

Supporting Information for

**Source identification of VOCs in a petrochemical complex by applying
open-path Fourier transform infrared spectrometry**

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Table S1 Detection limit of the mobile OPFTIR

Compounds	Detection limit (ppm-m)	Compounds	Detection limit (ppm-m)
carbon monoxide	0.67	ethyl acetate	0.10
ozone	1.21	ethyl benzene	2.77
methane	0.68	ethylene	0.62
acetylene	0.65	exxon 87 gasoline	4.33
ammonia	0.58	methanol	0.56
1,3-butadiene	1.10	nitrous oxide	0.12
butane	3.17	n-octane	0.91
2-butanone	0.57	propylene	1.60
chloromethane	9.58	styrene	3.33
cyclohexane	0.51	1,1,1,2-tetrafluoroethane	0.10
dichlorodifluoromethane	0.11	toluene	39.40
dimethyl ether	0.58	trichlorofluoromethane	0.22
DMF	2.08	vinyl acetate	0.05

Table S2 The coefficient of variation and accuracy of the mobile OPFTIR for five compounds

Compounds	ethyl acetate	1,3-butadiene	ethylene	2-butanone	methane	propylene
Coefficient of variation (%)	1.13	1.30	0.85	1.54	5.80	0.73
Accuracy (%)	89.6	111	103	100	102	103

Table S3 The detailed path lengths and heights of the OPFTIR settings

Types of OPFTIR	Plant	Location	Path length (m)	Height (m)	
Stationary	-	-	125	12	
Mobile	Plant A	western	155	5	
		eastern	100	11	
	Plant B	northern	95	5	
		southern	133	6	
	Plant C	northern	200	2	
		southern	125	3	
	Plant D	northern	135	2	
		southern	133	2	
	Three sections of Plant B	first monitoring path		82	5
		second monitoring path		137	9
third monitoring path			122	4	
fourth monitoring path			131	6	

Table S4 Manufacturing processes that use DMF as one of the raw materials in the plant B

Process	Notation	Raw materials	Products
Dry Polyurethane (PU) synthetic leather process	M1	PU resins, 2-Butanone, Toluene, DMF, Dye	Dry process PU synthetic leather
Wet PU synthetic leather process	M2	PU Resins, DMF	Wet process PU synthetic leather
PU resin manufacturing process	M3	Polyester, 2-Butanone, Toluene, DMF, 4,4'-diphenylmethane diisocyanate, Chain extenders, Toluene diisocyanate	PU resin
Synthetic fiber manufacturing process	M4	PU resin, DMF, Dye, Toluene	Microfiber
PU resin manufacturing process	M5	Polyester, 2-Butanone, Toluene, DMF, 4,4'-diphenylmethane diisocyanate, Chain extenders, Toluene diisocyanate	PU resin

Table S5 Odorous contribution of odorous species from the first section of plant B

Odorous species	Monitoring path	Maximum concentration (ppb)	Mean concentration (ppb)	Detection frequency	Air quality regulation (ppb)	Percentage of the concentrations over air quality regulation	Odor threshold (ppb)*	Percentage of the concentrations over odor threshold
DMF	First	3034	26.7	7.4%	200	2.7%	470	1.4 %
	Second	7652	1316	94.1%	200	81.0%	470	72.6 %
2-butanone	First	897	4.49	2.1%	4000	0 %	250	0.6 %
	Second	3333	293	64.4%	4000	0 %	250	39.6 %
ethyl acetate	First	1338	13.8	12.1%	8000	0 %	170	1.9 %
	Second	1542	319	72.7%	8000	0 %	170	54.1 %
toluene	First	174	0.09	0.05%	2000	0 %	160	0.1 %
	Second	380	1.45	0.8%	2000	0 %	160	0.4 %
isopropanol	First	ND	ND	--	8000	--	1000	--
	Second	1008	16.8	5.8%	8000	0 %	1000	0.1 %

notation

*Odor Thresholds for Chemicals with Established Occupational Health Standards, American Industrial Hygiene Association,1989.

Table S6 Odorous contribution of odorous species from the second section of plant B

Odorous species	Monitoring path	Maximum concentration (ppb)	Mean concentration (ppb)	Detection frequency	Air quality regulation (ppb)	Percentage of the concentrations over air quality regulation	Odor threshold (ppb)*	Percentage of the concentrations over odor threshold
DMF	Second	2912	844	94.1%	200	80.6%	470	61.8%
	Third	12078	935	83.6%	200	63.1%	470	51.5%
2-butanone	Second	1452	167	54.4%	4000	0.00%	250	25.7%
	Third	349	11.6	9.03%	4000	0.00%	250	0.48%
ethyl acetate	Second	1148	149	57.1%	8000	0.00%	170	30.1%
	Third	1020	23.0	15.7%	8000	0.00%	170	4.87%
toluene	Second	179	0.30	0.17%	2000	0.00%	160	0.17%
	Third	645	5.15	1.66%	2000	0.00%	160	0.95%
isopropanol	Second	568	7.00	2.20%	8000	0.00%	1000	0.00%
	Third	303	2.95	1.31%	8000	0.00%	1000	0.00%

notation

*Odor Thresholds for Chemicals with Established Occupational Health Standards, American Industrial Hygiene Association, 1989.

Table S7 Odorous contribution of odorous species from the third section of plant B

Odorous species	Monitoring path	Maximum concentration (ppb)	Mean concentration (ppb)	Detection frequency	Air quality regulation (ppb)	Percentage of the concentrations over air quality regulation	Odor threshold (ppb)*	Percentage of the concentrations over odor threshold
DMF	Second	3889	360	74.8%	200	48.6%	470	29.8%
	Fourth	4142	105	23.3%	200	11.4%	470	6.92%
2-butanone	Second	3987	57.1	22.3%	4000	0.00%	250	5.48%
	Fourth	418	3.70	2.68%	4000	0.00%	250	0.23%
ethyl acetate	Second	1185	40.8	29.6%	8000	0.00%	170	6.77%
	Fourth	208	1.20	1.72%	8000	0.00%	170	0.08%
toluene	Second	476	2.52	2.00%	2000	0.00%	160	0.50%
	Fourth	1555	7.26	2.60%	2000	0.00%	160	1.89%
isopropanol	Second	730	2.62	1.75%	8000	0.00%	1000	0.00%
	Fourth	228	0.16	0.11%	8000	0.00%	1000	0.00%

notation

*Odor Thresholds for Chemicals with Established Occupational Health Standards, American Industrial Hygiene Association, 1989.

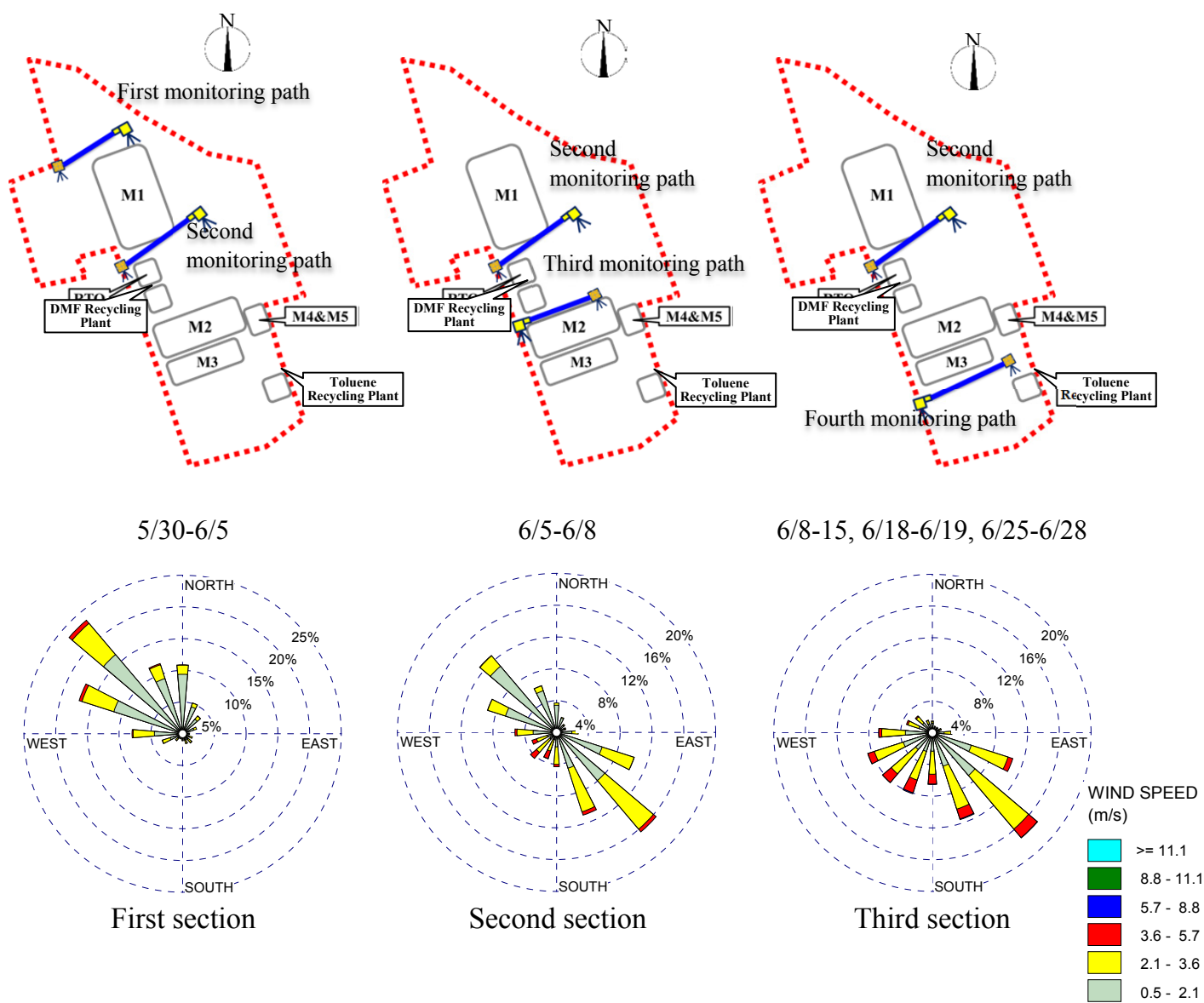


Figure S1 Locations of three sections and its DMF monitoring paths of the mobile open-path FTIR systems for factory B