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Observation-based analysis of ozone production sensitivity for two persistent ozone episodes in Guangdong, China

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Supplementary Equations

$$\text{fresh VOC} = (CO_8 - CO_{13}) \times \frac{\text{VOC}}{\text{CO}}(\text{inventory}) \quad \text{(S1)}$$

$$\text{leftover VOC} = CO_{13} \times \frac{\text{VOC}}{\text{CO}}(\text{inventory}) \times \exp(-\text{Kvoc}\int_8^{18}[\text{OH}]dt)(t = 10h) \quad \text{(S2)}$$

$$VOC_8 = \text{fresh VOC} + \text{leftover VOC} \quad \text{(S3)}$$

$$[\text{VOC}]_{13} = [\text{VOC}]_8 \times \exp(-K_{VOC}\int_8^{13}[\text{OH}]dt) \quad \text{(S4)}$$

$$\Delta\text{VOC} = [\text{VOC}]_8 - [\text{VOC}]_{13} \quad \text{(S5)}$$

$$\Delta\text{OVOC} = CO_{mean} \times \frac{\text{OVOC}}{\text{CO}}(\text{observed}) \times \exp(-\text{Kovoc}\int_8^{13}[\text{OH}]dt) \quad \text{(S6)}$$

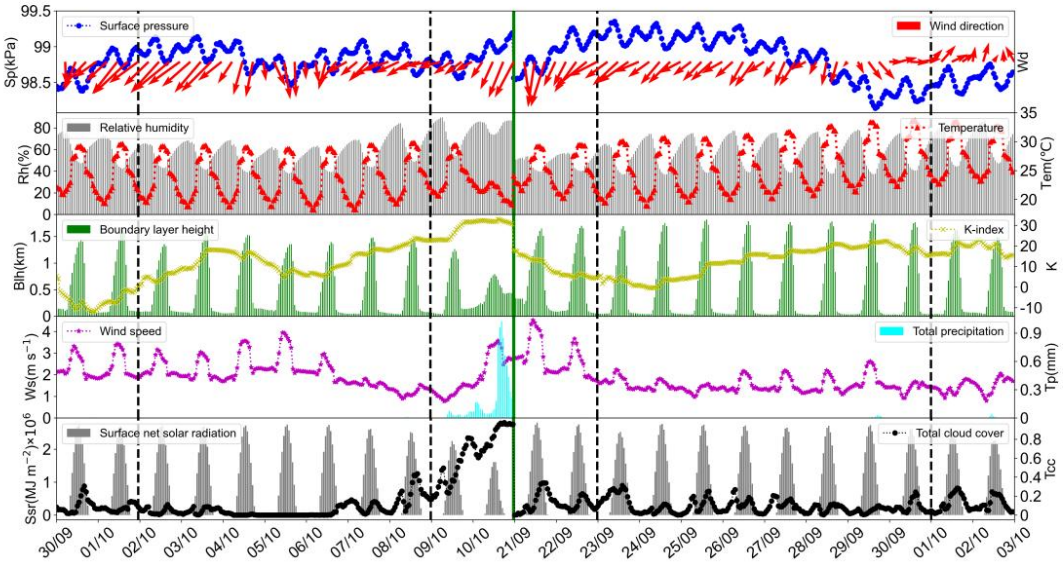
Supplementary Tables

Table S1. Ratios of VOC species to CO and the corresponding reaction rate constants of individual VOC_s with OH (Huang et al., 2021).

	VOC_S/CO	VOC_S/VOC_S (total)	molecular mass	$10^{-12}\times K_{OH}$
Methylbenzene	0.01266	0.0634	92	5.63
M/P-xylene	0.00965	0.04836	106	18.9
Formaldehyde	0.00900	0.0451	30	9.37
Ethylbenzene	0.00771	0.03863	106	7
N-hexane	0.00582	0.0292	86	5.2
Ethylene	0.00544	0.02728	28	8.52
Acrylic	0.00479	0.02399	42	26.3
Acetone	0.00475	0.02379	58	0.17
Benzene	0.00432	0.02166	78	1.22
O-xylene	0.00407	0.02038	106	13.6
Ethanol	0.00405	0.02032	46	3.2
Ethane	0.00397	0.01992	30	0.26
Butanone	0.00331	0.01662	72	1.22
Methanol	0.00326	0.01635	32	0.94
N-butane	0.00319	0.01601	58	2.36
Cyclohexane	0.00300	0.01504	84	6.97
Propane	0.00297	0.01489	44	1.09
N-pentane	0.00289	0.01451	72	3.8
2-methylpentane	0.00274	0.01377	86	5.2
Acetaldehyde	0.00272	0.01364	44	15
1-butene	0.00238	0.01193	56	31.4
1,2,4-Trimethylbenzene	0.00222	0.01114	120	32.5
M-xylene	0.00152	0.00761	106	23.1
N-heptane	0.00140	0.00706	100	6.76
4-Methyl-2-pentanone	0.00123	0.00616	100	13
N-dodecane	0.00101	0.00508	170	13.2
1,2,3-Trimethylbenzene	0.00089	0.00448	120	32.7
1,3,5-Trimethylbenzene	0.00086	0.00431	120	56.7
N-octane	0.00083	0.00419	114	8.11
2,3-Dimethylbutane	0.00080	0.00405	86	5.78

Hexanal	0.00075	0.00379	100	30
Undecane	0.00073	0.00367	156	12.3
O-ethyl toluene	0.00073	0.00367	120	11.9
Trans-2-butene	0.00070	0.00353	56	64
N-decane	0.00069	0.00346	142	11
P-ethyl toluene	0.00067	0.00336	120	11.8
2,2,4-Trimethyl pentane	0.00067	0.00335	114	3.34
Total	0.23547	0.6082	/	/

Supplementary Figures



25 **Figure S1: Hourly meteorological parameters during the study period. The green line is added to separate the two episodes, the black dashed lines indicate the two days before and two days after the episodes.**

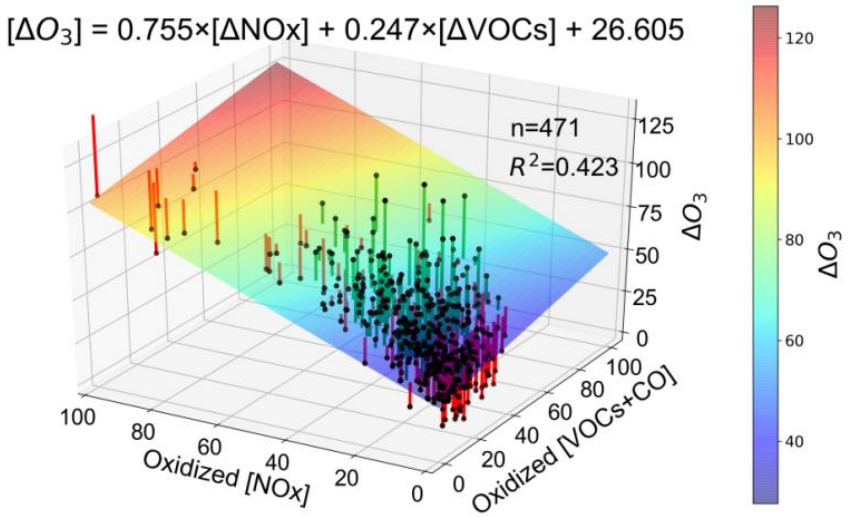


Figure S2: Three-dimensional depiction of ozone formation rate (ΔO_3, z-axis) plotted as a function of oxidized NOx (x-axis) and oxidized VOC (y-axis). The black dots denote values of ΔO_3, the colored plane is the best linear fit to the black dots, and the green and red bars denote positive and negative deviations from the plane, respectively. The equation listed represents the surface as a function of oxidized NOx and oxidized VOC. R^2 is the square of correlation coefficient of the linear regression.