Measurement report: Ambient volatile organic compounds (VOCs) at an urban site in Beijing: characteristics, sources, and implications for pollution control

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Figure S1. Map of the studying location

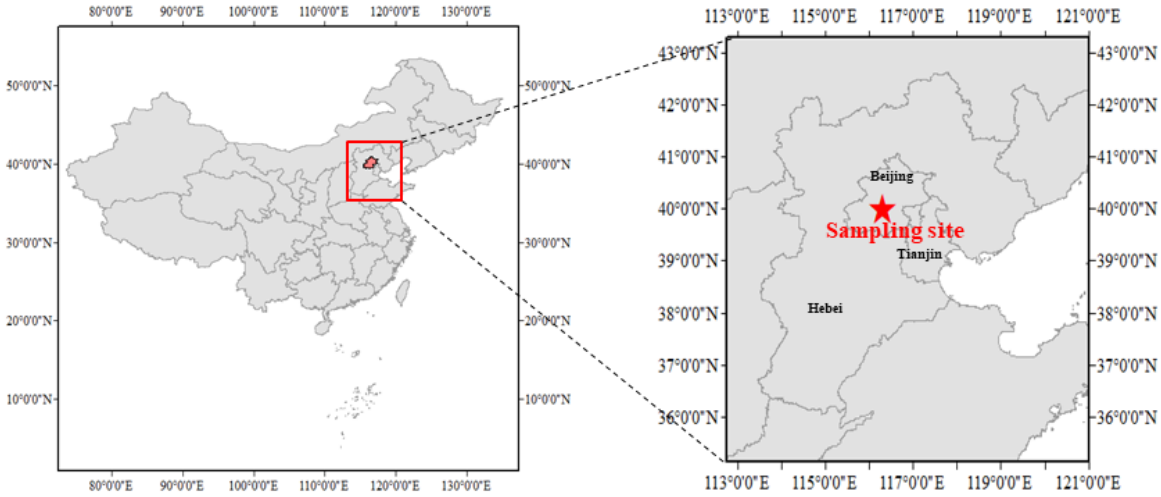

Figure S2. The performance of the random forest model in predicting the hourly concentrations of $PM_{2.5}$ and O_3. The model was constructed with 90% original data and the remained data was applied to validate the model.

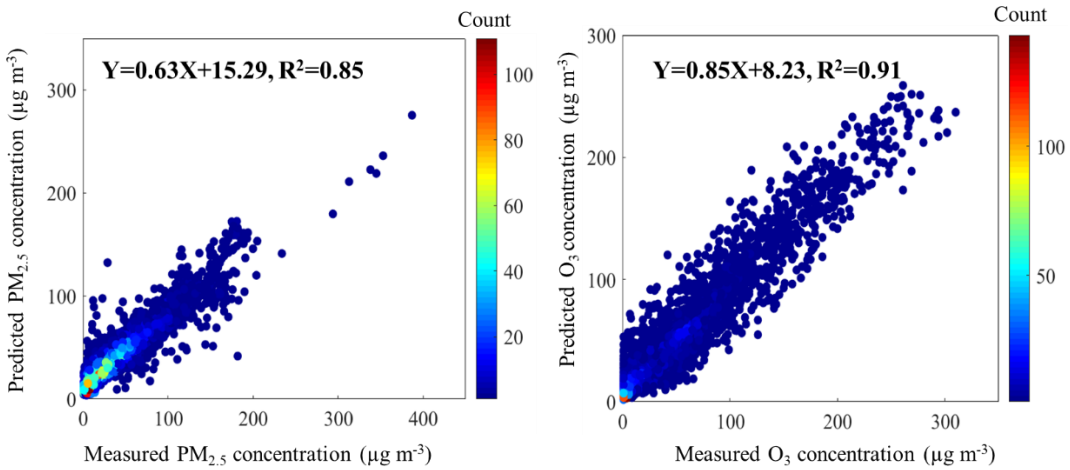

Table S1. List of VOCs and their MIR and SOA yield values used in this study.

No.	Species	MIR	SOA yield
1	Isobutane	1.23	0
2	n-butane	1.15	0
3	iso-pentane	1.45	0
4	n-pentane	1.31	0
5	2,2-dimethylbutane	1.17	0
6	2-methylpentane	1.50	0
7	3-methylpentane	1.80	0
8	n-hexane	1.24	0.0028
9	2,4-dimethylpentane	1.55	0
10	2-methylhexane	1.19	0
11	3-methylhexane	1.61	0
12	n-heptane	1.07	0.0066
13	2,2,4-trimethylpentane	1.26	0.0073
14	2,3,4-trimethylpentane	1.03	0.0073
15	2-methylheptane	1.07	0.003
16	3-methylheptane	1.24	0.005
17	n-octane	0.90	0.013
18	n-nonane	0.78	0.021
19	n-decane	0.68	0.033
20	n-undecane	0.61	0.05
21	n-dodecane	0.55	0.069
22	Cyclopentane	2.39	0.012
23	Methylcyclopentane	2.19	0.022
24	Cyclohexane	1.25	0.022
25	Methylcyclohexane	1.70	0.035
26	1-butene	9.73	0
27	trans-2-butene	15.16	0
28	cis-2-butene	14.24	0
29	1,3-butadiene	12.61	0
30	1-pentene	7.21	0.026
31	2-pentene	10.38	0.026
32	Isoprene	10.61	0.026
33	1-hexene	5.49	0.077
34	Benzene	0.72	0
35	Toluene	4.00	0.09
36	Ethylbenzene	3.04	0.049
37	m/p-xylene	7.80	0.049
38	o-xylene	7.64	0.049
39	Styrene	1.73	0.049
40	iso-Propylbenzene	2.52	0.073
41	n-Propylbenzene	2.03	0.073

42	m-Ethyltoluene	7.39	0.073
43	p-Ethyltoluene	4.44	0.073
44	o-Ethyltoluene	5.59	0.073
45	1,3,5-Trimethylbenzene	11.76	0.073
46	1,2,3-Trimethylbenzene	11.97	0.073
47	1,2,4-Trimethylbenzene	8.87	0.073
48	1,3-Diethylbenzene	7.10	0.1
49	1,4-Diethylbenzene	4.43	0.1
50	Freon11	0.00	0
51	Freon113	0.00	0
52	Freon114	0.00	0
53	Chloromethane	0.04	0
54	Methylene chloride	0.04	0
55	Trichloromethane	0.02	0
56	Trichloromethane	0.00	0
57	Bromodichloromethane	0.00	0
58	Dibromochloromethane	0.00	0
59	Bromomethane	0.02	0
60	Tribromomethane	0.00	0
61	1,1-Dibromoethane	0.10	0
62	Ethyl chloride	0.29	0
63	1,1-Dichloroethane	0.07	0
64	1,2-Dichloroethane	0.21	0
65	1,1,1-Trichloroethane	0.00	0
66	1,1,2-Trichloroethane	0.09	0
67	1,1,2,2-Tetrachloroethane	0.00	0
68	1,2-Dichloro-propane	0.29	0
69	Chloroethene	2.83	0
70	1,1-Dichloroethene	1.79	0
71	trans-1,2-dichloroethene	1.70	0
72	cis-1,2-dichloroethene	1.70	0
73	Trichloroethylene	0.64	0
74	cis-1,3-dichloropropene	3.70	0
75	trans-1,3-dichloropropene	5.03	0
76	Tetrachloroethylene	0.03	0
77	Hexachloro-1,3-butadiene	0.00	0
78	Chlorobenzene	0.32	0
79	1,2-dichlorobenzene	0.18	0
80	1,3-dichlorobenzene	0.18	0
81	1,4-dichlorobenzene	0.18	0
82	1,2,4-trichlorobenzene	0.09	0
83	Benzyl chloride	2.92	0
84	MTBE	0.73	0
85	Tetrahydrofuran	4.31	0

86	1,4-dioxane	2.62	0
87	Isopropyl alcohol	0.61	0
88	Acrolein	7.45	0
89	Acetone	0.36	0
90	MEK	1.48	0
91	MBK	3.14	0
92	MIBK	3.88	0
93	Vinyl acetate	3.20	0
94	Ethyl acetate	0.63	0
95	Methyl methacrylate	15.61	0

Text S1. Source appointment by PMF

Factor 1 was characterized with high loadings of SO_2 (72%), carbon tetrachloride (30%), methylchloride (27%), trichloromethane (20%), and benzene (20%). It was well known that SO_2 and trichloromethane were typical tracers of coal combustion and biomass burning, respectively(Ren et al., 2021; Zhang et al., 2018). Moreira dos Santos et al. (2004) also found that coal combustion could release significant amounts of benzene into the atmosphere(dos Santos et al., 2004). Especially in summer, open biomass burning in the rural regions of Beijing could release a large amount of Cl-containing VOC and aromatics to the atmosphere(Li et al., 2007). Therefore, this factor could be attributed to combustion source.

The predominant species found in factor 2 were O-ethyltoluene (65%), and styrene (58%). It is well documented that many aromatics such as benzene, ethyltoluene could be released from either vehicle emission or solvent use(Borbon et al., 2002; Shao et al., 2016). The poor correlation among these aromatics and other combustion tracers (e.g., SO_2) in this source further revealed that these species might be sourced from solvent usage. O-ethyltoluene was often used in the production of other chemical products(Shao et al., 2016), and thus the factor could be identified as the solvent use.

The most abundant species in factor 3 were 2,3,4-trimethylpentane, n-butane, and methyl cyclopentane with contributions of 54%, 47%, and 47%, respectively. It was reported that 2,3,4-trimethylpentane were released from petroleum products as a result of evaporation by refineries(Civan et al., 2011; Dumanoglu et al., 2014). Meanwhile, Mo et al. (2015) also verified that a high proportion of styrene was detected from petroleum refining emissions(Mo et al., 2015). Thus, the VOC species for factor 3 mainly originated from petrochemical industrial emissions.

Factor 4 was distinguished by high levels of 1-butene (84%) and trans-2-butene (78%). Guo et al. (2004) pointed out that low-carbon alkane could be considered to be the unburned fuel emissions(Guo et al., 2004). Geng et al. (2009a) also demonstrated that the C3-C5 alkenes were mainly emitted from the fuel evaporation(Geng et al., 2009). Hence, this factor represented the fuel evaporation.

Factor 5 was characterized by a large mass fraction of 1-hexene (62%), MTBE (53%), and vinyl acetate (46%). It was widely acknowledged that MTBE was a typical fingerprint of gasoline-powered vehicle emissions because it was often used as a fuel additive in motor gasoline (Liang et al., 2020). In addition, the poor correlation between the fuel evaporation factor and the MTBE are also observed ($r = 0.23$), indicating these factors shared with different origins. Hence, this factor was termed as the gasoline vehicle exhaust.

Factor 6 was dominated by N-undecanone (98%), N-dodecane (93%), and N-decane (73%). N-decane and N-undecanone were good markers of diesel exhaust emissions(Liu et al., 2008), indicating that this factor represented diesel engine emission.

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