**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:

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

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-$O_3$MDA8 and 90th-$O_3$MDA8 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.