

We greatly appreciate the comments and criticism of the 2 anonymous reviewers and Dr. Seth Lyman. These reviewers provided critical suggestions that have substantially improved the quality of our paper. The main criticisms from the reviewers focused on 1) disparities between options selected for the different simulations (e.g., dry deposition, photolysis, boundary conditions, etc.) and 2) a lack of understanding of the sensitivity to different VOC and NO_x emission scenarios. We have addressed both of these in detail in the revised manuscript. Specifically, we have done the following:

1. ensured consistency between options when running MOZART and RACM (when possible, as some namelist options do not work with one or the other chemistry mechanism)
2. identified dry deposition as a primary difference between the MOZART and RACM simulations such that when it is turned off in both cases, nearly identical levels of O₃ are produced
3. leveraged WYDEQ VOC and NO_x data to quantify model biases and then adjust the emissions by these biases, enabling us to understand the sensitivity of O₃ production in the UGRB to different VOC and NO_x conditions.

In addition to these major revisions to the manuscript, we have explicitly addressed all of the other comments from the reviewers and corrected minor grammatical errors that were overlooked in the original manuscript. We again thank the reviewers for the insightful feedback and hope that our revisions meet their expectations.

1. **Reviewer Comment:** The high wintertime O₃ pollution in the Upper Green River Basin (UGRB), Wyoming is simulated in the study. During some years in winter months high O₃ pollution in oil and gas producing basins of Utah and Wyoming have been observed. Numerous field campaigns and modeling studies have been conducted to understand the emissions and processes causing these high O₃ pollution events. It is important for the air quality models to accurately simulate the wintertime O₃ in UGRB, which could also help to develop mitigation strategies in the future. Here the authors deploy the-state-of-the-art WRF-Chem model to simulate high O₃ during March, 2017. There are several aspects of the study that could make an important contribution to the field. The authors also conduct rigorous evaluation of the meteorological simulations. However, there are some shortcomings of the study that need to be addressed.

Author Response: The authors thank the anonymous reviewer for the feedback provided.

Major Comments:

2. **Reviewer Comment:** The authors emphasize the importance of using the existing anthropogenic emission inventories to model the high winter O₃ in UGRB, and claim that this is the main strength of this study. While it's important to use the bottom-up emission inventories, the scientific community should not limit itself using the bottom-up inventories only. As Ahmadov et al. 2015 showed the EPA NEI inventory can grossly over/under-estimate

the NO_x/VOC emissions from an oil and gas producing region (Uintah Basin). Therefore, in my opinion it's an underestimation of the importance of the study by focusing on the use of the emission inventory.

Author Response: We thank the reviewer for pointing out the findings from the Ahmadov et al. (2015) study in the Uinta Basin (UB), UT. We agree that the scientific community should not limit themselves to the emission inventories only, but we would like to point out that the studies using 3-D photochemical models (Ahmadov et al., 2015; Matichuk et al., 2017) have focused on the high O₃ events occurring in the UB not in the Upper Green River Basin (UGRB), WY. Also, as noted by several studies cited in the paper (Schnell et al., 2009; Oltmans et al., 2014; Rappenglück et al., 2014; Field et al., 2015; Lyman and Tran, 2015), the formation of O₃ in basins with operating natural gas and oil extraction facilities depend on the topography, meteorology, and chemical processes specific to the basin. These studies have pointed out that high O₃ events occur during different months in different basin and also vary from year to year in the same basin. Thus, the results of one basin cannot be applied to other basins without validation and analysis. In addition, the 3-D photochemical models used to study high O₃ events in the UB used a previous version of National Emission Inventory (NEI 2011) data compared to our study (NEI 2014v2). We would like to emphasize the use of the NEI 2014v2 dataset as these data include emissions from natural gas and oil production fields, which are not included in prior inventories. Thus, for these reasons, we would like to put an emphasis on the importance of using the existing anthropogenic emission inventories to study a high O₃ event in the UGRB, WY.

- 3. Reviewer Comment:** Introduction: The statement about the shortfalls of other studies is somewhat misleading. Do the authors refer to the box modeling studies conducted in the past? The box models are designed to use measured concentrations of the chemical species, not emission inventories. As for the 3D air quality models Ahmadov et. al. (2015) demonstrated that the emission inventories can have huge uncertainties. Moreover, as I discuss below this study doesn't prove that the NEI-2014 inventory accurately represents the emissions for the UGRB during March, 2017.

Author Response: We do refer to previous studies that use box models, as mentioned on line 51. Further, on line 94, the findings of these box models have been discussed.

- 4. Reviewer Comment:** Here two different gas chemistry schemes are used, MOZART and RACM. As the WRF-Chem namelists provided in SI show the MOZART simulation included aerosols and their feedback on radiation. However, in the RACM simulations the authors turned off aerosols. In the paper differences in the meteorological simulations between these two model cases are presented and attributed to the aerosol feedback, though simulated aerosol fields aren't shown. I assume the aerosol concentrations in UGRB were relatively low.

Author Response: In the revised manuscript, we have updated all simulations used in this study. The major changes in the simulations include the use of the same namelist options

for both MOZART and RACM. Hence, in the revised MOZART simulation, aerosols and their feedback on radiation are not included. Despite this, there exists some differences in the meteorological fields, which is not due to the inclusion of aerosols and their feedbacks.

5. **Reviewer Comment:** The two gas chemistry mechanisms also use different photolysis schemes (`phot_opt`). Such difference makes it hard to compare the results of these two model cases.

Author Response: A discussion regarding the use of different photolysis options has been provided in the revised paper, line 221: *“Despite all the same namelist options used in these models, the simulations with MOZART use photolysis option 4, which is the updated TUV photolysis option that was setup to work with only few chemistry mechanism schemes in WRF-Chem v3.9.1. While the RACM simulations use photolysis option 1, which is the Madronich photolysis scheme. With the current setup for photolysis option 4 in the WRF-Chem v3.9.1 it does not work with RACM chemistry mechanism. This study uses photolysis option 4 for MOZART simulation as it produces higher O₃ compared to when photolysis option 1 was used (Figure not shown).”*

Furthermore, in Section 3.2, line 381, the difference in the results for the MOZART and RACM simulations owing to the use of different photolysis options has been discussed as follows: *“It is important to note that one difference between the MOZART and RACM simulations used in this study is the photolysis option (`phot_opt = 4` for MOZART and `phot_opt = 1` for RACM), which could affect O₃ production. As RACM is not coupled to `phot_opt = 4`, an addition sensitivity simulation was performed using option 1 with MOZART, which led to less O₃ compared with using option 4, albeit with better agreement with the observations. As such, we elected to use `phot_opt = 4` for subsequent simulations but note that some of the difference between RACM and MOZART may be attributed to the photolysis scheme used with the former leading to less O₃ production.”*

6. **Reviewer Comment:** Here the model simulations are presented for 5 days only. This is quite short. I suggest extending the model simulations to evaluate the model’s capability in simulating ozone and other chemical species other days in March, 2017. Even if O₃ levels were low those days it’s important to check the model’s ability to simulate O₃ and other species in different meteorological conditions by using the same model configuration and emission dataset.

Author Response: We agree that extending the model simulation could provide more information on the model’s capability at simulating O₃ and other chemical species. However, extending the simulation period is out of scope for this study as the model is computationally expensive and requires longer hours to run the simulations. Hence, a short period with one of the high O₃ events of the season was chosen for this study and the simulations were carried out in the finest resolution (in terms of model stability) possible. We do note that in lieu of extending the model period, considerable effort has been given to studying the sensitivity of O₃ formation to VOC and NO_x emissions, which has greatly improved the

impact of the study.

- Reviewer Comment:** 350: Ahmadov et al. (2015) found that the reduced dry deposition of ozone over snow covered ground is one of key processes leading to high wintertime ozone buildup. It seems that the model has this snow impact on dry deposition in the MOZART scheme, but not in the RACM scheme in the version of the model used here. This discussion of the dry deposition needs to be revised.

Author Response: The discussion on the dry deposition of gas species in both chemistry mechanisms has been updated in Section 3.2, line 387: “*To better understand the chemistry mechanisms’ sensitivity to dry deposition, we compare the diurnal variation of O₃ concentrations from MOZART and RACM with dry deposition turned on and off in both simulations at the 7 monitoring stations.*” The results of these sensitivity simulations have also been described in the revised manuscript.

- Reviewer Comment:** Although the model is able to simulate the high O₃, the simulated VOC mixing ratios are a factor of six lower than the observed ones. The NO_x simulations show underestimation too. This begs the question, does the model simulate high O₃ for the right reasons? It’d be helpful to conduct sensitivity simulations by adjusting the NO_x and VOC emissions to account for uncertainties in the NEI.

Author Response: Thank you for the great comment. We have performed a sensitivity study on VOC and NO_x emissions. The adjustment process for this portion of the study is discussed in Section 2.7, line 270.

- Reviewer Comment:** 360: This is missing in the community version of WRF-Chem.

Author Response: The line referenced in the original manuscript does not mention specific components of the WRF-Chem model, as such we are unsure what the reviewer is referencing.

- Reviewer Comment:** For the mitigation strategies it’s helpful to understand the NO_x/VOC sensitivity of the O₃ formation. I suggest conducting sensitivity simulations by adjusting the emissions to show how the simulated O₃ will respond to the NO_x and/or VOC emission adjustments in UGRB.

Author Response: Yes! Again, this is a great comment, which motivated us to explore the VOC and NO_x parameter space in more detail. Sensitivity simulations with increased VOC and NO_x emissions constrained to observations were conducted, and the results of these simulations are described in detail on line 495 of the revised manuscript.

- Reviewer Comment:** The advantage of using a tightly coupled meteorology-chemistry model such as WRF-Chem isn’t discussed here. As Ahmadov et al. showed this is essential to simulate the stagnation episodes and multi-day buildup of the pollutants in a basin.

Author Response: In Section 2.2, line 169, the benefit of using WRF-Chem has been updated as follows: “*This is beneficial over models such as CAMx and CMAQ where the*

meteorological and the atmospheric chemistry components are run separately. Ahmadov et al. (2015) also pointed out the benefit of WRF-Chem, which helped in the proper simulation of pollutant accumulation in shallow inversion layers.”

Minor Comments:

12. **Reviewer Comment:** The CMAQ modeling paper by Matichuk et al. (<https://doi.org/10.1002/2017>) isn't cited here.

Author Response: We have somehow missed to cite this CMAQ modeling paper and we would like to thank the reviewer for suggesting this article. We have added the citation for Matichuk et al. (2017) on line 119, “*Matichuk et al. (2017) used the WRF and Community Multiscale Air Quality (CMAQ) models to study a 10-day high-ozone episode in 2013 in the UB. Similar to Ahmadov et al. (2015), they also used the NEI2011 emission dataset, but they found that the CMAQ model did not reproduce the observed O₃, NO_x, and VOC levels in the UB. Matichuk et al. (2017) identified a positive temperature bias and overestimation of the daytime planetary boundary layer height in the WRF simulations, which was hypothesized to be the reason for underestimation of O₃, NO_x, and VOCs from the CMAQ model.*”

13. **Reviewer Comment:** The evaluation of the meteorological simulations can be moved to SI.

Author Response: The authors think that meteorological simulations be kept in the main manuscript and hence have not been moved to SI. The reason is that O₃ formation is highly sensitive to the meteorological conditions, and we feel that is is important to show the model's ability to simulate the conditions up front.

References

- Ahmadov, R., McKeen, S., Trainer, M., Banta, R., Brewer, A., Brown, S., Edwards, P., De Gouw, J., Frost, G., Gilman, J., et al.: Understanding high wintertime ozone pollution events in an oil-and natural gas-producing region of the western US, *Atmospheric Chemistry and Physics*, 15, 411–429, 2015.
- Field, R., Soltis, J., Pérez-Ballesta, P., Grandesso, E., and Montague, D.: Distributions of air pollutants associated with oil and natural gas development measured in the Upper Green River Basin of Wyoming, *Elem Sci Anth*, 3, 2015.
- Lyman, S. and Tran, T.: Inversion structure and winter ozone distribution in the Uintah Basin, Utah, USA, *Atmospheric Environment*, 123, 156–165, 2015.
- Matichuk, R., Tonnesen, G., Luecken, D., Gilliam, R., Napelenok, S. L., Baker, K. R., Schwede, D., Murphy, B., Helmig, D., Lyman, S. N., et al.: Evaluation of the community multiscale air quality model for simulating winter ozone formation in the Uinta Basin, *Journal of Geophysical Research: Atmospheres*, 122, 13–545, 2017.

- Oltmans, S., Schnell, R., Johnson, B., Pétron, G., Mefford, T., and Neely III, R.: Anatomy of wintertime ozone associated with oil and natural gas extraction activity in Wyoming and Utah, *Elementa: Science of the Anthropocene*, 2, 2014.
- Rappenglück, B., Ackermann, L., Alvarez, S., Golovko, J., Buhr, M., Field, R., Soltis, J., Montague, D. C., Hauze, B., Adamson, S., et al.: Strong wintertime ozone events in the Upper Green River basin, Wyoming, *Atmospheric Chemistry and Physics*, 14, 4909, 2014.
- Schnell, R. C., Oltmans, S. J., Neely, R. R., Endres, M. S., Molenaar, J. V., and White, A. B.: Rapid photochemical production of ozone at high concentrations in a rural site during winter, *Nature Geoscience*, 2, 120, 2009.