



Supplement of

Explicit modeling of isoprene chemical processing in polluted air masses in suburban areas of the Yangtze River Delta region: radical cycling and formation of ozone and formaldehyde

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11 Text S1. Conditional Probability Function (CPF)

The CPF was originally used to show the wind directions that dominate a high concentration
of a pollutant, showing the probability of such concentrations occurring by wind direction
(Ashbaugh et al. 1985). The CPF is defined as:

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$$CPF = \frac{m_{\theta,j}}{n_{\theta,j}}$$

16 Where $m_{\theta,j}$ is the number of samples in the wind sector θ and wind speed interval *j* with mixing 17 ratios greater than high O₃ concentration. In this study, we defined high O₃ concentration as the 18 95th percentile of observed O₃ concentration (131 ppbv). $n_{\theta,j}$ is the total number of samples in the 19 wind sector θ and wind speed interval *j*.

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21 Test S2. Sensitive study of HONO/NO₂ ratio.

To investigate the sensitivity of our simulation to HONO/NO₂ ratio, we conducted a series of simulations with different HONO/NO₂. The results were summarized in Table S2 and Figure S1. A lower HONO/NO₂ ratio (e.g. 0.005) can lead to 15.28% decrease of HO radical and a higher ratio (e.g. 0.04) can caused 14.08% increase in OH concentration. This could be explained by the importance role of HONO photolysis in OH sources.





Figure S1. Comparison of observed and simulated O3 concentrations in 5 episodes.



Figure S2. Comparison of observed and simulated HCHO concentrations in 5 episodes



Figure S3. Comparison of simulated and linear regression concentration of OVOC



Figure S4. Comparison of OH concentration under different HONO/NO2 ratios.





43 Figure S6. Sensitivity analysis of OBM modelled O₃, HCHO, and OH concentrations without alkenes 44 (including ethylene, propene, and acetylene), isoprene, and EXT (ethylbenzene, xylene, and toluene) 45 input.





Figure S7. Sensitivity analysis of OBM modelled O₃, HCHO, and OH concentrations with different 48 49 CH₄ concentrations.



vsis of OBM modelled O₃, HCHO, and OH concentrations with reduce NO₂ concentrations.



HONO/NO ₂ ratio	Change in OH (%)		
0.005	-15.3%		
0.01	-9.3%		
0.03	7.5%		
0.04	14.1%		

Table S2 Results of linear regression of OVOC

β ₀	β_1	β_2	β ₃	β_4	β5	Sig	R
-0.3425	0.027	0.623	0.820	1.091	0.205	0.000	0.853

65 **Reference:**

- 66 Lowell L. Ashbaugh, William C. Malm, Willy Z. Sadeh. A residence time probability analysis of
- 67 sulfur concentrations at grand Canyon National Park[J]. Atmospheric Environment, 1985,

68 19(8):1263-1270.