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Nighttime ozone in the lower boundary layer: insights from 3-year tower-based measurements in South China and regional air quality modeling

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Table S1. Statistical metrics of comparison between observed and simulated ozone and meteorological parameters

Parameters	$\overline{Obs}$	$\overline{\text{Sim}}$	r	NMB (%)[a]	MB[b]	RMSE[c]	IOA[d]
Ozone (ppbv)	24	22	0.70	-7.66	-1.81	13.55	0.83
T (℃)	28	27	0.95	0.93	0.11	1.05	0.96
RH (%)	54	53	0.69	-8.99	-2.11	7.79	0.79

[a]Normalized mean bias (NMB). Defined as $NMB = \frac{\sum_{i=1}^{n}(Sim_i - Obs_i)}{\sum_{i=1}^{n} Obs_i}$

[b]Mean bias (MB). Defined as $MB = \overline{Obs} - \overline{Sim}$

[c]Root mean square error (RMSE). Defined as $RMSE = \frac{\sum_{i=1}^{n}(Sim_i - \overline{Sim_i})(Obs_i - \overline{Obs_i})}{\sqrt{\sum_{i=1}^{n}(Sim_i - \overline{Sim_i})^2}\sqrt{\sum_{i=1}^{n}(Obs_i - \overline{Obs_i})^2}}$

[d]Index of agreement (IOA). Defined as $IOA = 1 - \frac{\sum_{i=1}^{n}(Sim_i - Obs_i)^2}{\sum_{i=1}^{n}(|Sim_i - \overline{Obs}| + |Obs_i - \overline{Obs}|)^2}$

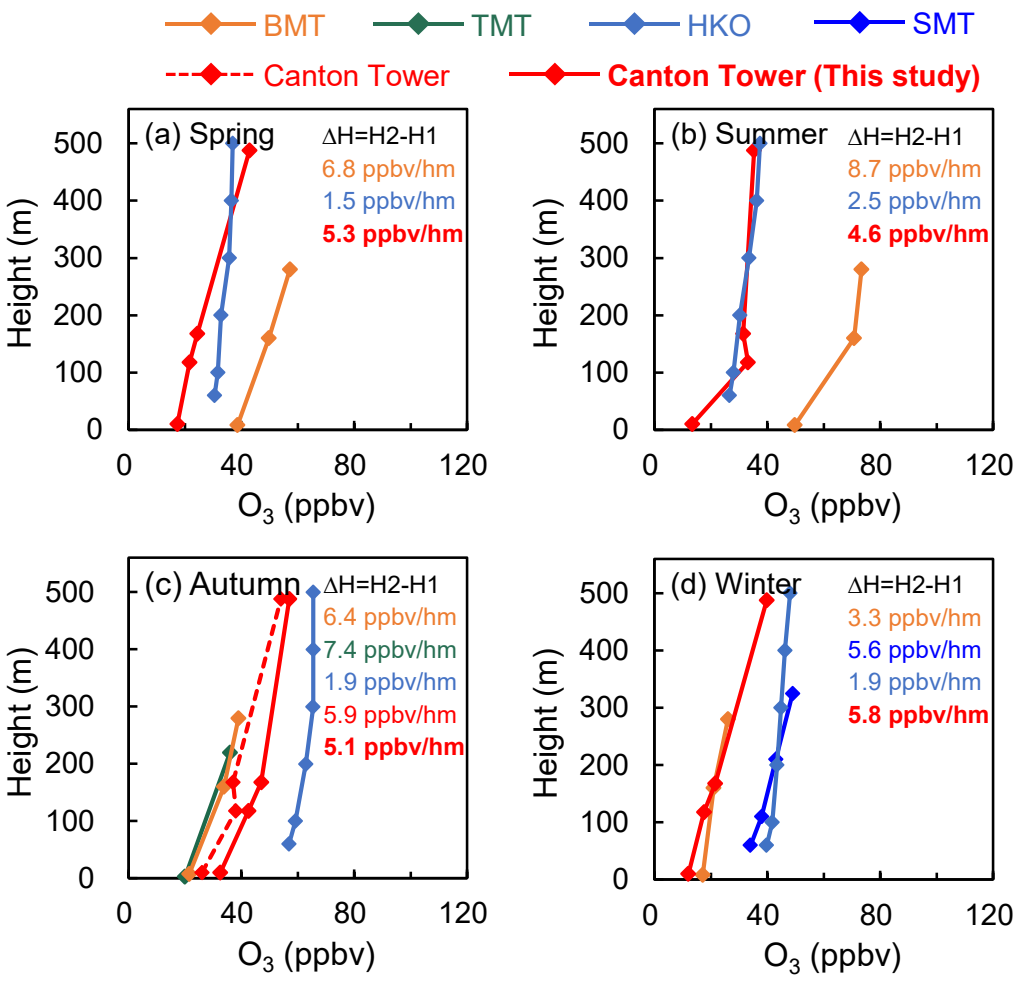

Figure S1. Comparison of the lower boundary layer ozone between the Canton Tower and nearby ozonesonde observations and other reported tower-based observations. H1, H2 represent the lowest and highest measuring point in each station, respectively. Measurements in the Beijing Meteorology Tower (BMT) is from Liu et al. (2022) (2019 to 2020), in the Tianjin Meteorological Tower (TMT) is from Han et al. (2020) (October 2018), in the Shenzhen Meteorology Tower (SMT) is from Li et al. (2019) (December 2017), in the Canton Tower is from Li et al. (2022) (August 18 to November 5, 2020), and in Hong Kong Observatory (January, April, July and October 2017 to 2019), respectively.

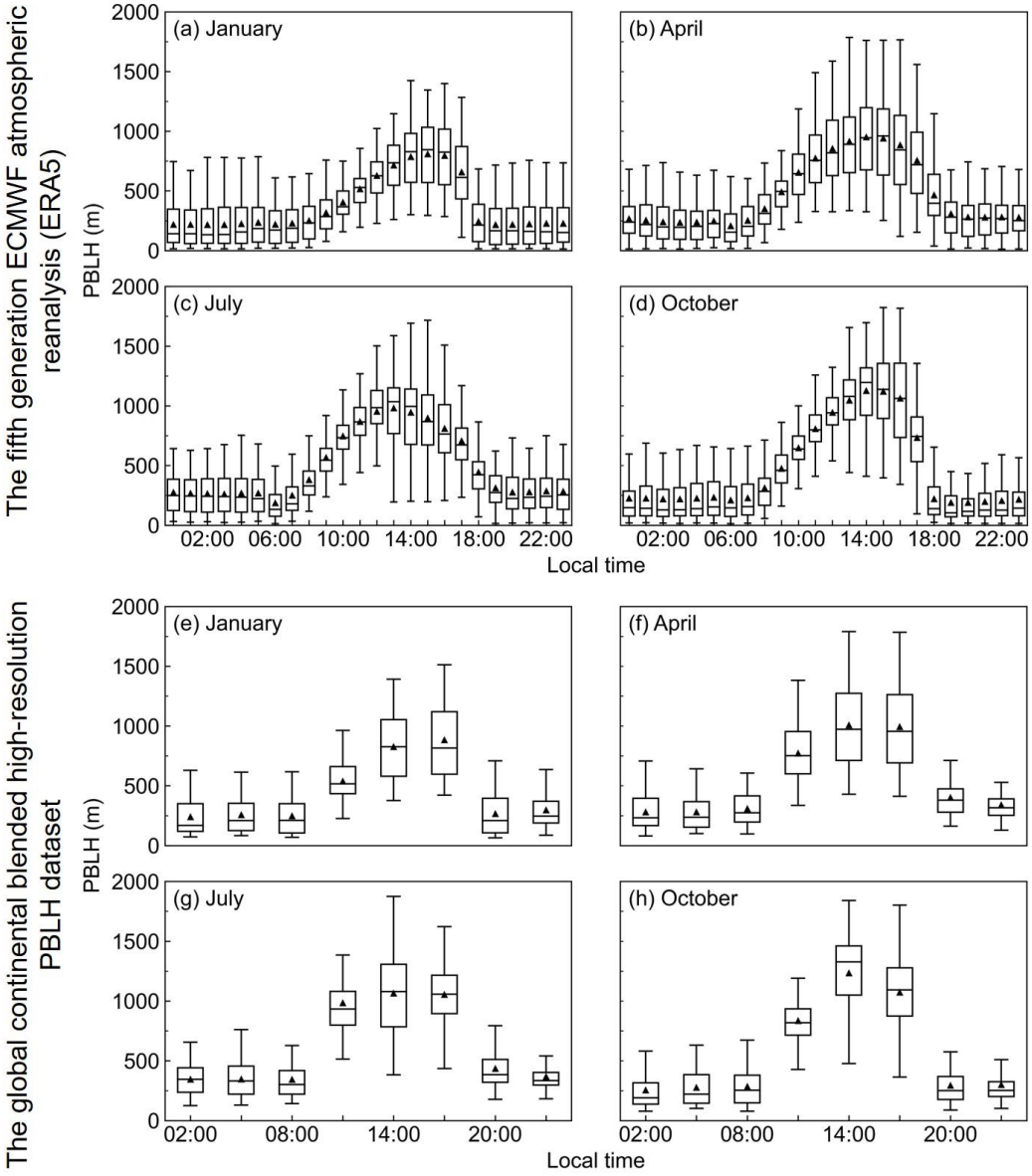

Figure S2. Time series of the planet boundary layer height (PBLH) at the Canton Tower. Panels (a) to (d) show the PBLH obtained from the ERA5 re-analysis dataset with 1-hour temporal resolution. Panels (e) to (h) show the PBLH obtained from the global continental blended high-resolution PBLH dataset (Guo. et al., 2022) with 3-hour temporal resolution.

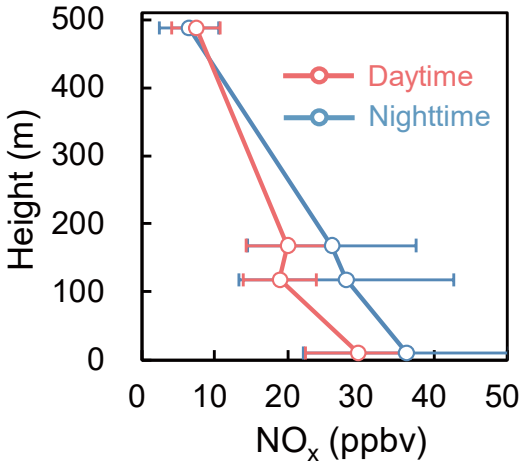

Figure S3. Mean NO_x vertical structure in the lower boundary layer observed at the Canton Tower, October 2017. Blue and rosy lines denote nighttime (20:00-07:00 LT) and daytime (08:00-19:00 LT) mean NO_x profiles.

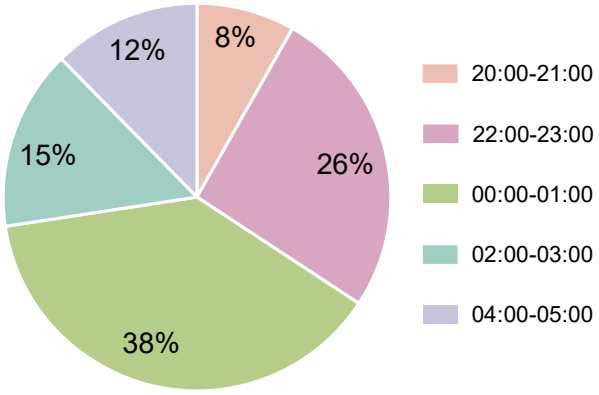

Figure S4. Occurrence time of nocturnal ozone enhancement (NOE) events among all the days in 2017-2019 with available observations. The occurrence time is defined as the time of maximum ($\Delta O_3/\Delta t$) during each NOE event.

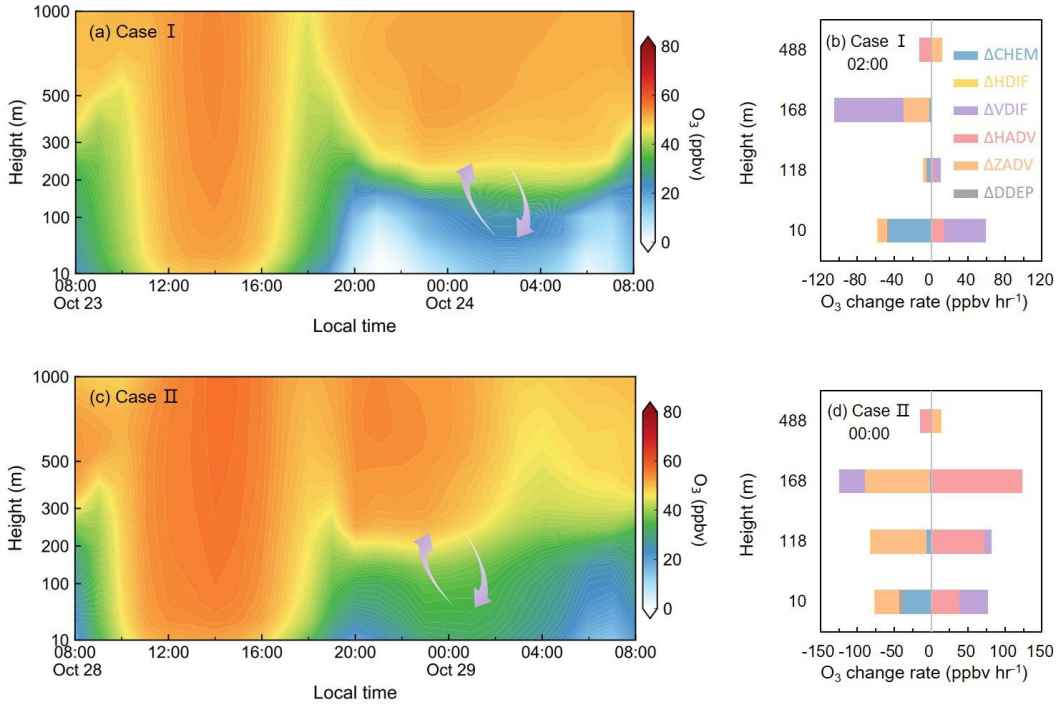

Figure S5. CMAQ model simulation of two NOE events. Panels (a) and (b) show the simulated ozone of case I from the surface to 1000 m at the Canton Tower and ozone budget terms diagnosed from the CMAQ IPR module at different measurement height. Panels (c) and (d) are the same as panels (a) and (b) but for case II. ΔCHEM represents change in chemistry, ΔVDIF represents change in vertical diffusion, ΔZADV represents change in vertical advection, ΔHDIF represents change in horizontal diffusion, ΔHADV represents change in horizontal advection, and ΔDDEP represents change in dry deposition.

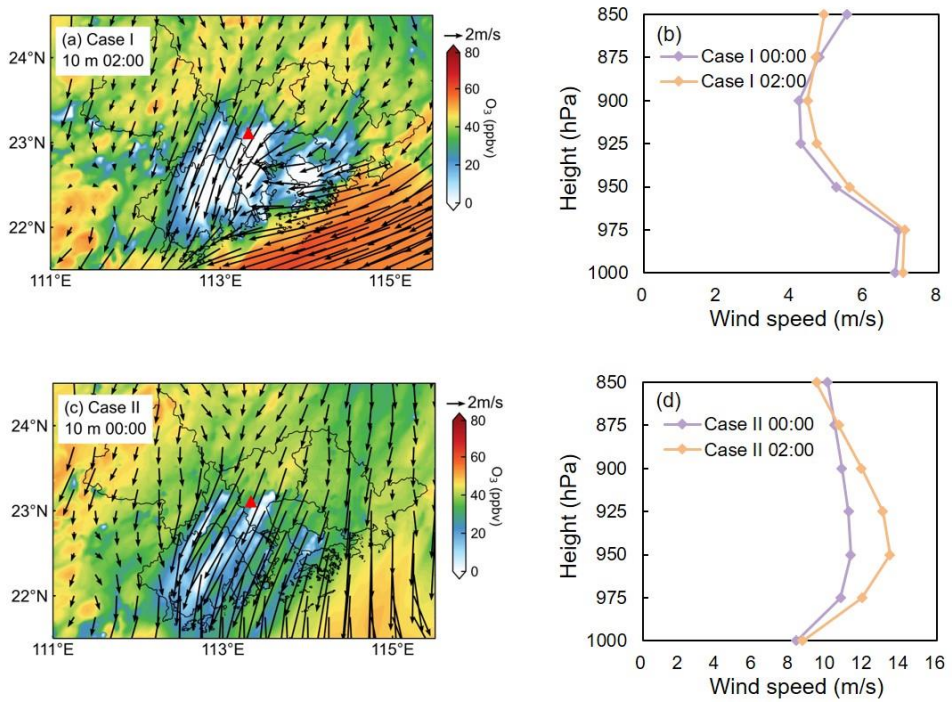

Figure S6. CMAQ model simulation of two NOE events. Panels (a) and (b) show the simulated surface ozone and the horizontal and vertical wind from the ERA5 dataset of case I. Panels (c) and (d) are the same as panels (a) and (b) but for case II. The triangle marks the location of the Canton Tower

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