How photochemically consumed volatile organic compounds affect ozone formation: a case study in Chengdu, China

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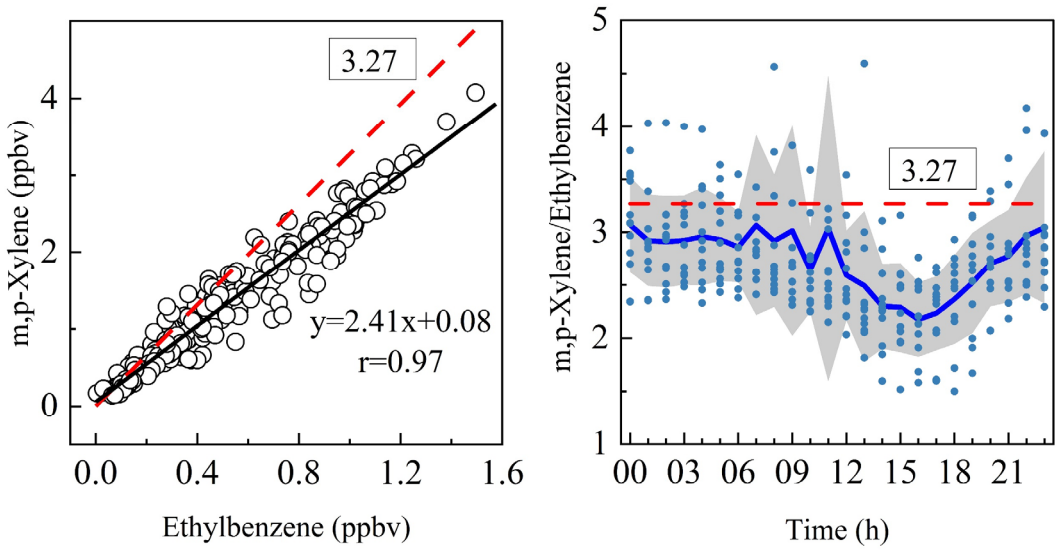

Figure S1. Scatterplot between m,p-xylene and ethylbenzene (left). Diurnal variation of m,p-xylene/ethylbenzene mixing ratio (right). The blue line represents the mean, and the gray area represents the standard deviation. The blue dots are the ratios of hourly measurements for each day during the observation period. The red dashed line shows the initial emission ratio of m,p-xylene/ethylbenzene estimated in this study (3.27 ppbv/ppbv).

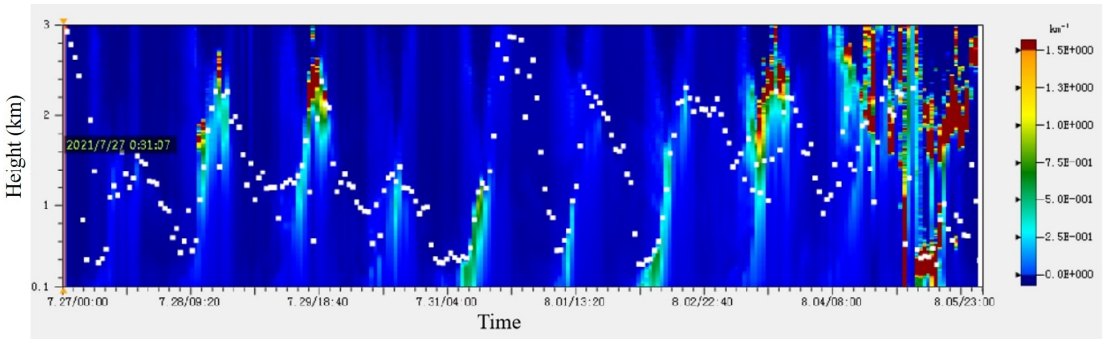

Figure S2. Inversion map of vertical diffusion data from aerosol lidar.

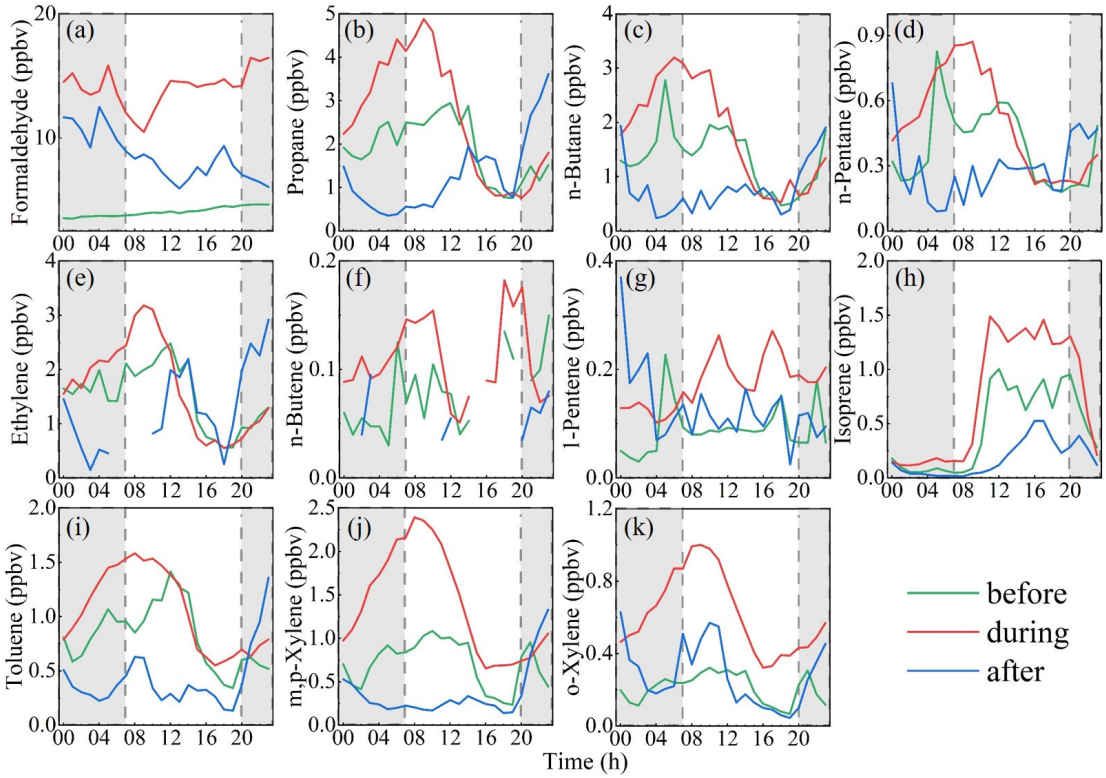

Figure S3. Diurnal and nocturnal variation of key VOC species (formaldehyde (**a**), alkanes (**b**—**d**), alkenes (**e**—**h**), aromatics (**i**—**k**)) before (25 July–26 July), during (27 July–4 August), and after (5 August) the pollution. The gray shaded area indicates nighttime (daytime: 7:00—20:00 (CNST); nighttime: 21:00—6:00 (CNST)).

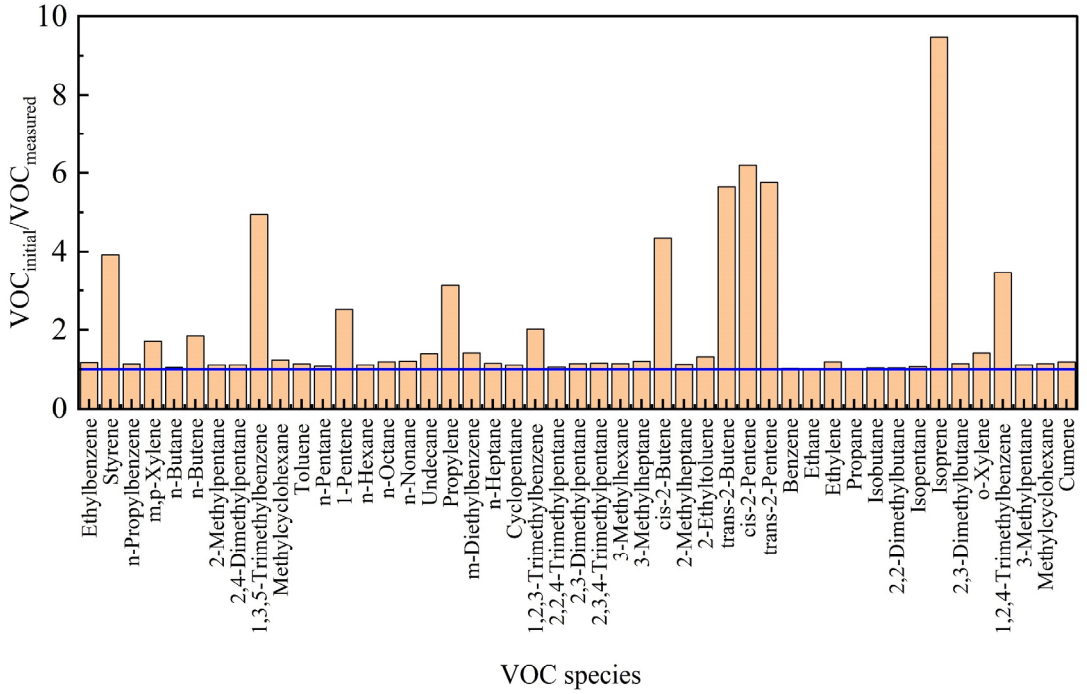

Figure S4. The ratios of initial/measured concentration of VOCs.

Table S1. The contributions of VOCs to OFP at Chengdu.

Species (n = 47)	MIR (g·O$_3$/g·VOC)	Concentration (μg/m^3)			OFP (μg/m^3)		
		Meas.	Cons.	PICs	Meas.	Cons.	PICs
Alkanes		30.768	2.179	32.894	34.504	2.912	37.355
Ethane	0.28	3.421	0.017	3.434	0.958	0.005	0.961
Propane	0.49	4.258	0.089	4.347	2.086	0.044	2.130
n-Butane	1.15	3.916	0.172	4.068	4.504	0.197	4.678
Isobutane	1.23	2.572	0.102	2.664	3.164	0.126	3.276
Cyclopentane	2.39	0.347	0.038	0.384	0.828	0.090	0.917
n-Pentane	1.31	1.338	0.100	1.436	1.752	0.132	1.880
Isopentane	1.45	5.082	0.363	5.437	7.368	0.527	7.884
Methylcyclohexane	2.19	1.041	0.153	1.199	2.280	0.335	2.625
2-Methylpentane	1.50	1.664	0.195	1.856	2.496	0.293	2.784
n-Hexane	1.24	1.518	0.175	1.688	1.882	0.216	2.093
2,2-Dimethylbutane	1.17	1.006	0.048	1.055	1.177	0.056	1.234
2,3-Dimethylbutane	0.97	0.872	0.134	1.006	0.846	0.130	0.976
3-Methylpentane	1.80	1.265	0.159	1.419	2.277	0.285	2.554
Methylcyclohexane	1.70	0.053	0.012	0.065	0.090	0.021	0.110
2,3-Dimethylpentane	1.34	0.063	0.007	0.070	0.097	0.011	0.108
2,4-Dimethylpentane	1.55	0.375	0.048	0.424	0.401	0.052	0.453
3-Methylhexane	1.61	0.157	0.023	0.180	0.210	0.031	0.241
n-Heptane	1.07	0.485	0.069	0.554	0.781	0.111	0.892

2,2,4-Trimethylpentane	1.26	0.257	0.053	0.310	0.231	0.048	0.279
2,3,4-Trimethylpentane	1.03	0.059	0.004	0.063	0.074	0.005	0.079
2-Methylheptane	1.07	0.423	0.061	0.484	0.435	0.063	0.499
3-Methylheptane	1.24	0.194	0.043	0.238	0.241	0.054	0.296
n-Octane	0.90	0.119	0.015	0.134	0.127	0.016	0.143
n-Nonane	0.78	0.137	0.029	0.164	0.107	0.022	0.128
Undecane	0.61	0.148	0.069	0.217	0.090	0.042	0.133
Alkenes		5.283	22.529	27.804	53.903	247.619	301.466
Ethylene	9.00	1.932	0.336	2.259	17.387	3.027	20.330
Propylene	11.66	0.198	0.181	0.379	2.308	2.109	4.417
n-Butene	9.73	0.231	0.192	0.423	2.251	1.864	4.113
cis-2-Butene	14.24	0.099	0.325	0.423	1.410	4.630	6.030
trans-2-Butene	15.16	0.476	2.287	2.764	7.212	34.667	41.908
Isoprene	10.61	1.538	16.910	18.448	16.318	179.412	195.731
1-Pentene	7.21	0.440	0.637	1.077	3.176	4.595	7.764
cis-2-Pentene	10.38	0.294	1.259	1.555	3.049	13.068	16.137
trans-2-Pentene	10.56	0.075	0.401	0.476	0.790	4.236	5.027
Aromatics		15.641	7.963	23.599	86.848	53.089	139.988
Benzene	0.72	1.306	0.034	1.336	0.940	0.024	0.962
Toluene	4.00	3.648	0.487	4.135	14.590	1.948	16.537
Styrene	1.73	0.472	1.428	1.902	0.817	2.470	3.290
Ethylbenzene	3.04	2.037	0.361	2.382	6.194	1.098	7.242
m,p-Xylene	7.80	5.229	3.605	8.849	40.781	28.115	69.023
o-Xylene	7.64	2.280	1.020	3.300	17.422	7.793	25.215
n-Propylbenzene	2.03	0.060	0.009	0.069	0.122	0.018	0.140
1,2,3-Trimethylbenzene	11.97	0.054	0.198	0.251	0.630	2.326	2.955
1,2,4-Trimethylbenzene	11.76	0.050	0.056	0.106	0.597	0.669	1.266
1,3,5-Trimethylbenzene	11.76	0.080	0.028	0.107	0.445	0.154	0.597
2-Ethyltoluene	5.59	0.313	0.699	1.011	3.683	8.225	11.886
Cumene	2.52	0.037	0.007	0.044	0.094	0.018	0.111
m-Diethylbenzene	7.10	0.075	0.032	0.107	0.530	0.229	0.758
NMHC		51.692	32.671	84.298	175.254	303.620	478.809

* Under normal temperature and pressure (25 °C, 101 kPa), the volume of 1 mol gas is 22.4 × (273 + 25) / 273 = 24.5 L/mol. We converted ppbv to μg/m^3 according to the following formula:
Mass concentration = Volume concentration × Relative molecule Mass / 24.5