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Supplement of

Meteorological conditions and aerosol-meteorology feedback drive divergent responses of co-occurring $PM_{2.5}$ and O_3 pollution to NO_x–VOC perturbations in Beijing–Tianjin–Hebei–Shandong

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Table S1 Statistics of the DHP samples at the reference thresholds ($PM_{2.5}$ > 35, MDA8 O_3 > 100 μg m^{-3}) and their ranges across the 25 perturbed threshold combinations. Medians are in μg m^{-3}.

condition	n	percentage	percentage range	$PM_{2.5}$ median	$PM_{2.5}$ median range	O_3 median	O_3 median range
Convective	87	5.8	5.2–6.1	41.6	38.7–44.1	153.1	151.4–153.4
Stable	192	12.7	12.3–13.3	46.3	43.4–47.7	153.7	150.7–157.0
WarmHumid	604	40.0	38.9–42.0	45.6	43.5–46.8	148.9	146.0–150.1
DryHot	242	16.0	14.6–18.8	39.7	38.1–41.0	163.7	162.9–164.0
Moderate	385	25.5	23.4–25.5	41.3	39.6–43.0	162.3	158.2–164.2
Total	1510	100.0	-	42.7	40.7–44.3	155.4	153.3–157.4

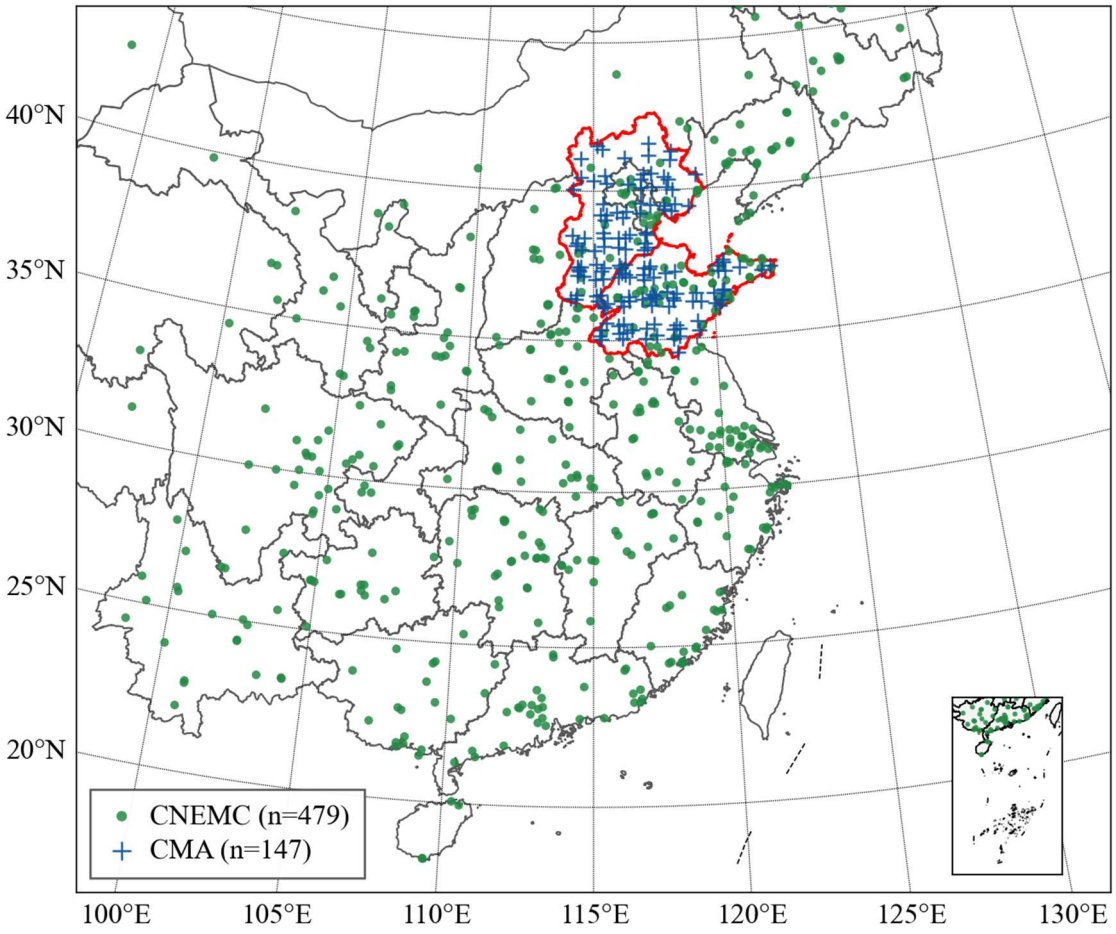


Figure S1 Model domain and the locations of two types of observation stations used in this study. Green circles denote CNEMC stations (n=479), while blue crosses denote CMA stations (n=147). The red outlines delineate the Beijing–Tianjin–Hebei–Shandong (BTHS) region.

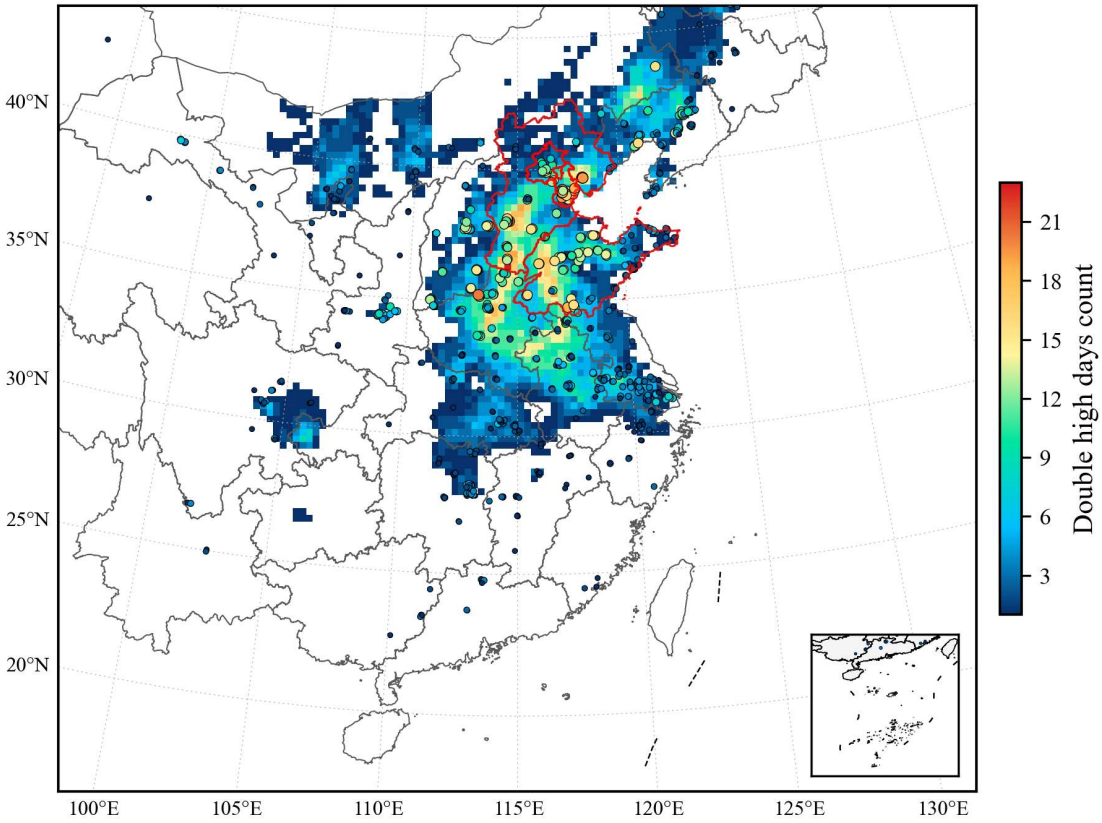


Figure S2 Spatial distribution of co-occurring $PM_{2.5}$ and O_3 pollution (DHP) days during 1–30 July 2020. A DHP day is defined as a day when the daily mean $PM_{2.5}$ exceeds 35 μg m^{-3} and the maximum daily 8-hour average (MDA8) O_3 exceeds 100 μg m^{-3} simultaneously. The color shading represents the number of DHP days at each WRF-Chem grid. Overlaid filled circles denote observed DHP days at surface observational stations, with the same color scale applied. The red outlines delineate the BTHS, where the most frequent co-pollution episodes are concentrated.

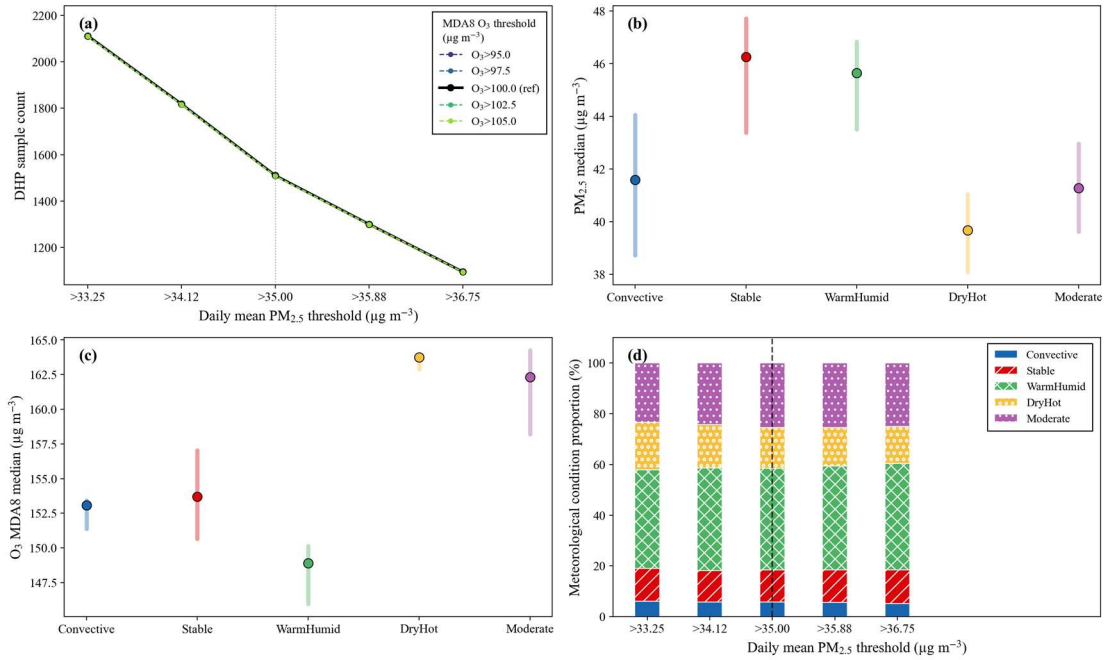


Figure S3 Sensitivity of DHP identification and meteorological condition classification to the threshold. (a) DHP sample count as a function of the $PM_{2.5}$ threshold; each line denotes one MDA8 O_3 threshold (95–105 μg m^{-3}), with the black solid line indicating the reference. (b) $PM_{2.5}$ and (c) MDA8 O_3 medians within each meteorological condition type: dots denote the reference threshold and vertical bars the range across all 25 combinations. (d) Meteorological condition proportions as a function of the $PM_{2.5}$ threshold with the O_3 threshold fixed at 100 μg m^{-3}; the dashed line marks the reference $PM_{2.5}$ threshold.

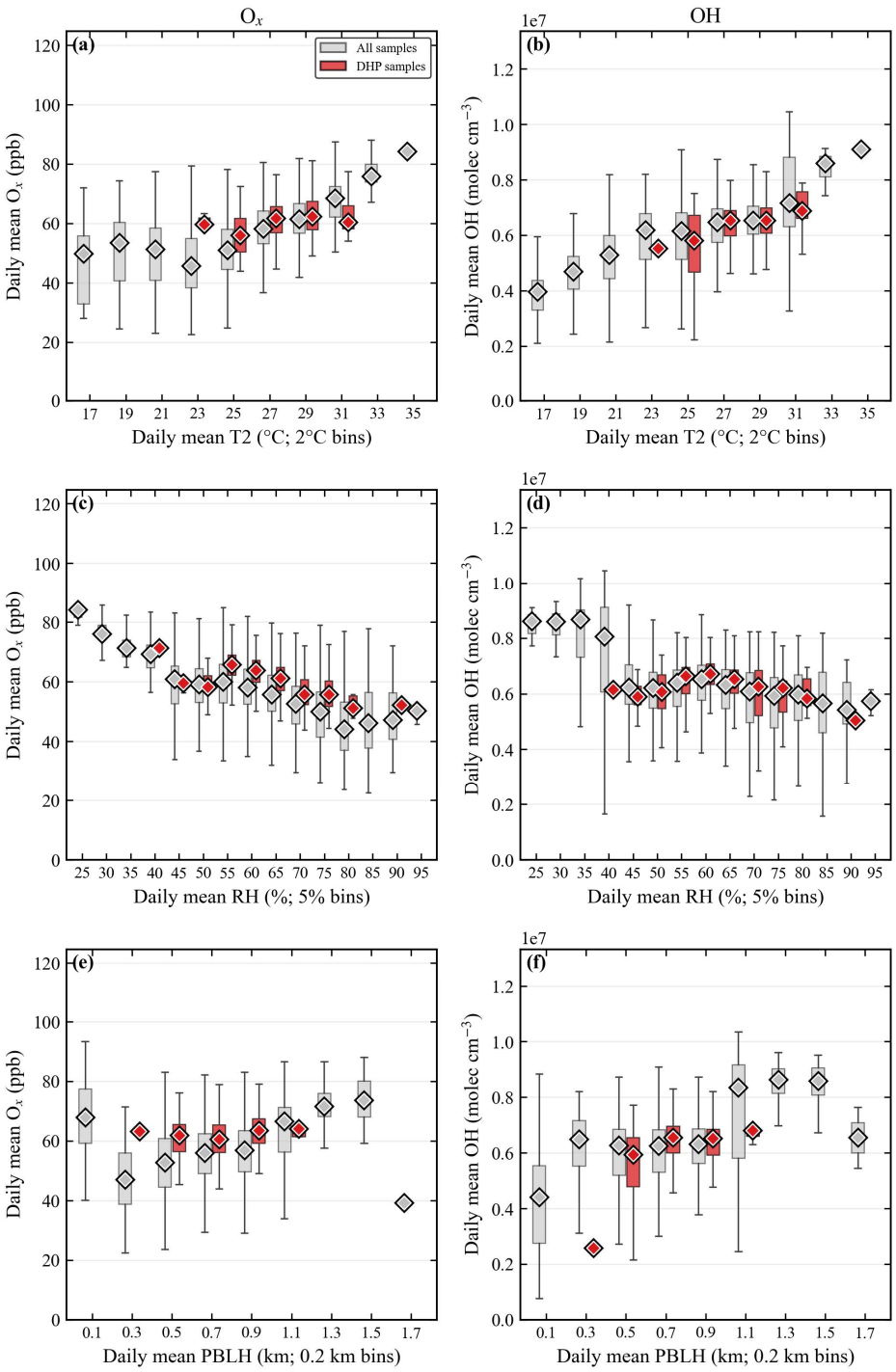


Figure S4 Boxplots of daily mean (a) (c) (e) O_x (O_3 + NO_2, ppb) and (b) (d) (f) OH (molecules cm^{-3}) in each 2-m air temperature (T2), 2-m relative humidity (RH2), and planetary boundary layer height (PBLH) bin of all samples and DHP samples from the EXP_W_BASE experiment. T2 is binned to 2°C intervals, RH2 to 5% intervals and PBLH to 0.2 km intervals. In each boxplot, the horizontal line inside the box represents the median, the box spans the interquartile range (25th–75th percentile), and the whiskers extend to the most extreme data points within 1.5 times the interquartile range from the box edges.

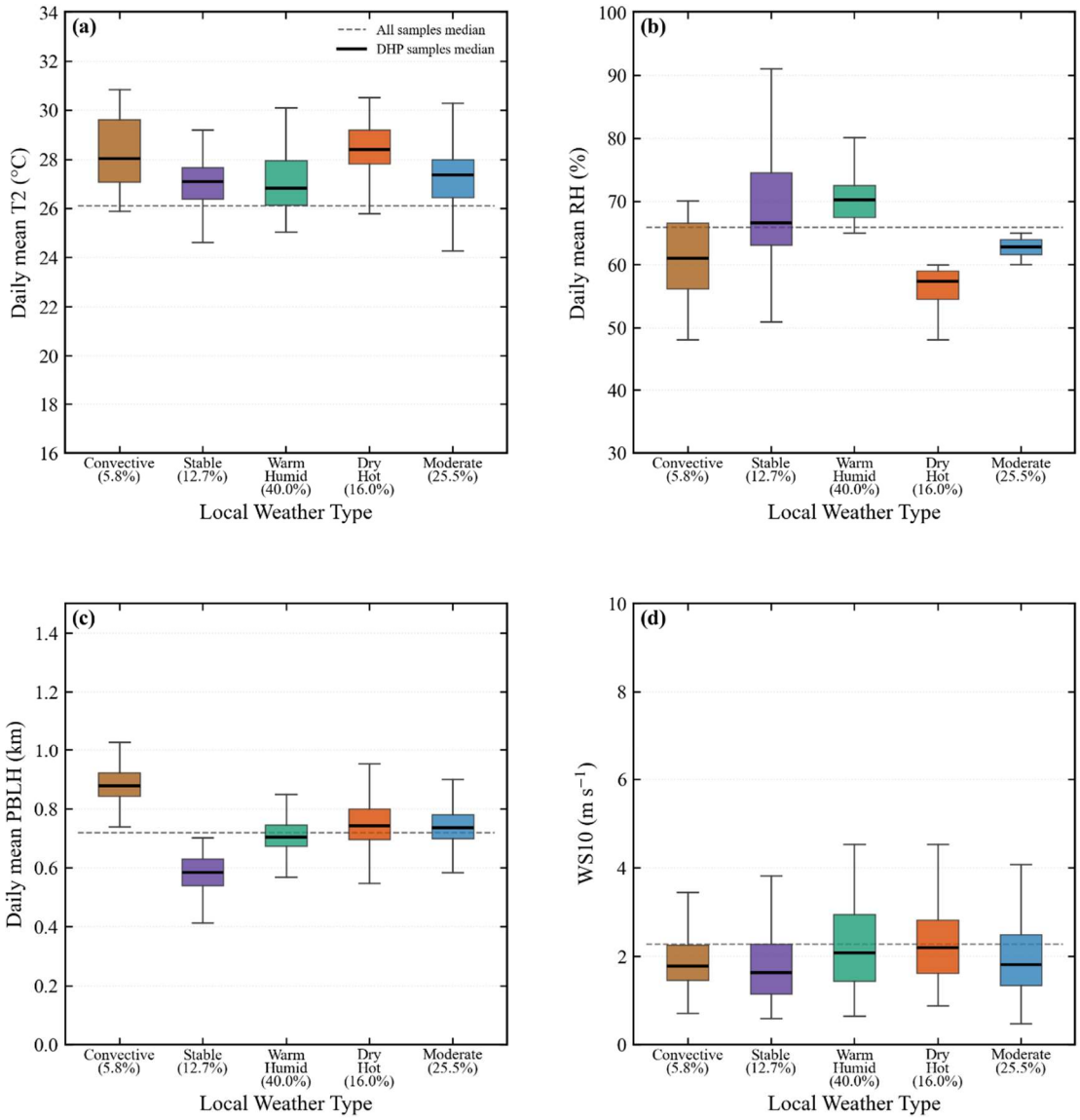


Figure S5 Boxplots of daily mean (a) T2 (°C), (b) RH2 (%), (c) PBLH (km), and (d) 10-m wind speed (WS10, m s^{-1}) for different meteorological condition types. The numbers in parentheses beneath each type indicate the proportion in the DHP samples and the gray dashed lines denote the median values for all samples.

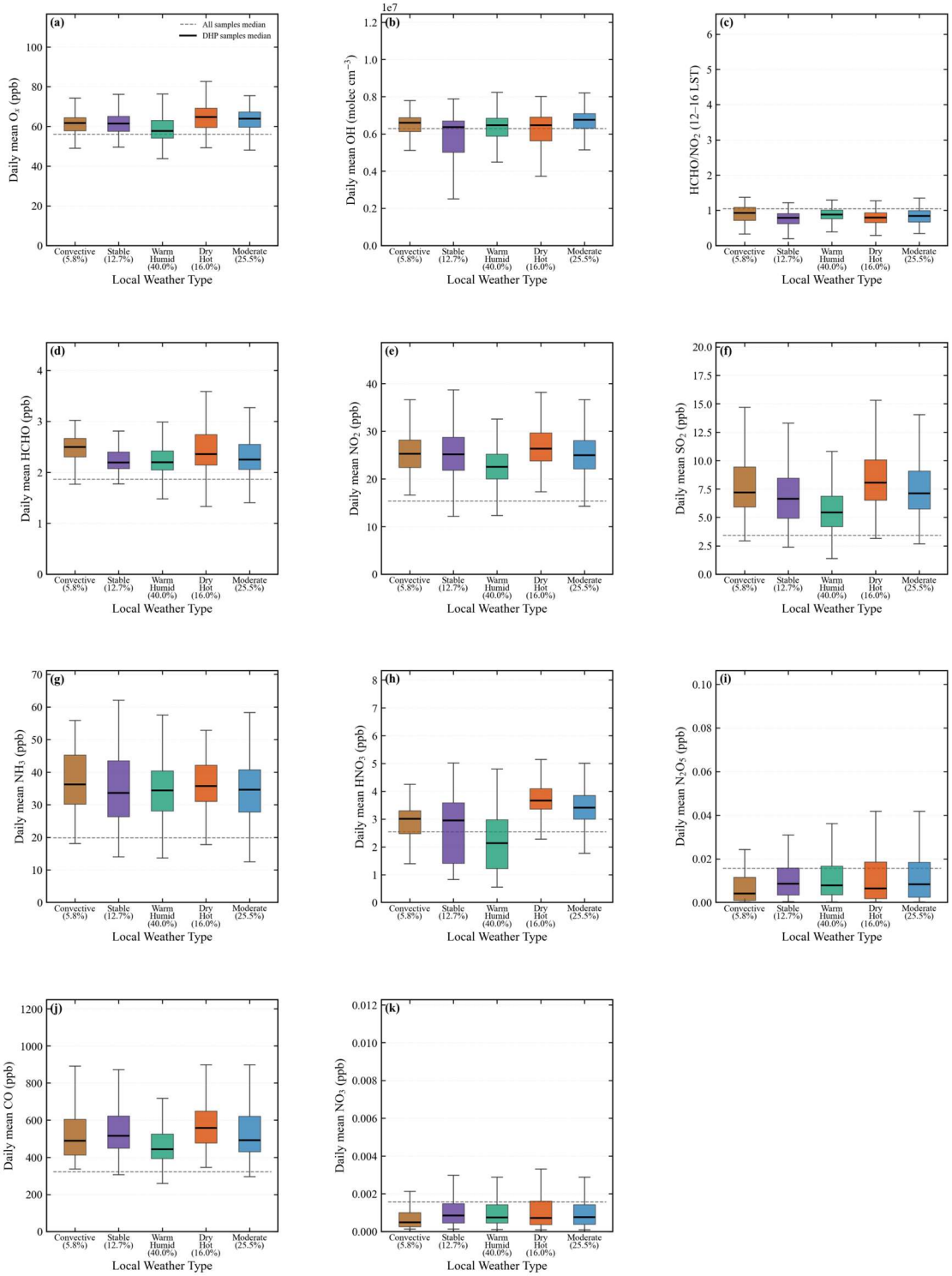


Figure S6 Boxplots of daily mean surface (a) total oxidants (O_x; ppb), (b) hydroxyl radicals (OH; molecules cm^{-3}), (c) HCHO/NO_2 ratio (unitless), (d) HCHO (ppb), (e) NO_2 (ppb), (f) SO_2 (ppb), (g) NH_3 (ppb), (h) HNO_3 (ppb), (i) N_2O_5 (ppb), (j) CO (ppb), and (k) nitrate radicals (NO_3; ppb) for different meteorological condition types. The numbers in parentheses beneath each type indicate the proportion in the DHP samples and the gray dashed lines denote the median values for all samples.

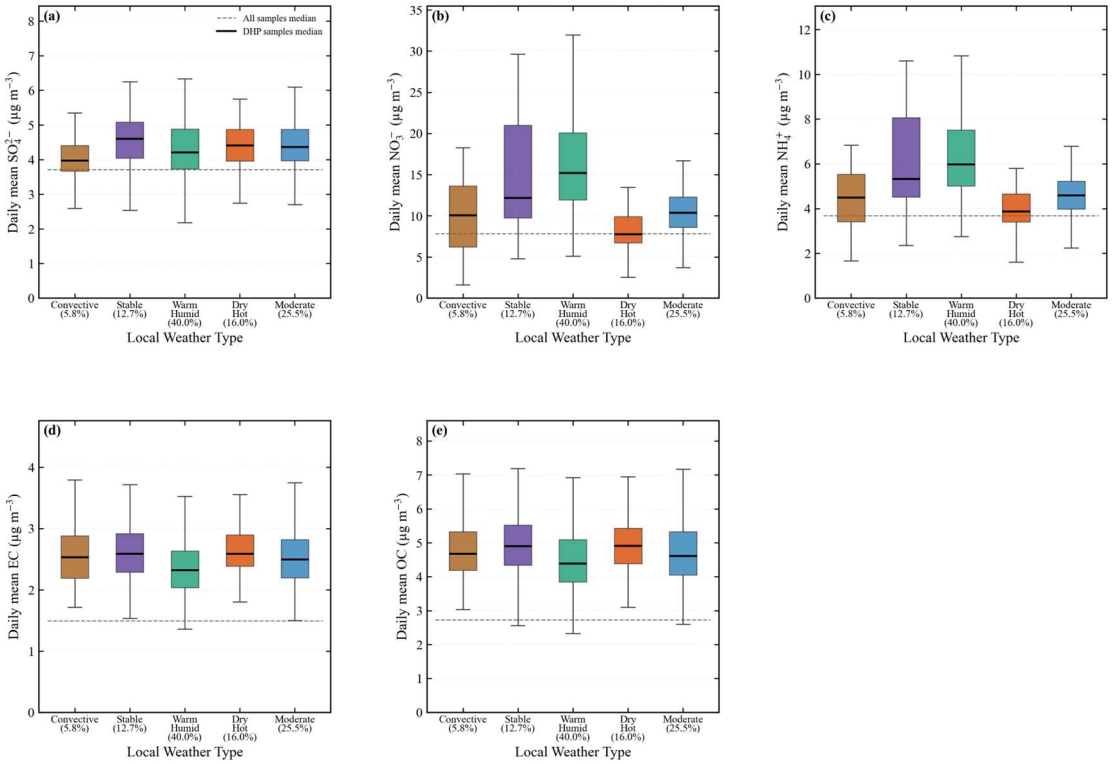


Figure S7 Boxplots of daily mean (a) SO_4^{2-} (μg m^{-3}), (b) NO_3^- (μg m^{-3}), (c) NH_4^+ (μg m^{-3}), (d) BC (μg m^{-3}), (e) OC (μg m^{-3}) for different meteorological condition types. The numbers in parentheses beneath each type indicate the proportion in the DHP samples and the gray dashed lines denote the median values for all samples.

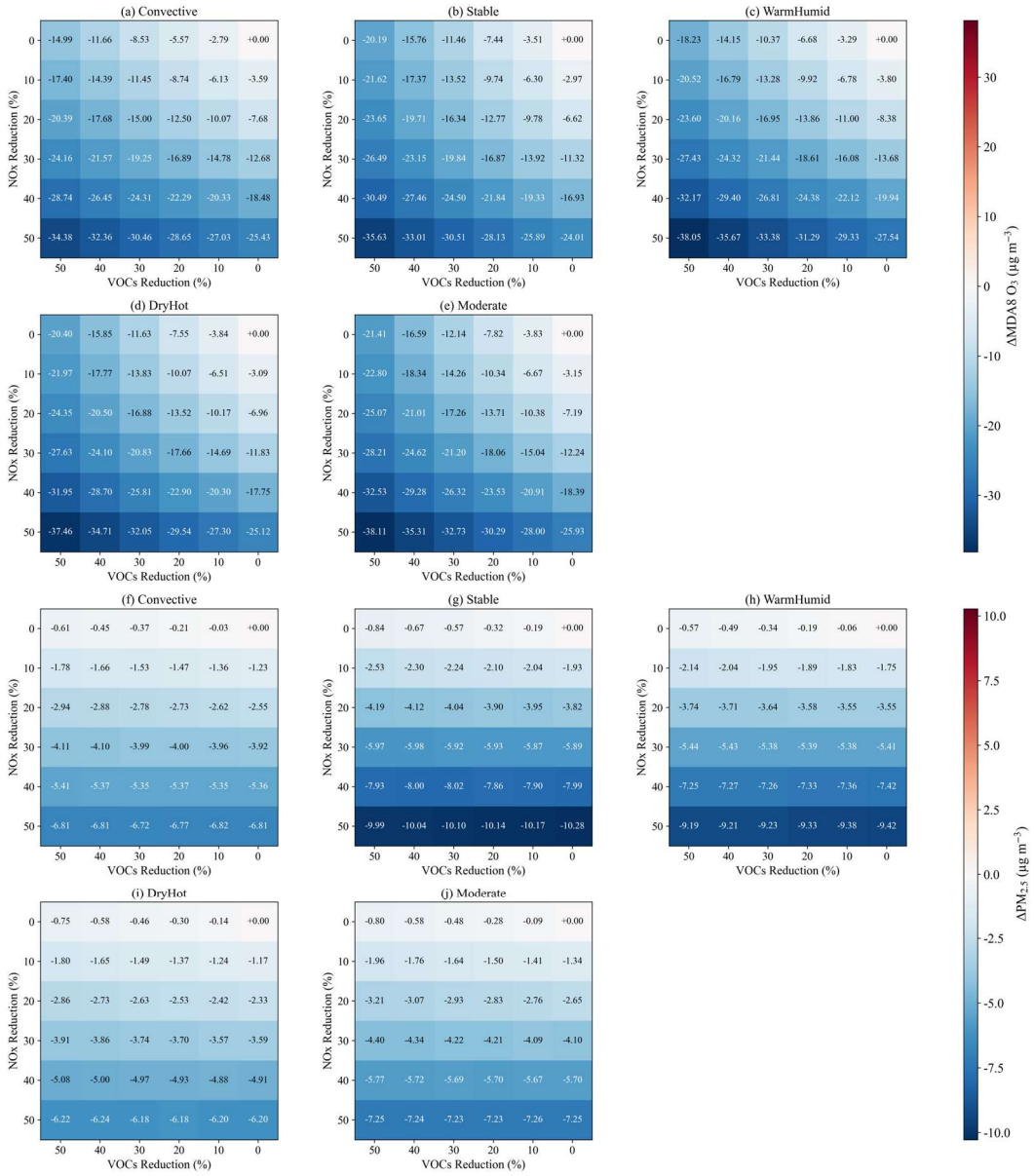


Figure S8 MDA8 O_3 and $PM_{2.5}$ response to NO_x and VOC reductions for DHP samples classified into different meteorological condition types. The absolute differences in MDA8 O_3 between each reduction scenario and the baseline scenario (ΔMDA8 O_3, μg m^{-3}) for (a) Convective, (b) Stable, (c) WarmHumid, (d) DryHot, and (e) Moderate, and the absolute differences in $PM_{2.5}$ between each reduction scenario and the baseline (Δ$PM_{2.5}$, μg m^{-3}) for (f) Convective, (g) Stable, (h) WarmHumid, (i) DryHot, and (j) Moderate. Rows and columns denote NO_x and VOC reduction levels (%).

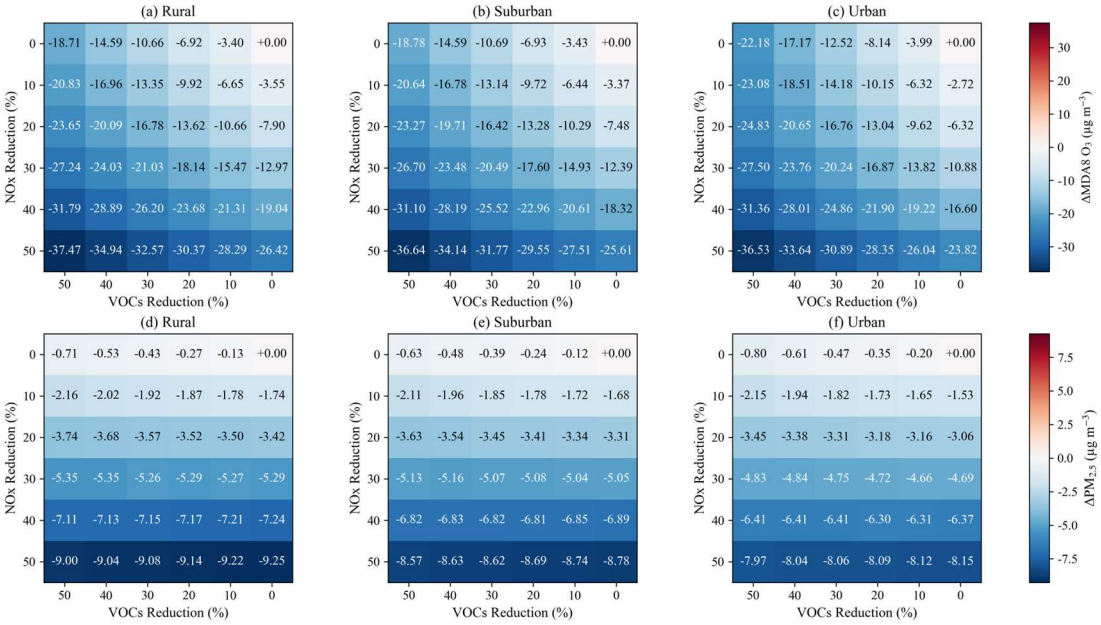


Figure S9 The absolute differences in MDA8 O_3 between each reduction scenario and the baseline scenario (ΔMDA8 O_3, μg m^{-3}) for (a) rural, (b) suburban, and (c) urban grid cells, and the absolute differences in $PM_{2.5}$ between each reduction scenario and the baseline (Δ$PM_{2.5}$, μg m^{-3}) for (d) rural, (e) suburban, and (f) urban grid cells for DHP samples. Rows and columns denote NO_x and VOC reduction levels (%).

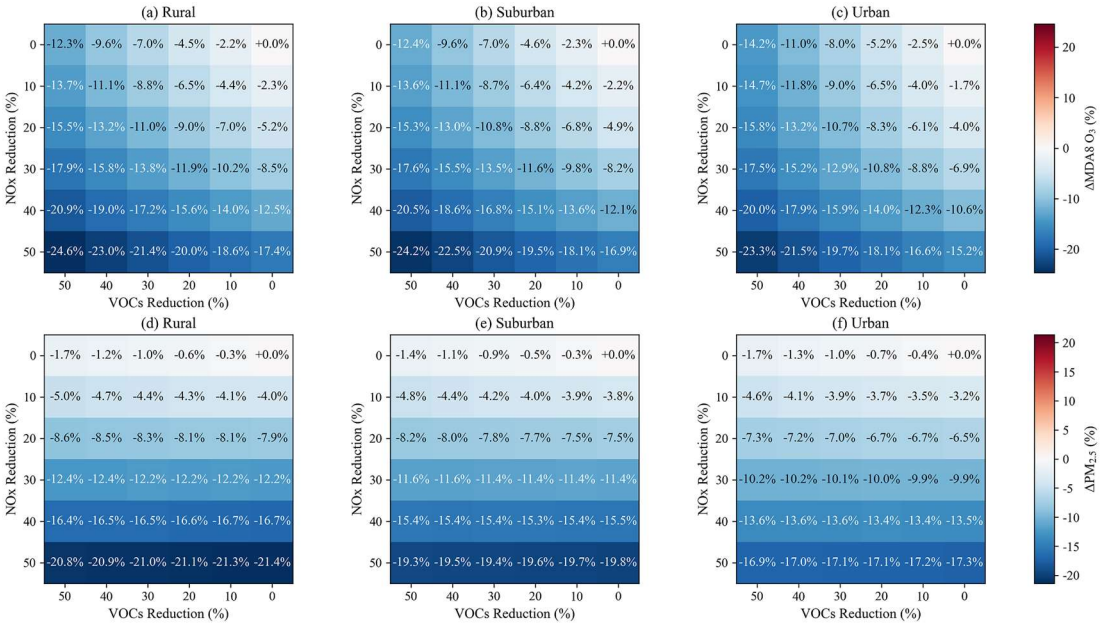


Figure S10 The percentage differences in MDA8 O_3 between each reduction scenario and the baseline scenario (ΔMDA8 O_3, %) for (a) rural, (b) suburban, and (c) urban grid cells, and the percentage differences in $PM_{2.5}$ between each reduction scenario and the baseline (Δ$PM_{2.5}$, %) for (d) rural, (e) suburban, and (f) urban grid cells for DHP samples. Rows and columns denote NO_x and VOC reduction levels (%).

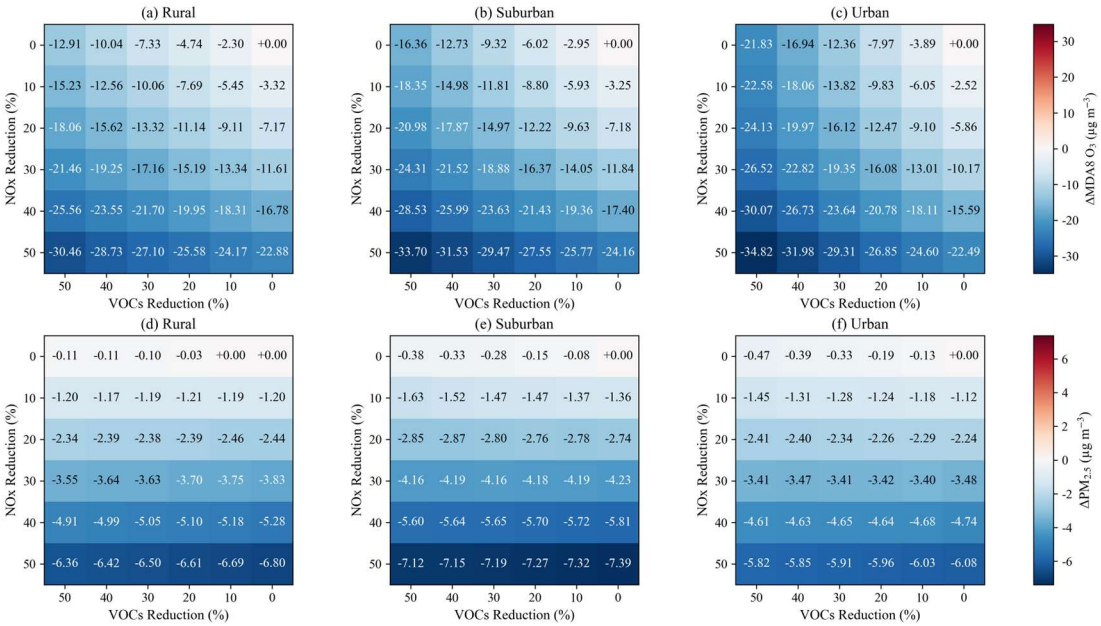


Figure S11 The absolute differences in MDA8 O_3 between each reduction scenario and the baseline scenario (ΔMDA8 O_3, μg m^{-3}) for (a) rural, (b) suburban, and (c) urban grid cells, and the absolute differences in $PM_{2.5}$ between each reduction scenario and the baseline (Δ$PM_{2.5}$, μg m^{-3}) for (d) rural, (e) suburban, and (f) urban grid cells for all samples. Rows and columns denote NO_x and VOC reduction levels (%).

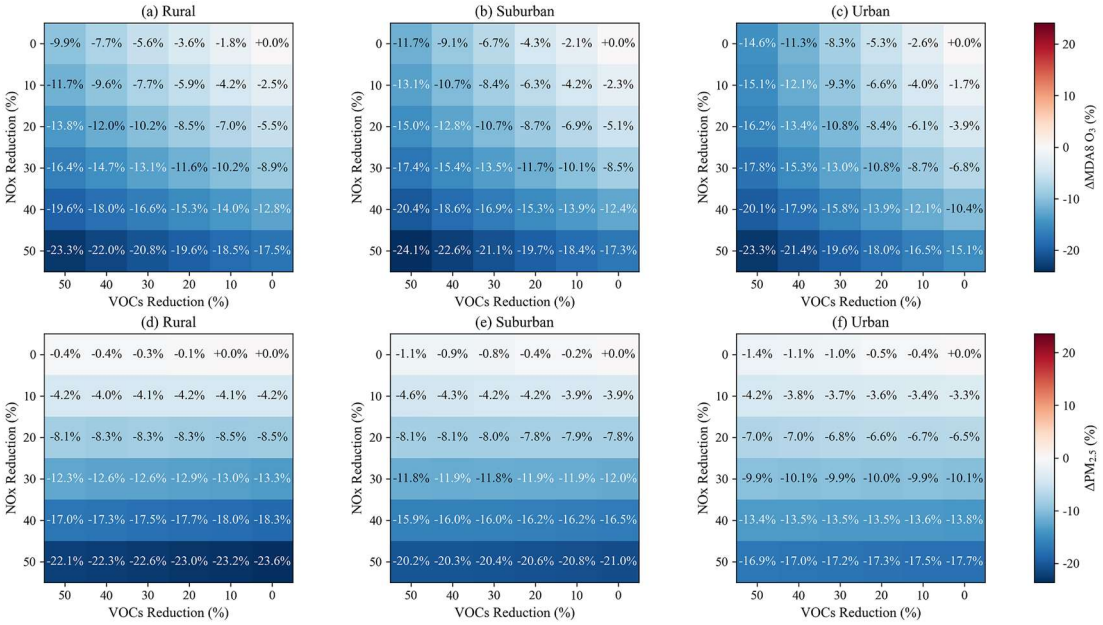


Figure S12 The percentage differences in MDA8 O_3 between each reduction scenario and the baseline scenario (ΔMDA8 O_3, %) for (a) rural, (b) suburban, and (c) urban grid cells, and the percentage differences in $PM_{2.5}$ between each reduction scenario and the baseline ($\Delta PM_{2.5}$, %) for (d) rural, (e) suburban, and (f) urban grid cells for all samples. Rows and columns denote NO_x and VOC reduction levels (%).

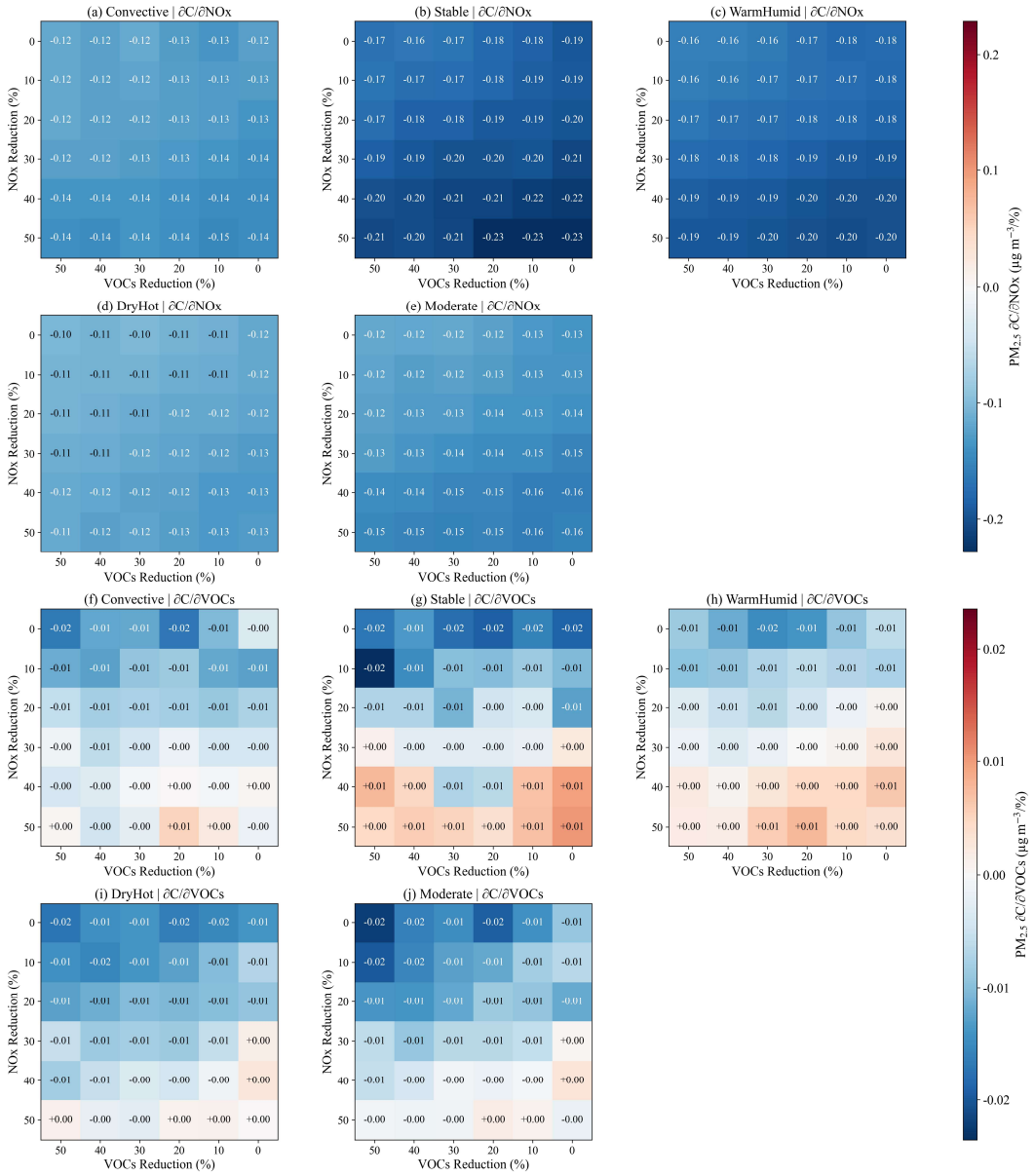


Figure S13 $PM_{2.5}$ response gradient to NO_x and VOC emission reductions for DHP samples classified into different meteorological condition types. $\partial(PM_{2.5})/\partial NO_x$ (μg m^{-3}/%) for (a) Convective, (b) Stable, (c) WarmHumid, (d) DryHot, and (e) Moderate, and $\partial(PM_{2.5})/\partial VOCs$ (μg m^{-3}/%) for (f) Convective, (g) Stable, (h) WarmHumid, (i) DryHot, and (j) Moderate. The gradients are computed by differentiating the absolute response matrices with respect to the reduction level at 10 percentage point intervals (0, 10, 20, 30, 40, 50%). Rows and columns denote NO_x and VOC reduction levels (%).

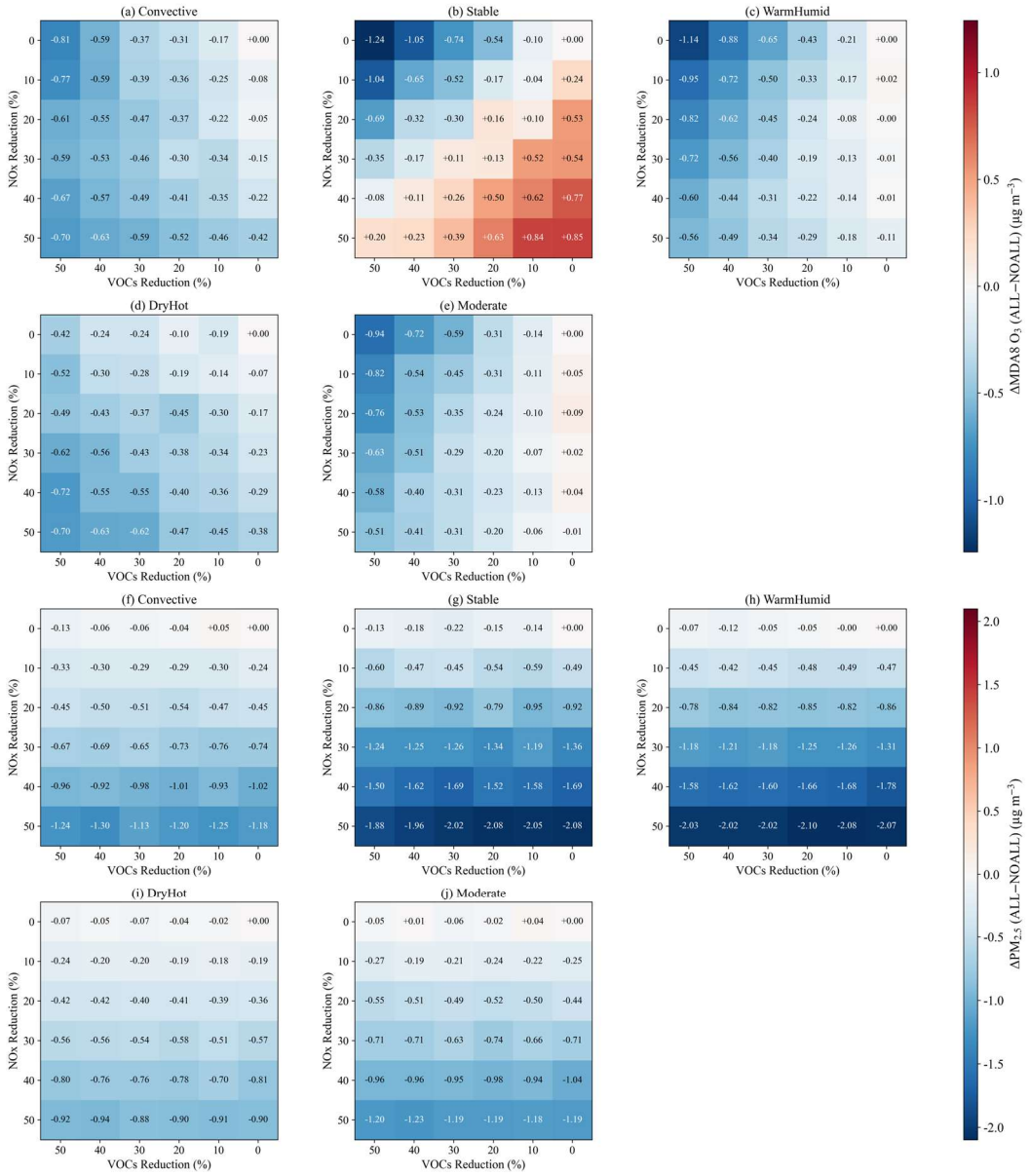


Figure S14 The impact of aerosol-meteorology feedback on MDA8 O_3 (Δ_{aer}MDA8 O_3, μg m^{-3}) and $PM_{2.5}$ ($\Delta_{aer}PM_{2.5}$, μg m^{-3}) responses to NO_x and VOC emission reductions for (a) (f) Convective, (b) (g) Stable, (c) (h) WarmHumid, (d) (i) DryHot, and (e) (j) Moderate. Rows and columns denote NO_x and VOC reduction levels (%), respectively.

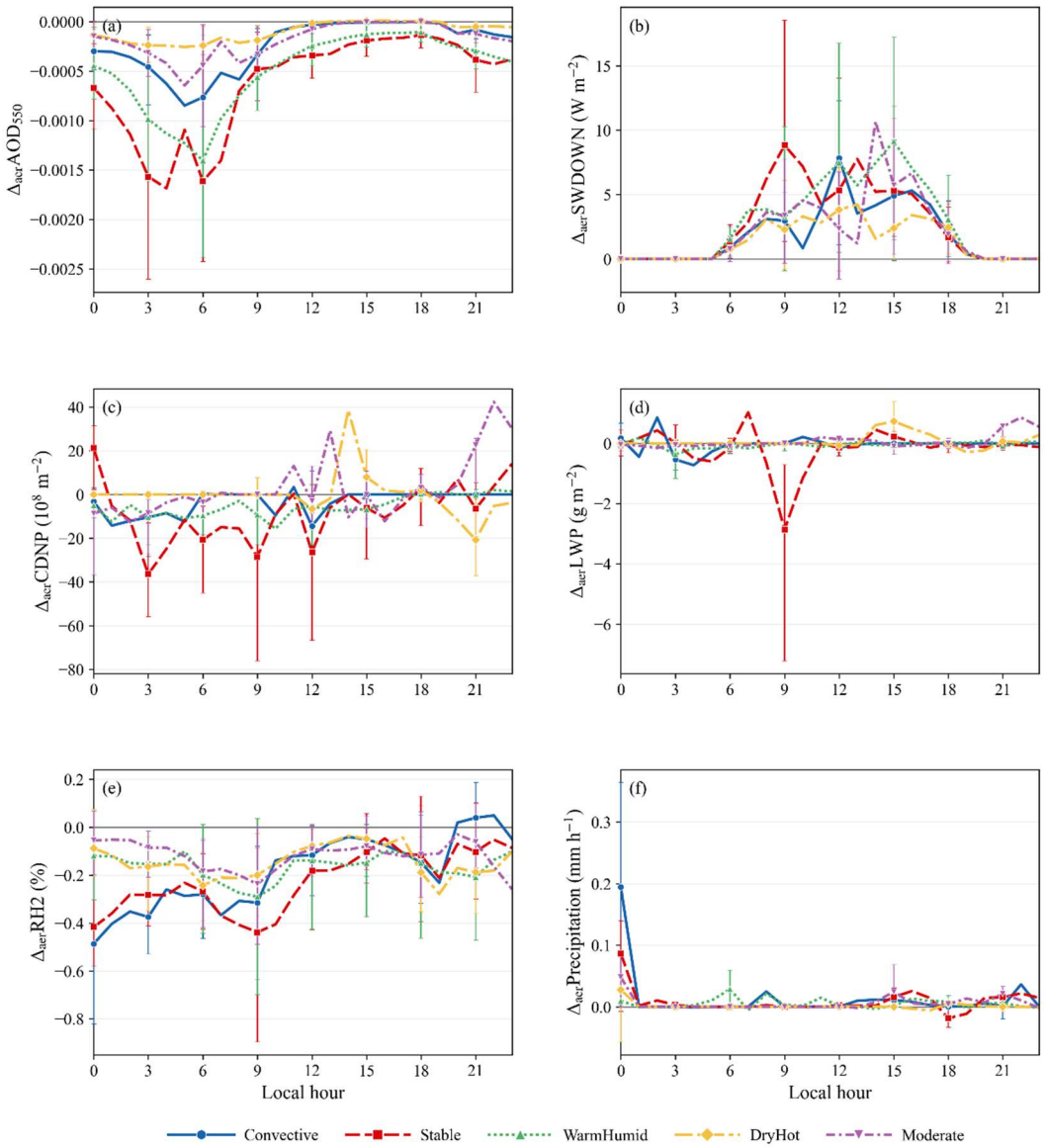


Figure S15 Diurnal profiles of the impact of aerosol-meteorology feedback ($\Delta_{aer}X$) on the response of (a) aerosol optical depth at 550 nm (AOD_{550}), (b) shortwave downward radiation (SWDOWN, W m^{-2}), (c) cloud droplet number path (CDNP, 10^8 m^{-2}), (d) liquid water path (LWP, g m^{-2}), (e) RH2 (%), and (f) precipitation (mm h^{-1}) to NO_x and VOC emission reductions under different meteorological condition types. The vertical bars plotted every 3 h indicate the p10–p90 range across emission reduction scenarios.

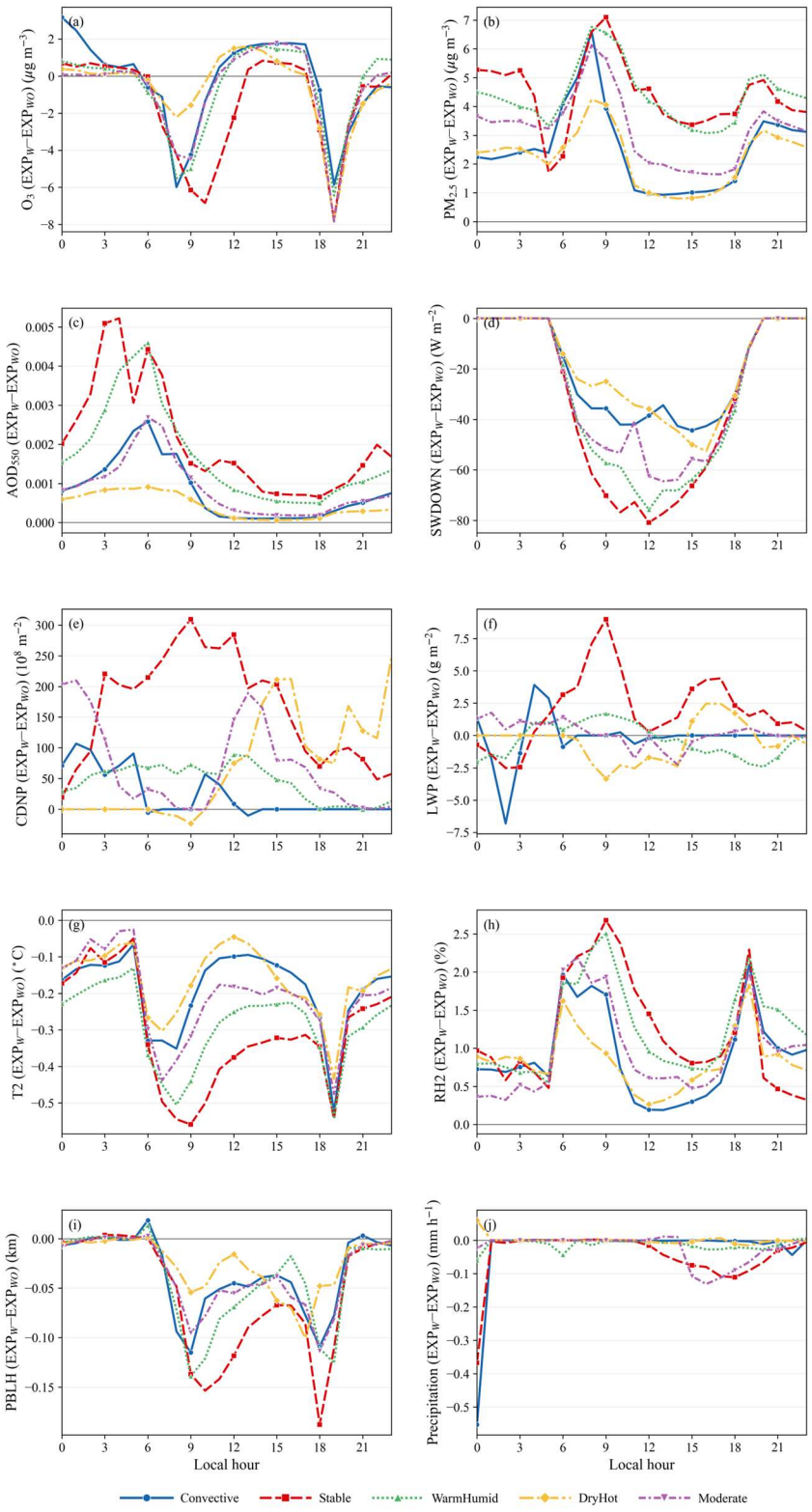


Figure S16 Diurnal profiles of the difference in (a) O_3 (μg m^{-3}), (b) $PM_{2.5}$ (μg m^{-3}), (c) AOD_{550}, (d) SWDOWN (W m^{-2}), (e) CDNP (10^8 m^{-2}), (f) LWP (g m^{-2}), (g) T2 (°C), (h) RH2 (%), (i) PBLH (km), and (j) precipitation (mm h^{-1}) between EXP_W_BASE and EXP_WO_BASE under different meteorological condition types.

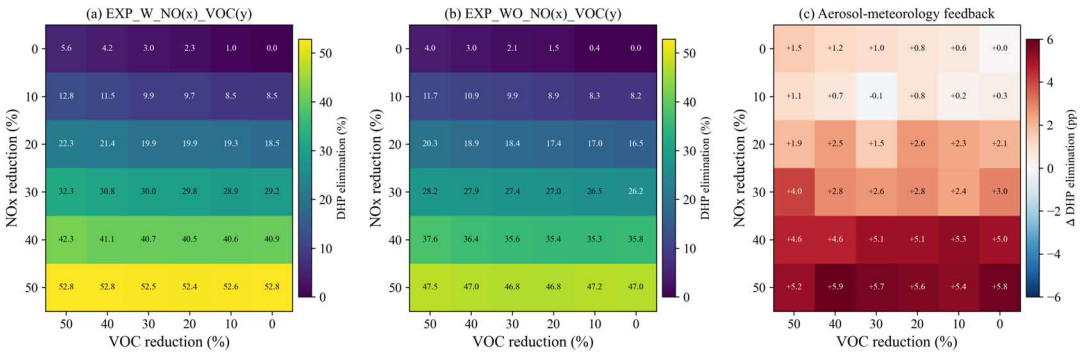


Figure S17 DHP elimination after NO_x and VOC emission reductions in (a) EXP_W_NO(x)_VOC(y) (%) and (b) EXP_WO_NO(x)_VOC(y) (%), and (c) the impact of aerosol-meteorology feedback on DHP elimination (percentage points). Elimination denotes the fraction of the 1510 baseline DHP samples that are removed by emission reductions.