

Supplementary Materials: Characterization and sources of VOCs during PM_{2.5} pollution periods in a typical city of the Yangtze River Delta

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Scheme S1. Relevant VOCs parameters used in this study.

Compound	MDL (ppt)	$K_{OH} \times 10^{12}$	A ^b	B ^b	n ^b	FAC (%)	FVOC _{ti} (%)
Alkanes							
Ethane *	64	0.20	1.49×10^{-17}	499	2	– ^d	–
Propane *	48	0.96	1.65×10^{-17}	87	2	–	–
<i>i</i> -Butane *	44	1.97	1.17×10^{-17}	–213	2	–	–
<i>n</i> -Butane *	30	2.14	1.81×10^{-17}	–114	2	–	–
<i>i</i> -Pentane *	12	3.60 ^c				–	–
<i>n</i> -Pentane *	30	3.49	2.52×10^{-17}	–158	2	–	–
2,2-Dimethylbutane *	3	1.89	3.37×10^{-11}	809		–	–
Cyclopentane	8	4.62	2.73×10^{-17}	–214	2	–	–
2,3-Dimethylbutane	9	5.58	1.66×10^{-17}	–407	2	–	–
2-Methylpentane *	8	5.20 ^c				–	–
3-Methylpentane *	12	5.20 ^c				–	–
<i>n</i> -Hexane	8	4.79	2.54×10^{-14}	112	1	–	–
2,3-Dimethylpentane	4	5.10 ^c				0.06	14
Methylcyclopentane	7	5.10 ^c				0.17	10
Cyclohexane	1	6.54	3.26×10^{-17}	–262	2	0.17	14
2,4-Dimethylpentane	1	4.77 ^c				0.06	14
3-Methylhexane	9	5.10 ^c				0.06	14
2,2,4-Trimethylpentane	4	3.05	2.35×10^{-17}	–140	2	0.06	17
<i>n</i> -Heptane	6	6.53	1.95×10^{-17}	–406	2	0.06	14
Methylcyclohexane	1	9.64 ^c				2.7	20
2,3,4-Trimethylpentane	2	6.60 ^c				0.06	17
2-Methylheptane	2	8.30 ^c				0.5	10
3-Methylheptane	2	8.60 ^c				0.5	10
<i>n</i> -Octane	6	7.76	2.72×10^{-17}	–361	2	0.06	17
<i>n</i> -Nonane	9	9.43	2.53×10^{-17}	–436	2	1.5	20
<i>n</i> -Decane	6	10.62	3.17×10^{-17}	–406	2	2	22
Alkenes							
Ethylene *	35	9.32	1.96×10^{-12}	–438		–	–
Propene *	41	29.15	4.85×10^{-12}	–504		–	–

Compound	MDL (ppt)	$K_{OH} \times 10^{12}$	A ^b	B ^b	n ^b	FAC (%)	FVOC _{ri} (%)
1-Butene *	4	34.51	6.55×10^{-12}	-467	-	-	-
trans-2-Butene	5	71.51	1.01×10^{-11}	-550	-	-	-
cis-2-Butene	8	62.24	1.10×10^{-11}	-487	-	-	-
3-Methyl-1-butene	2	35.46	5.32×10^{-12}	-533	-	-	-
1-Pentene	2	31.40 ^c			-	-	-
2-Methyl-1-butene	3	61.00 ^c			-	-	-
Isoprene *	6	108.17	2.70×10^{-11}	-390	2	50	
trans-2-Pentene	2	67.00 ^c			-	-	-
cis-2-Pentene	1	65.00 ^c			-	-	-
2-Methyl-2-butene	2	95.23	1.92×10^{-11}	-450	-	-	-
Cyclopentene	8	67.00 ^c			4	94	
4-Methyl-1-pentene	5	-			-	-	-
1-Hexene	1	37.00 ^c			-	-	-
trans-2-Hexene	3	-			-	-	-
cis-2-Hexene	2	-			-	-	-
3-Hexene	1	-			-	-	-
α -Pinene	1	57.10	1.21×10^{-11}	-436	-	-	-
β -Pinene	1	81.68	1.55×10^{-11}	-467	-	-	-
Alkyne							
Acetylene *	54	0.80 ^c			-	-	-
Aromatics							
Benzene *	15	1.17	2.33×10^{-12}	193	2.0	10	
Toluene *	9	3.93	1.18×10^{-12}	-338	5.4	12	
Ethylbenzene *	9	7.00 ^c			5.4	15	
<i>m,p</i> -Xylene *	15	18.65	1.87×10^{-11}	0	3.2	34	
<i>o</i> -Xylene *	7	13.60 ^c			5.0	26	
Styrene *	30	58.00 ^c			-	-	-
Isopropylbenzene	1	6.30 ^c			4.0	13	
<i>n</i> -Propylbenzene	1	5.80 ^c			1.6	12	
<i>m</i> -Ethyltoluene	4	18.60 ^c			6.3	31	
<i>p</i> -Ethyltoluene	1	11.80 ^c			2.5	21	
<i>o</i> -Ethyltoluene	1	11.90 ^c			5.6	23	
1,3,5-Trimethylbenzene	2	56.70 ^c			2.9	74	
1,2,4-Trimethylbenzene	6	32.50 ^c			2.0	58	
1,2,3-Trimethylbenzene	2	32.70 ^c			3.6	51	

^a K_{OH} represents the average reaction rates with OH from the calculated results ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), we calculated T dependent K_{OH} in this study, for alkanes, the recommended temperature-dependent expression is shown in Equation 1, while for alkenes, alkynes, and aromatics, Equation 2 is used.

$$K_{OH} = AT^n e^{-B/T} \quad (1)$$

$$K_{OH} = Ae^{-B/T} \quad (2)$$

^b A represents the Arrhenius constant ($\text{cm}^3 \text{ molecule}^{-1} \text{ s}^{-1}$), B is the ratio of apparent activation energy to molar gas constant (K), and n is a coefficient, the value of A, B, and n are obtained from Atkinson and Arey (2003).

^c The K_{OH} values at 298 K were used for compounds whose A and B parameters were not queried.

^d - represents that the relevant parameters for the compound were not calculated.

* Compounds used for PMF analysis.

Table S2. Comparison of meteorological parameters and air pollutants concentrations between morning time (6:00-10:00) of December 7 and 8, 2019.

	December 7	December 8
T (°C)	11.6 ± 2.3	13.1 ± 1.0
RH (%)	45.4 ± 12.3	45.5 ± 4.6
Wind speed (m s ⁻¹)	0.3 ± 0.2	0.8 ± 0.4
Wind direction	Southeast winds dominate	Southeast winds dominate
PM ₁₀ (µg m ⁻³)	63.4 ± 1.9	53.0 ± 5.1
PM _{2.5} (µg m ⁻³)	33.8 ± 1.3	35.8 ± 6.1
SO ₂ (µg m ⁻³)	7.8 ± 2.6	8.8 ± 3.9
CO (mg m ⁻³)	0.92 ± 0.1	0.94 ± 0.05
NO ₂ (µg m ⁻³)	49.4 ± 6.7	54.6 ± 3.9
O ₃ (µg m ⁻³)	7.0 ± 8.0	10.4 ± 14.0
Alkanes (ppb)	36.0 ± 16.3	18.3 ± 5.6
Alkenes (ppb)	6.7 ± 1.8	3.7 ± 0.7
Alkyne (ppb)	3.1 ± 0.3	2.7 ± 0.7
Aromatics (ppb)	13.7 ± 14.0	1.0 ± 0.5
TVOCs (ppb)	59.4 ± 31.9	25.7 ± 6.8

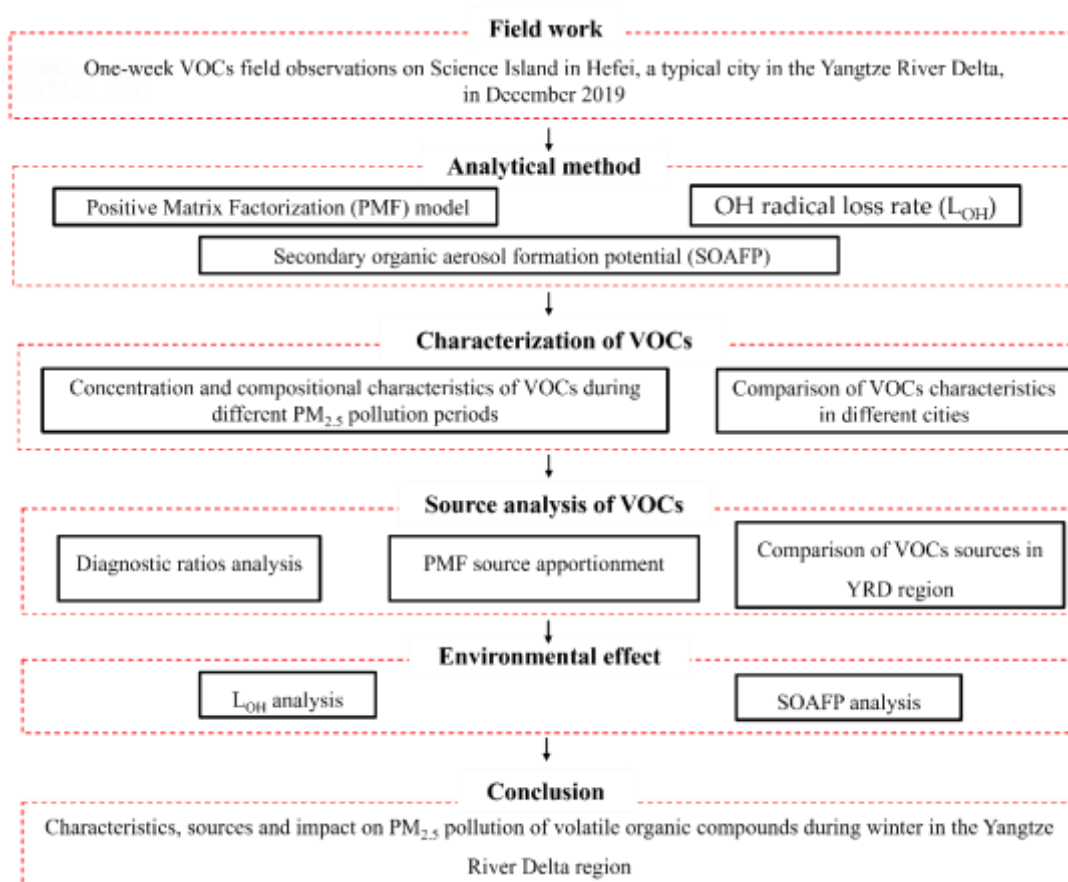


Figure S1. Flowchart for this study.

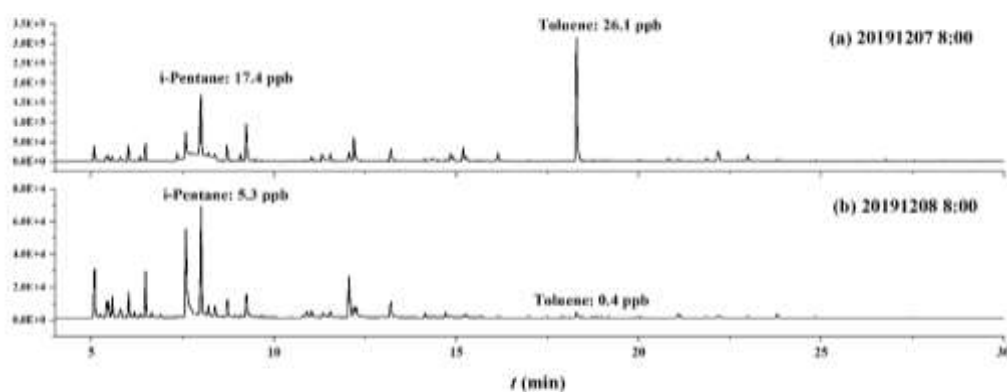


Figure S2. Chromatogram of the sample collected on December 7, 2019 at 8:00 (a), Chromatogram of the sample collected on December 8, 2019 at 8:00 (b).

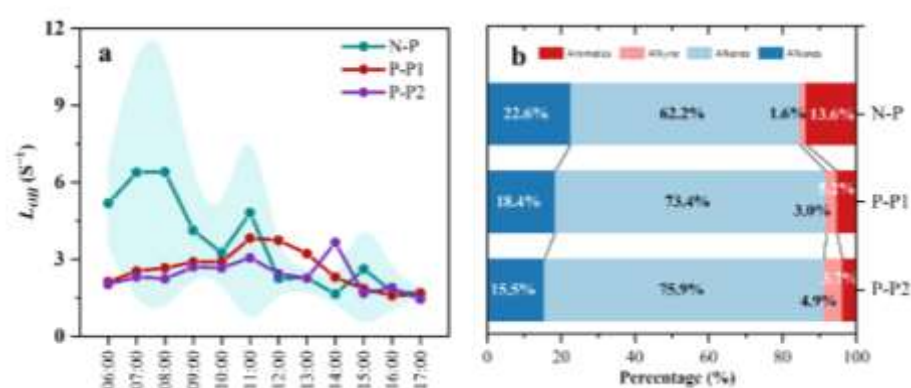


Figure S3. Diurnal variation (a) and composition (b) of OH loss rate (L_{OH}) in N-P, P-P1 and P-P2 period.