

Supplementary Materials

GEOS-CF Evidence for Regional Near-Neutral and Weak Day–Night Reversal Signals in Surface Ozone

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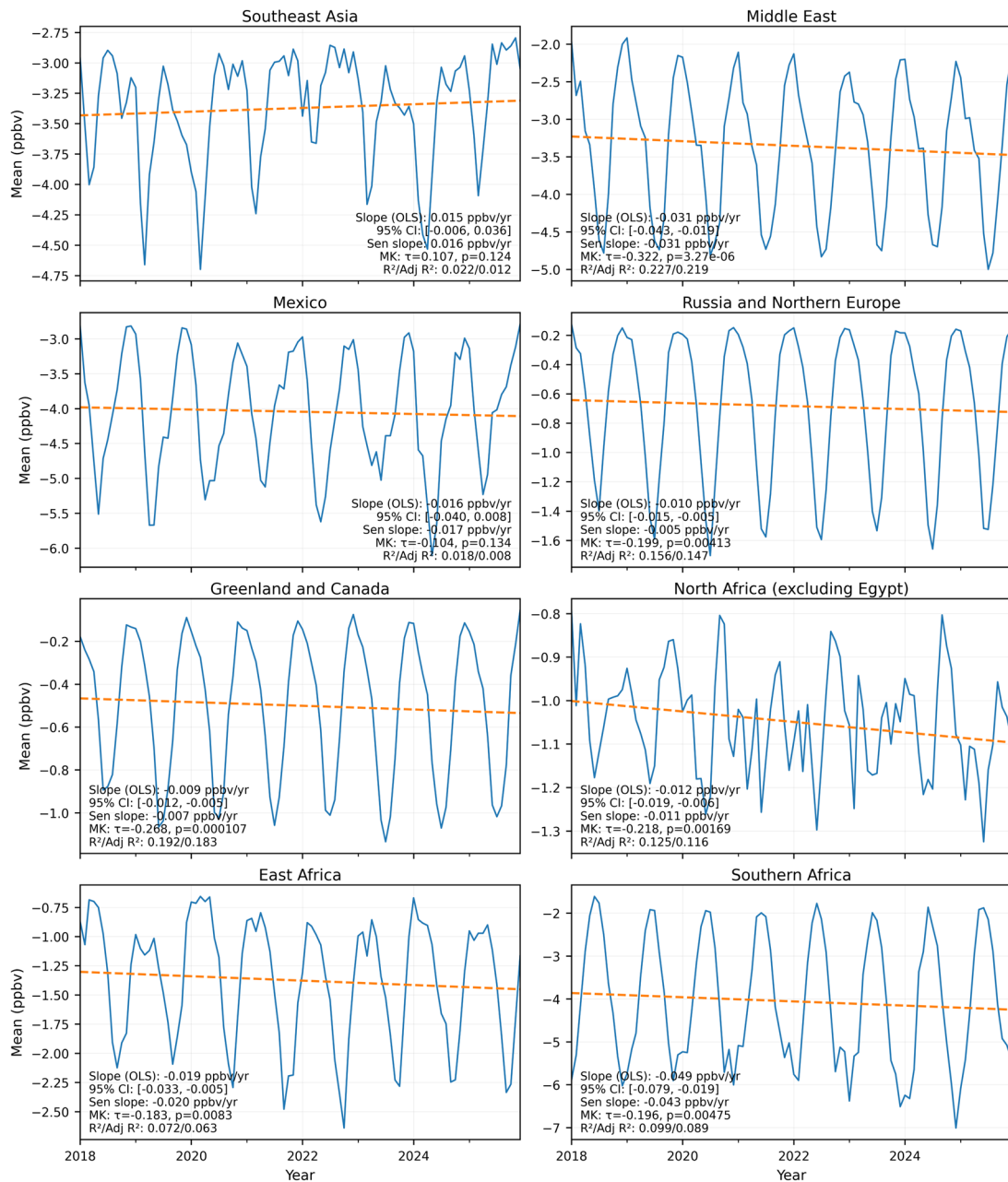


Figure S1. Regional time series and trends of mean ΔO_3 in other focus regions (2018–2025).

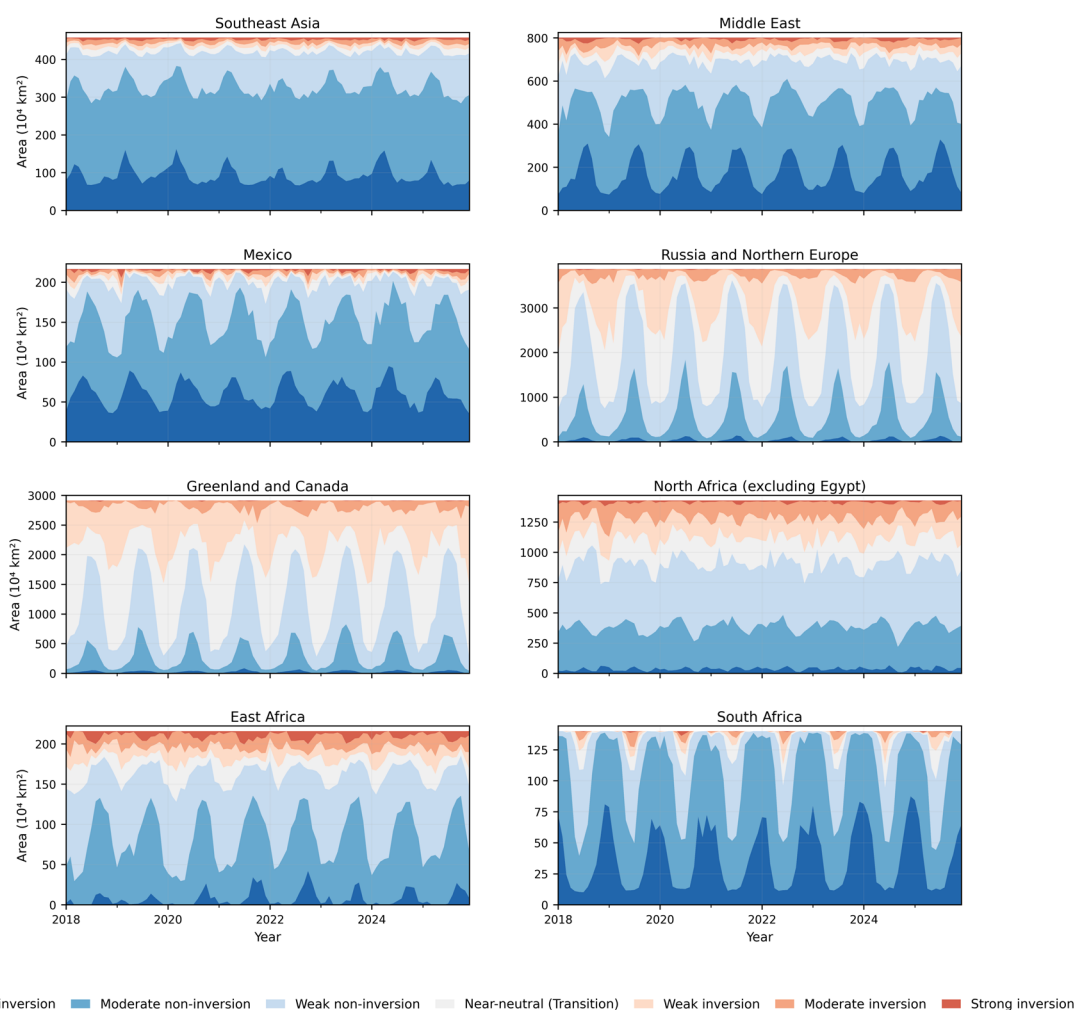


Figure S2. Seasonal evolution of regime areas in major focus regions (stacked monthly areas, seven classes).

Data Source

Surface ozone was obtained from the NASA GEOS Composition Forecast (GEOS-CF) v1 replay product NASA/GEOS-CF/v1/rpl/tavg1hr, accessed via Google Earth Engine. The product provides hourly time-averaged global replay fields on a 0.25° grid. The variable O_3 is reported as volume mixing ratio in dry air (mol mol^{-1}) and was converted to ppbv for analysis. Detailed descriptions of the aforementioned dataset can be found in Knowland et al. [1].

References

[1] Knowland, K.E.; Keller, C.A.; Lucchesi, R. *File Specification for GEOS-CF Products*; GMAO Office Note No. 17, Version 1.3, 54p; NASA Goddard Space Flight Center, Global Modeling and Assimilation Office: Greenbelt, MD, USA, 2022.

Supplementary validation of GEOS-CF surface O₃

To assess the reliability of GEOS-CF for this study, we compared hourly GEOS-CF surface O₃ with collocated hourly ground-based observations at four representative sites in the United States, Europe, and China. GEOS-CF values and observations were matched at the same site location and the same UTC hour. The comparison was quantified using the coefficient of determination (R^2), root mean square error (RMSE), mean bias (MB), and mean absolute error (MAE).

These four sites were selected to provide a compact but representative cross-regional validation of GEOS-CF surface O₃. US Big Bend represents a relatively remote arid background environment in North America, while Europe Paris and Europe Milan represent densely populated urban-background settings in Western/Central Europe, including a major metropolitan region and the Po Valley pollution environment. China Dingling represents a suburban/regional-background site near the North China Plain, a key region highlighted in the main analysis. Together, these sites cover different continents, emission environments, land-use settings, and meteorological regimes, while providing sufficiently long hourly O₃ records for direct time-matched comparison with GEOS-CF. They were therefore used to test whether GEOS-CF can reproduce hourly surface O₃ variability across representative background and urban-influenced conditions rather than at a single local site.

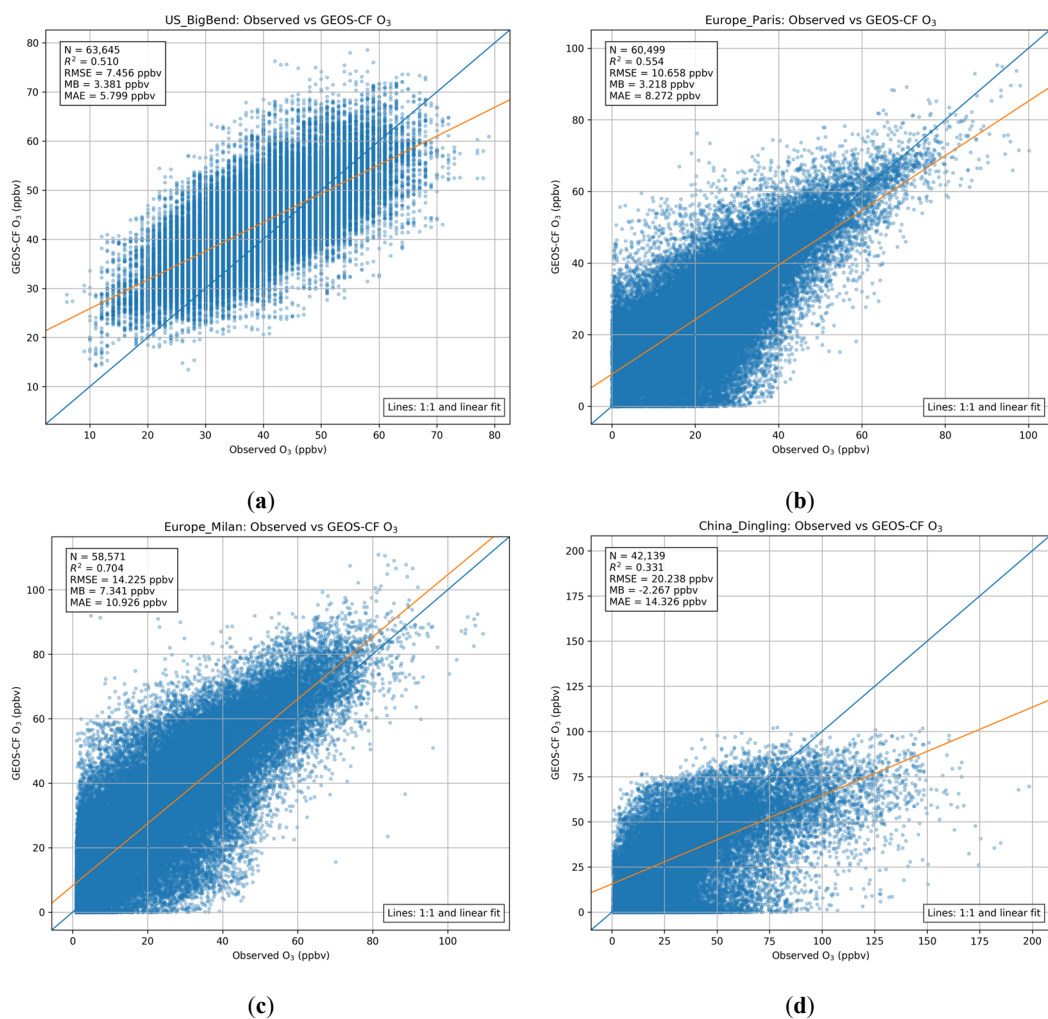


Figure S3. Validation of GEOS-CF hourly surface O₃ against collocated ground-based observations at four representative sites. (a) US Big Bend; (b) Europe Paris; (c) Europe Milan; and (d) China Dingling. Each panel shows hourly observed O₃ versus collocated GEOS-CF O₃ at the same site and UTC hour. The blue line denotes the 1:1 line, and the orange line denotes the linear regression fit. The inset in each panel reports the sample size (N), coefficient of determination (R^2), root mean square error (RMSE), mean bias (MB), and mean absolute error (MAE). O₃ is expressed in ppbv. Positive MB indicates that GEOS-CF is higher than the observed value on average.

As shown in Figure S3a–d, the validation indicates overall moderate-to-good agreement between GEOS-CF and ground observations. The four representative sites show R^2 values ranging from 0.331 to 0.704, with better agreement at Milan ($R^2 = 0.704$), Paris ($R^2 = 0.554$), and US Big Bend ($R^2 = 0.510$), and relatively larger uncertainty at Dingling ($R^2 = 0.331$). These results suggest that GEOS-CF can reasonably capture regional-scale temporal variability in surface O_3 , although site-level discrepancies and regional biases remain.

GEOS-CF is an official NASA GMAO atmospheric composition product, and the GEE dataset NASA/GEOS-CF/v1/rpl/tavg1hr provides hourly time-averaged replay fields from the 0.25° GEOS-CF global constituent prediction system. Nevertheless, the present study does not rely on product authority alone; we additionally provide independent station-based validation to support its application in regional-scale analysis of O_3 day–night variability. Therefore, GEOS-CF is considered suitable for the regional-scale diagnostic analysis conducted in this study, while the results should still be interpreted with appropriate caution.

Supplementary sensitivity analysis of station-based ΔO_3 validation

Because the main analysis used fixed local-time windows rather than solar-zenith-angle-based definitions, we tested whether the station-based ΔO_3 reversal agreement was sensitive to reasonable shifts in the day/night window. To further assess the robustness of GEOS-CF-based reversal detection, we performed a concise station-based sensitivity analysis using four representative sites: US Big Bend, Europe Paris, Europe Milan and China Dingling. Monthly ΔO_3 was recalculated as $O_{3, \text{night}} - O_{3, \text{day}}$ using three alternative local-time definitions of daytime/nighttime: 06:00–18:00 / 18:00–06:00, 07:00–19:00 / 19:00–07:00, and 08:00–20:00 / 20:00–08:00. We also tested two data-completeness criteria, requiring $\geq 75\%$ and $\geq 90\%$ valid daytime and nighttime hours per month.

For each site and month, reversal was defined as $\Delta O_3 > 0$. The monthly reversal agreement rate was calculated as the percentage of valid months in which GEOS-CF and ground observations gave the same reversal/non-reversal classification. Figure S4 shows the sensitivity of this agreement rate to the three daytime/nighttime definitions. Table S1 summarizes the corresponding agreement rate, median absolute ΔO_3 bias, mean observed ΔO_3 , and mean GEOS-CF ΔO_3 under different time-window and data-completeness settings.

Overall, the results are broadly consistent across alternative daytime/nighttime definitions and data-completeness thresholds. The agreement rate remains high for Europe Milan and China Dingling, moderate-to-high for Europe Paris, and more sensitive to the daytime/nighttime definition at US Big Bend. These results indicate that the station-based GEOS-CF ΔO_3 reversal signal is reasonably robust to common methodological choices, although site-level uncertainty remains.

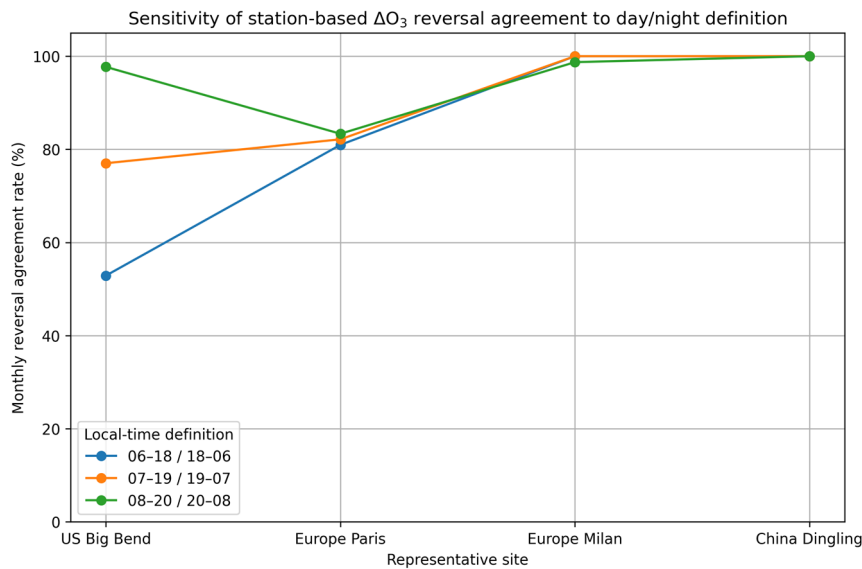


Figure S4. Sensitivity of station-based monthly ΔO_3 reversal agreement to daytime/nighttime definition. The monthly reversal agreement rate represents the percentage of valid months in which GEOS-CF and ground observations give the same reversal/non-reversal classification, where reversal is defined as $\Delta O_3 = O_{3, \text{night}} - O_{3, \text{day}} > 0$. Three local-time definitions were tested: 06:00–18:00 / 18:00–06:00, 07:00–19:00 / 19:00–07:00, and 08:00–20:00 / 20:00–08:00. The four representative sites are US Big Bend, Europe Paris, Europe Milan, and China Dingling.

Table S1. Sensitivity of station-based ΔO_3 validation to daytime/nighttime definitions and data-completeness thresholds.

Sensitivity Test	Scenario	Site	Valid Months	Reversal Agreement (%)	Median ΔO_3 Bias (ppbv)	Mean Observed ΔO_3 (ppbv)	Mean GEOS-CF ΔO_3 (ppbv)
Day/night definition	06:00–18:00 / 18:00–06:00	China Dingling	58	100	4.97	–5.69	–11.19
Day/night definition	07:00–19:00 / 19:00–07:00	China Dingling	58	100	3.1	–10.04	–12.84
Day/night definition	08:00–20:00 / 20:00–08:00	China Dingling	58	100	2.62	–13.54	–13.49
Day/night definition	06:00–18:00 / 18:00–06:00	Europe Milan	78	100	8.12	–6.26	–14.82
Day/night definition	07:00–19:00 / 19:00–07:00	Europe Milan	78	100	7.25	–9.44	–17.14
Day/night definition	08:00–20:00 / 20:00–08:00	Europe Milan	78	98.7	6.55	–11.92	–18.08
Day/night definition	06:00–18:00 / 18:00–06:00	Europe Paris	84	81	5.58	–2.6	–8.38
Day/night definition	07:00–19:00 / 19:00–07:00	Europe Paris	84	82.1	5.07	–4.7	–10.09
Day/night definition	08:00–20:00 / 20:00–08:00	Europe Paris	84	83.3	4.22	–6.54	–11.12
Day/night definition	06:00–18:00 / 18:00–06:00	US Big Bend	87	52.9	1.22	–1.17	0.06
Day/night definition	07:00–19:00 / 19:00–07:00	US Big Bend	87	77	1.62	–2.26	–0.5
Day/night definition	08:00–20:00 / 20:00–08:00	US Big Bend	87	97.7	1.79	–3.14	–1.11
Data completeness	$\geq 75\%$ valid day/night hours	China Dingling	58	100	4.97	–5.69	–11.19
Data completeness	$\geq 90\%$ valid day/night hours	China Dingling	52	100	5.25	–5.58	–11.23
Data completeness	$\geq 75\%$ valid day/night hours	Europe Milan	78	100	8.12	–6.26	–14.82
Data completeness	$\geq 90\%$ valid day/night hours	Europe Milan	72	100	8.15	–6.46	–15.13
Data completeness	$\geq 75\%$ valid day/night hours	Europe Paris	84	81	5.58	–2.6	–8.38
Data completeness	$\geq 90\%$ valid day/night hours	Europe Paris	80	80	5.44	–2.51	–8.16
Data completeness	$\geq 75\%$ valid day/night hours	US Big Bend	87	52.9	1.22	–1.17	0.06
Data completeness	$\geq 90\%$ valid day/night hours	US Big Bend	74	51.4	1.18	–1.13	0.08

To further assess the robustness of GEOS-CF-based reversal detection, we performed a concise station-based sensitivity analysis using four representative sites: US Big Bend, Europe Paris, Europe Milan and China Dingling. Monthly ΔO_3 was recalculated as $O_{3, \text{night}} - O_{3, \text{day}}$ using three alternative local-time definitions of daytime/nighttime: 06:00–18:00 / 18:00–06:00, 07:00–19:00 / 19:00–07:00, and 08:00–20:00 / 20:00–08:00. We also tested two data-completeness criteria, requiring $\geq 75\%$ and $\geq 90\%$ valid daytime and nighttime hours per month.

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Overall, the results are broadly consistent across alternative daytime/nighttime definitions and data-completeness thresholds. The agreement rate remains high for Europe Milan and China Dingling, moderate-to-high for Europe Paris, and more sensitive to the daytime/nighttime definition at US Big Bend. These results indicate that the station-based GEOS-CF ΔO_3 reversal signal is reasonably robust to common methodological choices, although site-level uncertainty remains.

Definition and classification thresholds of ΔO_3 regimes

The day–night O_3 contrast was defined as $\Delta O_3 = O_{3, \text{night}} - O_{3, \text{day}}$. To avoid interpreting very small differences around zero as robust reversal or non-reversal, we introduced a near-neutral buffer of ± 1 ppbv. The remaining categories were defined using symmetric thresholds of 5 and 10 ppbv to distinguish weak, moderate, and strong day–night contrasts. The classification thresholds are listed in Table S2.

Table S2. Thresholds used to classify the seven ΔO_3 regimes.

Regime	Threshold
Strong non-reversal	$\Delta O_3 \leq -10$ ppbv
Moderate non-reversal	$-10 < \Delta O_3 \leq -5$ ppbv
Weak non-reversal	$-5 < \Delta O_3 \leq -1$ ppbv
Near-neutral transition	$-1 < \Delta O_3 < 1$ ppbv
Weak reversal	$1 \leq \Delta O_3 < 5$ ppbv
Moderate reversal	$5 \leq \Delta O_3 < 10$ ppbv
Strong reversal	$\Delta O_3 \geq 10$ ppbv