Principal component analysis and mapping to characterize the emission of volatile organic compounds in a typical petrochemical industrial park

Supplementary material

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Tables S1 through S3 provide the information regarding the VOCs emitted from 20 companies including 519,442 sources in the study site from 2012 and 2014.

Table S1. VOCs emitted from 20 companies including 519,442 sources in the study site in 2012

	Emission (ton/year)																				MDL (ppbv)
	F01	F02	F03	F04	F05	F06	F07	F08	F09	F10	F11	F12	F13	F14	F15	F16	F17	F18	F19	F20	
1,2-Dichloroethane	1.02E+00	2.72E+00	9.21E-01	1.61E-02	3.71E-01	9.66E-02	8.04E-03	1.06E+01	2.30E-02	3.01E-01	9.02E-03	ND	1.66E-01	7.00E-03	3.43E-04	2.15E-02	ND	1.30E-02	5.00E-03	5.42E-03	0.14
Tetrachloroethylene	2.70E-02	ND	1.40E-02	1.60E-02	3.28E-04	1.50E-01	1.30E-02	2.03E-01	3.80E-02	3.01E-01	1.50E-02	ND	2.21E-01	5.00E-03	1.78E-04	2.90E-02	ND	2.10E-02	2.25E-04	6.00E-03	0.28
Ethanal	2.33E+00	5.40E-02	ND	7.71E-01	5.00E-03	ND	ND	1.69E-01	6.50E-02	2.60E-02	5.10E-02	2.55E-01	ND	ND	ND	1.50E-02	ND	2.20E-02	ND	9.30E-02	6.20
Acrylonitrile	4.90E-06	ND	4.00E-03	ND	3.41E-04	5.83E-01	4.52E-03	6.20E-02	1.30E-02	ND	2.31E+00	ND	5.10E-02	1.00E-03	1.61E-04	1.40E-02	ND	7.00E-03	3.01E-03	2.00E-03	0.22
Benzene	5.28E+01	1.00E-03	2.66E-02	3.02E-02	5.68E-04	9.26E-02	3.96E-01	5.41E-01	9.48E+00	3.01E-01	4.40E-02	9.42E-03	5.02E-01	2.82E-03	7.53E-03	1.81E-02	ND	1.00E-02	2.10E-02	6.11E-02	0.24
Carbon tetrachloride	ND	ND	1.30E-02	1.60E-02	3.41E-04	1.45E-01	1.20E-02	2.62E+00	3.70E-02	3.01E-01	1.40E-02	ND	2.16E-01	4.00E-03	1.83E-04	2.80E-02	ND	2.00E-02	2.17E-04	6.00E-03	0.23
Chloroform	1.47E+00	4.81E-01	1.59E-01	4.74E-02	2.24E-02	1.96E-01	8.40E-02	ND	9.11E-01	3.01E-01	2.40E-02	2.80E-04	9.94E-01	4.00E-03	6.18E-03	1.03E-01	2.00E-02	2.70E-02	1.72E-04	5.90E-02	0.24
Ethylbenzene	1.04E+01	7.76E-04	2.47E+00	1.80E-02	4.65E-04	1.08E-01	7.03E-01	1.67E-01	2.10E+00	3.01E-01	1.77E+00	8.73E-04	1.75E-01	3.19E-03	2.46E-03	2.25E-02	ND	1.40E-02	7.37E-03	1.30E-02	0.24
Ethylene oxide	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	1.41E+00	ND	9.78E-02	ND	9.84E-02	ND	ND	ND	0.14
Formaldehyde	1.80E+00	6.20E-02	ND	1.40E-02	7.10E-04	ND	ND	2.66E-01	1.26E-01	6.40E-02	1.01E-01	2.25E-01	ND	ND	ND	2.20E-02	ND	4.90E-01	ND	7.30E-02	7.90
Dichloromethane	2.20E-02	2.00E-02	4.12E-02	1.60E-02	2.24E-02	9.60E-02	2.30E-01	3.00E-03	2.00E-02	3.01E-01	8.04E-03	ND	1.54E-01	ND	1.15E-03	1.92E-02	1.01E-03	1.20E-02	1.03E-03	1.38E-02	0.26
Epoxypropane	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	8.81E-03	ND	1.02E+00	ND	ND	ND	0.18
Styrene	4.69E-01	4.56E-07	1.02E+00	1.60E-02	3.55E-04	3.22E-01	1.20E-02	1.34E-01	1.21E+00	3.01E-01	3.94E+00	1.66E-04	1.75E-01	3.19E-03	1.62E-03	2.20E-02	ND	1.40E-02	1.53E-04	1.59E-02	0.19
Trichloroethene	ND	3.30E-02	1.10E-02	1.60E-02	3.38E-04	1.23E-01	1.00E-02	1.61E-01	3.10E-02	3.01E-01	1.20E-02	ND	1.93E-01	4.00E-03	1.76E-04	2.50E-02	ND	1.70E-02	1.84E-04	5.00E-03	0.21
Chloroethene	6.20E-01	6.57E-01	5.15E-01	1.60E-02	3.14E-04	5.55E-02	5.64E-03	7.70E-02	1.40E-02	3.01E-01	5.00E-03	ND	1.24E-01	7.02E-01	1.50E-04	1.30E-02	ND	7.00E-03	5.19E-04	3.05E-03	0.27
1,3-Butadiene	2.76E+01	4.27E-06	4.72E-02	2.98E-06	3.16E-04	4.96E+00	2.01E-02	6.40E-02	1.26E-02	2.13E-05	8.23E-01	1.10E-02	5.20E-02	1.00E-03	1.61E-04	7.20E-02	ND	7.00E-03	7.63E-05	3.52E-03	0.44
Vinyl acetate	ND	ND	6.00E-03	ND	1.10E+00	8.36E-02	9.04E-03	9.30E-02	2.10E-02	ND	8.00E-03	3.00E-03	8.40E-02	2.00E-03	1.70E-04	1.90E-02	6.35E-05	1.10E-02	2.11E+00	3.00E-03	0.24
Cumene	2.15E-01	ND	7.01E-02	1.62E-02	3.85E-04	1.24E-01	9.00E+00	2.50E-04	3.60E-02	1.20E-02	2.07E-01	2.81E-07	1.87E-01	4.36E-04	4.65E-04	2.42E-02	ND	1.60E-02	2.03E-04	1.61E-02	0.15

- Numbers represented by the emissions in ton/year.
- ND and MDL denote non-detected and method detection limit, respectively.

Table S2. VOCs emitted from 20 companies including 519,442 sources in the study site in 2013

	Emission (ton/year)																				MDL (ppbv)
	F01	F02	F03	F04	F05	F06	F07	F08	F09	F10	F11	F12	F13	F14	F15	F16	F17	F18	F19	F20	
1,2-Dichloroethane	4.39E+00	7.39E+00	1.26E+00	1.44E-02	2.36E-04	7.33E-02	6.90E-03	1.08E+01	2.06E-02	2.30E-02	1.18E-02	ND	8.60E-02	8.18E-03	3.36E-04	8.11E-01	6.62E-04	3.00E-02	3.54E-03	2.30E-02	0.14
Tetrachloroethylene	2.55E-02	ND	1.32E-02	ND	2.20E-04	1.14E-01	1.14E-02	2.86E-01	3.39E-02	1.74E-01	1.72E-02	ND	1.35E-01	5.00E-03	2.05E-04	9.94E-02	ND	4.59E-02	1.62E-04	6.58E-03	0.28
Ethanal	3.46E+00	4.57E-02	ND	1.35E+00	2.27E-03	ND	ND	1.83E-02	4.96E-02	1.72E-02	4.40E-02	1.56E-01	ND	ND	ND	6.26E-02	ND	5.05E-02	ND	2.76E-01	6.20
Acrylonitrile	4.84E-06	ND	4.00E-03	ND	2.29E-04	5.30E-01	3.90E-03	8.73E-02	1.15E-02	ND	1.11E+00	ND	4.52E-02	1.00E-03	1.61E-04	3.68E-02	ND	1.59E-02	2.13E-02	2.25E-03	0.22
Benzene	4.35E+01	9.67E-04	4.26E-02	2.91E-02	6.11E-04	7.46E-02	2.27E-01	2.82E-01	2.21E+00	1.74E-01	3.01E-02	5.52E-03	3.83E-01	3.06E-03	7.04E-03	5.18E-02	ND	2.29E-02	2.06E-01	2.94E-01	0.24
Carbon tetrachloride	ND	ND	1.22E-02	ND	2.29E-04	1.10E-01	1.03E-02	2.83E+00	3.08E-02	1.74E-01	1.72E-02	ND	1.30E-01	4.00E-03	2.08E-04	9.58E-02	ND	4.41E-02	1.56E-04	5.53E-03	0.23
Chloroform	1.83E+00	3.85E+00	9.60E-02	2.40E-02	5.80E-01	1.66E-01	1.08E+00	2.15E-01	2.55E-02	1.70E-01	3.10E-02	1.44E-04	3.12E-01	4.29E-03	2.44E-02	2.15E-01	4.13E-03	5.03E-02	1.23E-04	1.96E-01	0.24
Ethylbenzene	7.58E+00	5.65E-04	2.41E+00	3.56E-03	3.41E-04	8.89E-02	4.21E-01	2.03E-01	3.82E-01	1.79E-01	2.05E+00	2.05E-06	9.27E-02	3.24E-03	4.68E-03	7.02E-02	ND	3.23E-02	4.37E-02	5.30E-02	0.24
Ethylene oxide	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	3.83E+00	ND	4.65E-02	ND	8.85E-02	ND	ND	ND	0.14
Formaldehyde	4.82E+00	5.22E-02	ND	1.13E-02	3.22E-04	ND	ND	2.87E-02	1.10E-01	4.22E-02	8.72E-02	1.24E-01	ND	ND	ND	8.85E-02	ND	1.10E+00	ND	1.93E-01	7.90
Dichloromethane	1.86E-02	ND	9.06E-02	2.80E-01	2.53E-04	7.59E-02	8.44E-03	8.46E-09	1.61E-02	1.75E-01	1.02E-02	ND	7.49E-02	ND	1.10E-03	5.55E-02	6.14E-06	2.55E-02	1.45E-03	4.14E-03	0.26
Epoxypropane	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	4.22E-03	ND	1.07E+00	ND	ND	ND	0.18
Styrene	3.44E-01	3.45E-03	1.05E+00	3.04E-07	2.38E-04	2.67E-01	1.07E-02	1.89E-01	1.02E+00	1.75E-01	4.45E+00	ND	9.26E-02	3.24E-03	3.07E-03	6.99E-02	ND	3.18E-02	1.10E-04	1.48E-02	0.19
Trichloroethene	ND	ND	1.05E-02	ND	2.27E-04	9.28E-02	8.86E-03	2.27E-01	2.68E-02	1.74E-01	1.35E-02	ND	1.10E-01	4.00E-03	1.95E-04	8.08E-02	ND	3.71E-02	1.32E-04	4.43E-03	0.21
Chloroethene	2.61E+00	2.62E+00	1.25E+00	ND	2.11E-04	4.29E-02	4.84E-03	1.08E-01	1.19E-02	1.74E-01	6.75E-03	ND	4.87E-02	7.96E-01	1.52E-04	3.62E-02	ND	1.59E-02	3.73E-04	2.60E-03	0.27
1,3-Butadiene	2.04E+01	2.81E-02	1.00E-01	2.85E-06	2.14E-04	3.77E+00	5.20E-02	8.73E-02	1.13E-02	1.17E-05	9.44E-01	4.09E-03	4.61E-02	1.00E-03	1.89E-03	7.01E-02	ND	1.59E-02	5.48E-05	1.04E-02	0.44
Vinyl acetate	ND	ND	5.85E-03	ND	1.51E+00	6.32E-02	6.82E-03	1.30E-01	1.73E-02	ND	1.02E-02	1.08E-03	7.44E-02	2.00E-03	1.79E-04	5.54E-02	6.85E-05	2.47E-02	1.21E+00	3.29E-03	0.24
Cumene	1.49E-01	ND	8.48E-02	1.48E-04	2.54E-04	9.56E-02	8.33E+00	9.05E-05	1.25E-03	1.78E-06	2.44E-01	3.58E-07	1.04E-01	5.64E-04	6.86E-04	7.72E-02	ND	3.53E-02	4.15E-04	2.17E-02	0.15

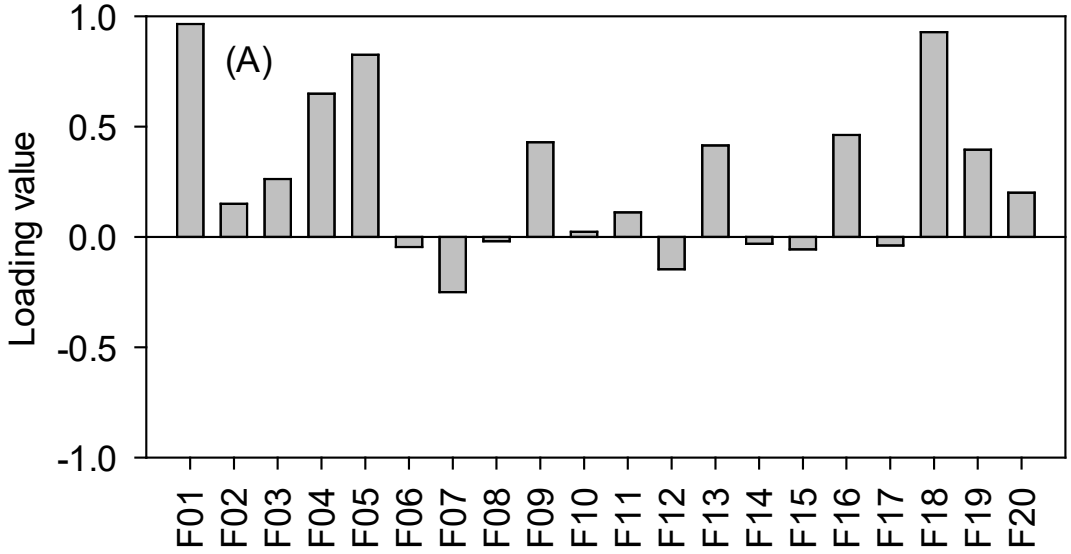
- Numbers represented by the emissions in ton/year.
- ND and MDL denote non-detected and method detection limit, respectively.

Table S3. VOCs emitted from 20 companies including 519,442 sources in the study site in 2014

	Emission (ton/year)																				MDL (ppbv)
	F01	F02	F03	F04	F05	F06	F07	F08	F09	F10	F11	F12	F13	F14	F15	F16	F17	F18	F19	F20	
1,2-Dichloroethane	1.84E+00	1.04E+00	1.79E+00	2.25E-02	3.53E-04	7.26E-02	9.49E-03	1.18E+01	1.56E-02	1.51E-03	1.11E-02	ND	9.01E-02	8.88E-03	6.89E-03	5.05E-02	ND	1.92E-02	3.54E-03	3.81E-02	0.14
Tetrachloroethylene	9.77E-01	ND	2.06E-01	ND	3.29E-04	1.12E-01	1.58E-02	2.16E-01	2.55E-02	1.61E-01	1.62E-02	ND	1.41E-01	5.00E-03	6.74E-03	7.50E-02	ND	2.94E-02	1.62E-04	2.98E-02	0.28
Ethanal	2.98E+00	3.99E-02	ND	6.03E-01	1.35E-02	ND	ND	1.83E-02	1.98E-02	ND	7.45E-02	2.15E-01	ND	ND	ND	4.69E-02	ND	3.24E-02	0.00E+00	2.07E-01	6.20
Acrylonitrile	4.60E-06	ND	3.99E-03	ND	3.42E-04	5.09E-01	5.23E-03	6.60E-02	8.68E-03	ND	1.21E+00	ND	4.73E-02	1.00E-03	2.02E-04	2.81E-02	ND	1.02E-02	9.12E-04	1.90E-03	0.22
Benzene	4.18E+01	9.67E-04	3.89E-01	2.75E-02	1.12E-03	7.06E-02	2.59E-01	2.07E-01	1.89E+00	1.61E-01	3.00E-02	5.93E-03	4.01E-01	3.21E-03	1.46E-02	3.94E-02	ND	1.47E-02	2.20E-03	2.09E-01	0.24
Carbon tetrachloride	9.53E-01	ND	3.64E-01	ND	3.42E-04	1.09E-01	1.43E-02	3.07E+00	2.27E-02	1.61E-01	1.62E-02	ND	1.36E-01	4.00E-03	6.77E-03	7.23E-02	ND	2.83E-02	1.56E-04	2.90E-02	0.23
Chloroform	5.05E+00	5.29E+00	5.90E-01	2.28E-02	1.17E+00	1.69E-01	9.33E-01	1.14E-01	1.92E-02	1.61E-01	1.26E-02	1.44E-04	1.41E+00	4.47E-03	4.97E-02	1.29E-01	2.60E-03	2.26E-02	1.23E-04	3.05E-02	0.24
Ethylbenzene	8.34E+00	4.37E-04	2.76E+00	1.60E-03	5.34E-04	8.73E-02	4.15E-01	1.50E-01	3.60E-01	1.61E-01	1.94E+00	3.39E-06	9.71E-02	3.27E-03	1.75E-02	5.32E-02	ND	2.07E-02	2.88E-03	5.66E-02	0.24
Ethylene oxide	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	2.05E+00	ND	8.86E-02	ND	8.77E-02	ND	ND	ND	0.14
Formaldehyde	3.65E+00	4.59E-02	0.00E+00	2.32E-04	1.92E-03	ND	ND	2.87E-02	8.89E-02	ND	1.47E-01	2.37E-01	ND	ND	ND	6.63E-02	ND	7.04E-01	ND	1.52E-01	7.90
Dichloromethane	2.28E+00	ND	4.23E-01	ND	3.72E-04	7.65E-02	2.29E-01	2.23E-03	1.19E-02	1.61E-01	9.63E-03	ND	7.86E-02	ND	7.94E-03	4.22E-02	6.51E-06	1.63E-02	4.85E-04	2.80E-02	0.26
Epoxypropane	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	ND	8.04E-03	ND	1.13E+00	ND	ND	ND	0.18
Styrene	1.23E+00	1.78E-07	1.07E+00	3.20E-07	3.56E-04	2.18E-01	1.36E-02	1.43E-01	9.97E-01	1.61E-01	4.21E+00	ND	9.71E-02	3.27E-03	1.03E-02	5.29E-02	ND	2.04E-02	1.10E-04	4.51E-02	0.19
Trichloroethene	9.53E-01	ND	3.62E-01	ND	3.38E-04	9.18E-02	1.23E-02	1.72E-01	2.00E-02	1.61E-01	1.27E-02	ND	1.15E-01	4.00E-03	6.72E-03	6.10E-02	ND	2.38E-02	1.32E-04	2.79E-02	0.21
Chloroethene	1.36E+00	4.31E-01	9.77E-01	ND	3.15E-04	4.25E-02	6.48E-03	8.20E-02	9.10E-03	1.61E-01	6.36E-03	ND	5.10E-02	1.08E+00	6.67E-03	2.75E-02	ND	1.02E-02	3.73E-04	2.63E-02	0.27
1,3-Butadiene	2.07E+01	1.67E-06	4.33E-01	3.00E-06	3.20E-04	3.46E+00	1.74E-02	6.75E-02	8.25E-03	1.10E-05	2.57E-01	1.90E-02	4.82E-02	1.00E-03	6.55E-03	6.30E-02	ND	1.02E-02	5.48E-05	3.04E-02	0.44
Vinyl acetate	ND	ND	5.83E-03	ND	2.81E+00	6.26E-02	8.09E-03	9.92E-02	1.25E-02	ND	9.59E-03	5.00E-03	7.79E-02	2.00E-03	2.38E-04	4.21E-02	7.27E-05	1.59E-02	6.56E-01	2.82E-03	0.24
Cumene	1.10E+00	ND	4.33E-01	1.81E-04	3.74E-04	9.43E-02	2.69E+01	4.56E-05	1.19E-03	1.33E-06	2.31E-01	5.93E-07	1.10E-01	6.40E-04	1.61E-03	5.84E-02	ND	2.26E-02	1.28E-04	2.78E-02	0.15

- Numbers represented by the emissions in ton/year.
- ND and MDL denote non-detected and method detection limit, respectively.

In Fig. S1A that depicts the result of PC4 accounting for 11.5% of the total data variance, the companies with the loading value greater than 0.6 comprised F10, F12, and F14. Figs. S1B through S1D further illustrate the ratios of different sources contributing to the VOC emissions in the critical companies from 2012 to 2014. The VOC emitted from the wastewater treatment plants (WWTPs) appeared to be relatively more important in these companies (the contribution ratios ranged from 53.9% to 74.6%, from 39.7% to 66.9%, and from 23.7% to 54.9% in 2012, 2013, and 2014, respectively). In the result of PC5 (9.0% of the data variance), the critical company was F11 (Fig. S2A). It was indicated in Figs. S2B through S2D, the stack was the dominant source (the contribution ratios ranged from 44.6% to 60.9% during the period of 2012 to 2014).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F01
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F03
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F05
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F18
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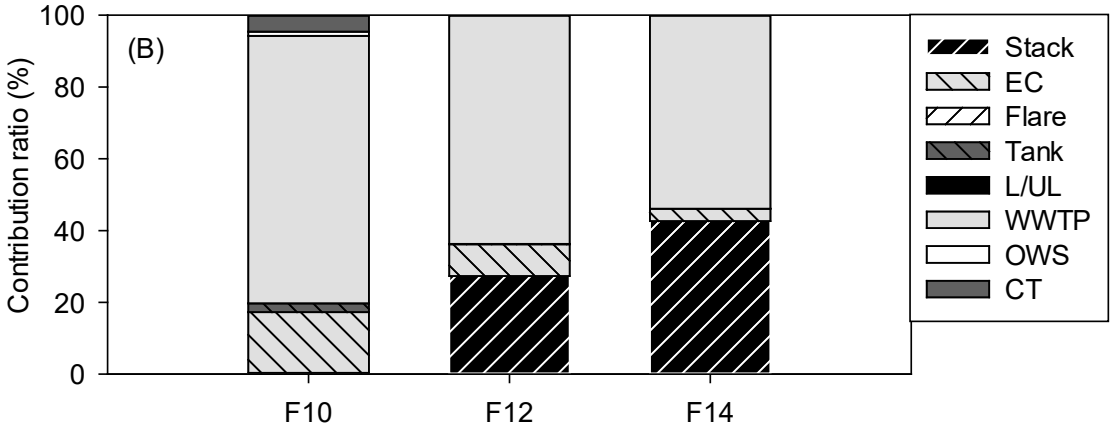
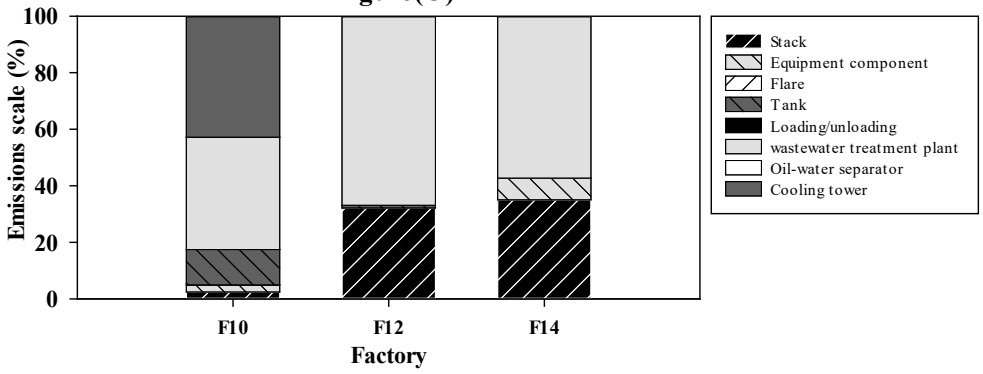

(B)
Contribution ratio (%)
100
80
60
40
20
0
F10
F12
F14
Stack
EC
Flare
Tank
L/UL
WWTP
OWS
CT

Figure(O)


Emissions scale (%)
100
80
60
40
20
0
F10
F12
F14
Factory
Stack
Equipment component
Flare
Tank
Loading/unloading
wastewater treatment plant
Oil-water separator
Cooling tower

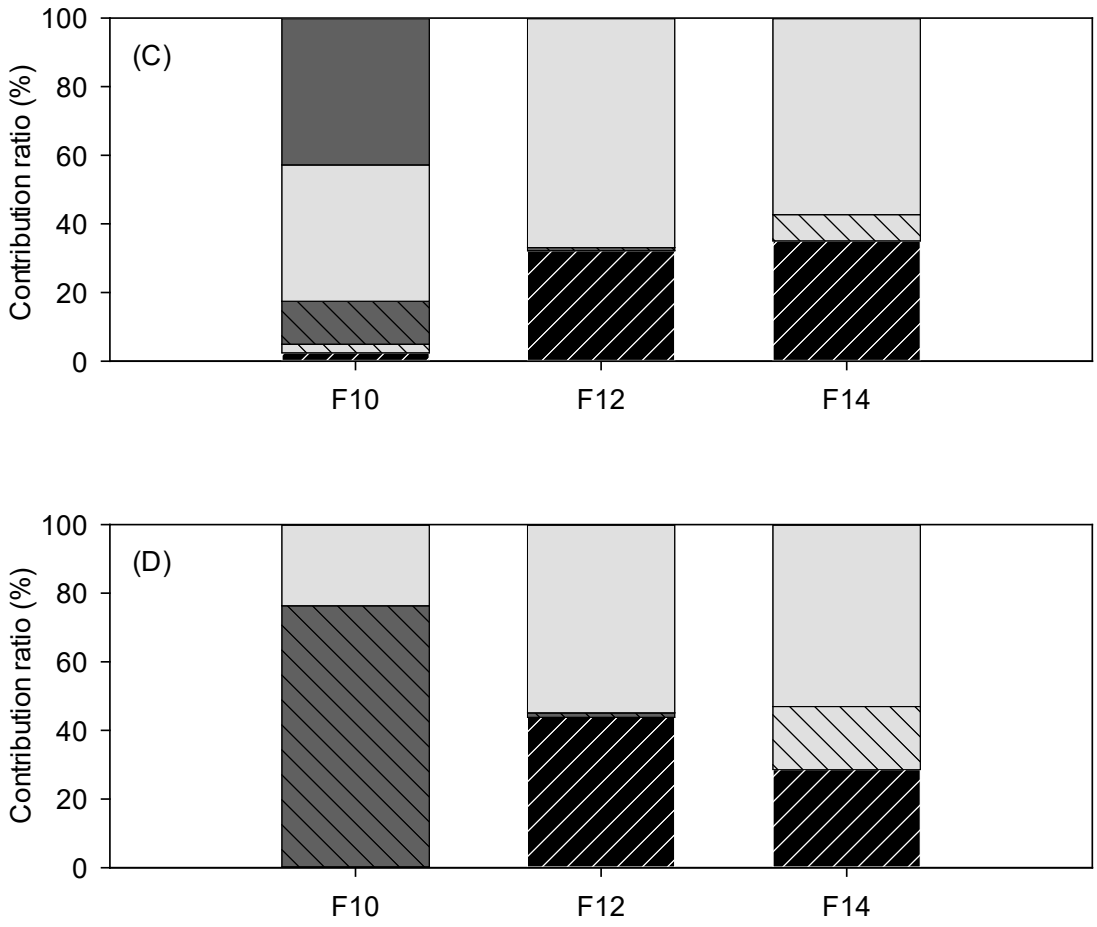
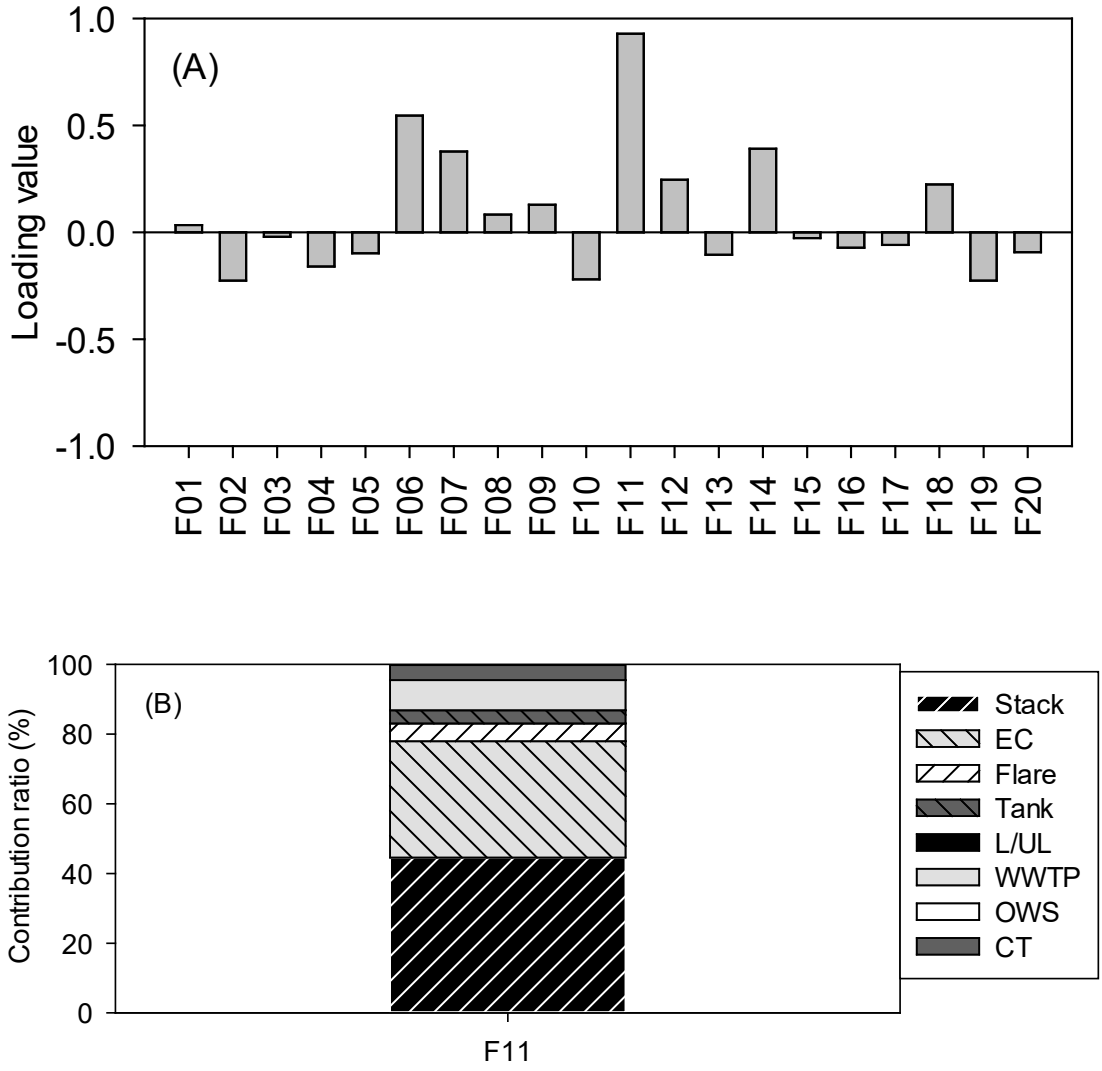


Figure S1. (A) Loading values of 20 companies in the 4th principal component (PC4) and contribution ratios of different sources in the critical companies in PC1 in (B) 2012, (C) 2013, and (D) 2014. EC, L/UL, WWTP, OLS, and CT denote equipment component, loading/unloading, wastewater treatment plant, oil-water separator, and cooling tower, respectively.


(A)
Loading value
1.0
0.5
0.0
-0.5
-1.0
F01
F02
F03
F04
F05
F06
F07
F08
F09
F10
F11
F12
F13
F14
F15
F16
F17
F18
F19
F20
(B)
Contribution ratio (%)
100
80
60
40
20
0
F11
Stack
EC
Flare
Tank
L/UL
WWTP
OWS
CT

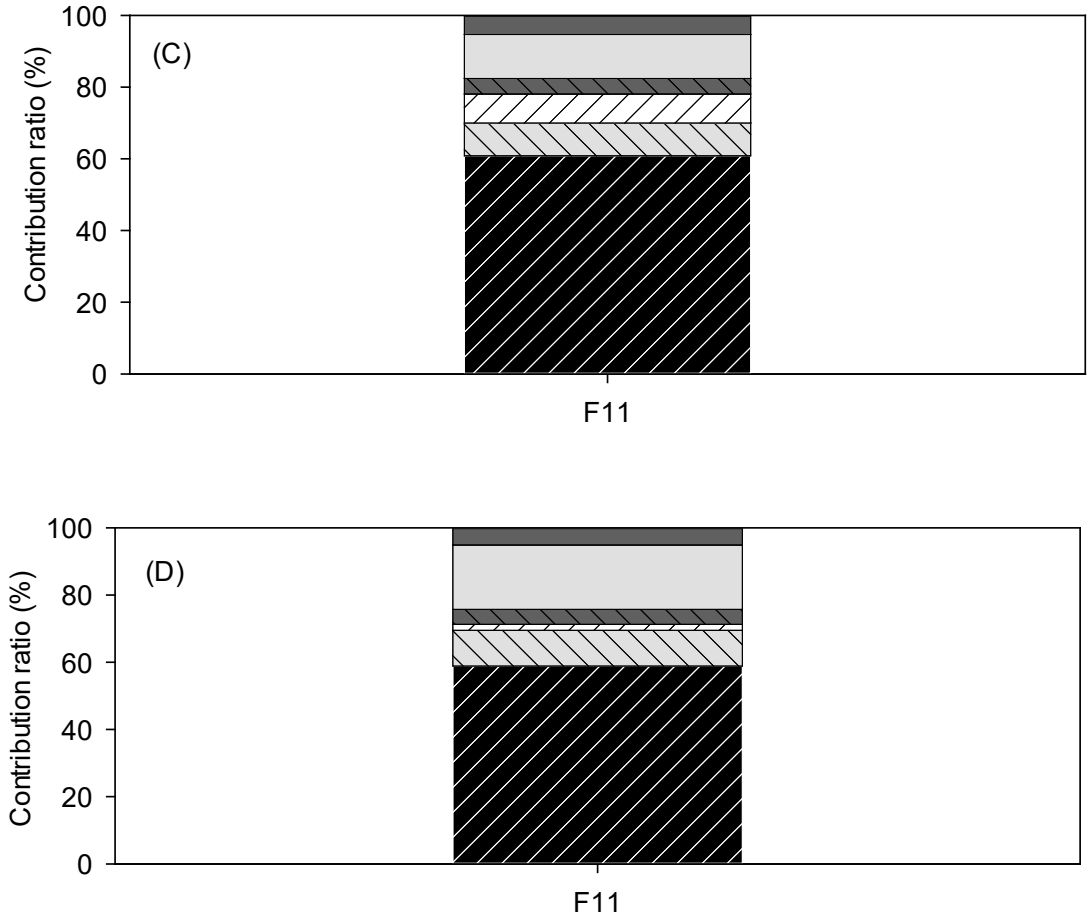


Figure S2. (A) Loading values of 20 companies in the 5th principal component (PC5) and contribution ratios of different sources in the critical companies in PC5 in (B) 2012, (C) 2013, and (D) 2014. EC, L/UL, WWTP, OLS, and CT denote equipment component, loading/unloading, wastewater treatment plant, oil-water separator, and cooling tower, respectively.