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Supplementary Materials: Health Risk Assessment of Toxic and Harmful Air Pollutants Discharged by a Petrochemical Company in the Beijing-Tianjin-Hebei Region of China

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1. Total amount of pollutants and typical monomer test results

Due to various reasons, this study cannot perform sampling at the boundary of each emission source after diffusion. Therefore, Table S1 is a sample taken at the chimney opening of a stationary emission source according to the requirements of the China Environmental Protection Agency.

According to the test results, in the company's organized emissions, the main substances that constituted HAPs were benzene, toluene, and xylene. The sum of the mass concentrations of these three types of substances accounted for more than 75% of the total concentration of VOCs, and the sum of detection frequencies accounted for more than 85% of the total number of detections, far greater than the sum of other detected monomers. Among other VOC monomers, substances such as ethylbenzene, trimethylbenzene, dichlorobenzene, styrene, etc. were detected, appearing randomly and accidentally and therefore with no statistical value. Therefore, this study took benzene, toluene, and xylene as the main pollutants to participate in the statistics. The test results were shown in Table S1 below:

Table S1. The total amount of organized emissions of fixed sources of VOC and the test results of major pollutants.

Point	Type	Result	Mar	Jun	Sept	Min	Max	Average
A	VOCs	Concentration (mg/m³)	0.059	0.142	0.221	0.059	0.221	0.141
		Emission rate (kg/h)	2.4×10^{-3}	4.5×10^{-3}	7.8×10^{-3}	2.1×10^{-3}	7.9×10^{-3}	5.2×10^{-3}
	Benzene	Concentration (mg/m³)	0.013	0.007	0.019	0.007	0.019	0.013
		Emission rate (kg/h)	4.7×10^{-4}	2.5×10^{-4}	6.9×10^{-4}	2.5×10^{-4}	6.9×10^{-4}	4.7×10^{-4}
	Toluene	Concentration (mg/m³)	ND	0.007	0.019	ND	0.019	0.009
		Emission rate (kg/h)	7.3×10^{-5}	2.5×10^{-4}	6.9×10^{-4}	7.3×10^{-5}	6.9×10^{-4}	3.4×10^{-4}
	Xylene	Concentration (mg/m³)	ND	ND	0.130	ND	0.130	0.045
		Emission rate (kg/h)	7.3×10^{-5}	7.2×10^{-5}	4.6×10^{-3}	7.2×10^{-5}	4.6×10^{-3}	1.6×10^{-3}
B	VOCs	Concentration (mg/m³)	0.075	0.005	0.948	0.005	0.948	0.343
		Emission rate (kg/h)	2.1×10^{-3}	1.4×10^{-4}	2.5×10^{-2}	1.4×10^{-4}	2.5×10^{-2}	9.1×10^{-3}

Point	Type	Result	Mar	Jun	Sept	Min	Max	Average
	Benzene	Concentration (mg/m³)	0.026	0.005	0.100	0.005	0.100	0.044
		Emission rate (kg/h)	7.2×10^{-5}	1.6×10^{-5}	2.5×10^{-4}	1.6×10^{-5}	2.5×10^{-4}	1.1×10^{-4}
	Toluene	Concentration (mg/m³)	0.007	ND	0.060	ND	0.060	0.023
		Emission rate (kg/h)	2.0×10^{-4}	5.4×10^{-5}	1.6×10^{-3}	5.4×10^{-5}	1.6×10^{-3}	6.2×10^{-4}
	Xylene	Concentration (mg/m³)	0.011	0.109	ND	ND	0.109	0.041
		Emission rate (kg/h)	3.1×10^{-4}	2.9×10^{-3}	5.4×10^{-5}	5.4×10^{-5}	2.9×10^{-3}	1.1×10^{-3}
C	VOCs	Concentration (mg/m³)	0.220	ND	0.181	ND	0.223	0.138
		Emission rate (kg/h)	7.0×10^{-3}	6.3×10^{-5}	5.7×10^{-3}	6.3×10^{-5}	7.0×10^{-3}	4.3×10^{-3}
	Benzene	Concentration (mg/m³)	0.054	ND	0.160	ND	0.160	0.072
		Emission rate (kg/h)	1.7×10^{-3}	6.3×10^{-5}	5.1×10^{-4}	6.3×10^{-5}	5.1×10^{-4}	7.6×10^{-4}
	Toluene	Concentration (mg/m³)	0.004	ND	0.160	ND	0.160	0.055
		Emission rate (kg/h)	1.2×10^{-4}	6.3×10^{-5}	5.1×10^{-4}	6.3×10^{-5}	5.1×10^{-4}	2.3×10^{-4}
	Xylene	Concentration (mg/m³)	0.096	ND	ND	ND	0.096	0.033
		Emission rate (kg/h)	2.9×10^{-4}	6.3×10^{-4}	6.3×10^{-4}	6.3×10^{-4}	2.9×10^{-4}	1.0×10^{-4}
D	VOCs	Concentration (mg/m³)	0.079	ND	1.48	ND	1.48	0.52
		Emission rate (kg/h)	2.8×10^{-3}	7.0×10^{-5}	5.2×10^{-2}	7.0×10^{-5}	5.2×10^{-2}	1.8×10^{-2}
	Benzene	Concentration (mg/m³)	0.035	ND	0.105	ND	0.105	0.047
		Emission rate (kg/h)	1.3×10^{-3}	7.0×10^{-5}	3.7×10^{-3}	7.0×10^{-5}	3.7×10^{-3}	1.7×10^{-3}
	Toluene	Concentration (mg/m³)	ND	ND	0.091	ND	0.091	0.032
		Emission rate (kg/h)	7.1×10^{-5}	7.0×10^{-5}	3.2×10^{-3}	7.0×10^{-5}	3.2×10^{-3}	1.1×10^{-3}
	Xylene	Concentration (mg/m³)	ND	0.221	ND	ND	0.202	0.077
		Emission rate (kg/h)	7.1×10^{-5}	7.9×10^{-3}	7.0×10^{-5}	7.0×10^{-5}	7.9×10^{-3}	2.7×10^{-3}
E	VOCs	Concentration (mg/m³)	0.038	1.84	0.178	0.036	1.93	0.706
		Emission rate (kg/h)	2.1×10^{-3}	0.13	1.3×10^{-2}	2.1×10^{-3}	0.13	4.2×10^{-2}
	Benzene	Concentration (mg/m³)	0.013	0.009	0.014	0.009	0.014	0.012
		Emission rate (kg/h)	7.8×10^{-4}	5.5×10^{-4}	8.3×10^{-4}	5.5×10^{-4}	8.3×10^{-4}	7.2×10^{-4}
	Toluene	Concentration (mg/m³)	ND	0.051	0.019	ND	0.051	0.024

Point	Type	Result	Mar	Jun	Sept	Min	Max	Average
F		Emission rate (kg/h)	1.3×10^{-4}	3.2×10^{-3}	1.2×10^{-3}	1.3×10^{-4}	3.2×10^{-3}	1.5×10^{-3}
	Xylene	Concentration (mg/m^3)	ND	ND	1.50	ND	1.50	0.501
		Emission rate (kg/h)	1.1×10^{-4}	1.3×10^{-4}	9.0×10^{-2}	1.3×10^{-4}	9.2×10^{-2}	3.1×10^{-2}
	VOCs	Concentration (mg/m^3)	0.071	1.42	0.243	0.071	1.40	0.565
		Emission rate (kg/h)	1.1×10^{-3}	1.6×10^{-2}	2.8×10^{-3}	1.2×10^{-3}	1.6×10^{-2}	7.1×10^{-3}
	Benzene	Concentration (mg/m^3)	0.011	0.007	0.023	0.007	0.023	0.014
		Emission rate (kg/h)	1.5×10^{-5}	8.4×10^{-4}	2.7×10^{-5}	8.7×10^{-4}	2.6×10^{-5}	1.8×10^{-5}
	Toluene	Concentration (mg/m^3)	ND	0.026	0.028	ND	0.028	0.019
		Emission rate (kg/h)	2.9×10^{-5}	3.2×10^{-4}	3.4×10^{-4}	2.9×10^{-5}	3.4×10^{-4}	2.3×10^{-4}
	Xylene	Concentration (mg/m^3)	ND	ND	1.14	ND	1.14	0.381
		Emission rate (kg/h)	2.9×10^{-5}	2.4×10^{-5}	1.4×10^{-2}	2.4×10^{-5}	1.4×10^{-2}	4.7×10^{-3}
G	VOCs	Concentration (mg/m^3)	0.049	0.791	0.893	0.049	0.893	0.578
		Emission rate (kg/h)	4.2×10^{-3}	8.7×10^{-5}	5.9×10^{-2}	4.2×10^{-3}	5.9×10^{-2}	2.1×10^{-2}
	Benzene	Concentration (mg/m^3)	0.047	0.005	0.069	0.005	0.069	0.04
		Emission rate (kg/h)	4.0×10^{-3}	8.7×10^{-5}	4.6×10^{-3}	8.7×10^{-5}	4.6×10^{-3}	2.9×10^{-3}
	Toluene	Concentration (mg/m^3)	ND	0.018	0.059	ND	0.059	0.026
		Emission rate (kg/h)	8.8×10^{-5}	8.7×10^{-5}	3.3×10^{-3}	8.8×10^{-5}	3.3×10^{-3}	1.1×10^{-3}
	Xylene	Concentration (mg/m^3)	ND	0.118	0.636	ND	0.636	0.252
		Emission rate (kg/h)	8.8×10^{-5}	8.7×10^{-5}	9.4×10^{-3}	8.8×10^{-5}	9.4×10^{-3}	3.2×10^{-3}
H	VOCs	Concentration (mg/m^3)	0.394	1.58	1.42	0.394	1.58	1.131
		Emission rate (kg/h)	6.1×10^{-3}	2.4×10^{-2}	2.2×10^{-2}	6.1×10^{-3}	2.4×10^{-2}	1.7×10^{-2}
	Benzene	Concentration (mg/m^3)	0.089	0.007	0.112	0.007	0.112	0.069
		Emission rate (kg/h)	1.3×10^{-3}	1.2×10^{-3}	1.6×10^{-3}	1.2×10^{-3}	1.6×10^{-3}	1.5×10^{-3}
	Toluene	Concentration (mg/m^3)	0.006	0.038	0.079	0.008	0.078	0.03
		Emission rate (kg/h)	1.2×10^{-4}	5.6×10^{-4}	1.3×10^{-3}	1.2×10^{-4}	1.3×10^{-3}	6.2×10^{-4}
	Xylene	Concentration (mg/m^3)	0.200	0.195	1.24	0.195	1.24	0.545
		Emission rate (kg/h)	3.3×10^{-3}	3.1×10^{-3}	1.8×10^{-2}	3.1×10^{-3}	1.8×10^{-2}	8.3×10^{-3}

Point	Type	Result	Mar	Jun	Sept	Min	Max	Average
I	VOCs	Concentration（mg/m³）	0.062	0.145	0.950	0.062	0.950	0.386
		Emission rate（kg/h）	6.3×10^{-3}	0.14	8.9×10^{-2}	6.3×10^{-3}	0.14	7.8×10^{-2}
	Benzene	Concentration（mg/m³）	0.012	0.007	0.071	0.007	0.071	0.03
		Emission rate（kg/h）	1.2×10^{-3}	6.3×10^{-4}	6.6×10^{-3}	6.3×10^{-4}	6.6×10^{-3}	2.8×10^{-3}
	Toluene	Concentration（mg/m³）	ND	0.032	0.059	ND	0.059	0.031
		Emission rate（kg/h）	2.0×10^{-4}	3.1×10^{-3}	5.4×10^{-3}	2.0×10^{-4}	5.4×10^{-3}	2.9×10^{-3}
	Xylene	Concentration（mg/m³）	0.015	1.14	0.158	0.015	1.14	0.438
		Emission rate（kg/h）	1.6×10^{-3}	0.11	1.5×10^{-2}	1.6×10^{-3}	0.11	4.2×10^{-2}
J	VOCs	Concentration（mg/m³）	1.48	0.205	0.255	0.205	1.48	0.647
		Emission rate（kg/h）	0.14	1.9×10^{-2}	2.3×10^{-2}	1.9×10^{-2}	0.14	6.1×10^{-2}
	Benzene	Concentration（mg/m³）	1.17	0.205	0.198	0.205	1.17	0.524
		Emission rate（kg/h）	0.11	1.9×10^{-2}	1.8×10^{-2}	1.8×10^{-2}	0.11	4.9×10^{-2}
	Toluene	Concentration（mg/m³）	0.158	ND	0.016	ND	0.158	0.059
		Emission rate（kg/h）	1.4×10^{-2}	1.8×10^{-4}	1.4×10^{-3}	1.6×10^{-4}	1.3×10^{-2}	5.5×10^{-3}
	Xylene	Concentration（mg/m³）	0.013	0.016	ND	ND	0.016	0.01
		Emission rate（kg/h）	1.2×10^{-3}	1.5×10^{-3}	1.9×10^{-4}	1.9×10^{-4}	1.5×10^{-3}	9.6×10^{-4}
K	VOCs	Concentration（mg/m³）	0.300	2.21	0.329	0.300	2.21	0.946
		Emission rate（kg/h）	1.8×10^{-3}	1.4×10^{-2}	2.1×10^{-3}	1.6×10^{-3}	1.2×10^{-2}	5.7×10^{-3}
	Benzene	Concentration（mg/m³）	0.063	0.007	0.025	0.007	0.063	0.032
		Emission rate（kg/h）	3.7×10^{-4}	4.2×10^{-5}	1.5×10^{-4}	4.2×10^{-5}	3.7×10^{-4}	1.9×10^{-4}
	Toluene	Concentration（mg/m³）	0.006	0.048	0.033	0.008	0.047	0.030
		Emission rate（kg/h）	4.1×10^{-5}	3.0×10^{-4}	1.9×10^{-4}	4.1×10^{-5}	3.0×10^{-4}	1.8×10^{-4}
	Xylene	Concentration（mg/m³）	0.143	0.011	1.84	0.011	1.84	0.665
		Emission rate（kg/h）	8.3×10^{-4}	6.6×10^{-5}	1.1×10^{-2}	6.6×10^{-5}	1.1×10^{-2}	4.0×10^{-3}

Note: "ND" was not detected. The detection limit of this method was 0.004mg/m³. For undetected items, the emission rate and average value will be calculated based on half of the detection limit.

2. Statistics of test results of main pollutants from stationary sources

According to the survey results, the average total emission concentration of VOCs from 11 fixed pollution sources was between 0.138mg/m³ and 1.310mg/m³. According to the single test result, the emission concentration was between ND ~2.210mg/m³. The two pollution sources with the highest average concentration were H and K, and their concentrations were 1.310mg/m³ and 0.946mg/m³ respectively. The highest concentrations of a single test were K and E, and their concentrations were 2.210 mg/m³ and 1.930 mg/m³ respectively. As shown in Figure S1:

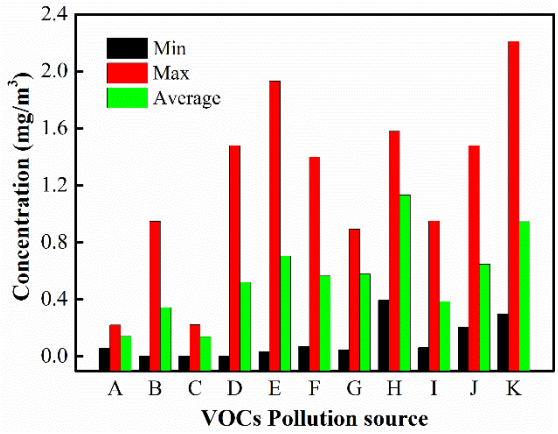

Figure S1. Distribution of VOCs emission concentration.

The average emission concentration of benzene in 11 fixed pollution sources was between 0.012mg/m³ and 0.524mg/m³. The distribution range of the single test result was between ND ~ 1.170mg/m³. The two pollution sources with the highest average concentration were J and C, and their concentrations were respectively 0.524mg/m³ and 0.072mg/m³. The highest concentrations in a single detection were J and C, and their concentrations were 1.170 mg/m³ and 0.160 mg/m³ respectively. As shown in Figure S2:

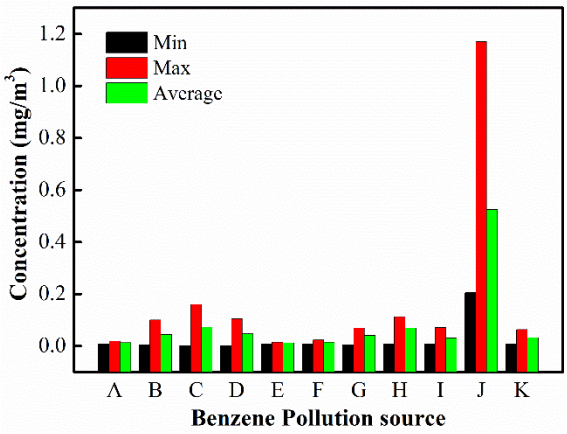

Figure S2. Distribution of benzene emission concentration.

The average emission concentration of toluene in the 11 fixed pollution sources was between 0.009mg/m³~0.059mg/m³. The distribution range of this single test result was between ND ~0.160mg/m³. The two pollution sources with the highest average concentration were J and C, and their concentrations were respectively 0.059mg/m³ and 0.055mg/m³. The highest concentrations in a single detection were J and C, and their concentrations were 0.158mg/m³ and 0.160mg/m³, respectively. As shown in Figure S3:

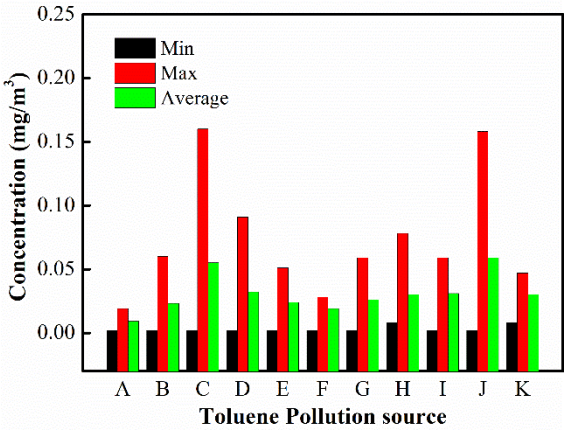

Figure S3. Concentration distribution of toluene emission.

The average emission concentration of xylene from the 11 fixed pollution sources was between 0.010mg/m^3 and 0.665mg/m^3. The distribution range of this single test result was between ND ~1.840mg/m^3. The two pollution sources with the highest average concentration were K and H, and their concentrations were 0.665mg/m^3 and 0.545mg/m^3 respectively. The highest concentrations in a single detection were K and E, and their concentrations were 1.840mg/m^3 and 1.500mg/m^3 respectively. As shown in Figure S4:

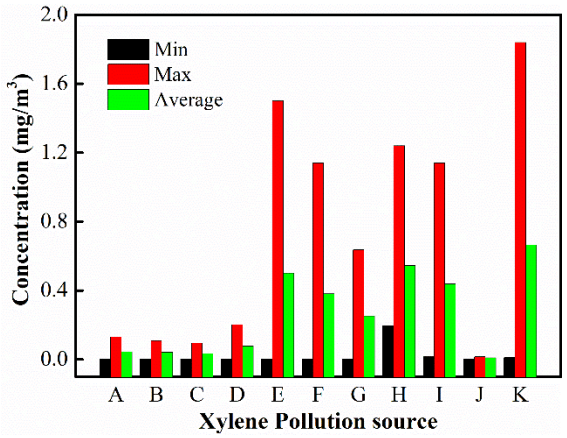

Figure S4. Distribution of xylene emission concentration.

According to Figure S5, it could be seen that the average VOC emission rate of 11 fixed pollution sources ranges from 4.3×10^{-3}kg/h to 7.8×10^{-2}kg/h. The single test result was between 6.3×10^{-5}kg/h~0.14kg/h. The two pollution sources with the highest average emission rate were I and J, with emission rates of 7.8×10^{-2}kg/h and 6.1×10^{-2}kg/h respectively. The highest concentrations in a single test were I and J, and their concentrations were both 0.14 kg/h.

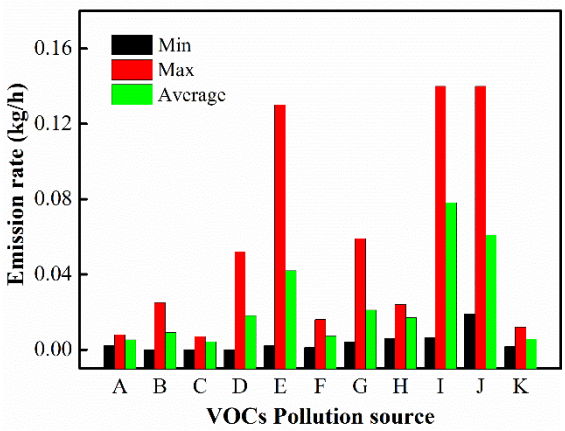

Figure S5. Distribution of VOCs emission rate.

According to Figure S6, it could be seen that the average emission rate of benzene from the 11 fixed pollution sources was between 1.8×10^{-5}kg/h and 4.9×10^{-2}kg/h. The single test result was between 1.6×10^{-5}kg/h~0.11kg/h. The two pollution sources with the highest average emission rate were J and G, and their emission rates were 4.9×10^{-2}kg/h and 2.9×10^{-3}kg/h respectively. The highest concentrations in a single test were J and I, and their concentrations were 0.11kg/h and 6.6×10^{-3}kg/h respectively.

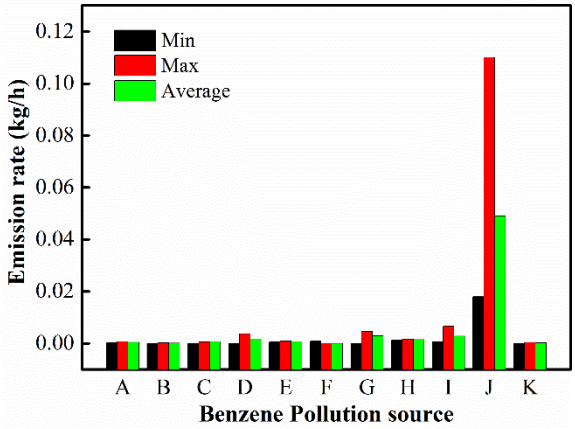

Figure S6. Distribution of benzene emission rate.

According to Figure S7, it could be seen that the average toluene emission rate of 11 fixed pollution sources was between 1.8×10^{-4}kg/h~5.5×10^{-3}kg/h. The result of a single test was between 2.9×10^{-5}kg/h and 1.3×10^{-2}kg/h. The two pollution sources with the highest average emission rate were J and I, and their emission rates were 5.5×10^{-3}kg/h and 2.9×10^{-3}kg/h respectively. The highest concentration in a single test was J and I, and their concentrations were 1.3×10^{-2}kg/h and 5.4×10^{-3}kg/h respectively.

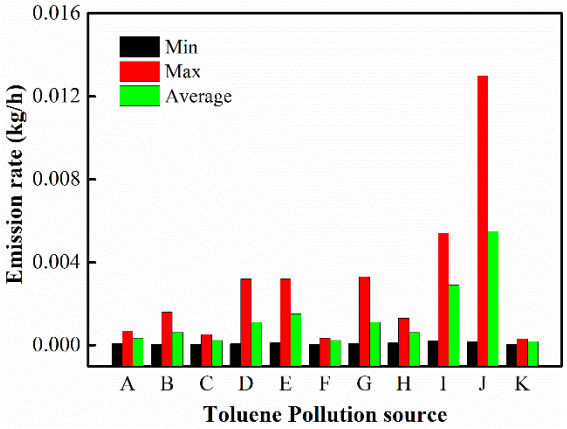

Figure S7. Distribution of toluene emission rate.

According to Figure S8, it could be seen that the average emission rate of xylene from the 11 fixed pollution sources was between 1×10^{-4}kg/h and 4.2×10^{-2}kg/h. The result of a single test was between 2.4×10^{-5}kg/h~0.11kg/h. The two pollution sources with the highest average emission rate were I and E, and their emission rates were 4.2×10^{-2}kg/h and 3.1×10^{-2}kg/h, respectively. The highest concentrations in a single test were I and E, and their concentrations were 0.11kg/h and 9.2×10^{-2}kg/h respectively.

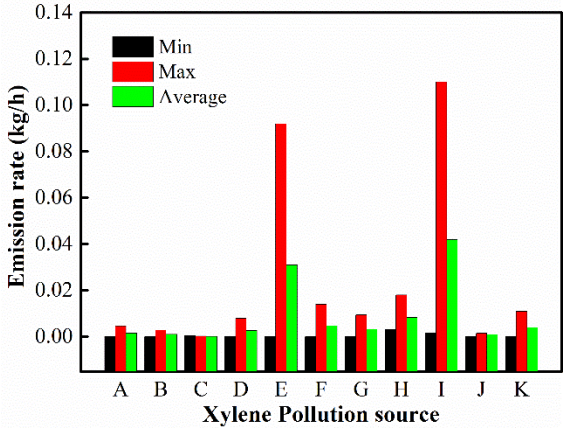

Figure S8. Xylene emission rate distribution.

3. Statistics of typical pollutant emissions

According to the emission concentration and emission intensity, the maximum emission values of benzene, toluene, and xylene were counted. The situation was shown in Table S2 and Table S3:

Table S2. Statistics of the maximum emission concentration of benzene, toluene and xylene.

Type	Benzene		Toluene		Xylene	
	Point	Concentration (mg/m³)	Point	Concentration (mg/m³)	Point	Concentration (mg/m³)
Max average	J	0.524	J	0.059	K	0.665
	C	0.072	C	0.055	H	0.545
Single Max	J	1.170	J	0.158	K	1.840
	C	1.600	C	0.160	E	1.500

Table S3. Statistics of maximum emission intensity of benzene, toluene and xylene.

Type	Benzene	Toluene	Xylene

	Point	Rate（kg/h）	Point	Rate（kg/h）	Point	Rate（kg/h）
Max average	J	4.9×10^{-2}	J	5.5×10^{-3}	I	4.2×10^{-2}
	G	2.9×10^{-3}	I	2.9×10^{-3}	E	3.1×10^{-2}
Single Max	J	0.11	J	1.3×10^{-2}	I	0.11
	I	6.6×10^{-3}	I	5.4×10^{-3}	E	9.2×10^{-2}

4. Discharge points of fixed pollution sources in the factory

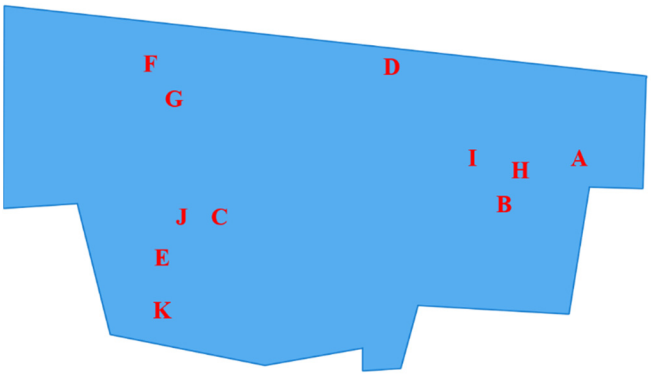

Figure S9. Stationary pollution source discharge point.