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Supplement of

VOC species and emission inventory from vehicles and their SOA formation potentials estimation in Shanghai, China

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Supplement for "VOC species and emission inventory from vehicles and their SOA formation potentials estimation in Shanghai, China"

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1. Measured VOC species of different vehicle types and gas evaporation

Table S1 lists the weight percentage of individual VOC from different vehicle types and gas evaporation. The top 5 major species from LDGV were m,p-xylene, toluene, o-xylene, ethylbenzene, and n-decane, occupying 7.5%, 7.4%, 5.5%, 4.3%, and 3.9% of the total VOC, respectively. The top 5 major species from taxi were toluene, m,p-xylene, o-xylene, ethylbenzene, and 1,2,4-trimethylbenzene, occupying 7.7%, 5.9%, 4.9%, 4.5%, and 3.5% of the total VOC, respectively. The top 5 major species from HDDT were n-dodecane, n-undecane, propene, acetone, and n-decane, occupying 11.4%, 9.8%, 9.8%, 7.5%, and 6.6% of the total VOC, respectively. The top 5 major species from bus were n-dodecane, propene, n-undecane, n-decane, and acetone, occupying 15.9%, 11.9%, 7.6%, 7.1%, and 6.5% of the total VOC, respectively. 2-methylhexane, m,p-xylene, ethylbenzene, o-xylene, and methyl-tertbutyl-ether were major species in the exhaust of motorcycle, which contributed 23.4%, 9.3%, 5.5%, 4.4%, and 4.0% of the total VOC. Propane, isopentane, isobutene, 1-pentene, and n-butane were major species of gas evaporation, contributing 15.99%, 11.87%, 9.69%, 8.87%, and 6.51% of the total VOCs,

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respectively.

Table S1. Weight percentage (wt.%) of individual VOC from different vehicle types and gas evaporation.

VOC species	LDGV	Taxi	HDDT	Bus	Motorcycle	Gas evaporation
Ethane	0.45±0.07	0.41±0.03	0.82±0.51	0.46±0.15	2.88±1.20	ND
Propane	0.03±0.03	0.04±0.02	2.35±1.55	1.26±1.19	1.09±0.75	19.59±2.68
n-butane	0.53±0.08	0.48±0.06	0.25±0.14	0.27±0.13	1.33±0.45	7.89±3.41
n-pentane	2.31±0.23	2.52±0.27	0.51±0.21	0.34±0.05	0.87±1.24	5.27±1.54
n-hexane	3.04±0.55	2.97±0.17	0.53±0.19	0.98±0.74	2.88±1.22	1.32±0.56
n-heptane	1.60±0.21	1.47±0.09	1.04±0.33	0.92±0.38	2.33±1.21	0.54±0.50
n-octance	2.51±0.31	3.06±1.11	1.69±0.62	1.20±1.08	0.58±0.30	ND
n-nonane	0.96±0.12	0.98±0.18	3.79±1.11	3.56±1.17	0.25±0.23	ND
n-decane	3.95±0.47	3.51±0.71	6.62±1.27	7.10±2.66	0.15±0.14	ND
n-undecane	0.38±0.08	0.52±0.41	9.78±3.27	7.60±0.44	0.06±0.10	ND
n-dodecane	0.16±0.02	0.29±0.07	11.36±2.61	15.94±11.44	0.06±0.09	ND
Isobutene	0.24±0.05	0.27±0.03	0.35±0.12	0.59±0.72	1.47±0.43	11.73±5.85
Isopentane	2.97±0.20	2.85±0.29	2.02±0.67	1.60±1.30	2.54±2.32	14.27±2.94
2,2-dimethylbutane	0.72±0.40	0.86±0.44	ND	ND	0.43±0.15	1.30±0.98
2,3-dimethylbutane	1.02±0.17	1.16±0.10	1.41±1.57	ND	1.29±0.48	0.60±0.18
2-methylpentane	2.27±0.15	1.9±0.31	0.52±0.33	ND	1.90±0.97	1.96±0.50
3-methylpentane	2.05±0.51	1.84±0.41	1.43±0.50	0.58±0.73	2.00±0.83	0.90±0.30
2-methylhexane	1.26±0.38	1.31±0.31	0.52±0.40	0.43±0.10	23.43±10.72	1.28±0.88
3-methylhexane	1.10±0.23	0.90±0.10	0.89±0.86	0.68±0.22	1.55±0.29	0.35±0.10
2,4-dimethylpentane	0.02±0.01	0.05±0.01	ND	0.35±0.26	0.61±0.30	0.13±0.16
2,3-dimethylpentane	1.02±0.32	0.68±0.08	0.61±0.41	0.18±0.00	1.36±0.51	0.06±0.07
2,3,4-trimethylpentane	0.11±0.04	0.16±0.02	ND	0.60±0.57	0.48±0.64	0.07±0.14
3-methylheptane	1.61±0.19	1.61±0.23	1.01±0.32	1.01±0.58	0.68±0.46	ND
2,2,4-trimethylpentane	1.39±0.52	1.03±0.17	1.04±0.67	0.60±0.01	0.91±0.85	0.87±0.88
2-methylheptane	1.96±0.18	1.96±0.23	1.00±0.24	1.04±0.90	0.55±0.31	ND
Cyclopentan	1.36±0.44	1.28±0.14	0.03±0.01	0.04±0.02	1.17±0.33	0.04±0.04
Cyclohexane	0.48±0.12	0.35±0.04	ND	ND	0.98±0.70	1.41±1.74
Methylcyclopentane	2.63±0.15	2.62±0.82	0.07±0.02	0.10±0.06	1.31±0.48	0.68±0.20
Methylcyclohexane	1.68±0.66	0.95±0.17	0.24±0.06	0.34±0.26	0.77±0.48	0.07±0.09
Ethene	0.40±0.08	0.37±0.05	0.75±0.47	0.43±0.13	3.13±1.49	2.94±2.07
Propene	1.18±0.68	1.92±0.34	9.78±1.33	11.92±0.18	0.79±0.42	2.05±0.15
1,3-butadiene	0.01±0.00	0.02±0.02	ND	ND	0.04±0.02	0.04±0.02
1-butene	2.05±0.25	2.03±0.34	1.17±0.61	0.88±0.10	1.76±0.65	3.90±1.09
trans-2-butene	0.19±0.13	0.24±0.05	0.24±0.10	0.22±0.08	0.40±0.53	3.64±0.84
cis-2-butene	0.27±0.01	0.86±1.27	0.15±0.06	0.16±0.06	0.54±0.36	1.79±0.72
isoprene	0.03±0.01	0.03±0.02	ND	ND	0.05±0.02	0.06±0.08
trans-2-pentene	0.95±0.24	0.53±0.07	0.16±0.11	0.13±0.01	0.36±0.22	0.64±0.09
cis-2-Pentene	0.38±0.18	0.76±0.13	0.08±0.04	0.07±0.00	0.27±0.27	2.68±0.22

1-pentene	0.35±0.12	0.27±0.02	1.10±0.77	0.72±0.02	0.65±0.33	10.13±2.77
1-hexene	0.74±0.21	1.26±0.59	1.78±1.51	1.32±0.27	1.59±0.98	1.10±0.59
Ethyne	0.40±0.05	0.36±0.02	0.74±0.46	0.42±0.15	2.54±1.23	ND
Benzene	2.90±0.53	2.88±0.33	3.37±0.75	2.92±0.55	1.34±0.33	0.09±0.02
Toluene	7.37±0.1	7.72±0.71	3.02±0.61	2.3±2.11	2.50±0.81	0.34±0.09
Styrene	2.09±0.23	2.21±0.31	0.12±0.02	0.24±0.13	0.23±0.10	0.01±0.01
Ethylbenzene	4.3±0.23	4.53±0.37	0.95±0.13	0.94±0.79	5.53±5.26	0.03±0.01
m,p-Xylene	7.53±0.56	5.88±0.52	2.13±0.33	2.44±0.78	9.34±6.48	0.02±0.02
o-Xylene	5.55±0.46	4.85±0.38	0.74±0.07	0.91±0.26	4.37±5.00	0.02±0.00
1,3,5-trimethylbenzene	1.82±0.07	1.91±0.31	0.35±0.06	0.45±0.14	0.55±0.49	0.01±0.01
1,2,4-trimethylbenzene	3.48±0.26	3.55±0.32	1.15±0.31	1.56±0.73	0.65±0.53	ND
isopropylbenzene	0.49±0.11	0.63±0.04	0.08±0.02	0.10±0.02	0.12±0.07	ND
n-propylbenzene	0.71±0.09	0.72±0.08	0.24±0.04	0.30±0.10	0.30±0.16	ND
m-ethyltoluene	0.49±0.19	0.57±0.15	0.55±0.24	0.93±0.44	0.37±0.32	ND
p-ethyltoluene	2.32±0.99	3.52±0.40	0.32±0.09	0.49±0.22	0.20±0.15	ND
o-ethyltoluene	1.15±0.34	1.49±0.37	0.20±0.14	0.20±0.07	0.31±0.23	ND
1,2,3-trimethylbenzene	1.77±0.24	2.11±0.43	0.73±0.15	1.04±0.43	0.29±0.3	ND
m-diethylbenzene	0.69±0.16	0.79±0.47	0.22±0.06	0.42±0.26	ND	ND
p-diethylbenzene	0.87±0.18	1.11±0.18	0.56±0.84	2.58±3.26	ND	ND
Acetone	0.63±0.12	0.42±0.07	7.53±4.57	6.47±1.26	0.55±0.54	ND
isopropanol	0.06±0.03	0.04±0.01	ND	1.09±1.17	0.01±0.01	ND
methyl-ethyl-ketone	0.05±0.01	0.05±0.03	1.83±1.24	1.42±0.64	ND	ND
Tetrahydrofuran	0.07±0.01	0.07±0.01	0.21±0.07	0.19±0.04	ND	ND
Vinylacetate	0.01±0.01	0.01±0.01	2.32±0.81	1.41±0.04	ND	ND
Dioxane	0.01±0.00	0.02±0.01	ND	ND	ND	ND
Ethylacetate	0.09±0.01	0.10±0.02	0.87±0.21	1.07±0.06	1.12±0.47	ND
Methyl-tertbutyl-ether	0.08±0.00	0.11±0.03	0.28±0.06	0.46±0.28	3.96±1.96	ND
4-methyl-2-pentanone	0.14±0.03	0.10±0.02	0.2±0.04	0.25±0.01	ND	ND
2-hexanone	0.03±0.02	0.10±0.02	0.55±0.21	0.39±0.11	ND	ND

2. Observation data of meteorological condition and air pollutant concentration

Fig. S1 shows time series observation data of meteorology parameters and CO, O_3, VOCs species, OC, and EC concentration in summer (from January 1 to January 31) and winter (from August 1 to August 31) in the atmosphere of Shanghai urban in 2013. Detail information of the monitoring site was introduced by Qiao et al. (2014). During the winter observation, air temperature varied in the range of -0.8-18.0°C and the average temperature was 5.5±3.8°C. Relative humidity (RH) fluctuated in the range of 23.3-84.9% and the average RH was 59.8±12.9%. Wind speed was in the range of 0.6-4.5m·s^{-1} and the average wind speed was 2.0±0.7m·s^{-1}. The average concentrations of CO, ethylbenzene, and m,p-xylene in winter were 993±544ppb, 1.16±1.09ppb, and 1.27±1.11ppb. The maximum O_3 concentration was 74ppb. The average concentrations of OC and EC were 13.40±8.68μg·m^{-3} and 2.72±2.17μg·m^{-3}.

During the summer observation, air temperature varied in the range of 23.7-43.0°C and the average temperature was 31.9±3.8°C. Relative humidity (RH) fluctuated in the range of 22.6-80.4% and the average RH was 58.2±12.8%. Wind speed was in the range of 0.6-5.4m·s^{-1} and the average wind speed was 1.2±0.8 m·s^{-1}. The average concentrations of CO, ethylbenzene, and m,p-xylene in summer were 721±140ppb, 0.73±0.57ppb, and 0.26±0.21ppb. The maximum O_3 concentration was 164ppb. The average concentrations of OC and EC were 7.44±4.81μg·m^{-3} and 1.37±0.86μg·m^{-3}.

Concentrations of CO, ethylbenzene, xylene, OC and EC showed good consistency in the observation period. The photochemical exposure (Δt·[OH]) was calculated using Eq. (1). The figure indicates during the period with high ozone, the OC/EC ratio and Δt·[OH] is much higher than during the other periods. More secondary formation of OC can be expected during the high ozone period.

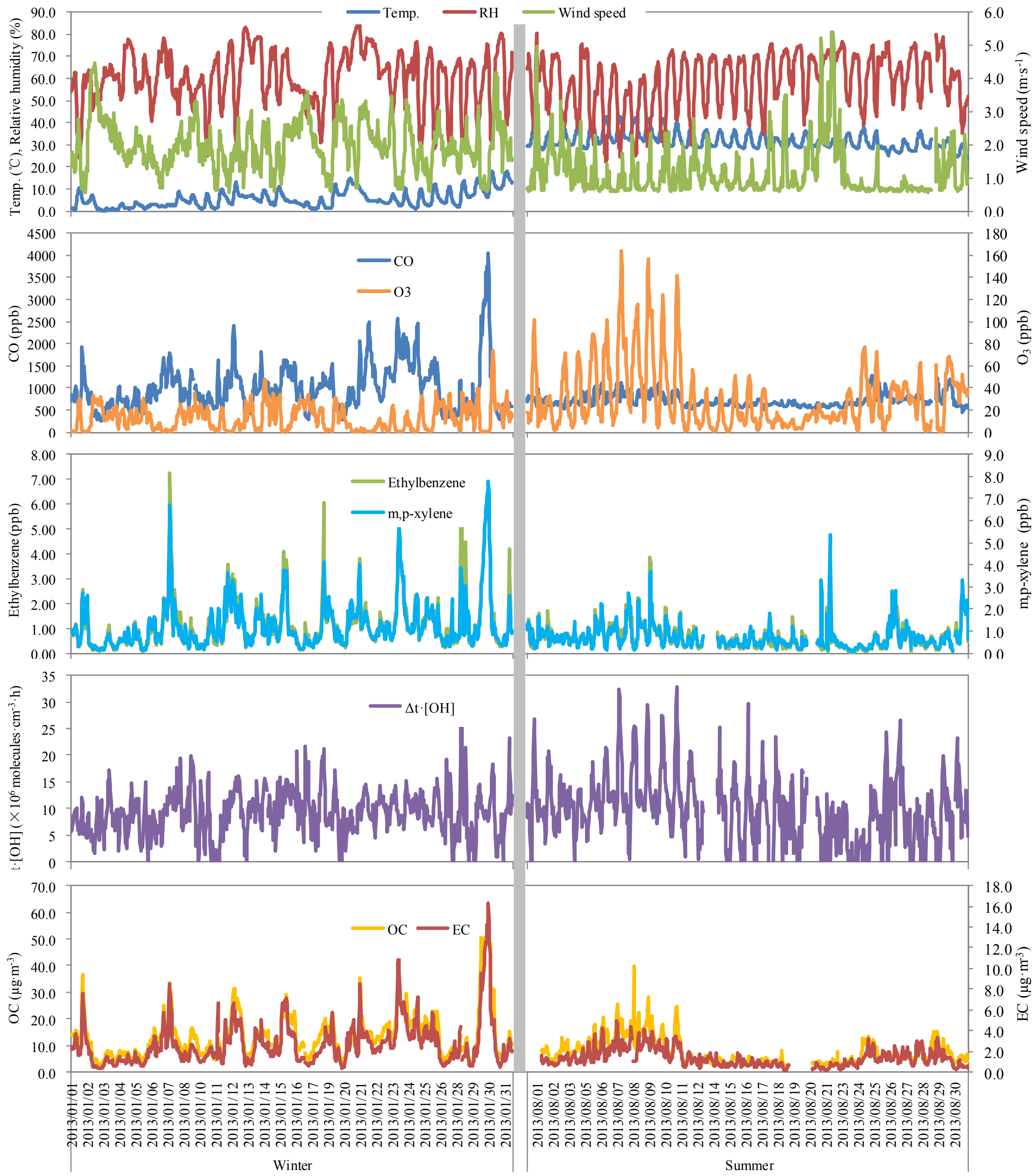


Fig. S1. Time series observation data of meteorological condition and CO, O_3, ethylbenzene, m,p-xylene, OC, and EC concentration in Shanghai urban in 2013.

3. Correlationship of ethylbenzene and m,p-xylene during the observation period

Fig. S2 shows the correlationship of hourly ethylbenzene and m,p-xylene concentration in the urban atmosphere during the observation period in Shanghai. It was indicated that these two species presented strong correlationship whether in summer or winter. The ratios of m,p-xylene to ethylbenzene were 1.09 and 1.04, and the correlation coefficients were 0.88 and 0.96 in summer and winter, respectively.

The correlationship implied that two species mainly came from the same source. According to the measured VOCs profiles from vehicle exhaust, vehicle emission could be the major source of m,p-xylene to ethylbenzene.

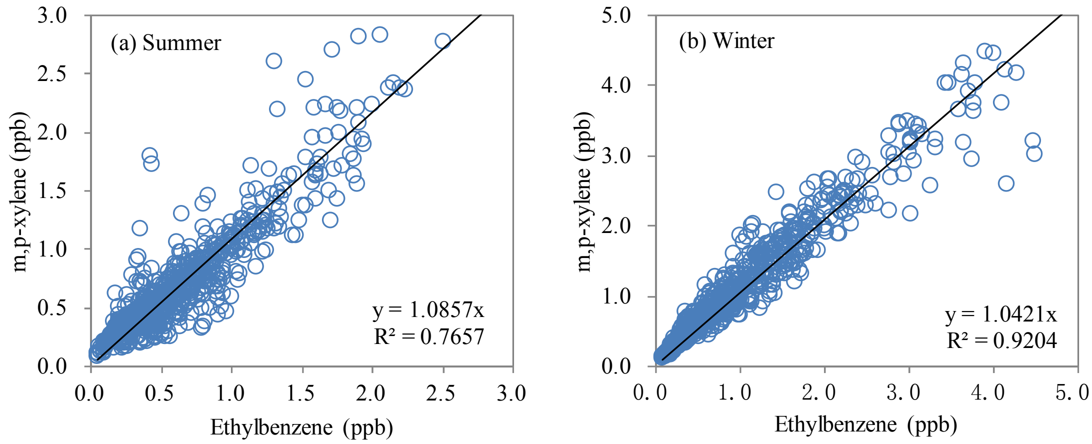
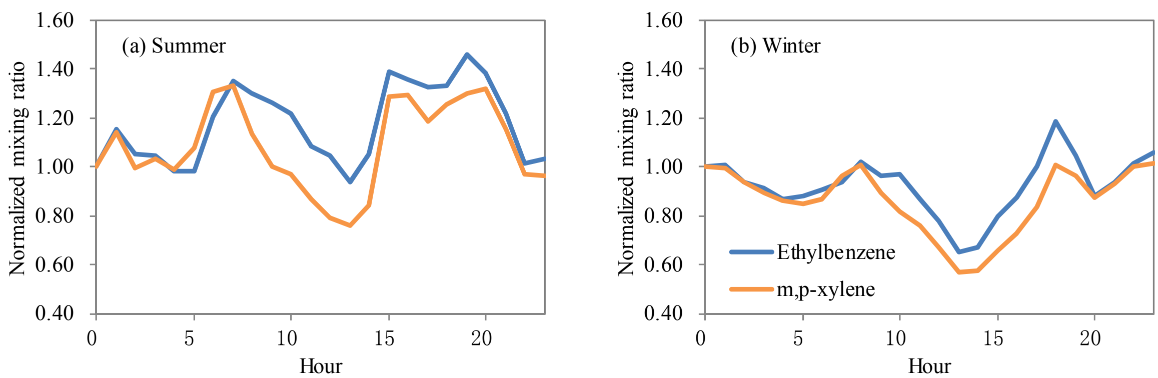


Fig. S2. Correlation between ethylbenzene and m,p-xylene mixing ratios in summer and winter in 2013.

Fig. S3 shows the diurnal distribution of average concentrations of ethylbenzene and m,p-xylene in summer and winter during the observation period. The average concentrations of ethylbenzene and m,p-xylene were normalized to 1 at 0:00 am. It was indicated that there was an obvious depletion of m,p-xylene compared with ethylbenzene in daytime. And more m,p-xylene depletion was observed in summer than in winter. On this account, we used the ratios of m,p-xylene to ethylbenzene to characterize the photochemical age.



(a) Summer (b) Winter

Fig. S3. Diurnal distribution of average concentrations of ethylbenzene and m,p-xylene in summer and winter in 2013.

4. CO emission inventory in Shanghai

Fig. S4 shows CO emission contribution of different sources in Shanghai in 2012. The methodology of CO emission inventory compilation has been introduced by Huang et al. (2011). The emission sources covered industry, transportation, residential and agriculture sectors. The industry sectors include fuel combustion processes of power plants, boilers, furnaces, kilns, and non-combustion processes such as iron and steel manufacturing, oil refining, cement producing, etc. Transport emission sources mainly consist of on-road and off-road vehicle exhaust and road dust emissions. The residential emission sources cover most of the emissions associated with daily life, such as residential fuel combustion emissions, domestic paint and solvent use, gas evaporation in service stations and so on. The agriculture emission sources mainly include the emissions from livestock feeding, fertilizer application and biomass burning. The activity data were updated to the year of 2012 from pollution source census data, national key pollution source list, and statistical yearbook. Total CO emission amount was 1236.1 tons in Shanghai in 2012. Vehicle was the second major source, taking up 27.8% of the total CO emission.

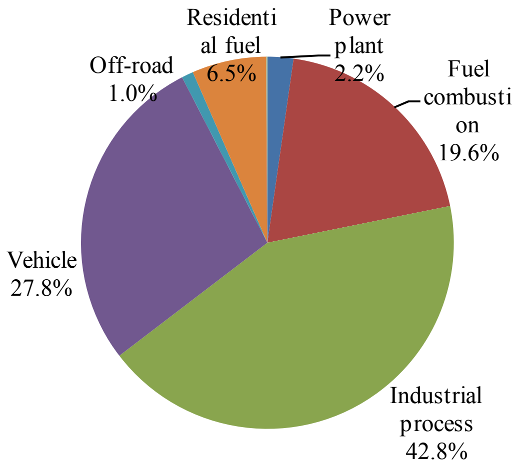


Fig. S4. CO emission contribution of different sources in Shanghai in2012.

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