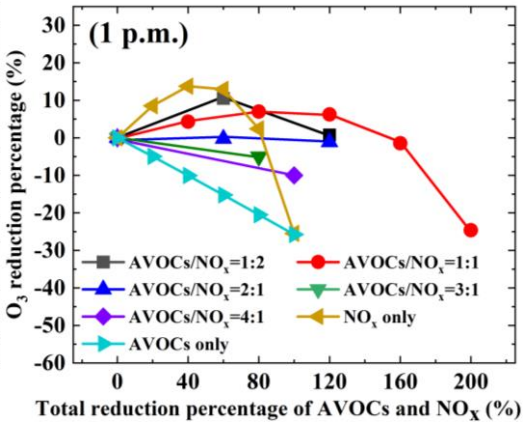
O3 reduction percentage (%)
NOx reduction percentage (%)
AVOCs reduction percentage (%)
0%
25%
50%
75%
100%


(1 p.m.)
O3 reduction percentage (%)
Total reduction percentage of AVOCs and NOX (%)
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AVOCs/NOx=2:1
AVOCs/NOx=3:1
AVOCs/NOx=4:1
NOx only
AVOCs only

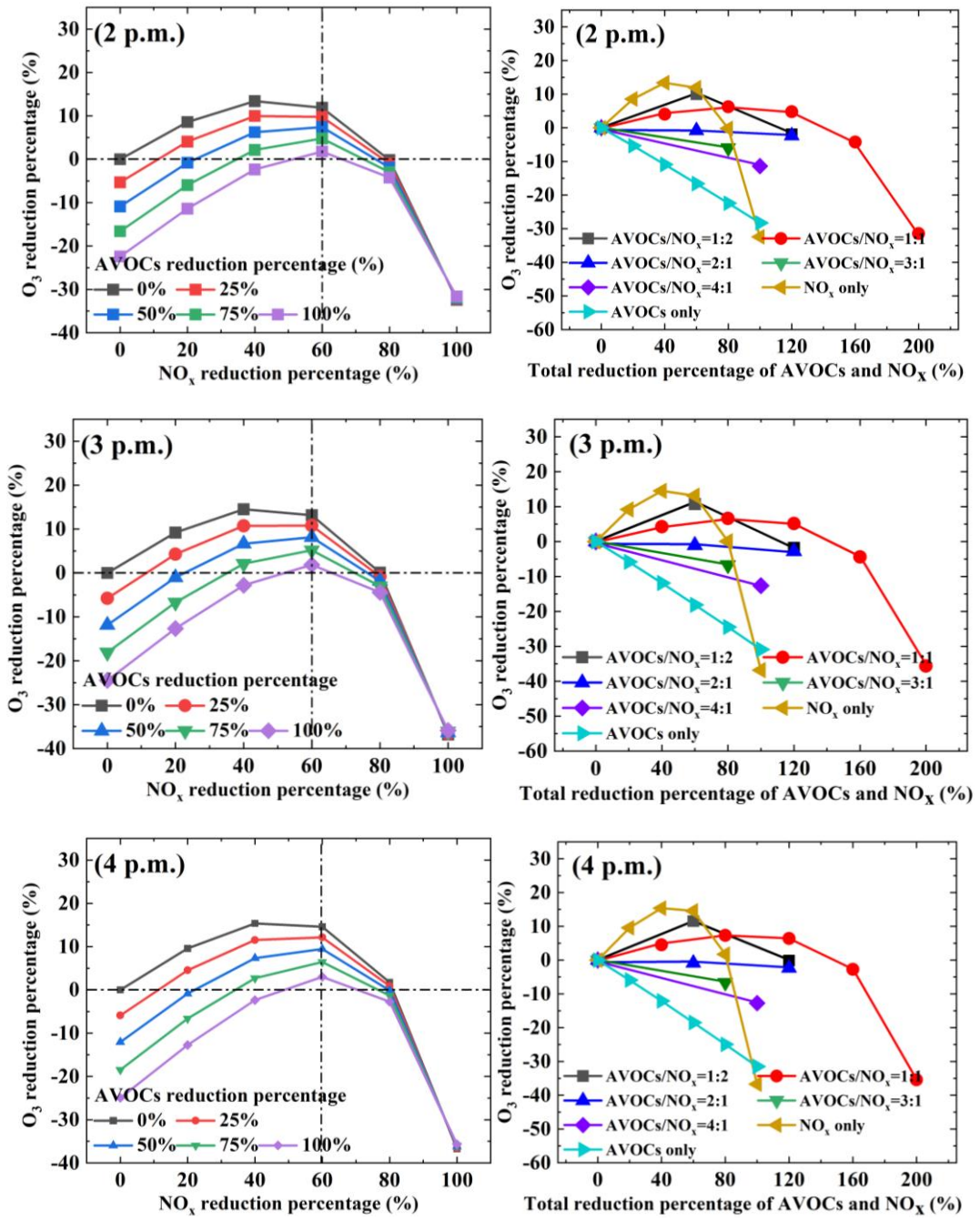

Fig. S9. Response of the O_3 concentration to different AVOCs and NO_x reduction percentages.

References:

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