Authors' Final response

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Evaluation of the WRF-Chem Performance for gaseous pollutants over the United Arab Emirates

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Reviewer 2

Reviewer: The paper "Evaluation of the WRF-Chem Performance for gaseous pollutants over the United Arab Emirates" by Yarragunta et al. present an evaluation of the WRF-Chem chemistry transport model implemented by the United Arab Emirates. This is done against in situ measurements for surface windspeed and temperature, another model for other meteorological variables and TROPOMI-derived satellite measurements for trace gas chemical species. While the application of the WRF-Chem model over this area has certain scientific and applicative interest, the data and methodology of comparison is clearly limited. The only objective of evaluation of a model is better fitted to other more methodological journals such as "Atmospheric Measurements and Techniques" than "Atmospheric Chemistry and Physics" in which actual geophysical results are to be presented (and this is not the case of the current manuscript).

Reply: Thank you for your valuable feedback and for emphasizing the importance of applying the WRF-Chem model in the United Arab Emirates. We understand your concern regarding the manuscript's suitability for publication in the journal "Atmospheric Chemistry and Physics". However, we strongly believe our findings offer significant insights into regional air quality dynamics, particularly in a region characterized by high aerosol loads and extreme meteorological conditions. Our study aims to enhance the scientific understanding of atmospheric processes in the hyper-arid UAE, a country representative of those in the Middle East. This is crucial for informing future research in atmospheric chemistry and physics in arid/semi-arid regions, which are projected to expand in a warming climate. The evaluation against in situ measurements and TROPOMI-derived satellite data provides a robust assessment of the model's performance, serving as a critical foundation for further refinement and application in operational and research atmospheric studies in the Middle East and similar hyper-arid regions. We are committed to expanding the manuscript to include a more in-depth discussion of the geophysical implications of our findings and their relevance to broader atmospheric chemistry research. We believe these additions will align the manuscript more closely with the scope of "Atmospheric Chemistry and Physics" and enhance its quality so as to meet the journal's high standards. We appreciate your thoughtful review and consideration.

Reviewer: Moreover, the paper needs substantial major revisions to be publishable. I strongly recommend the full revision of the three major aspects:

Reply: Thank you for your comprehensive review and valuable feedback on our manuscript. We greatly appreciate your time and effort in evaluating our work. We recognize the importance of addressing the significant revisions the reviewer has suggested to improve our study's overall quality and robustness. Below, we provide our detailed responses and outline the specific actions we intend to take to address the reviewer's concerns.

Reviewer: Ozone total column: The paper only evaluates ozone simulations by comparing with total column ozone retrievals from TROPOMI. The ozone total column is largely dominated by stratospheric ozone, that accounts for 90% of the total column ozone or more. The influence of tropospheric ozone in these measurements is negligible. This is not a validation of tropospheric ozone which is the only part of ozone that affects air quality, which is the aim of the paper. Stratospheric ozone is only linked with stratospheric chemistry and transport (not mentioned in the paper). Moreover, it is unclear why there is a long paragraph (lines 721-746) describing the phenomena exclusivity driving the variability of tropospheric ozone (anthropogenic precursors, NOx or COV limited photochemical regimes).

Reply: Thank you for your insightful comment. Our focus is indeed on the tropospheric column of ozone, which is directly relevant to surface air quality. We acknowledge that the total column ozone measurements are predominantly influenced by stratospheric ozone, which accounts for approximately 90% of the total column. In comparison, tropospheric ozone contributes only about 10% as stated by the reviewer. Given this, we understand that total column ozone is unsuitable for validating ground-level ozone. Due to the unavailability of TROPOMI data for June and December 2018, we have decided to refine our simulation period to more recent years, in particular June and December 2022, for which TROPOMI ozone profile data is available (product name: S5P_L2__O3__PR_HiR), allowing for a direct evaluation of the tropospheric ozone.

Furthermore, the updated simulation period aligns with the EDGAR anthropogenic emissions data availability of up to 2022. We will ensure that the revised manuscript reflects our focus on tropospheric ozone and remove any content related to stratospheric ozone that is outside the scope of our study. Thank you again for pointing out this important distinction.

Reviewer: This part of the paper should be fully revised. It is mandatory to include a validation of tropospheric ozone (from the surface up to the tropopause) from WRF-Chem, which is an available ozone product from TROPOMI. Also, variability of total ozone columns should be linked with stratospheric ozone and pollution-related phenomena with only tropospheric ozone.

Reply: Thank you for your valuable comments. We have carefully considered your suggestions and revised the manuscript accordingly. We have now included validation of tropospheric ozone (from the surface up to the tropopause) using WRF-Chem, leveraging the available tropospheric ozone data from TROPOMI. Additionally, we have clarified the distinction between total ozone column variability and tropospheric ozone variability in the manuscript. As the variability in the total ozone column is primarily associated with stratospheric ozone changes, we have acknowledged that this falls outside the scope of our current study. Instead, we have focused on tropospheric ozone variability directly linked to pollution-related phenomena. We have conducted simulations for the year 2022, as stated in the reply to the reviewer's previous comment, and incorporated these revisions into the relevant sections of the manuscript.

Reviewer: The comparison method : authors evaluate WRF-Chem by only comparing a single monthly average maps (for 2 months) for different variables, which does not consider any information on diurnal variation. This is not sufficient for a model that is expected to provide diagnostics of air quality, since air pollution outbreaks strongly vary at daily scale and they only last for a few days (1 to 10 days). This method of validation gaseous pollution should be completed with comparisons including the daily evolution (temporal evolution within the month) and it also illustrate with a comparison of the description of at least one air pollution outbreak. More in details, strong biases should be very justified (only general arguments are provided) and statistic estimators such as RMSE should be calculated again since their values are not consistent with their definition.

Reply: Thank you for your valuable comments. We understand the importance of considering diurnal variation when evaluating WRF-Chem for air quality diagnostics. Initially, our simulations did not include a diurnal component because TROPOMI satellite retrievals are available only once daily, limiting our ability to capture daily variability. However, based on the reviewer's suggestions, we are now incorporating idealized diurnal profiles into our simulations using the updated EDGAR emission inventory, available up to 2022. Additionally, we have included a detailed analysis of the temporal evolution of gaseous pollutants within the month and provide a case study of a high-pollution event to illustrate the model's performance in capturing short-lived pollution outbreaks. Furthermore, we will provide a more detailed justification for any strong biases observed and recalculate the statistical estimators, such as RMSE, to ensure they are consistent with their definitions. These updates will be reflected in the revised manuscript.

Reviewer: Validation of the planetary boundary height: Given that this variable is only forecasted in models or reanalysis such as ERA5, a comparison between models is not a sufficient validation. I strongly suggest adding a comparison against measurements (typically from radiosondes or lidar). ERA5 PBL height are useful to compare its relative spatial distribution, but a validation should include absolute comparisons against measurements. It would also be important to analyze the influence of the PBL in surface air pollutant concentrations.

Reply: Thank you for your valuable feedback on our manuscript. We agree that a more comprehensive validation of the planetary boundary layer (PBL) height is necessary. While our initial comparison of the PBL height from model simulations with ERA5 data helped to understand its relative spatial distribution, we acknowledge that this approach does not provide absolute validation. Following the Reviewer's suggestion, we have incorporated comparisons against measurements, specifically using radiosonde data available twice daily at the Abu Dhabi International Airport, the only location in the UAE where such data is collected. We extracted PBL height data from WRF-Chem for the grid point nearest the airport (24.45ºN, 54.64ºE) and compared the summer and winter of 2022. We will also examine how variations in PBL height influence surface air pollutant concentrations beyond the inverse relationship between PBL depth and a given pollutant concentration seen in a daytime-nighttime comparison to better understand its impact on air quality. These revisions have been made and are reflected in the revised manuscript.

Reviewer: These additional minor aspects are to be revised:

Reply: Thank you for your thorough review and valuable feedback on our manuscript.

Reviewer: Line 318 : the definition of the AK vector should be revised; they describe the vertical sensitivity concerning the true vertical profile of the target variable in the atmosphere

Reply: Thank you for your comment. We appreciate your attention to detail. We have revised the definition of the averaging kernel (AK) vector in line 318 to accurately reflect its role in describing the vertical sensitivity to the true vertical profile of the target variable in the atmosphere. This clarification has been made to ensure the manuscript correctly represents the vertical sensitivity information provided by the AK vector. The updated definition is included in the revised manuscript.

Reviewer: Equation 3 : Xret seems to be related to the "retrieved variable", which is not the "model profile". Subindexes should be renamed for consistency. The same for Xtrue.

Reply: Thank you for your comment. We appreciate your careful review. In response, we have revised the notation in Equation 3 for clarity and consistency. We acknowledge that X_{ret} should represent the "retrieved profile or smoothed model profile" rather than the "model profile", and X_{true} should correspond to the "true model profile (raw)" of the target variable. We have updated the sub-indices throughout the manuscript to ensure consistency and accurately reflect their meanings. The clarification regarding X_{ret} as the retrieved or smoothed model profile, as mentioned in line 332, has also been maintained. These changes are reflected in the revised manuscript.

Reviewer: Figures : each panel of all figures should have a label (a), (b), etc.. otherwise it is unclear

Reply: Thank you for your comment and your careful review. In response, we have revised all the figures in the manuscript to include labels for each panel (e.g., (a), (b), etc.) as per the reviewer's suggestion. This addition aims to improve clarity and make it easier to reference specific panels within the figures. These revisions have been incorporated into the updated manuscript.

Reviewer: A figure of Group for High Resolution Sea Surface Temperature can be provided. It is actually a valuable comparison against measurements. We strongly need a graphic support for the long description of this comparison in a paragraph (near line 523).

Reply: Thank you for your comment. In response to the reviewer's suggestion, we have included a figure showing the Group for High-Resolution Sea Surface Temperature (GHRSST) data in the revised manuscript. This figure provides valuable visual support for the detailed comparison discussed in the paragraph in lines 522-538. We believe this addition enhances the clarity and effectiveness of the manuscript.

Reviewer: Cities, locations in the figures: We need to point out at least in one map the geographical location of the cities or places described in the paragraphs.

Reply: Thank you for your comment and thorough review. In response to the reviewer's suggestion, we have revised Fig. 1b to include the geographical locations of the cities and places mentioned in the manuscript. This addition aims to enhance clarity and provide a better geographical context for the study area. We hope this revision improves the overall readability and effectiveness of the manuscript.

Reviewer: Lines 534-536 : we need wind vectors overlaid in the figure to understand these circulation aspects.

Reply: Thank you for your comment and thorough review. In response to the reviewer's suggestion, we have revised Figs. 3 and 4 by overlaying surface wind vectors on each plot to better illustrate the circulation aspects discussed in the manuscript. We believe this addition enhances the clarity and understanding of the figures and improves the overall readability and effectiveness of the manuscript.

Reviewer: Line 566: there is not "trend" between two months, but a variation. We use the term "trend" for clear multiyear evolution with many time steps.

Reply: Thank you for your comment. In response to the reviewer's suggestion, we have replaced the term "trend" with "variation" in line 566 to accurately reflect the two months' comparison. We hope this revision improves the precision and clarity of the manuscript.

Reviewer: Line 572 : too many digits are used to described the PBL height comparisons (e.g. 646.7 m ?) as compared to its precision.

Reply: In response to the reviewer's suggestion, we have revised the manuscript to remove excessive digits from the PBL height comparisons, ensuring that the values are presented without decimal places to better reflect their precision. We believe this revision enhances the clarity and accuracy of the manuscript.

Reviewer: Line 655 : It should be clearly stated that the WRF-Chem model overestimates (positive bias) by a factor of 2 both background and peaks of NO2

Reply: We have revised the manuscript to clearly state that the WRF-Chem model overestimates peaks of NO_2 by a factor of 2, indicating a positive bias. This overestimation is observed when comparing the average values between the TROPOMI NO2 and the model over the UAE. This clarification has been incorporated into the revised manuscript.

Reviewer: Line 690 : these RMSE values are not compatible with the actual differences seen visually in the maps. If it is an unbiased RMSE that is calculated, the definition and name of the quantity should be revised.

Reply: Thank you for your comment and thorough review. Our analysis used the standard RMSE computation, not the unbiased RMSE. The RMSE values in our study represent the average error across the entire UAE, which may not always correspond directly to the visual differences observed in the maps. The maps in Figs. 5, 6, and 7 show absolute differences, while the RMSE values in line 690 summarize the overall model error. We will clarify this distinction in the revised manuscript to prevent any confusion. Thank you for highlighting this point.

Reviewer: How are the biases, RMSE, R of WRF-Chem in other regions in literature (East Asia and India) compare to those found in this study? Provide this comparison in percentage and the comparison with the results of the paper should be explicitly stated.

Reply: Thank you for your comment and thorough review. In response to the reviewer's suggestion, we will incorporate a comparison of the biases, RMSE, and R of WRF-Chem from other geographical regions, such as East Asia and India, as reported in the literature. This comparison will be presented as a percentage and explicitly discussed concerning the results of our study. We believe this addition will enhance the clarity and comprehensiveness of the manuscript.

Reviewer: Ozone columns are often express in Dobson Units. For comparison, this unit should be used.

Reply: Thank you for your comment. In response to the reviewer's suggestion, we have revised the manuscript to express the ozone columns in Dobson Units (DU) for consistency and ease of comparison. We believe this modification will improve the clarity and comprehensiveness of the manuscript.

Reviewer: What is the influence of the altitude in the comparison between gaseous pollutants ? Where do averaging kernels peak? Model values without AVK should be shown as well to understand its influence.

Reply: Thank you for your comment. In response to the reviewer's suggestion, we have revised the manuscript to include the raw model values in the corresponding tables to understand better the influence of averaging kernels on comparing gaseous pollutants. Additionally, we have incorporated a figure showing the averaging kernel matrix to illustrate where the averaging kernels peak in the revised manuscript. These revisions have been made to enhance the clarity and comprehensiveness of the manuscript.