Supplement of Atmos. Chem. Phys., 21, 4939–4958, 2021
https://doi.org/10.5194/acp-21-4939-2021-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Spatiotemporal variation, sources, and secondary transformation potential of volatile organic compounds in Xi'an, China

Mengdi Song et al.

Correspondence to: Xin Li (li_xin@pku.edu.cn)

Table S1: Measured VOC species in CB, DHS, and QL sites.

Classification	VOC Species		
Alkanes	Ethane	3-Methylpentane	Methylcyclohexane
	Propane	n-Hexane	2,3,4-Trimethylpentane
	Iso-butane	2,4-Dimethylpentane	2-Methylheptane
	n-Butane	Methylcyclopentane	3-Methylheptane
	Cyclopentane	2-Methylhexane	n-Octane
	Iso-pentane	Cyclohexane	n-Nonane
	n-Pentane	2,3-Dimethylpentane	n-Decane
	2,2-Dimethylbutane	3-Methylhexane	n-Undecane
	2,3-Dimethylbutane	2,2,4-Trimethylpentane	n-Dodecane
	2-Methylpentane	n-Heptane	
Alkenes	Ethylene	Cis-butene	Isoprene
	propene	1,3-Butadiene	cis-2-Pentene
	Trans-2-butene	1-Pentene	1-Hexene
	1-Butene	trans-2-Pentene	
Alkynes	Ethyne		
Aromatics	Benzene	iso-Propylbenzene	1,2,4-Trimethylbenzene
	Toluene	n-Propylbenzene	1,2,3-Trimethylbenzene
	Ethylbenzene	m-ethyltoluene	m-diethylbenzene
	m/p-Xylene	p-ethyltoluene	p-diethylbenzene
	o-Xylene	1,3,5-Trimethylbenzene	
	Styrene	o-Ethyltoluene	
Halohydro-carbons	Freon114	cis-1,2-Dichloroethylene	1,1,2-trichloroethane
	Chloromethane	Chloroform	Tetrachloroethene
	Vinylchloride	1,1,1-Trichloroethane	1,2-Dibromoethane
	Bromomethane	Tetrachloromethane	Chlorobenzene
	Chloroethane	1,2-Dichloroethane	1,3-Dichlorobenzene
	Freon11	Trichloroethylene	1,4-Dichlorobenzene
	1,1-Dichloroethene	1,2-Dichloropropane	Benzylchloride
	Freon113	Bromodichloromethane	1,2-Dichlorobenzene
	Dichloromethane	trans-1,3-Dichloropropene	
	1,1-Dichloroethane	cis-1,3-Dichloropropene	
OVOCs	Acetaldehyde	Methyl Vinyl Ketone	3-Pentanone
	Acrolein	Methyl Ethyl Ketone	n-Hexanal
	Propanal	n-Butanal	MTBE
	Acetone	2-Pentanone	
	Methacrolein	n-Pentanal	
Others	Acetonitrile		

Table S2: Measured VOC species in VOC grid sampling sites.

Classification	VOC Species		
Alkanes	Ethane	3-Methylpentane	Methylcyclohexane
	Propane	n-Hexane	2,3,4-Trimethylpentane
	Iso-butane	2,4-Dimethylpentane	2-Methylheptane
	n-Butane	Methylcyclopentane	3-Methylheptane
	Cyclopentane	2-Methylhexane	n-Octane
	Iso-pentane	Cyclohexane	n-Nonane
	n-Pentane	2,3-Dimethylpentane	n-Decane
	2,2-Dimethylbutane	3-Methylhexane	n-Undecane
	2,3-Dimethylbutane	2,2,4-Trimethylpentane	n-Dodecane
	2-Methylpentane	n-Heptane	
Alkenes	Ethylene	Cis-butene	Isoprene
	propene	1,3-Butadiene	cis-2-Pentene
	Trans-2-butene	1-Pentene	1-Hexene
	1-Butene	trans-2-Pentene	
Alkynes	Ethyne		
Aromatics	Benzene	iso-Propylbenzene	1,2,4-Trimethylbenzene
	Toluene	n-Propylbenzene	1,2,3-Trimethylbenzene
	Ethylbenzene	m-ethyltoluene	m-diethylbenzene
	m/p-Xylene	p-ethyltoluene	p-diethylbenzene
	o-Xylene	1,3,5-Trimethylbenzene	Naphthalene
	Styrene	o-Ethyltoluene	
Halohydro-carbons	Freon114	Tetrachloromethane	Bromodicloromethane
	Freon11	1,2-Dichloroethane	Benzyl chloride
	Freon113	Trichloroethylene	1,2-Dichlorobenzene
	Chloromethane	1,2-Dichloropropane	trans-1,2-Dichloroethylene
	Vinylchloride	cis-1,3-Dichloropropene	Freon12
	Bromomethane	trans-1,3-Dichloropropene	Trichloromethane
	Chloroethane	1,2,4-trichlorobenzene	Dibromo-monochloro-methane
	1,1-Dichloroethene	1,1,2-trichloroethane	Tribromomethane
	Dichloromethane	Tetrachloroethene	1,1,2,2-tetrachloroethane
	1,1-Dichloroethane	1,2-Dibromoethane	1,3-Dichlorobenzene
	cis-1,2-Dichloroethylene	Chlorobenzene	Hexachloro-1,3-butadiene
	1,1,1-Trichloroethane	1,4-Dichlorobenzene	
OVOCs	Acrolein	2-Propanol	Tetrahydrofuran
	Methyl isobutyl ketone	Vinyl Acetate	Methyl methacrylate
	Acetone	Methyl Ethyl Ketone	1,4-Dioxane
	MTBE	Ethyl Acetate	2-Hexanone
Others	Carbon Disulfide		

Table S3: Concentrations of seven VOCs groups in VOC grid sampling sites.

site	Alkanes	Alkenes	Alkynes	Aromatics	Halohydrocarbons	OVOCs	Others	TVOCs
XF	19.2	8.4	2.3	4.4	4.9	14.6	0.2	54.0
CT	16.1	3.6	1.8	3.3	5.1	11.5	0.1	41.4
HC	15.2	2.4	1.2	2.8	4.5	12.1	0.1	38.2
ZYT	13.7	5.0	1.8	3.0	2.0	9.7	0.1	35.4
YT	8.7	3.3	1.1	1.1	3.4	16.1	0.2	33.9
XS	12.3	2.4	1.2	2.6	3.5	10.5	0.2	32.6
GYL	10.1	2.5	1.3	2.5	3.6	9.8	0.1	29.9
LTC	10.5	4.8	2.3	2.4	2.4	6.7	0.1	29.4
XY	11.6	2.7	1.5	1.7	3.4	8.3	0.1	29.1
JFT	9.8	2.8	1.1	1.4	2.5	10.6	0.1	28.2
RS	10.6	2.4	1.4	1.3	3.5	8.6	0.1	27.9
LT	8.7	3.2	0.9	0.9	3.4	10.5	0.2	27.7
GZ	10.1	2.6	1.4	1.7	3.6	7.2	0.1	26.6
ZZC	9.8	2.0	1.2	1.2	2.5	8.3	0.1	25.0
JDT	7.5	2.9	1.1	1.3	2.9	7.0	0.1	22.8
CAT	7.3	2.3	0.8	0.9	2.7	7.9	0.1	22.2
XX	8.0	1.8	1.3	0.9	2.9	5.5	0.1	20.6
YST	5.8	1.9	1.1	1.3	2.7	7.0	0.1	19.9
WQ	7.3	0.9	0.8	0.6	3.1	6.8	0.1	19.6
XHT	5.9	1.7	1.0	0.9	2.1	6.3	0.1	18.0

Table S4. The weather parameter on July 1 and July 14 in Xi'an

Date	Area	WS (m/s)	WD (°)	T (℃)	RH (%)
2019/7/1	urban	0.6	205.4	28.9	53.3
2020/7/14		0.6	199.7	31.3	50.9
2020/7/1	rural	1.1	209.8	27.7	54.1
2020/7/14		1.5	201.1	29.8	50.6

Table S5. Toluene to benzene ratio (T/B) of different source profiles in different researches (unit: ppb/ppb).

Category	Sub Category	Location	T/B	Reference	Sub Category average	Min	Max
Transportation	Gasoline vehicle exhaust	Tianjin	1.08	Wang et al.,2013; Dai et al.,2013	1.08	0.93	2.21
	Motorcycle exhaust	Taiwan	1.46	Yao et al,2013	1.46		
	Diesel vehicle exhaust	Beijing	1.77	Yao et al,2015a	0.93		
		Beijing	1.04	Yao et al,2015a			
		Beijing	1.05	Yao et al,2015a			
		Beijing	1.28	Yao et al,2015a			
		Xiamen	0.21	Mo, et al.,2016			
		Xiamen	0.22	Mo, et al.,2016			
	LPG vehicle exhaust	Shanghai	1.05	Qiao et al..,2012	1.05		
	Rural vehicle exhaust	Beijing	2.21	Yao et al.,2015b	1.64		
		Beijing	1.07	Yao et al.,2015b			
	Fuel evaporation	Guangzhou	1.71	Zhang et al.,2013	2.21		
		Guangzhou	2.71	Zhang et al.,2013			
	Tunnel	Hefei	1.52	Deng et al., 2018	1.48		
		Hefei	1.48	Deng et al., 2018			
		Hefei	1.31	Deng et al., 2018			
		Hefei	1.56	Deng et al., 2018			
		PRD	1.52	Liu et al., 2008a			
Burning	Coaling burning	Beijing	0.24	Mo, et al.,2016	0.24	0.23	0.38
	Coaling burning	Beijing	0.38	Liu et al.,2008a	0.38		
	Wheat	Beijing	0.23	Mo, et al.,2016	0.23		
	Maize	Beijing	0.30	Mo, et al.,2016	0.30		
	Wood	Beijing	0.27	Li et al., 2011	0.27		
Solvent use	Architecture paint	Shanghai	15.34	Wang et al.,2014	8.82	8.82	51.43
		Beijing	2.30	Yuan et al.,2010			
	Furniture paint	Beijing	32.44	Yuan et al.,2010	31.35		
		Shanghai	42.13	Wang et al.,2014			
		PRD	15.08	Zheng et al.,2013			
		PRD	34.68	Zheng et al.,2013			
		Beijing	32.44	Yuan et al.,2010			
	Surface paint	PRD	8.17	Zheng et al.,2013	12.63		
		PRD	17.09	Zheng et al.,2013			
	Paint manufacturing	PRD	6.10	Zheng et al.,2013	15.94		
		PRD	25.78	Zheng et al.,2013			
	Shoemaking	PRD	21.28	Zheng et al.,2013	25.38		

		PRD	29.47	Zheng et al.,2013			
	Printing	PRD	38.15	Zheng et al.,2013	51.43		
		PRD	64.71	Zheng et al.,2013			
Industrial processes	Petrochemical industry	YRD	0.95	Mo, et al.,2015	1.37	1.37	5.76
		YRD	2.20	Mo, et al.,2015			
		YRD	3.20	Mo, et al.,2015			
		YRD	0.42	Mo, et al.,2015			
		YRD	0.95	Mo, et al.,2015			
		YRD	1.88	Mo, et al.,2015			
		YRD	0.39	Mo, et al.,2015			
		YRD	0.98	Mo, et al.,2015			
		YRD	1.80	Mo, et al.,2015			
		YRD	1.98	Mo, et al.,2015			
		YRD	1.13	Mo, et al.,2015			
		YRD	0.75	Mo, et al.,2015			
		YRD	1.21	Mo, et al.,2015			
	Chemical industry	YRD	2.37	Mo, et al.,2015	5.76		
		YRD	9.14	Mo, et al.,2015			
	Power plant	Liaoning	2.89	Shi et a..,2015	3.39		
		Liaoning	5.29	Shi et a..,2015			
		Liaoning	0.48	Shi et a..,2015			
		Liaoning	4.89	Shi et a..,2015			

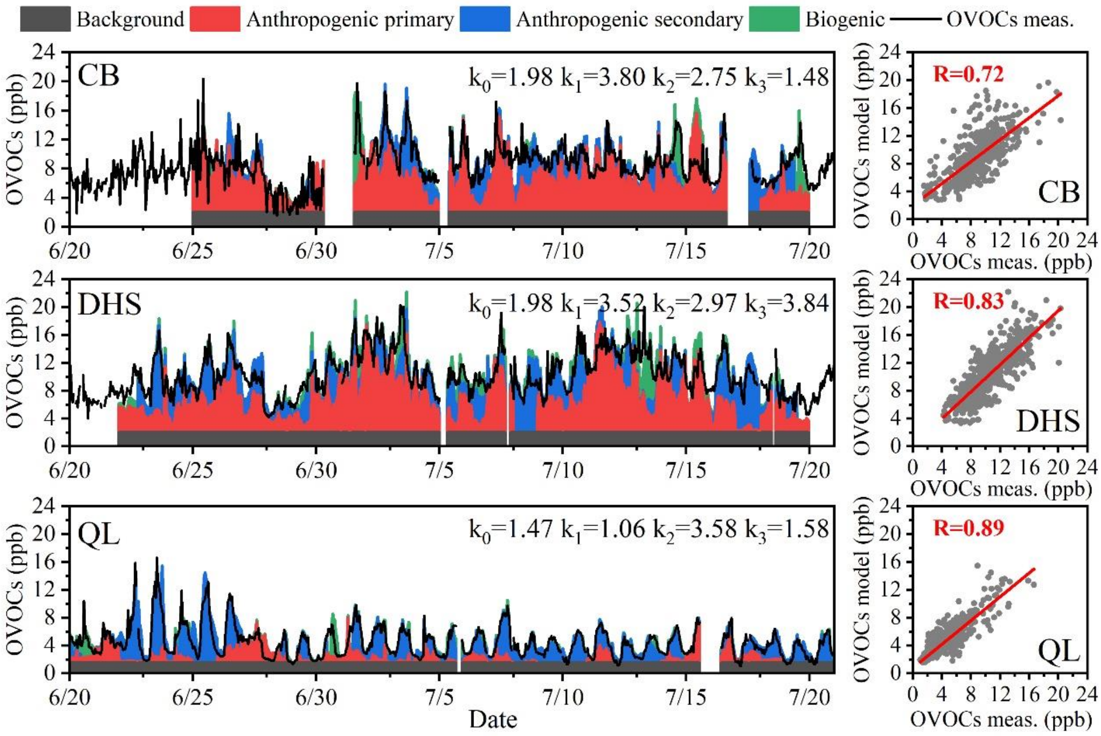

Figure S1. Time series of measured OVOCs concentrations and OVOCs calculated from the multi-linear regression model.

Note. The equation of the multi-linear regression model is:

$$[OVOCs]=k_0+k_1\times[Ethyne]+k_2\times[PAN]+k_3\times[Isoprene]$$

where [Ethyne] represents the concentration of ethyne, [PAN] represents the concentration of PAN, [Isoprene] represents the concentration of isoprene, k_0 represents the background concentration, k_1, k_2 and k_3 are the corresponding coefficients, meas. represents measure.

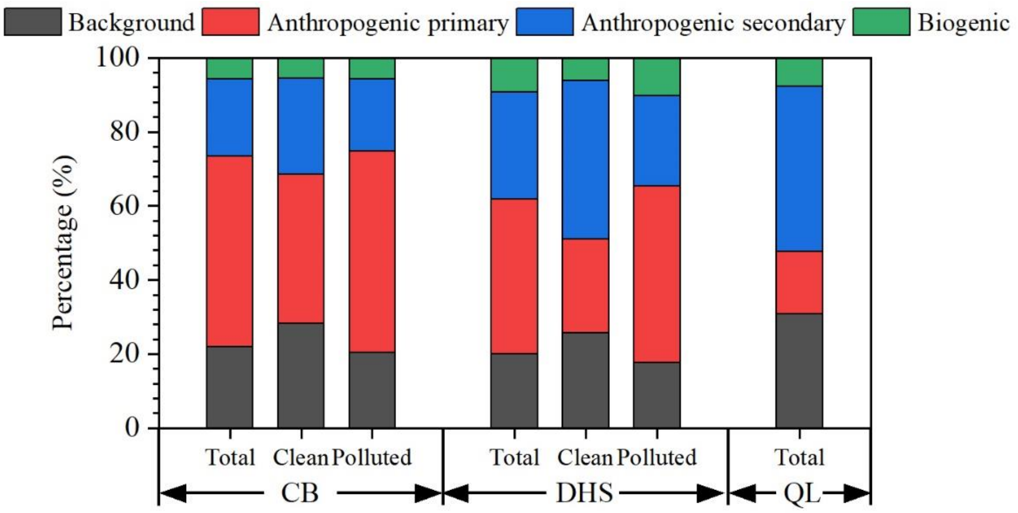

Figure S2. Contributions of different sources of OVOCs in different sites in Xi'an base on the multi-linear regression model. "Total" represent the entire observation period. The "Polluted" represent the period of ozone pollution event at CB and DHS sites (from June 23 to 26, 2019 and from June 30 to July 15, 2019), and the rest of the period as a "Clean" condition.

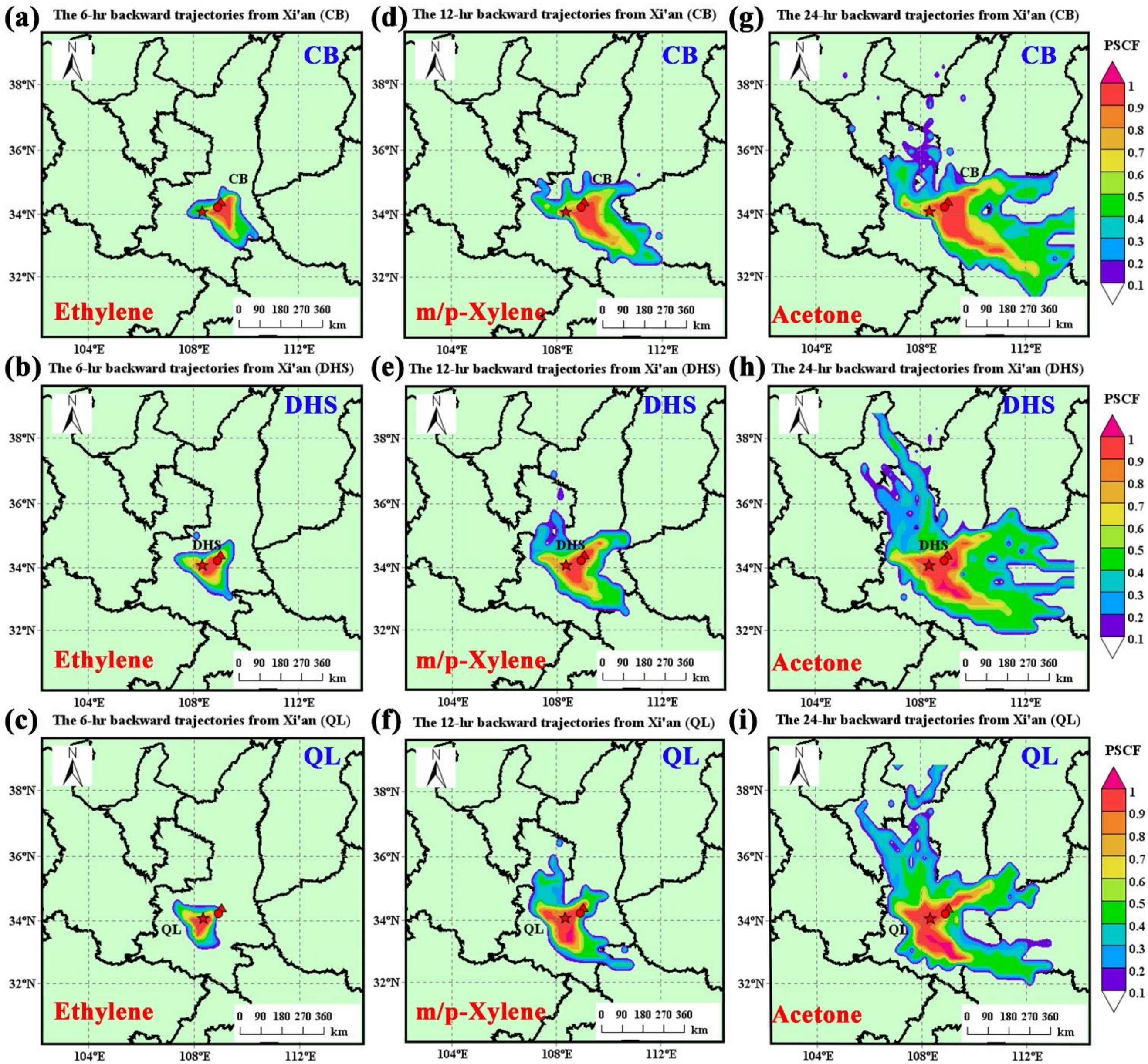

Figure S3: (a)-(c) 6-h backward trajectory PSCF analysis of ethylene in the CB, DHS, and QL sites, (d)-(f) 12-h backward trajectory PSCF analysis of m/p-Xylene in the CB, DHS, and QL sites, (g)-(i) 24-h backward trajectory PSCF analysis of acetone in the CB, DHS, and QL sites.

References

Dai, P., Ge, Y., Lin, Y., Su, S., and Liang, B.: Investigation on characteristics of exhaust and evaporative emissions from passenger cars fueled with gasoline/methanol blends, Fuel, 113, 10-16, 10.1016/j.fuel.2013.05.038, 2013.

Deng, C. X., Jin, Y. J., Zhang, M., Liu, X. W., and Yu, Z. M.: Emission Characteristics of VOCs from On-Road Vehicles in an Urban Tunnel in Eastern China and Predictions for 2017-2026, Aerosol and Air Quality Research, 18, 3025-3034, 10.4209/aaqr.2018.07.0248, 2018.

Jiun-Horng, T., Kuo-Hsiung, L., Chih-Yu, C., Nina, L., Sen-Yi, M., and Hung-Lung, C.: Volatile organic compound constituents from an integrated iron and steel facility, Journal of Hazardous Materials, 157, 569-578, 10.1016/j.jhazmat.2008.01.022, 2008.

Li, X.-h., Wang, S.-x., and Hao, J.-m.: Characteristics of Volatile Organic Compounds (VOCs) Emitted from Biofuel Combustion in China, Huanjing Kexue, 32, 3515-3521, 2011.

Liu, Y., Shao, M., Fu, L., Lu, S., Zeng, L., and Tang, D.: Source profiles of volatile organic compounds (VOCs) measured in China: Part I, Atmos. Environ., 42, 6247-6260, 10.1016/j.atmosenv.2008.01.070, 2008.

Mo, Z., Shao, M., and Lu, S.: Compilation of a source profile database for hydrocarbon and OVOC emissions in China, Atmos. Environ., 143, 209-217, 10.1016/j.atmosenv.2016.08.025, 2016.

Mo, Z., Shao, M., Lu, S., Qu, H., Zhou, M., Sun, J., and Gou, B.: Process-specific emission characteristics of volatile organic compounds (VOCs) from petrochemical facilities in the Yangtze River Delta, China, Science of the Total Environment, 533, 422-431, 10.1016/j.scitotenv.2015.06.089, 2015.

Qiao, Y.-z., Wang, H.-l., Huang, C., Chen, C.-h., Su, L.-y., Zhou, M., Xu, H., Zhang, G.-f., Chen, Y.-r., Li, L., Chen, M.-h., and Huang, H.-y.: Source Profile and Chemical Reactivity of Volatile Organic Compounds from Vehicle Exhaust, Huanjing Kexue, 33, 1071-1079, 2012.

Shi, J., Deng, H., Bai, Z., Kong, S., Wang, X., Hao, J., Han, X., and Ning, P.: Emission and profile characteristic of volatile organic compounds emitted from coke production, iron smelt, heating station and power plant in Liaoning Province, China, Science of the Total Environment, 515, 101-108, 10.1016/j.scitotenv.2015.02.034, 2015.

Wang, H., Qiao, Y., Chen, C., Lu, J., Dai, H., Qiao, L., Lou, S., Huang, C., Li, L., Jing, S., and Wu, J.: Source Profiles and Chemical Reactivity of Volatile Organic Compounds from Solvent Use in Shanghai, China, Aerosol and Air Quality Research, 14, 301-310, 10.4209/aaqr.2013.03.0064, 2014.

Wang, J., Jin, L., Gao, J., Shi, J., Zhao, Y., Liu, S., Jin, T., Bai, Z., and Wu, C.-Y.: Investigation of speciated VOC in gasoline vehicular exhaust under ECE and EUDC test cycles, Science of the Total Environment, 445, 110-116, 10.1016/j.scitotenv.2012.12.044, 2013.

Yao, Y.-C., Tsai, J.-H., and Wang, I. T.: Emissions of gaseous pollutant from motorcycle powered by ethanol-gasoline blend, Applied Energy, 102, 93-100, 10.1016/j.apenergy.2012.07.041, 2013.

Yao, Z., Shen, X., Ye, Y., Cao, X., Jiang, X., Zhang, Y., and He, K.: On-road emission characteristics of VOCs from diesel trucks in Beijing, China, Atmos. Environ., 103, 87-93, https://doi.org/10.1016/j.atmosenv.2014.12.028, 2015a.

Yao, Z., Wu, B., Shen, X., Cao, X., Jiang, X., Ye, Y., and He, K.: On-road emission characteristics of VOCs from rural vehicles and their ozone formation potential in Beijing, China, Atmos. Environ., 105, 91-96, 10.1016/j.atmosenv.2015.01.054, 2015b.

Yuan, B., Shao, M., Lu, S., and Wang, B.: Source profiles of volatile organic compounds associated with solvent use in Beijing, China, Atmos. Environ., 44, 1919-1926, 10.1016/j.atmosenv.2010.02.014, 2010.

Zhang, Y., Wang, X., Zhang, Z., Lu, S., Shao, M., Lee, F. S. C., and Yu, J.: Species profiles and normalized reactivity of volatile organic compounds from gasoline evaporation in China, Atmos. Environ., 79, 110-118, 10.1016/j.atmosenv.2013.06.029, 2013.

Zheng, J., Yu, Y., Mo, Z., Zhang, Z., Wang, X., Yin, S., Peng, K., Yang, Y., Feng, X., and Cai, H.: Industrial sector-based volatile organic compound (VOC) source profiles measured in manufacturing facilities in the Pearl River Delta, China, Science of the Total Environment, 456, 127-136, 10.1016/j.scitotenv.2013.03.055, 2013.