

Transport-dominated ozone pollution suppresses heat-ozone hotspots in a receptor basin

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41 Table S1. WRF-Chem configuration for September 2022.

Category	Setting
Model	WRF-Chem v3.9.1
Domains	d01: 36 km, 100×100 (Most of East Asia); d02: 12 km, 100×100 (Twain-Hu Basin centered); 31 vertical levels (top 50 hPa)
Meteorological IC/BC	NCEP FNL (1°×1°, 6-hourly); FDDA applied to d02
Chemical IC/BC	CAM-Chem (6-hourly)
Gas-phase chemistry	CBMZ
Aerosol scheme	MOSAIC (8 bins)
Anthropogenic emissions	MEIC (2022 version)
Biogenic emissions	MEGAN v2.1
Microphysics	Lin
Longwave radiation	RRTMG
Shortwave radiation	RRTMG
Surface layer	MM5 Monin-Obukhov
Land surface	Noah
Boundary layer	YSU
Cumulus	Grell 3D
Spin-up	First 2 days of September excluded
Timestep	180 s (d01), 60 s (d02)

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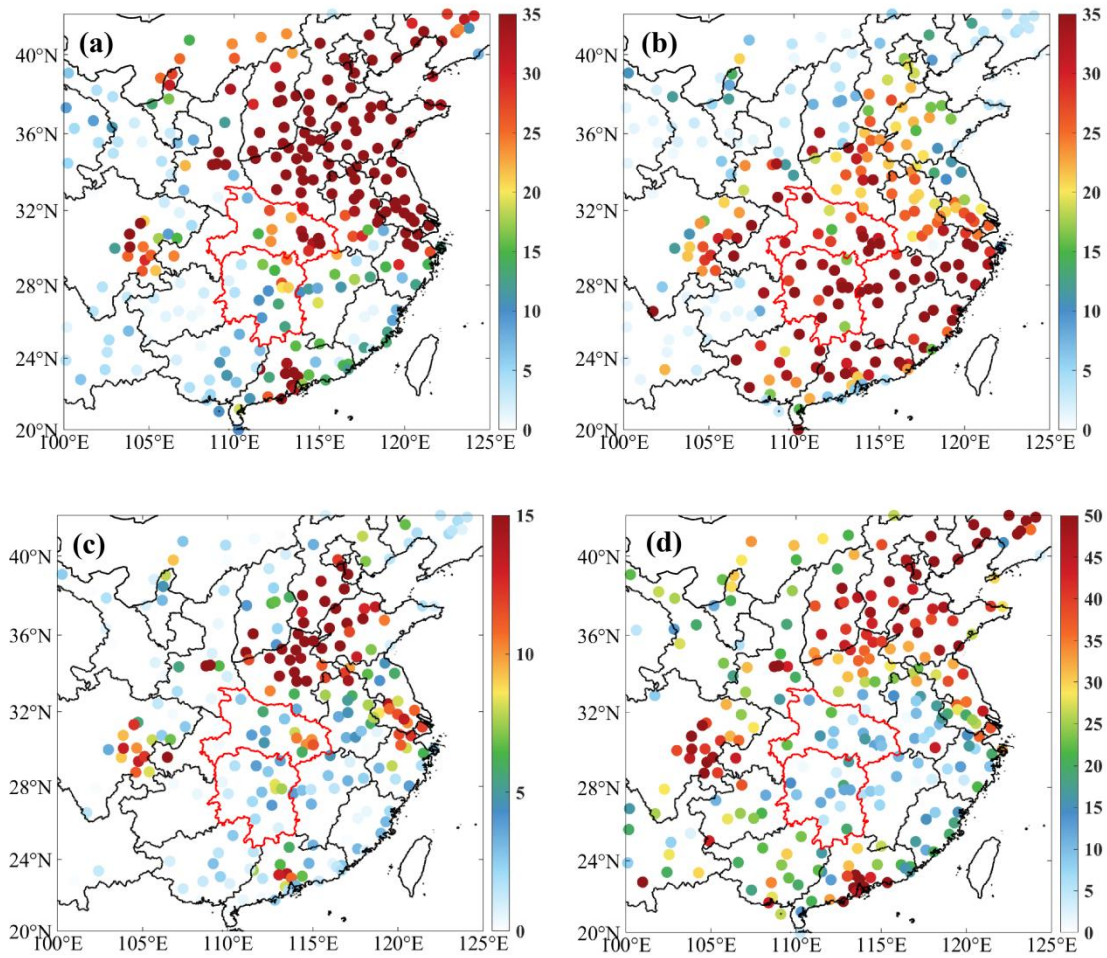


Figure S1. Spatial distribution of (a) ozone exceedance days (MDA8 $O_3 > 160 \mu g m^{-3}$), (b) extreme heat days (daily $T_{max} \geq 35^\circ C$), (c) compound heat-ozone days (same-day co-occurrence) and (d) the difference in MDA8 O_3 concentrations ($\mu g m^{-3}$) between extreme heat days and non-heat days across China during May–September 2016–2024. The Twain-Hu Basin is outlined in red.

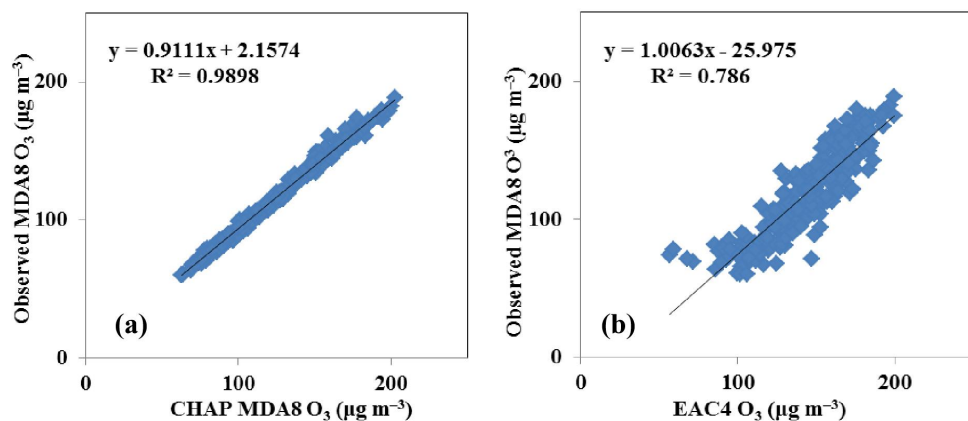


Figure S2. Evaluation ozone data consistency for September 2016–2023. (a) Twain-Hu Basin-averaged observed versus CHAP MDA8 O₃. (b) Basin-averaged observed MDA8 O₃ vs. EAC4 daytime 1000-hPa O₃.

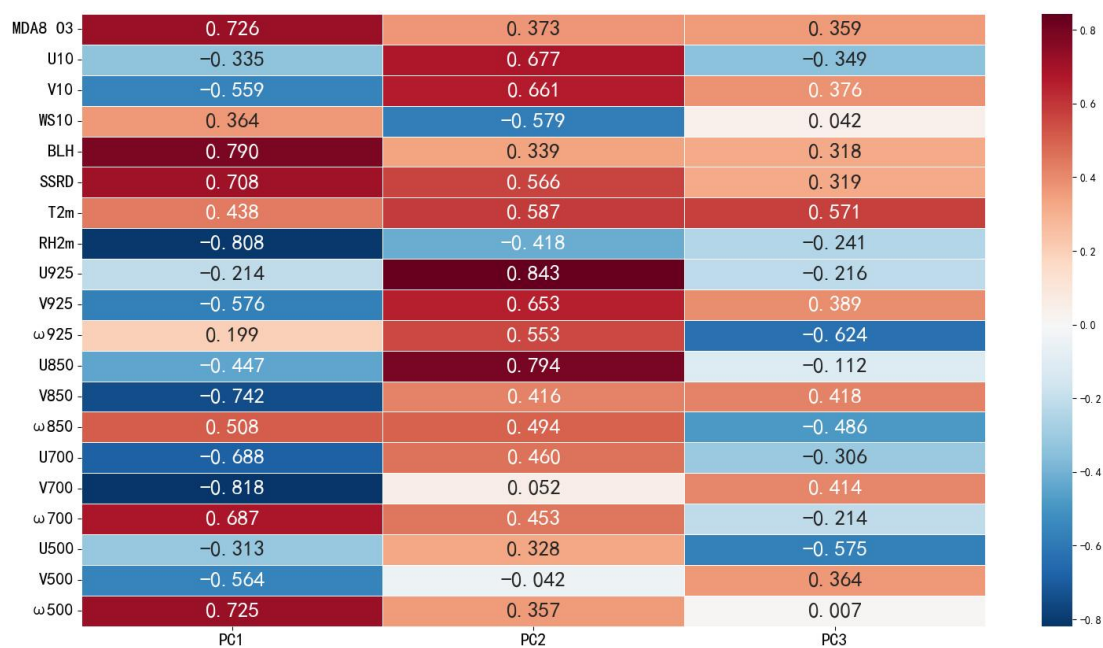


Figure S3. Heatmap of the loadings for the first three principal components (PC1–PC3).

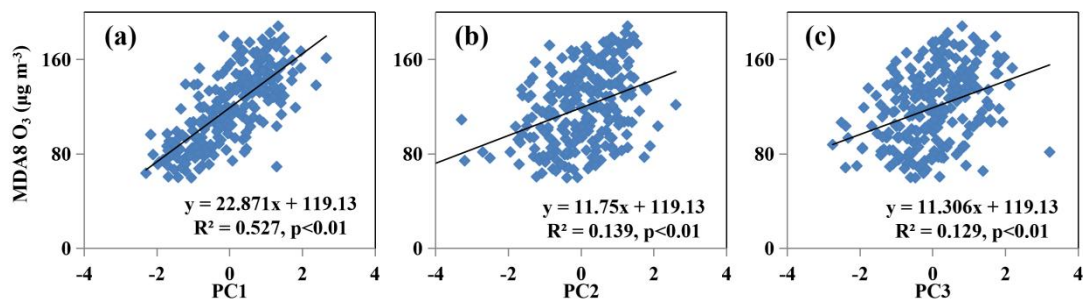


Figure S4. Scatter plots of (a) PC1, (b) PC2, and (c) PC3 versus MDA8 O₃ over the Twain-Hu Basin during September 2016–2023.

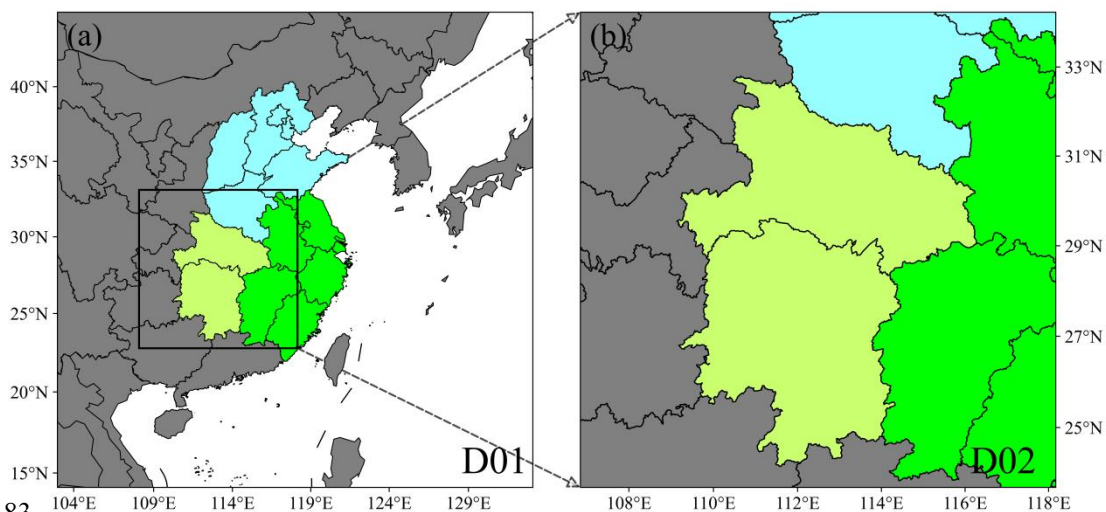


Figure S5. WRF-Chem simulation domains (a) d01 and (b) d02. Source-tagged regions: yellow – Twain-Hu Basin; cyan – North China; green – East China; gray – other areas.

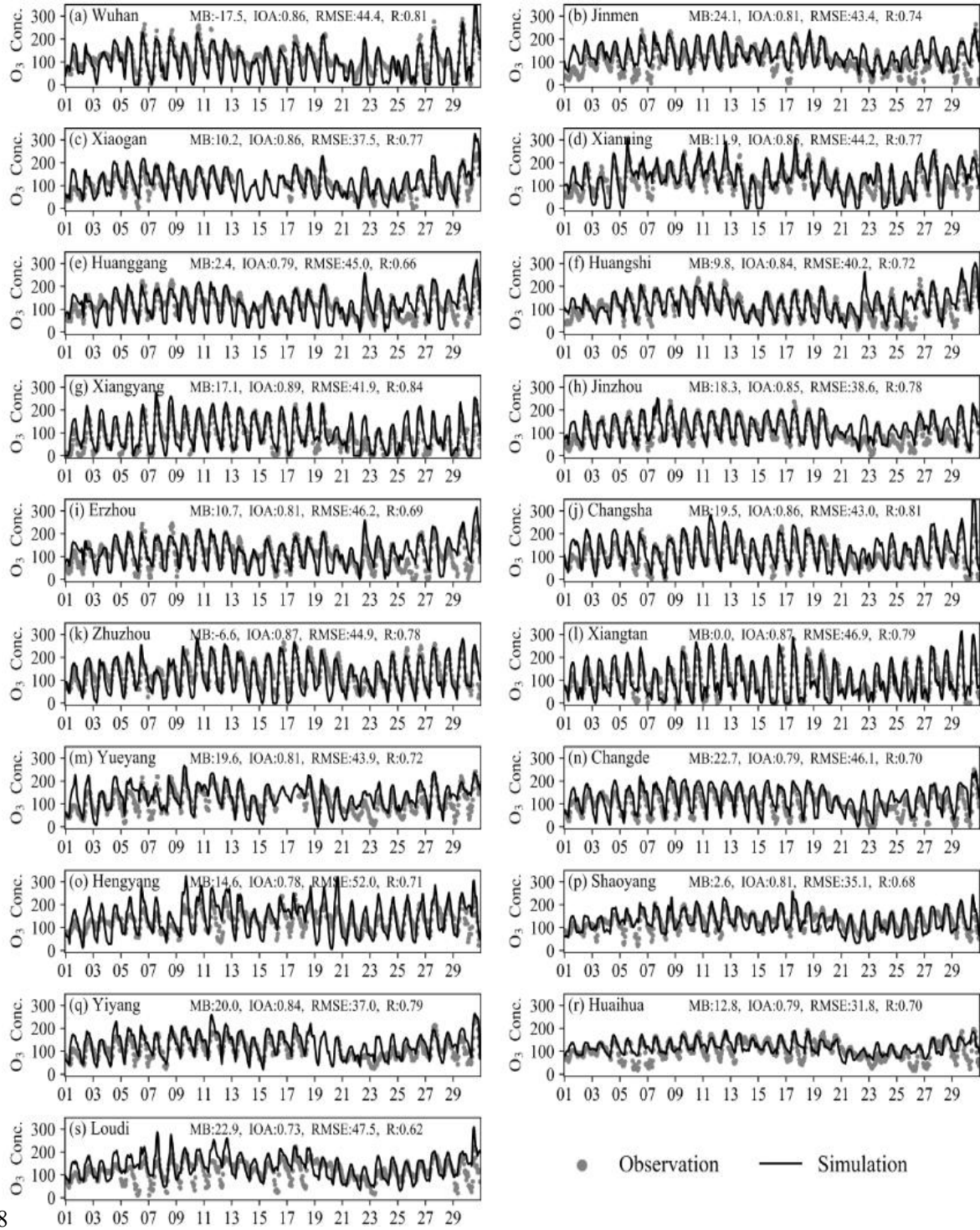


Figure S6. Comparison of simulated and observed ozone concentrations at multiple monitoring stations in the Twain-Hu Basin in September 2022.

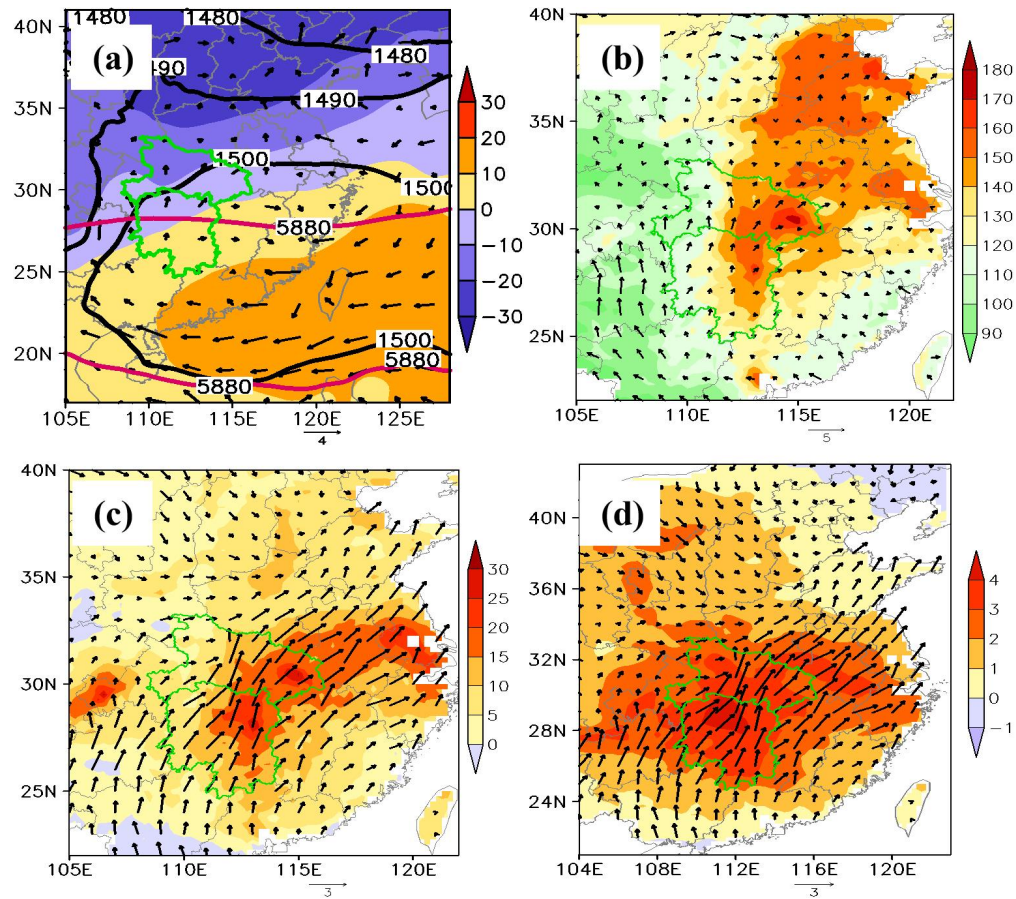


Figure S7. Composite for the P2 (local-accumulation type): (a) 850-hPa geopotential height (contours; gpm) and anomalies (shading) with 1000-hPa winds (vectors; m s^{-1}); (b) MDA8 O₃ (shading; $\mu\text{g m}^{-3}$) with 10-m winds (vectors; m s^{-1}); (c) as in (b) but for anomalies; (d) 2-m temperature anomalies overlaid with 10-m wind anomalies (vectors; m s^{-1}). All anomalies are relative to the 2016–2023 September mean.

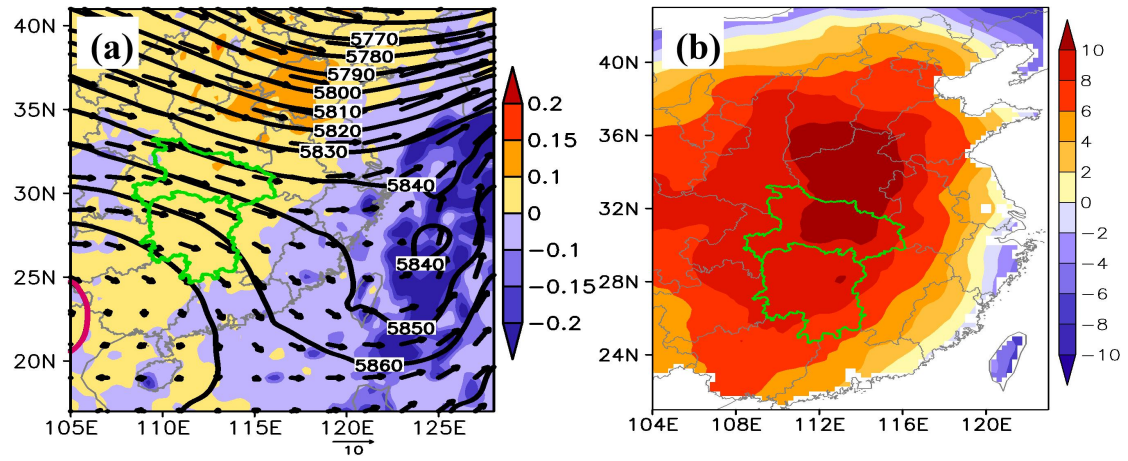


Figure S8. Composite for the P1: (a) 500-hPa geopotential height (contours; gpm), vertical velocity (shading), and winds (vectors; m s^{-1}); (b) total column ozone anomalies ($10^{-5} \text{ kg m}^{-2}$) relative to the September 2016–2023 mean.

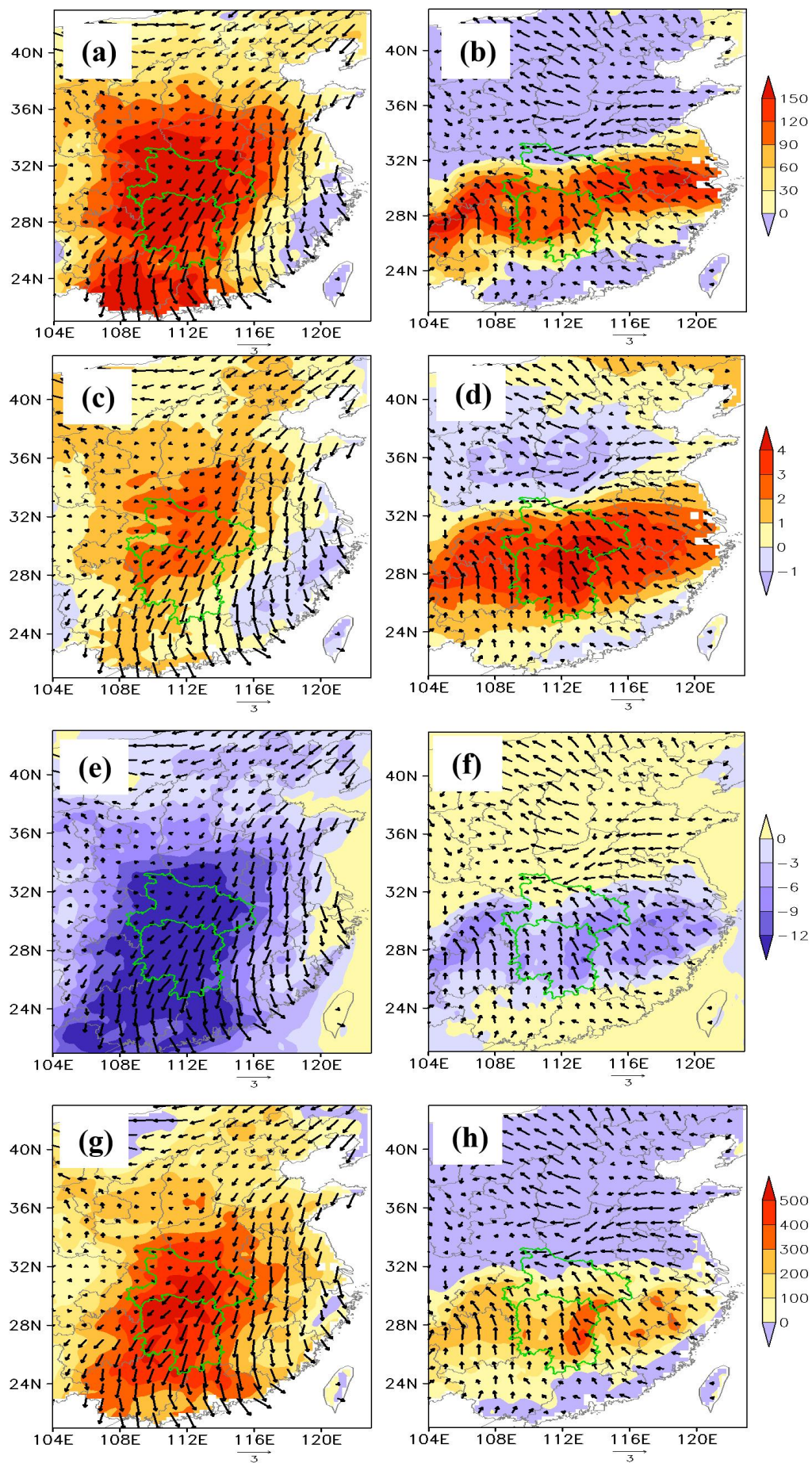


Figure S9. Composite anomalies (relative to 2016–2023 September mean) of (a,b) downward surface solar radiation (W m^{-2}), (c,d) 2-m temperature (K), (e,f) 2-m relative humidity (%), and (g,h) boundary layer height (m), overlaid with 10-m wind anomalies (vectors; m s^{-1}), for P1 (a,c,e,g) and P3 (b,d,f,h).

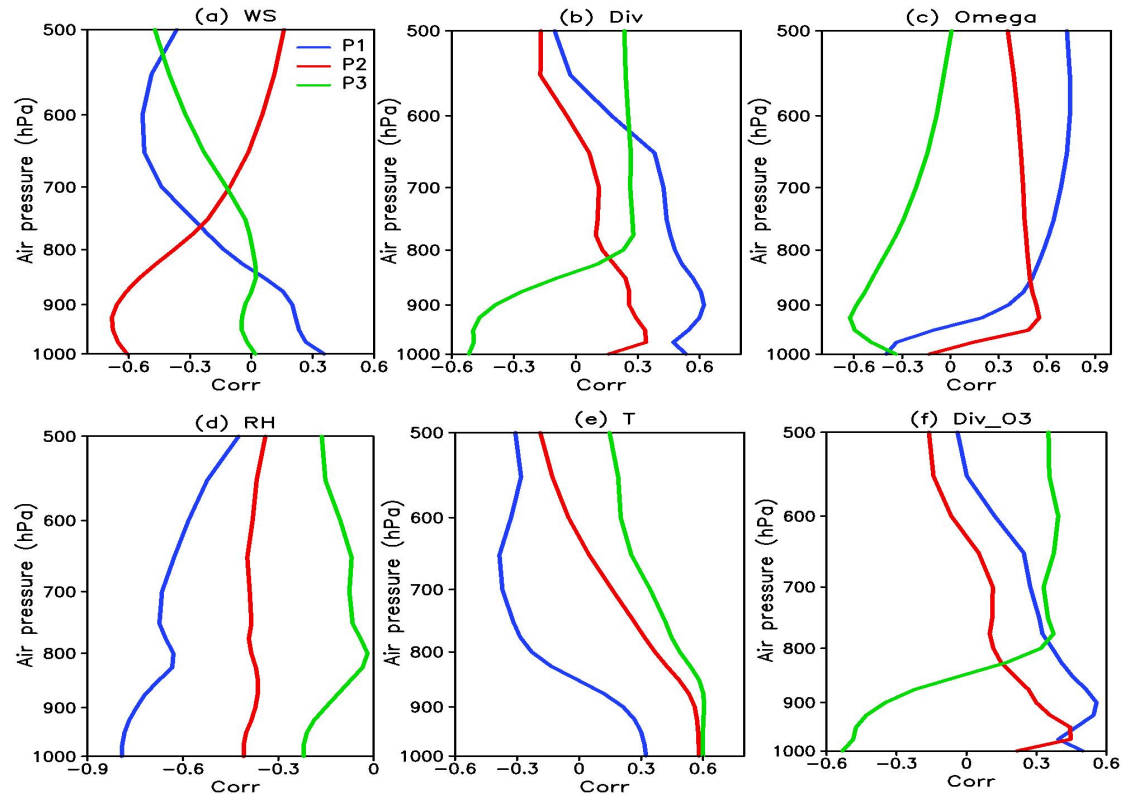


Figure S10. Vertical profiles of correlation coefficients between PCA-derived regimes (P1, P2, P3) and the Twain-Hu basin-averaged atmospheric structure: (a) wind speed, (b) divergence, (c) vertical velocity, (d) relative humidity, (e) temperature, (f) ozone flux divergence.

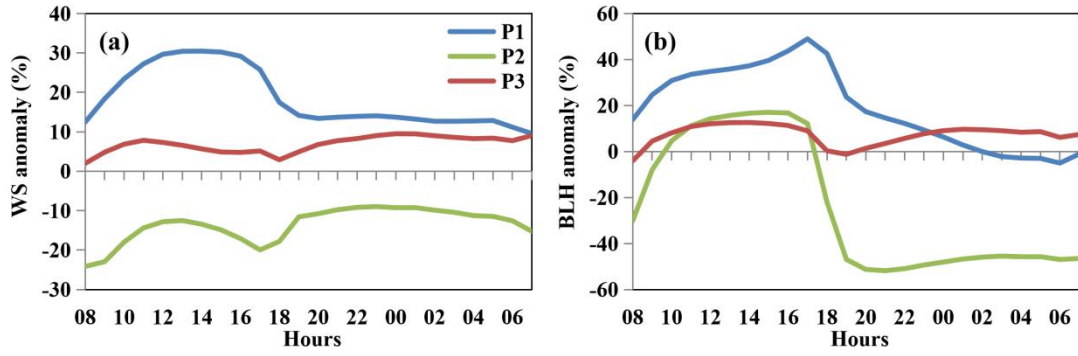


Figure S11. Basin-averaged diurnal anomalies (%) of (a) 10-m wind speed and (b) boundary layer height for P1, P2, and P3 regimes, relative to September 2016–2023 mean.

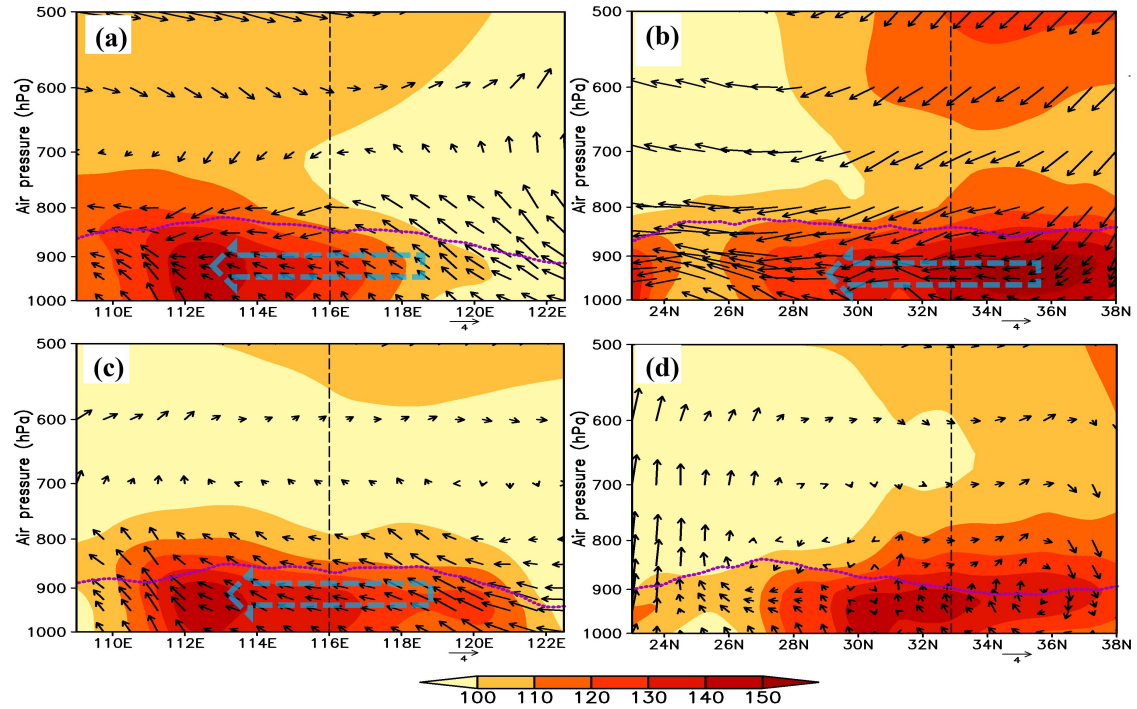


Figure S12. Vertical cross-sections of the Twain-Hu basin-averaged O_3 mixing ratio (10^9 kg kg^{-1}) overlaid with wind vectors (vertical velocity multiplied by 50), for P1 (a,b) and P3 (c,d) regimes. Thick arrows indicate transport direction.

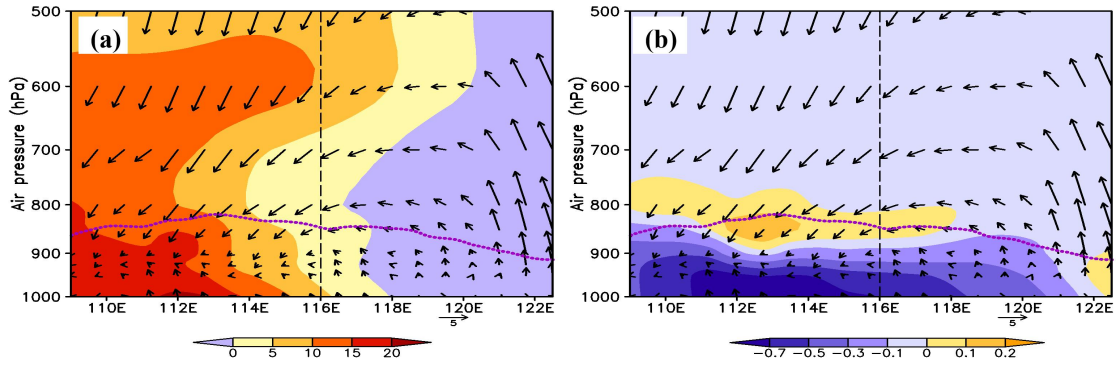


Figure S13. Vertical cross-sections of the Twain-Hu basin-averaged (a) O₃ and (b) HCHO mixing ratio anomalies (10⁹ kg kg⁻¹) overlaid with wind vectors anomalies (vertical velocity multiplied by 100), relative to September 2016–2023 mean, for the P1 regimes.

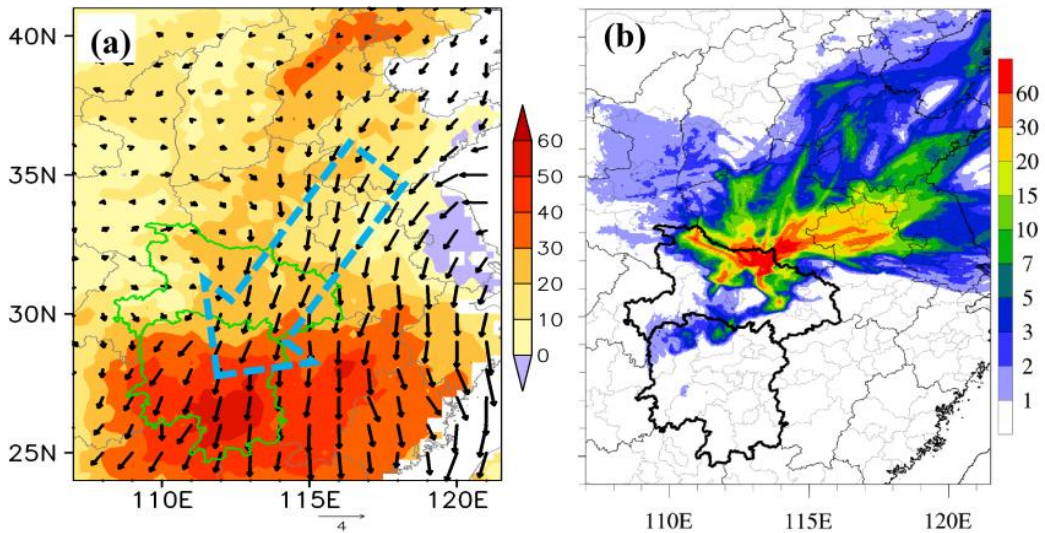


Figure S14. (a) MDA8 O₃ anomalies (shading, $\mu\text{g m}^{-3}$) and 850 hPa wind anomalies (vectors, m s⁻¹) in September 2022 relative to the 2016–2023 September mean. (b) Potential transport influence (residence times, s) derived from FLEXPART-WRF during September 2022.