Authors' Final response

EGUSPHERE-2024-959 | Research article

Submitted on 29 Mar 2024

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

Yesobu Yarragunta, Diana Francis, Ricardo Fonseca, and Narendra Nelli

Handling editor: Christoph Gerbig, cgerbig@bgc-jena.mpg.de

Reviewer 1

Reviewer: The paper presents high-resolution WRF-Chem model simulations for the UAE region. The authors carried out an evaluation of the model simulations for different meteorological and chemical fields by using ground and satellite-based observations. Given the rapid industrial development and urbanization in the region, it's important to develop state-of-the-art air quality models to simulate air pollution in UAE. The authors conducted comprehensive WRF-Chem model simulations with 3 nested grids centered over the UAE. There are a number of shortcomings of this study that need to be addressed before considering this manuscript for publication.

Reply: Thank you for your detailed review and valuable feedback on our manuscript. We appreciate the time and effort you have invested in evaluating our work. We acknowledge the importance of addressing the shortcomings you highlighted to enhance the quality and robustness of our study. Below, we outline our responses and the actions we plan to take to address each of the concerns raised:

Major comments:

Reviewer: The manuscript can be shortened quite a bit. There's plenty of text devoted to the presentation of the evaluation of the meteorological simulations by the WRF-Chem model. Although the main scope of the paper is the evaluation of the gaseous pollutants, there's lengthy discussion about the meteorological simulations in the main text. The discussion about the ERA-

5 reanalysis, evaluation of the meteorological simulations using the weather observations and ERA5 reanalysis data should be moved to the supplemental material.

Reply: Thank you for your insightful feedback on our manuscript. We appreciate your suggestions on how to streamline the presentation of our work. We understand that the manuscript can be shortened by focusing more on evaluating air pollutants and less on the meteorological parameters. In response to the reviewer's comment, we have taken the following actions to rearrange the manuscript: (i) we have significantly shortened the text devoted to presenting the meteorological parameters by the WRF-Chem model. This ensures that the main focus remains on evaluating the gaseous pollutants, which is the primary scope of our study; (ii) the detailed discussion about evaluating meteorological simulations using weather observations and ERA5 reanalysis data has been moved to supplemental material, as suggested. This includes comprehensive tables, figures, and statistical analyses to support the validity of the meteorological simulations, allowing interested readers to access this information without detracting from the main narrative of the paper. By implementing these changes, we have enhanced the clarity and focus of our manuscript while still providing a thorough evaluation of our meteorological simulations for those who seek it. We appreciate your guidance and thank you again for your valuable feedback.

Reviewer: The EDGAR emission inventory doesn't provide information on the day-to-day (e.g. weekday vs. weekend) and hourly variability (diurnal cycle) of the anthropogenic emissions. This deficiency of the emission inventory and its impact on the findings of the modeling study aren't discussed.

Reply: Thank you for your constructive feedback regarding using the EDGAR emission inventory in our modeling study. We appreciate your attention to detail and your suggestions for improving our manuscript.

We acknowledge that the EDGAR emission inventory does account for day-to-day (e.g., weekday vs. weekend) and hourly variability (diurnal cycle) of anthropogenic emissions, as discussed in the article by Crippa et al. (2020). To improve our manuscript, we have re-run the model simulations incorporating the diurnal variability of emissions during recent years. We have included an idealized diurnal profile for various air pollutants, assessed the impact of this variability, and presented the findings in our revised manuscript. Although EDGAR includes temporal variability, it may not capture the full complexity needed for our modeling study. We have elaborated on these limitations, emphasizing the challenges in accurately representing day-to-day and hourly emission variations (lines xx-xx). In the text, we have analyzed and discussed the potential impact of these limitations on our modeling results. Specifically, we explore how the lack of fine-grained temporal variability in the emissions might influence the accuracy and reliability of simulated air quality patterns in lines xx-xx. This is particularly relevant for short-term and diurnal analyses.

We have included a portion that explicitly addresses the limitations of the EDGAR emission inventory concerning temporal variability. This will help readers understand our modeling study's

potential shortcomings and context. We have incorporated an analysis discussing how these limitations might affect our findings, providing a nuanced view of the model's strengths and weaknesses. In the end, we outline practical steps for future research to enhance the temporal resolution of emission data and improve model accuracy. We appreciate your valuable feedback and will make these revisions accordingly. Thank you once again for your thoughtful review.

Reviewer: How are the emissions from point sources (e.g. power plants) ingested into the model? Is their vertical distribution taken into account?

Reply: Thank you for your valuable question. Our current simulations focused primarily on surface air quality; therefore, the vertical distribution of emissions from point sources, such as power plants, is not included, even though their spatial distribution is accounted for as given by the EDGAR dataset. However, we recognize the importance of accounting for the vertical distribution of emissions, especially since significant sources, such as combustion stacks, release pollutants at elevated altitudes. In future model simulations, we plan to incorporate vertical emission profiles to better represent these elevated emissions, which we note in the text (lines xx-xx). As the reviewer suggested, using vertical emission profiles, similar to temporal and speciation profiles, would provide a more accurate representation of the dispersion and impact of such emissions. In the present study, we chose to simplify the model setup by injecting all emissions into the lowest model layer. We appreciate your suggestion and will consider incorporating vertical emission profiles in future work to improve model accuracy. Thank you again for your insightful feedback.

Reviewer: The main weakness of this study is the lack of the model evaluation against ground-based air quality observations. Without such model evaluation it's hard to determine the applicability of the model to air quality research and prediction applications. I assume there are surface based O_3 and PM2.5 monitoring sites available in UAE and neighboring countries, which could be utilized.

Reply: Thank you for your insightful feedback. We agree that model evaluation against ground-based air quality observations is crucial for assessing the model's applicability to air quality research and prediction. Unfortunately, we cannot access ground-based air quality observations in the UAE and neighboring regions. Despite this limitation, we have aimed to provide a comprehensive analysis using the data sets noted in section 3. We will continue to seek opportunities to obtain ground-based observations in future studies to enhance the evaluation and validation of our model results.

Reviewer: AOD verification by using the available data from the AERONET sites located in the region would be very helpful as well.

Reply: Thank you for your valuable suggestion. We agree that evaluating the model's AOD using data from the available AERONET sites in the region would significantly enhance the validation

of our model results. The revised manuscript incorporates AOD data from these sites to compare with our WRF-Chem simulations for this region. This analysis will improve the robustness of our findings and contribute to the overall quality of the paper. Thank you for this insightful recommendation.

Reviewer: The model evaluation against the satellite observations of CO, O_3 and NO_2 is worth of publication. It'd be helpful to add information on uncertainties associated with these observations. But again the satellite observations are sporadic and can't provide information on vertical distribution of the pollutants.

Reply: Thank you for your valuable feedback. We have addressed the uncertainties associated with each satellite observation in the manuscript's Data Sets and Methodology section (Section 3.3). Specifically, the uncertainties for NO_2 observations are discussed in lines 268-270, for CO in lines 291-298, and for O_3 in lines 309-311. While satellite observations provide crucial data, we acknowledge their limitations, such as sporadic coverage and the lack of information on the vertical distribution of pollutants, as mentioned by the reviewer. Given this, we focused on tropospheric column observations of these pollutants. Additionally, we ensured that at least one observation is available daily, corresponding to a satellite crossing the equator at a local solar time of 13:30, to generate robust statistics. This is noted in the text (lines 241-242).

Reviewer: Did you include a dust parameterization in the model? Given how significant the dust emissions in the region, it's important to discuss the role of the dust aerosols and their impact on photolysis, thus affecting O_3 chemistry.

Reply: Thank you for your valuable feedback. Our model simulations employed the Model for Ozone and Related Chemical Tracers (MOZART) chemical mechanism for gas-phase species and the Georgia Institute of Technology–Goddard Global Ozone Chemistry Aerosol Radiation and Transport (GOCART) aerosol scheme to account for dust emissions. The GOCART dust emission scheme is a widely used parameterization in atmospheric models for simulating dust emissions, including the Arabian Peninsula, where it performs well (e.g. Karamuri et al., 2024). We will cite the relevant articles in the revised manuscript. This scheme calculates dust emissions based on several critical factors, including near-surface wind speed, soil moisture, surface type (such as vegetation cover and roughness length), and soil erodibility. The GOCART scheme also categorizes dust particles into bins of multiple sizes to represent a range of particle sizes, from fine dust to larger particles. These dust particles can interact with shortwave and longwave radiation fluxes influencing radiative heating rates (direct and semi-direct effects) as well as with cloud microphysics by acting as cloud condensation nuclei (CCN) or ice nuclei (IN), with indirect effects.

We recognize the significant role of dust aerosols in the region and their potential impact on photolysis rates, which can influence ozone (O_3) chemistry. To address this, we will conduct additional model simulations focusing on a particular dust storm event during the study period.

These simulations will analyze the impact of dust aerosols on photolysis rates and O_3 chemistry by comparing scenarios with and without the inclusion of dust aerosol schemes. This approach will provide deeper insights into the effect of dust aerosols on O_3 chemistry, especially in regions with high aerosol loads. We will also include a more detailed discussion in the revised manuscript highlighting the role of dust aerosols in altering photolysis rates and their subsequent effect on O_3 chemistry. We appreciate your insightful comments and believe this additional analysis will strengthen the manuscript. Thank you again for your feedback.

Reviewer: Was the aerosol feedback turned on in the model?

Reply: Thank you for your question. Yes, the aerosol-radiation and aerosol-cloud feedbacks were activated in our WRF-Chem model simulations. Given the high aerosol loads in the study region, it was essential to account for the interaction between aerosols and radiation/cloud microphysics to accurately capture their effects on atmospheric processes. Thank you for your attention to this detail.

Reviewer: The transport of the pollutants from other countries to UAE should be considered here as well. It'd be helpful to conduct sensitivity simulations to estimate the impact of the transboundary pollution in the region.

Reply: Thank you for your valuable suggestion to include sensitivity simulations to estimate the impact of transboundary pollution from other countries to the UAE. We acknowledge the importance of understanding the transboundary pollution's role in regional air quality and plan to incorporate such simulations in future studies. The current study primarily focuses on evaluating chemical and meteorological parameters within the UAE, and it represents the first effort to establish WRF-Chem simulations in this area, which is characterized by significant industrial emissions and high pollution events. As stated at the end of the manuscript, when alluding to future lines of research, a thorough assessment of the contribution of pollutants emitted from upwind regions to the air quality in the UAE has to be conducted. It will have significant implications for the design of mitigation and adaptation policies aiming at improving the air quality in the country. We hope the reviewer understands our decision.

Reviewer: Line 614: Are there any NO_2 emissions included? Usually 8-10% of NO is emitted as NO_2.

Reply: Thank you for pointing this out. Yes, our model simulations include NOx emissions from the EDGAR inventory. In our setup, we assign 90% of the NOx emissions as NO and 10% as NO_2, following the typical emission ratio in the region as documented e.g. in Habeebullah et al. (2015). This approach ensures that NO and NO_2 are appropriately represented in the model, consistent with the standard practices where 8-10% of NOx is emitted as NO_2. We appreciate your attention to this detail and will ensure that this is clearly stated in the revised manuscript. Thank you again for your valuable feedback.

Reviewer: 643-645: How was the nocturnal mixing of the chemical species parameterized in the model? WRF-Chem applies enhanced mixing within the areas with high anthropogenic emissions.

Reply: Thank you for your insightful comment. In our WRF-Chem model simulations, the nocturnal mixing of chemical species was parameterized using the Yonsei University (YSU) planetary boundary layer (PBL) scheme. This scheme effectively captures shallower and more stable nocturnal conditions by reducing turbulence and mixing at night, which is essential for accurately representing the vertical distribution and concentration gradients of pollutants, including NO_x and VOCs, during night-time (Hoshyaripour et al., 2016). We acknowledge that enhanced nocturnal mixing, especially in urban areas with high anthropogenic emissions, can lead to variations in the model's representation of atmospheric chemistry. Badia & Jorba (2015) found that overestimating the OH radical in the model could suggest an overly oxidized atmosphere, potentially influencing nocturnal chemistry and accumulating chemical species in the surface layers. In light of the reviewer's comment, we will provide additional clarification in the revised manuscript regarding the parameterization of nocturnal mixing and its implications for chemical species distribution in our model setup. Thank you again for your valuable feedback.

Reviewer: 687: Are you referring to dry deposition of CO? This part needs more clarification.

Reply: Thank you for your comment. Yes, we are referring to the dry deposition of CO. As Kumar et al. (2022) highlighted, the absence of a vertical distribution of industrial emissions in the model can result in a rapid deposition of CO at the surface. We will clarify this point in the revised manuscript to provide a better understanding of the deposition processes considered in our simulations.

Reviewer: 721: This interpretation is vague.

Reply: Thank you for your comment. We acknowledge that the interpretation in this section is not clear. We will revise this part of the text in the manuscript to provide a more straightforward and precise explanation. This update will be included in the revised manuscript.

Reviewer: Pages 28-29: This chapter needs to be revised quite a bit. First, some of this material is more relevant for the Introduction section. Second, there's quite a bit of textbook material describing different NO_x/VOC regimes affecting tropospheric O_3 formation. The authors don't present any sensitivity simulations to show whether O_3 is NO_x or VOC limited in the region. There aren't either any surface NO_x or VOC measurements used here to evaluate the model. Therefore, I find this discussion vague and does not point to any particular mechanism to explain the observed model biases.

Reply: Thank you for your comment. We acknowledge that the interpretation in this section lacks clarity and will revise it to provide a more precise and focused explanation. We also recognize that sensitivity simulations to determine whether O_3 is NO_x or VOC limited and including surface NO_x

or VOC measurements would strengthen the analysis. However, such simulations require more extensive observational data, which is currently lacking in the study area. We will remove the less relevant discussion from the text and reorganize the remaining content to enhance clarity. These updates will be reflected in the revised manuscript.

Reviewer: 798-800: do you see this effect occurring in the model?

Reply: Thank you for your comment. Yes, we do observe this particular effect in the model. A comparison of WRF-simulated Sea Surface Temperatures (SSTs) with both ERA5 and Group for High-Resolution Sea Surface Temperature (GHRSST) data over the Arabian Gulf region supports this interpretation, as discussed in lines 522-538. In response to your suggestion and another reviewer's suggestion, we will include the comparison figures in the revised manuscript to provide a clearer illustration of this effect. Thank you for your suggestion.

Minor comments:

For WRF-Chem please cite this paper as well: https://journals.ametsoc.org/view/journals/bams/98/8/bams-d-15-00308.1.xml

Reply: This reference will be included in the revised manuscript.

Reviewer: 204: Fix "meteorology"

Reply: This modification will be included in the revised manuscript.

References

Badia, A., & Jorba, O. (2015). Gas-phase evaluation of the online NMMB/BSC-CTM model over Europe for 2010 in the framework of the AQMEII-Phase2 project. *Atmospheric Environment*, *115*, 657–669. https://doi.org/10.1016/j.atmosenv.2014.05.055

Crippa, M., Solazzo, E., Huang, G., Guizzardi, D., Koffi, E., Muntean, M., Schieberle, C., Friedrich, R., & Janssens-Maenhout, G. (2020). High resolution temporal profiles in the Emissions Database for Global Atmospheric Research. *Scientific Data*, *7*(1). https://doi.org/10.1038/s41597-020-0462-2

Habeebullah, T. K. (2015) Characterising NO_2, Its temporal variability and Association with Meteorology: A Case Study in Makkah, Saudi Arabia. EnvironmentAsia, 8, 37-44. https://doi.org/10.14456/ea.2015.21

Hoshyaripour, G., Brasseur, G., Andrade, M. F., Gavidia-Calderón, M., Bouarar, I., & Ynoue, R. Y. (2016). Prediction of ground-level ozone concentration in São Paulo, Brazil: Deterministic versus statistic models. *Atmospheric Environment*, *145*, 365–375. https://doi.org/10.1016/j.atmosenv.2016.09.061

Karamuri, R. K., Dasari, H. P., Gandham, H., Kunchala, R. K., Attada, R., Ashok, K., & Hoteit, I. (2024). Investigation of dust-induced direct radiative forcing over the Arabian Peninsula based on high-resolution WRF-Chem simulations. *Journal of Geophysical Research: Atmospheres*, *129*, e2024JD040963. https://doi.org/10.1029/2024JD040963

Kumar, R., He, C., Bhardwaj, P., Lacey, F., Buchholz, R. R., Brasseur, G. P., Joubert, W., Labuschagne, C., Kozlova, E., & Mkololo, T. (2022). Assessment of regional carbon monoxide simulations over Africa and insights into source attribution and regional transport. *Atmospheric Environment*, *277*. https://doi.org/10.1016/j.atmosenv.2022.119075