Supplement of Atmos. Chem. Phys., 22, 2173–2190, 2022
https://doi.org/10.5194/acp-22-2173-2022-supplement

Atmospheric Chemistry and Physics
Open Access

Supplement of

Atmospheric oxidation capacity and ozone pollution mechanism in a coastal city of southeastern China: analysis of a typical photochemical episode by an observation-based model

Taotao Liu et al.

Correspondence to: Jinsheng Chen (jschen@iue.ac.cn) and Likun Xue (xuelikun@sdu.edu.cn)

Captions:

Figure S1. The concentrations of monthly and annual MDA8h O_3 in Xiamen from 2016 to 2020.

Figure S2. 72h back trajectories were calculated at 100 m altitude during 20-29 Sep. 2019.

Figure S3. Daytime (06:00-18:00 LT) variations of the simulated concentration, production, and loss rate of (a)OH, (b)HO_2, and (c)RO_2 in Xiamen.

Figure S4. Synoptic situations of surface wind field from 20 to 29 Sep. 2019. Arrows in the figure represent the surface wind speed and direction. The blue square is the study site.

Table S1. Comparison of NO, NO_2 and total VOCs levels in cities between China and other countries.

Table S2. Dry deposition velocity (cm s^{-1}) for chemical species.

Table S3. Estimated degree of freedom (Edf), degree of reference (Ref. df), P-value, F-value, deviance explained (%), adjusted R^2 for the smoothed variables (including UV, T, RH, P, and WS) in the GAM model.

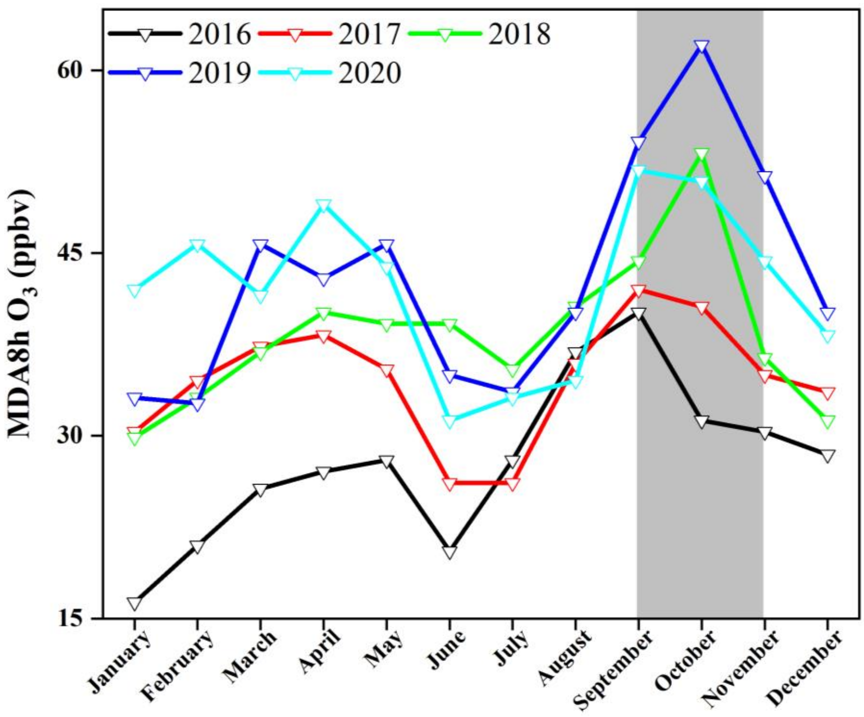

Figure S1. The concentrations of monthly and annual MDA8h O_3 in Xiamen from 2016 to 2020.

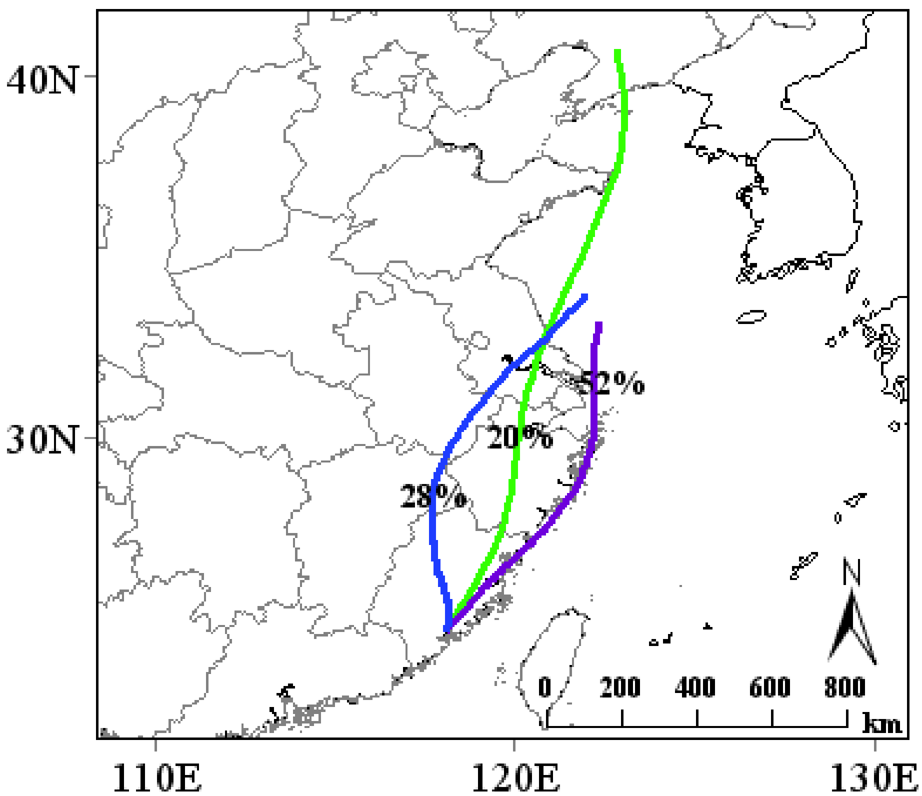

Figure S2. 72h back trajectories were calculated at 100 m altitude during 20-29 Sep. 2019.

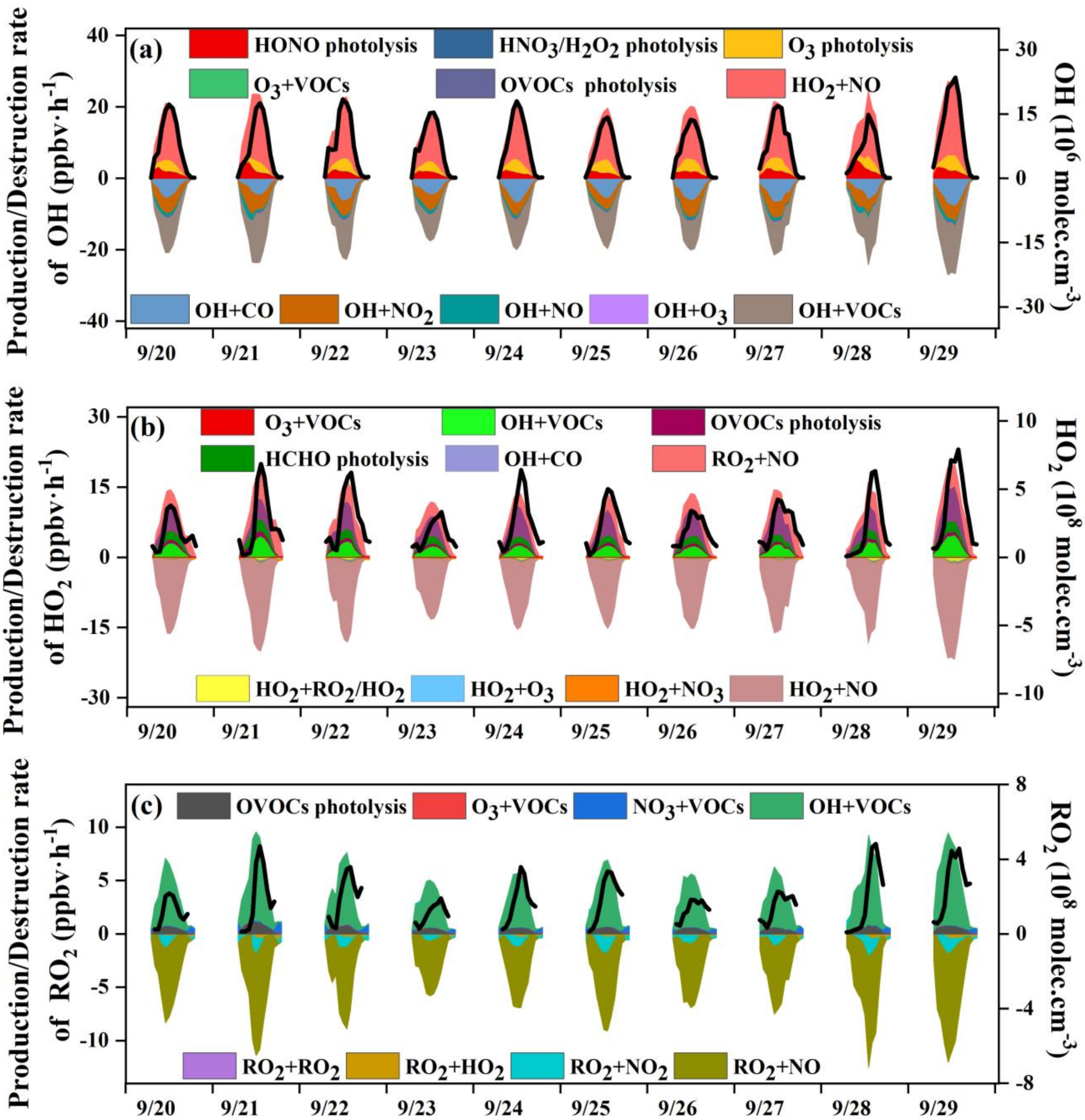

Figure S3. Daytime (06:00-18:00 LT) variations of the simulated concentration, production, and loss rate of (a)OH, (b)HO_2, and (c)RO_2 in Xiamen.

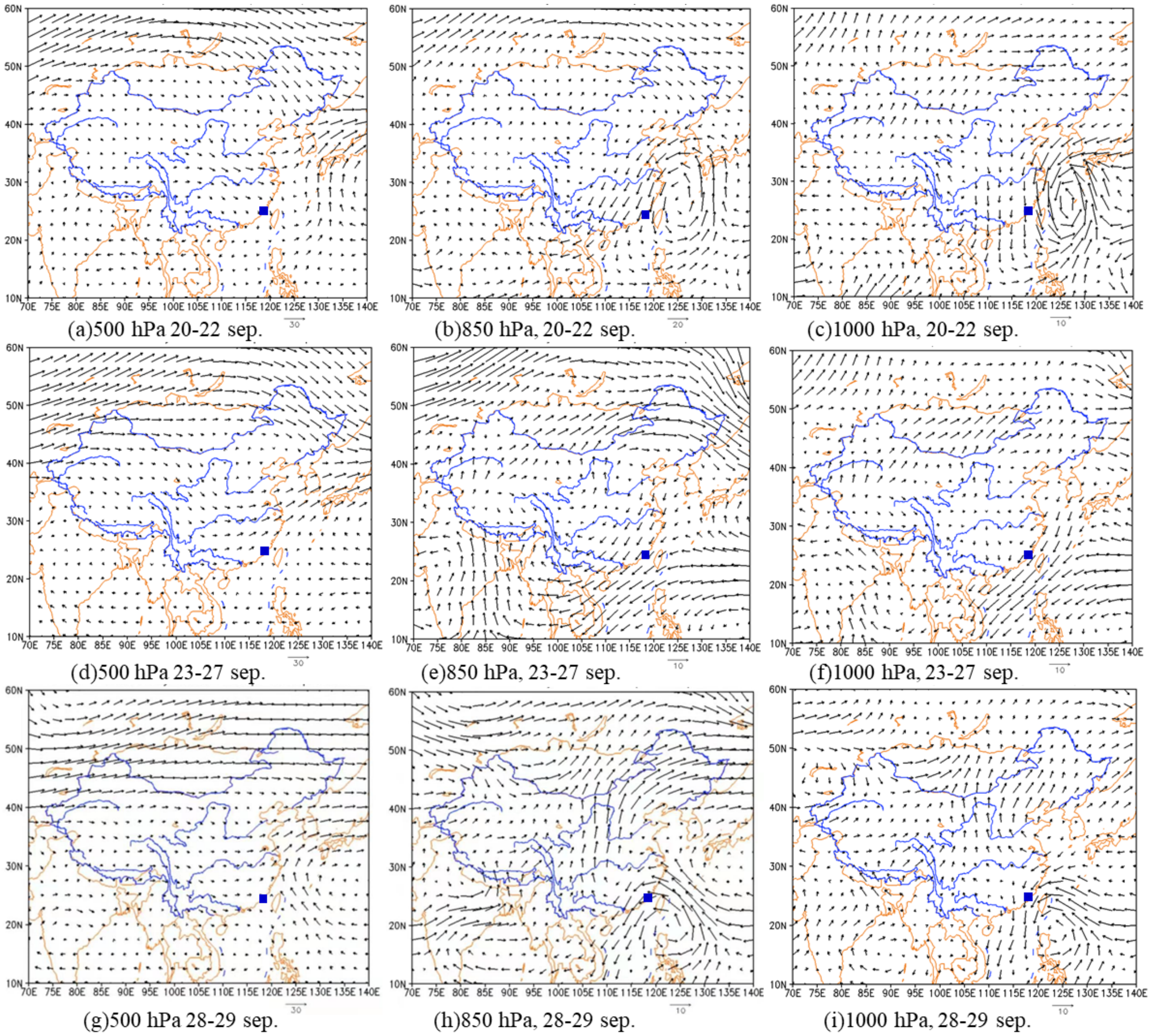

Figure S4. Synoptic situations of surface wind field from 20 to 29 Sep. 2019. Arrows in the figure represent the surface wind speed and direction. The blue square is the study site.

Table S1. Comparison of NO, NO_2 and total VOCs levels in cities between China and other countries (Units: ppbv).

Location	NO_2	NO	VOCs	Site category	Observation periods	Reference
Xiamen	15.4	1.4	17.2	Urban	Sep. 2019 (episode)	This study
Beijing	16.8	2.1	44.2	Urban		Liu et al., 2021b
Wuhan	17.5	3.2	30.2	Urban	Summer 2018 (episode)	Liu et al., 2021b
Lanzhou	15.8	2.9	45.3	Urban		Liu et al., 2021b
Shanghai	14.2	3.38	25.3	Urban	Jun. 2019 (episode)	Zhu et al., 2020
Chengdu	39.0	3.6	36.0	Urban	Jul. 2017 (episode)	Yang et al., 2020
Los Angeles	-	-	41.3	Urban	May.–Jun. 2010	Warneke et al., 2012
London	-	-	22.1	Urban	1998–2008	Von Schneidemesser et al., 2010
Tokyo	-	-	43.4	Urban	2003–2005	Hoshi et al., 2008

Beijing	11.5	4.8	28.1	Suburban	Aug. 2018	Yang et al., 2021
Hong Kong	25.0	14.0	26.9	Suburban	Aug. to Nov. 2013	Wang et al., 2018
Chengdu	11.4	8.0	28.0	Suburban	Summer 2019	Yang et al., 2021a
Qingdao	16.7	1.6	7.6	Rural	Oct.–Nov. 2019	Liu et al., 2021a
The Pearl River Delta	39.9	4.2	38.0	Rural	Octo.–Nov. 2014	He et al., 2019
Hong Kong	12.2	1.9	10.9	Regional background	Aug.–Dec. 2012	Li et al., 2018
Mt. Wuyi	-	-	4.7	Background	Dec. 2016	Hong et al., 2019
Mt. Tai	-	-	8.8	Background	Jun. 2006	Suthawaree et al., 2010
Mt. Waliguan	-	-	2.6	Remote region	Jul.–Aug. 2003	Xue et al., 2013

Note: “-” means that the data was not mentioned in the relevant studies.

Table S2. Dry deposition velocity (cm s^{-1}) for chemical species (Zhang et al., 2003).

Symbol	Name	dry deposition velocity
O_3	Ozone	0.6
NO_2	Nitrogen dioxide	0.6
HONO	Nitrous acid	1.9
HNO_3	Nitric acid	4.7
HNO_4	Pernitric acid	3.3
NH_3	Ammonia	1
SO_2	Sulphur dioxide	0.8
H_2SO_4	Sulphuric acid	1.1
H_2O_2	Hydrogen peroxide	1.2
PAN	Peroxyacetylnitrate	0.4
PPN	Peroxypropylnitrate	0.4
APAN	Aromatic acylnitrate	0.5
MPAN	Peroxymethacrylic nitric anhydride	0.3
HCHO	Formaldehyde	0.9
MCHO	Acetaldehyde	0.2
PALD	C3 Carbonyls	0.2
C4A	C4-C5 Carbonyls	0.2
C7A	C6-C8 Carbonyls	0.2
ACHO	Aromatic carbonyls	0.2
MVK	Methyl-vinyl-ketone	0.2
MACR	Methacrolein	0.2
MGLY	Methylgloxal	0.2
MOH	Methyl alcohol	0.7
ETOH	Ethyl alcohol	0.6
POH	C3 alcohol	0.5
CRES	Cresol	0.2
FORM	Formic acid	1.4
ACAC	Acetic acid	1.1
ROOH	Organic peroxides	0.6
ONIT	Organic nitrates	0.4
INIT	Isoprene nitrate	0.3

Table S3. Estimated degree of freedom (Edf), degree of reference (Ref. df), P-value, F-value, deviance explained (%), adjusted R^2 for the smoothed variables (including UV, T, RH, P, and WS) in the GAM model.

Smoothed variables	[a]Edf	[a]Ref.df	[b]F	[c]P-value	[d]Adjust R^2	[e]Deviance explained (%)
UV ($W \cdot m^{-2}$)	3.1	3.8	3.0	0.0	0.0	5.4
T (°C)	5.3	6.5	10.9	0.0	0.2	24.1
RH (%)	2.9	3.6	40.1	0.0	0.4	38.9
WS ($m \cdot s^{-1}$)	2.9	3.6	26.9	0.0	0.3	29.3
P (hPa)	6.9	8.0	3.9	0.0	0.1	13.4

Note: [a] The degree of freedom (edf, ref.df) of the explanatory variable is 1, indicating the linear relationships between the explanatory variable and the response variable, and a non-linear relationship is shown when the degree>1; [b] a high F-value indicates the great importance of the influencing factor; [c] the P-value is used to judge the significance of the model result; [d] the adjusted R^2 is the value of the regression square ranging from 0 to 1; [e] the deviance explained represents the fitting effect.

References:

Liu, Z., Wang, Y., Hu, B., Lu, K., Tang, G., Ji, D., Yang, X., Gao, W., Xie, Y., Liu, J., Yao, D., Yang, Y., and Zhang, Y.: Elucidating the quantitative characterization of atmospheric oxidation capacity in Beijing, China, Sci Total Environ, 771, 145306, 10.1016/j.scitotenv.2021.145306, 2021a.

Liu, X., Guo, H., Zeng, L., Lyu, X., Wang, Y., Zeren, Y., Yang, J., Zhang, L., Zhao, S., Li, J., and Zhang, G.: Photochemical ozone pollution in five Chinese megacities in summer 2018, Sci Total Environ, 149603, 10.1016/j.scitotenv.2021.149603, 2021b.

Yang, X., Wu, K., Wang, H., Liu, Y., Gu, S., Lu, Y., Zhang, X., Hu, Y., Ou, Y., Wang, S., and Wang, Z.: Summertime ozone pollution in Sichuan Basin, China: Meteorological conditions, sources and process analysis, Atmos. Environ., 226, 117392, 10.1016/j.atmosenv.2020.117392, 2020.

Warneke, C., Gouw, J.A., Holloway, J.S., Peischl, J., Ryerson, T.B., Atlas, E., Blake, D., Trainer, M., Parrish, D.D.: Multiyear trends in volatile organic compounds in Los Angeles, California: five decades of decreasing emissions. J. Geophys. Res.-Atmos. 117 (D21). http://dx.doi.org/10.1029/2012JD017899, 2012.

Von Schneidemesser, E., Monks, P.S., Plass-Duelmer, C.: Global comparison of VOC and CO observations in urban areas. Atmos. Environ. 44 (39), 5053–5064, 2010.

Hoshi, J.Y., Amano, S., Sasaki, Y., Korenaga, T.: Investigation and estimation of emission sources of 54 volatile organic compounds in ambient air in Tokyo. Atmos.

Environ. 42 (10), 2383–2393, 2008.

Wang, H., Lyu, X., Guo, H., Wang, Y., Zou, S., Ling, Z., Wang, X., Jiang, F., Zeren, Y., Pan, W., Huang, X., and Shen, J.: Ozone pollution around a coastal region of South China Sea: interaction between marine and continental air, Atmos. Chem. Phys., 18, 4277–4295, 10.5194/acp-18-4277-2018, 2018.

Yang, Y., Wang, Y., Huang, W., Yao, D., Zhao, S., Wang, Y., Ji, D., Zhang, R., and Wang, Y.: Parameterized atmospheric oxidation capacity and speciated OH reactivity over a suburban site in the North China Plain: A comparative study between summer and winter, Sci Total Environ, 773, 145264, 10.1016/j.scitotenv.2021.145264, 2021.

Yang, X., Lu, K., Ma, X., Liu, Y., Wang, H., Hu, R., Li, X., Lou, S., Chen, S., Dong, H., Wang, F., Wang, Y., Zhang, G., Li, S., Yang, S., Yang, Y., Kuang, C., Tan, Z., Chen, X., Qiu, P., Zeng, L., Xie, P., and Zhang, Y.: Observations and modeling of OH and HO2 radicals in Chengdu, China in summer 2019, Sci Total Environ, 772, 144829,2021a 10.1016/j.scitotenv.2020.144829, 2021a.

Tiwari, V., Hanai, Y., Masunaga, S., 2010. Ambient levels of volatile organic compounds in the vicinity of petrochemical industrial area of Yokohama, Japan. Air Qual. Atmos. Health 3 (2), 65–75.

He, Z., Wang, X., Ling, Z., Zhao, J., Guo, H., Shao, M., and Wang, Z.: Contributions of different anthropogenic volatile organic compound sources to ozone formation at a receptor site in the Pearl River Delta region and its policy implications, Atmospheric Chemistry and Physics, 19, 8801-8816, 10.5194/acp-19-8801-2019, 2019.

Li, Z., Xue, L., Yang, X., Zha, Q., Tham, Y. J., Yan, C., Louie, P. K. K., Luk, C. W. Y., Wang, T., and Wang, W.: Oxidizing capacity of the rural atmosphere in Hong Kong, Southern China, Sci Total Environ, 612, 1114-1122, 10.1016/j.scitotenv.2017.08.310, 2018.

Suthawaree, J., Kato, S., Okuzawa, K., Kanaya, Y., Pochanart, P., Akimoto, H., Wang, Z., and Kajii, Y.: Measurements of volatile organic compounds in the middle of Central East China during Mount Tai Experiment 2006 (MTX2006): observation of regional background and impact of biomass burning, Atmos. Chem. Phys., 10, 1269–1285, doi:10.5194/acp-10-1269-2010, 2010.

Xue, L. K. , Wang, T. , Guo, H. , Blake, D. R. , Tang, J. , & Zhang, X. C. , et al.: Sources and photochemistry of volatile organic compounds in the remote atmosphere of western China: results from the Mt. Waliguan Observator, Atmos. Chem. Phys., 10.5194/acp-13-8551-2013, 2013.

Hong, Z., Li, M., Wang, H., Xu, L., Hong, Y., Chen, J., Chen, J., Zhang, H., Zhang, Y., Wu, X., Hu, B., and Li, M.: Characteristics of atmospheric volatile organic compounds (VOCs) at a mountainous forest site and two urban sites in the southeast of China, Sci Total Environ, 10.1016/j.scitotenv.2018.12.132, 2019.

Zhu, J., Wang, S., Wang, H., Jing, S., Lou, S., Saiz-Lopez, A., and Zhou, B.:

Observationally constrained modeling of atmospheric oxidation capacity and photochemical reactivity in Shanghai, China, Atmos. Chem. Phys., 20, 1217-1232, 10.5194/acp-20-1217-2020, 2020.