

Dear Chief Editor,

We sincerely thank you for handling our manuscript and for providing us with the opportunity to revise our work.

We have now received the comments from the two anonymous reviewers. We are grateful for their thorough evaluation and constructive suggestions, which have been invaluable in improving the quality and clarity of our manuscript.

We have carefully considered all the comments and revised the manuscript accordingly. Point-by-point responses to each reviewer's comment are provided in detail in the accompanying document.

We hope that the revisions have adequately addressed all concerns raised by the reviewers, and we respectfully submit the revised manuscript for your consideration.

Thank you very much for your time and continued support.

Sincerely,

Dr. Nan Wang

College of Carbon Neutrality Future Technology

Sichuan University

Response to Reviewer 1,

Thank you very much for your thoughtful and constructive comments on our manuscript. We greatly appreciate the time and effort you have dedicated to reviewing our work. We have carefully considered all the suggestions/questions and have revised the manuscript accordingly. Below, we provide a point-by-point response to each comment. All changes in the revised manuscript are highlighted in **red text**.

Response to reviewer 1

We appreciate the reviewer's positive feedback on the scientific significance of our study and the recognition of its potential value for research and policymaking. We have carefully considered the comments regarding the need for further evidence and explanation in the Introduction and Discussion sections to provide a more comprehensive analysis of factors influencing O_3 distribution and to strengthen the validation of model simulations.

We agree that a more comprehensive discussion of the factors governing O_3 distributions and a clearer articulation of the uncertainties in regional chemical transport models (CTMs) would strengthen the foundation of our study. Following your suggestion, we have substantially revised the Introduction section as follows:

Comment 1: *In the manuscript, the term chemical boundary conditions (CBCs) suffers from redundant redefinition or inconsistent use of its abbreviation after initial definition. For example, chemical boundary condition (CBCs) is first defined on line 34; therefore, the abbreviation “CBCs” should be used directly in subsequent mentions (e.g., lines 127–128, 148, and 256). Conversely, the redefinition of chemical boundary condition (CBCs) on line 457 is unnecessary and should be removed. Moreover, both “chemical boundary condition” and “CBC” appear multiple times in the manuscript, and their usage is inconsistent with “CBCs” in meaning. It is recommended to define the term as CBC (singular form) upon its first appearance (i.e., “chemical boundary condition (CBC)”) and maintain consistent terminology throughout the manuscript.*

Response:

We sincerely thank the reviewer for this important observation. We agree that consistent terminology is crucial. In the revised manuscript, we have:

- Defined the term as **“chemical boundary condition (CBC)”** (singular form) at its first appearance (Line 34);
- Replaced all subsequent occurrences of “chemical boundary condition(s)” or “CBCs” with **“CBC”** throughout the text (e.g., Lines 35–36, 41, and other instances mentioned above and elsewhere in the text);
- Removed the redundant redefinition on Lines 141–142 and 512.

Comment 2: Line 270: *Although there are several definitions for the calculation formula of the Index of Agreement (IOA), the IOA formula presented in the manuscript differs from other established definitions. The authors are requested to verify and revise the IOA calculation formula accordingly, and to re-examine the IOA values reported in the paper.*

Response:

We appreciate this important comment. Regarding the IOA formula, we would like to note that during the earlier Access Review stage, we had already identified and corrected a typographical error in the IOA equation. As documented in our previous author response (under “Minor Font Errors and Typographical Corrections”), we stated:

- In addition, we have corrected a typographical error in the formula for the Index of Agreement (IOA) in **Section 2.2.1 (Line 301)**. We have carefully cross-checked the updated formula against established literature to ensure its technical accuracy. This correction ensures the methodological description is consistent with the actual statistical calculations performed in our study and does not change any of the evaluation results or conclusions.
- After consulting authoritative sources—particularly Willmott (1981), who originally proposed the Index of Agreement (*Physical Geography*, 2(2), 184–194; <https://doi.org/10.1080/02723646.1981.10642213>)—we confirm that the correct formulation of the IOA is:

$$IOA = 1 - \frac{n * RMSE^2}{\sum_{i=1}^n (|S_i - OBS| + |O_i - OBS|)^2}$$

The formula now in the manuscript has been verified and is now consistent with this standard definition.

Comment 3: *On Line 404, the performance ranking of the dynamic CBC scenarios should be clarified. Please explicitly state that the ranking is based on all monitoring sites across China. Given that the NMB-based performance differs between avg-O₃MDA8 and 90th-O₃MDA8, separate rankings for these two metrics are recommended. Additionally, a discussion on the NMB performance across different regional subdivisions would strengthen this section.*

Response:

Thank you for this excellent suggestion. We have:

- Clarified in the revised manuscript (now Line 441-443) that the performance ranking is based on all monitoring sites across China.
- Added separate performance rankings for avg-O₃MDA8 and 90th-O₃MDA8 in Lines 444–446.
- In Lines 455–464, we have included a comparative analysis of NMB performance across different regional subdivisions, with particular emphasis on the differences between the GEOS-Chem and CESM2.2 boundary condition scenarios. This enhanced regional discussion strengthens the model intercomparison and interpretation.

Comment 4: *Regarding Figure 4, the label "GEOSChem" is inconsistent with the text, which uses "GEOS-Chem". The figure should be revised to ensure consistency in nomenclature.*

Response:

We apologize for this inconsistency. The figure has been revised and regenerated, and the label in Figure 4 has been corrected to “GEOS-Chem” to ensure consistency with the standard nomenclature used throughout the manuscript.

Comment 5: *On Section 3.2.3 and Section 2.2.2: There is an inconsistency in the vertical data range described. The analysis in Section 3.2.3 is based on the 0-16 km range, whereas the description of the Vertical Observation Data in Section 2.2.2 states that all data were processed to 0-20 km. For consistency and clarity, the methodological description in Section 2.2.2 should be revised to reflect the 0-16 km range used in the subsequent analysis.*

Response:

We thank the reviewer for identifying this apparent inconsistency. After carefully reviewing the descriptions in Sections 2.2.2 and 3.2.3, as well as the associated figures and analyses, we would

like to clarify our rationale.

The ozonesonde data were originally processed and archived up to **20 km**, which is accurately reflected in Section 2.2.2 (Line 327). However, for the purpose of model evaluation, we focused our quantitative analysis on the **0–16 km layer**, as stated in Section 3.2.3. This choice was made to align with the vertical extent relevant to tropospheric and lower-stratospheric ozone dynamics over China and to ensure robust comparison with model outputs.

To facilitate interpretation, we explicitly define the following vertical layers in the text:

“the lower troposphere (0–3 km), the middle-to-upper troposphere (3–10 km), and the lower stratosphere (10–16 km).”

Figure 5 extends slightly beyond 16 km (up to ~18 km) for visual completeness, but all statistical evaluations are strictly confined to 0–16 km (Table 3).

Given that Section 2.2.2 describes the **full data processing range** (0–20 km), while Section 3.2.3 specifies the **analysis domain** (0–16 km), we believe retaining “0–20 km” in Section 2.2.2 provides a more accurate account of the raw observational data handling. To avoid any potential confusion, we have added a clarifying sentence in Section 2.2.2 (Line 324):

“and data within the 0–16 km layer were used in the model evaluation.”

Comment 6: *Table S1: According to the regional subregions description provided in the manuscript, the definition of the “Southwest China”—including its constituent provinces—is missing from Supplementary Table S1 and should be added to the table.*

Response:

We have added the missing entry for **“Southwest China”** in Supplementary Table S1, which now includes the provinces: **Sichuan, Chongqing, Guizhou, Yunnan, and Xizang.**

Comment 7: *Table S4: There is a minor error in the table caption—a comma “,” is missing between “IOA” and “r”.*

Response:

This typo has been corrected. The caption of **Table S4** now reads: “*using the metrics MB, and RMSE (in ppbv), and IOA, r and NMB (unitless)*”.

We believe these revisions fully address the reviewer's concerns and significantly enhance the comprehensiveness and robustness of our analysis. We hope the revised manuscript now meets the journal's publication standards, and we sincerely thank the reviewers once again for their time and insightful feedback.

Response to Reviewer 2,

We would like to express our sincere gratitude to Reviewer 2 for their thorough evaluation and constructive comments on our manuscript. We appreciate the reviewer's positive assessment of the study's scientific soundness and methodological robustness. The suggestions provided have helped us significantly improve the clarity, rigor, and reproducibility of our work.

Below, we provide a point-by-point response to the specific comments and technical corrections raised. All changes in the revised manuscript are highlighted **in red** for easy reference.

Response to General Comments

Comment: *Overall, this study appears scientifically sound and methodologically robust... I would recommend it for publication after addressing a few minor comments.*

Response: We thank the reviewer for this encouraging assessment. We have carefully addressed all the minor comments and technical corrections below to ensure the manuscript meets the high standards of ACP.

Response to Specific Comments

Comment 1 (Lines 42-43): *The statement referring to the “highest agreement (0.85 and 0.83)” for GEOS-Chem may be unclear to readers at this stage, as the specific metric is not yet defined. It would be helpful to clarify here whether these values correspond to the index of agreement (IOA), which is introduced later in the manuscript.*

Response: We agree that this clarification is necessary for better readability. We have revised the text in the Abstract to explicitly state that these values refer to the **Index of Agreement (IOA)**. Please see **Line 43** in the revised manuscript: “*...highest agreement (IOA = 0.85 and 0.83)...*”

Comment 2 (Lines 208-211): *The description includes the names of specific individuals alongside their institutions in relation to the MIX v1.1 inventory, which seems unnecessary in this context. It would likely be sufficient and more consistent with common practice to cite the inventory itself, along with an appropriate reference or weblink, rather than listing various individual contributors.*

Response: We fully agree with the reviewer that listing individual contributors is unnecessary and deviates from standard citation practices. We have removed the names and institutions from the manuscript. Instead, we have updated the text to provide a concise technical description of the MIX v1.1 inventory's specifications (resolution, sectors, and pollutants) to ensure reproducibility, citing the primary reference.

Please see our revisions in **Section 2.1, Lines 207-212**: “*...anthropogenic emissions were based on the MIX v1.1 inventory (Li et al., 2017b). This dataset provides monthly grid-based emission data at a 0.25° spatial resolution across five key sectors (power, industry, residential, transport, and agriculture), meeting the requirements for multi-scale atmospheric chemical transport modeling (<http://meicmodel.org.cn>, last access:13 Apr. 2026).*”

Comment 3 (Lines 294-300): *While most of the verification statistics introduced here are widely used and clearly understood, the index of agreement (IOA) may not be familiar to all readers (it was not to me). It would be helpful to include a brief explanation of what IOA represents and how it should be interpreted.*

Response: We have added a brief definition and interpretation guide for IOA in the **Observation data section** to assist readers unfamiliar with this metric. Please see our revisions in **Section 2.2.1, Lines 291-293:** *"...The IOA ranges from 0 to 1, where 1 indicates a perfect match between simulated and observed values, while values approaching 0 indicate poor model performance (Willmott, 1981)."*

Comment 4 (Lines 453 and 458): *For Figs. 3 and 4, which present the first statistical comparisons in the manuscript, it would be helpful to explicitly state in the captions the time period covered by the analysis as well as the number of data points (e.g., monitoring sites and/or days) included. This would clarify the statistical basis of the results and make the figures more self-contained for readers.*

Response: We thank the reviewer for this constructive suggestion. We have updated the captions for both Figure 3 and Figure 4 to explicitly state the analysis period (July–August 2019) and the number of monitoring sites included in the statistics. This addition clarifies the statistical basis of our results and makes the figures more self-contained.

Please see our revisions updated in **Fig. 3 caption (Line 474):** *"... at 1480 monitoring sites during July–August 2019..."* and **Fig. 4 caption (Lines 483-484):** *" Statistics are based on daily data from July -August 2019; number of monitoring sites: China (1480), E (319), N (181), S (256), C (204), NE (166), NW (154), and SW (200)."*

Comment 5 (Lines 487-493): *In Section 3.2.3, it would be helpful if the authors could state explicitly which vertical coordinate was used for the ozone-profile comparison (e.g., height above ground level, altitude above sea level, or geopotential height). This could be particularly relevant for high-altitude sites such as Lhasa, where differences in vertical coordinate might*

introduce an apparent vertical shift in the profiles. Figure 5 seems to indicate that HAGL was used, in which case the comparison may already be handled appropriately, but this should be clarified explicitly in the text or figure caption.

Response: We thank the reviewer for highlighting this critical methodological detail. We confirm that **Height Above Ground Level (HAGL)** was used for all vertical profile comparisons to ensure consistency across sites with varying topography (e.g., Lhasa). We have revised **Section 2.2.2 (Vertical Observation Data)** to explicitly state that sonde data were processed and interpolated based on HAGL, thereby eliminating potential biases caused by elevation differences.

The followings have been revised in the manuscript:

(1) Revised in Section 2.2.2, Lines 321-325: *"To ensure consistency across datasets and comparability with the model output, all sonde data were processed for the 0–20 km **height above ground level (HAGL)** range and interpolated to match the model vertical structure, with data within the 0–16 km **HAGL** layer used in the model evaluation."*

(2) Revised Section 3.2.3, Figure 5 caption: *"Figure 5. Comparison of vertical O₃ profiles between four CBC scenario simulations (BASE, H-CMAQ, GEOS-Chem, and CESM2.2) and sounding observations at five stations across China. All profiles are plotted against **Height Above Ground Level (HAGL)**; statistics are based on vertical profile data summarized in **Table S2 (including observation periods and site-specific information)**."*

Comment 6 (Line 568): *The comparisons in Section 3.3 demonstrate the clear benefit of dynamic CBCs relative to the static BASE scenario. However, I wonder whether the BASE setup is somewhat overly simplified as a benchmark, since it uses a spatially uniform and temporally constant profile. Could the authors comment on whether this remains common practice in regional CTM applications, and whether more realistic 3-D climatological boundary conditions are available and might constitute a more appropriate benchmark?*

Response: We appreciate this insightful comment. First of all, using the default profile-based chemical boundary conditions in CMAQ **does remain a common and practical choice** for baseline, sensitivity, and resource-limited regional applications, particularly because such

profiles are distributed with the model and are straightforward to implement. Secondly, we agree that more realistic three-dimensional, time-varying climatological boundary conditions are available. For example, the CMAQ community provides historical boundary condition datasets derived from global chemical transport models, which can better represent the variability of inflow chemical composition. However, in practice, **many previous regional CMAQ applications have adopted the default profile-based boundary conditions as a baseline configuration**, particularly in sensitivity analyses or methodological studies, due to their simplicity and consistency. In this study, we followed this common practice to establish a controlled benchmark (BASE) that isolates the impact of boundary condition representation. To support this statement on common practices, we have incorporated a recent comprehensive review (Zhu et al., 2024), which quantifies that approximately 70% of recent regional modeling studies still rely on default or unspecified (static) boundary conditions. We have revised the **Conclusion (Section 4)** to explicitly acknowledge this point, cite this evidence, and clarify the scientific rationale for using the simplified BASE scenario in this study.

Please see our revisions in Section 4 (Conclusion), Lines 778-785:

*"Our findings demonstrate that the choice of CBCs is not merely a technicality but a dynamic determinant of simulated O₃ levels for regional CTM, especially when facing synoptic regimes that favor long-range transport or vertical exchange. This underscores the necessity of moving beyond static boundary conditions in regional air quality modeling. **Static BCs remain a common baseline in regional modeling, with recent assessments indicating that a majority of studies still rely on default or unspecified boundary conditions (e.g., Zhu et al., 2024). While the simplified BASE scenario may not represent the most realistic boundary condition, it serves as a controlled baseline to isolate the incremental value of time-varying CBC, which is the primary focus of this study.** To advance predictive capability, future efforts should pursue multi-model ensembles to quantify CBC uncertainty, **evaluate 3-D climatological boundary conditions as a refined benchmark**, and explore the integration of real-time global fields into regional CTM forecasting systems. By elucidating the critical interplay between large-scale transport and regional pollution, this study provides a scientific foundation not only for improving O₃ forecasting but also for designing effective transboundary air quality management strategies."* We believe this revision provides quantitative evidence for the prevalence of static BCs while maintaining the original flow of our discussion on future research directions.

Comment 7 (Lines 729-738): *Related to the broader implications discussed here, I wonder to what extent conclusions drawn from the July–August 2019 study period can be generalized to other summers, other seasons, and other regions outside China. The discussion of two contrasting synoptic situations is helpful, but some explicit comment on how representative this study period is of typical summertime meteorological conditions would strengthen the manuscript.*

Response: We thank the reviewer for raising this important point regarding the generalizability of our findings. We agree that clarifying the representativeness of the study period strengthens the interpretation of our results. We have added a dedicated paragraph in the Conclusion (Section 4) to explicitly address this issue, drawing on the mechanistic insights already established in Section 3.3.

Our justification for the representativeness of the July–August 2019 period rests on three aspects:

1. **Meteorological Representativeness:** The study period covers the peak of the East Asian summer monsoon, capturing the canonical dipole between southeasterly marine inflows (associated with the Western Pacific Subtropical High) and northwesterly continental inflows. These two regimes dominate summer ozone transport patterns over eastern China.
2. **Synoptic Representativeness:** The inclusion of two typhoon events (Lekima and Krosa) and their associated circulation transitions (cyclonic scavenging vs. anticyclonic accumulation) reflects frequent and impactful synoptic disturbances during Chinese summers. The two phases analyzed (P1 and P2) effectively bracket the end-member meteorological conditions that modulate transboundary ozone influence.
3. **Pollution Representativeness:** Both phases exhibited significant ozone pollution episodes, ensuring that the identified CBC mechanisms are relevant to high-pollution scenarios of policy interest, rather than being confined to clean background conditions.

We clarify that while *quantitative magnitudes* of CBC influence may vary with interannual climate variability or across different seasons, the *mechanisms* identified—particularly the heightened sensitivity of ozone simulations to dynamic CBCs under transport-favorable synoptic regimes—are robust and applicable to typical summer pollution episodes in monsoon-affected regions. We have also tempered claims regarding applicability to other seasons or regions outside the East Asian monsoon domain to avoid overgeneralization.

Please see our revisions added to **Section 4 (Conclusion), Lines 748-756:**

"Regarding the representativeness of these findings, while this study focuses on summer 2019, the selected period captures representative meteorological regimes of the East Asian summer monsoon, including typical southeasterly marine flows and northwesterly continental inflows. The inclusion of typhoon-induced circulation changes (e.g., Lekima and Krosa) further ensures that the findings reflect common synoptic disturbances affecting regional air quality. Although quantitative magnitudes may vary with interannual climate variability, the identified mechanisms regarding CBC sensitivity under transport-favorable conditions are applicable to typical summer pollution episodes in monsoon-affected regions."

Comment 8 (Lines 772-774): *Please check whether the present Data Availability statement is fully in line with ACP/Copernicus requirements. It currently indicates that simulation results are available from the corresponding author, but it may be preferable to archive at least the key output in a public repository with a DOI. The manuscript does specify the WRF and CMAQ versions used, together with the relevant model websites, which is helpful, but for a modelling study of this kind it might also be worth considering whether a brief explicit code-availability statement would be appropriate, especially for any custom processing scripts used to generate the boundary-condition inputs.*

Response: We thank the reviewer for this important reminder regarding data transparency and reproducibility. We have carefully reviewed the ACP/Copernicus data policy and have added a dedicated Data Availability section at the end of the manuscript to fully comply with journal requirements.

Specifically, we have:

1. **Catalogued all third-party data sources:** We explicitly listed the access URLs or DOIs for all observational datasets (surface meteorology, O₃ monitoring, ozonesondes, satellite products), reanalysis data (ERA5), emission inventories (MEIC v1.4, MIX v1.1), and global model outputs (H-CMAQ, GEOS-Chem, CESM2.2) used in this study.
2. **Archived custom preprocessing scripts:** Following the reviewer's suggestion, we have uploaded the custom scripts developed for converting global model outputs into CMAQ-compatible boundary conditions to the **Zenodo** public repository, assigned DOI: 10.5281/zenodo.19447294, to ensure long-term accessibility and citability.

3. **Clarified model code availability:** We explicitly stated that the WRF v3.9.1 and CMAQ v5.3.3 source codes are open-source and publicly accessible via their official GitHub repositories.
4. **Provided access pathway for large outputs:** We clarified that additional large-volume model results are stored on the Shuguang high-performance computing system and available from the corresponding author upon reasonable request.

Please see our revisions in **Data Availability** section at the end of the manuscript (before References):

"The observational datasets used in this study are publicly available from the following sources: surface meteorological data from the China Meteorological Administration (<http://data.cma.cn>, last access: 4 Apr. 2026); surface O₃ concentrations from the China National Environmental Monitoring Center (<https://air.cnemc.cn:18007>, last access: 4 Apr. 2026); ozonesonde profiles from the World Ozone and Ultraviolet Radiation Data Centre (WOUDC, <https://woudc.org>, last access: 4 Apr. 2026), the China Air Pollution Data Center (CAPDC, <https://www.capdatabase.cn>, last access: 4 Apr. 2026), and the National Tibetan Plateau Data Center (TPDC, <https://data.tpsc.ac.cn>, last access: 4 Apr. 2026); and tropospheric O₃ column data from the EMI/GF-5 product (Zhao et al., 2024). Meteorological boundary conditions data derived from the ERA5 reanalysis dataset (Hersbach et al., 2023) are available at <https://doi.org/10.24381/cds.adbb2d47>. The MEIC v1.4 and MIX v1.1 emission inventories are available at <http://meicmodel.org>. Global chemical model outputs used as boundary conditions are available from the EQUATES project (H-CMAQ, <https://www.epa.gov/cmaq/EQUATES>, last access: 4 Apr. 2026), GEOS-Chem (<https://geoschem.github.io/>, last access: 4 Apr. 2026), and CESM2.2/CAM-chem (<https://www2.acom.ucar.edu/gcm/cam-chem>, last access: 4 Apr. 2026). The WRF v3.9.1 (<https://github.com/wrf-model/WRF>, last access: 4 Apr. 2026) and CMAQ v5.3.3 (<https://github.com/USEPA/CMAQ>) model source codes are open-source and publicly accessible via their official GitHub repositories. The custom scripts developed for processing global model outputs into CMAQ-compatible boundary conditions have been archived in the Zenodo repository under DOI: [10.5281/zenodo.19447294]. Additional model results are stored on Shuguang high-performance computing system and available from the corresponding author upon reasonable request (nan.wang@scu.edu.cn)."

Response to Technical Corrections

We have carefully proofread the manuscript and corrected all the technical issues pointed out by the reviewer.

- **Line 72:** Corrected to "China has". (**Now line 72**)
- **Line 151:** Added missing space in "...distributions (Zhu...)". (**Now line 151**)
- **Line 200:** Removed extra character/data. (**Now line 200**)
- **Line 203:** Removed extra blank space before the period. (**Now line 205**)
- **Line 254:** Removed "the" in "All three global model outputs". (**Now line 253**)
- **Line 336:** Corrected capitalization in "...tropospheric...". (**Now line 338**)
- **Line 339:** Reformatted to "36 x 36 km²". (**Now line 341**)
- **Line 346 & throughout:** Ensured "Figure" is spelled out at the beginning of sentences. (**Now lines 349 and 419**)
- **Line 387:** Corrected to "of the CMAQ modeling domain". (**Now line 390-391**)
- **Line 416:** Standardized tense. We have carefully reviewed tense usage throughout the Results and Discussion sections. Following academic conventions, we now consistently use present tense for describing figures, tables, statistical results, and scientific conclusions (e.g., 'Figure 3 illustrates...', 'The results indicate...', 'GEOS-Chem exhibits...'), while retaining past tense only for specific data collection procedures. This revision improves logical clarity and aligns with ACP style guidelines. (**Now line 423 ...**)
- **Line 479:** Corrected to "in those areas". (**Now line 484**)
- **Line 533:** Ensured O₃ uses subscript formatting. (**Now line 548**)

We believe these revisions fully address the reviewer's concerns and significantly enhance the comprehensiveness and robustness of our analysis. We hope the revised manuscript now meets the journal's publication standards, and we sincerely thank the reviewers once again for their time and insightful feedback.