

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:** This paper looks at high ozone events that occur in wintertime in the Upper Green River Basin. High wintertime ozone concentrations have been discussed in previous studies and are attributed to emissions from oil and gas extraction in combination with temperature inversions and enhanced photolysis fluxes due to snow covered ground. This paper discusses to what extent a regional chemical transport model (WRF-Chem) is able to represent these conditions by conducting sensitivity simulations with two different chemical mechanisms as well as a simulation where dry deposition has been turned off. The authors find that despite a significant underestimate in the modeled VOC concentrations, either chemical mechanism was able to represent the enhanced ozone concentrations.

This paper provides a good overview of previous work and in general the approaches and results are well presented. What I see missing is, however, a more in-depth analysis of the model results and an attempt to shed light into why the model despite a significant low bias in VOCs simulates ozone concentrations relatively well. The paper could be strengthened significantly by including more information on the NO_x and VOC sensitivities in the model (e.g. looking at HCHO/NO₂ ratios, modeled chemical tendencies etc.) and how they vary between the model simulations and also vary temporally and spatially. The model could also be compared to HCHO/NO₂ ratios at the Boulder site if speciated VOCs are available (from the data set description it is not clear what type of VOC measurements were collected). It further would be valuable to focus on individual VOC species and not just the total VOCs

since the reactivity of different VOCs and their role in ozone production varies widely. The modeled VOC bias might be driven by only a few VOCs that have abundant emissions but play little role in ozone production.

Author Response: We thank the reviewer for the suggestions. As suggested, an in-depth VOC and NO_x sensitivity analysis has been conducted. In the revised manuscript, the sensitivity simulations have been described in detail in Section 2.7, and the results have been discussed in Section 4. We are appreciative of this suggestion as the added results have strengthened the paper substantially.

Specific Comments:

2. **Reviewer Comment:** Line 143: I would disagree in that a valuable model should be able to represent conditions under any emission scenarios and VOC:NO_x levels

Author Response: The statement has been reworded on line 145 to read “*It is most useful to simulate O₃ events from recent years (versus modeling events in 2011) because basin-wide emission estimates from the State DEQ have decreased significantly over the last decade with potential impacts on both ozone precursor concentrations and VOC:NO_x ratios. Also, we do not have emissions for oil and gas from 2011.*”

3. **Reviewer Comment:** Section Model Setup: Table 2 lists only a few of the settings and Figures A2 and A3 will only be meaningful to readers who are very familiar with WRF-Chem. I suggest extending Table 2 and explicitly stating some of the main information there. Additional information is also needed on the model configuration, e.g. what was used as chemical boundary conditions, was the meteorology in the model constrained and if so how, ...

Author Response: Table 2 has been updated and now includes information regarding the chemical boundary conditions, dry deposition of gas species, lateral boundary conditions, and photolysis option used in the WRF-Chem simulations. The Community Atmosphere Model with Chemistry (CAM-Chem) data were used to update the chemical initial and boundary conditions in the model simulations, and this information has also been included in the revised paper. Specifically, in Section 2.3, line 189, the following has been added: “*To account for the transport of chemical species into the model domain, data from the Community Atmosphere Model with Chemistry (CAM-CHEM; Emmons et al. (2020)) were used in the simulations.*” Moreover, we have also added the following on line 248: “*The initial and boundary conditions of the simulations were updated every 24 hours for each simulations using the CAM-Chem data.*”

4. **Reviewer Comment:** Some questions to A2 and A3: The RACM setup does not use biogenic and fire emissions and also have_bcs_chem is set to false? There are a number of other differences between the MOZART and RACM simulation, so this means that the seen differences are not just related to the chemical scheme. Please elaborate on this and also provide justification behind these settings.

Author Response: We thank the reviewer for pointing this out. The simulations in the paper have been updated. Now, the biogenic and fire emissions along with aerosol radiation feedbacks have been turned off and `have_bcs_chem` has been set to true in all the simulations used in the revised version of the paper.

5. **Reviewer Comment:** In addition, this is a fairly small domain and I wonder how do chemical boundary conditions influence the ozone concentrations in the Basin? How were the chemical initial and boundary conditions treated (related also to comment above)?

Author Response: As mentioned in the response for a comment above (comment #3), the chemical initial and boundary conditions were updated every 24-hr using the CAM-CHEM dataset.

6. **Reviewer Comment:** Section 2.3: More detail on the measurement techniques and the accuracy of the measurements is needed.

Author Response: We agree we have not provided details on the measurement techniques. As mentioned on line 192, we have used the data provided by the Wyoming Department of Environmental Quality (WYDEQ), which was readily available on their website (www.wyvisnet.com) at the time this research was started.

7. **Reviewer Comment:** Line 198: MOZ17 has not yet been defined

Author Response: The authors thank the reviewer for pointing this out. In the revised manuscript, MOZ17 is not mentioned until Section 3.2 on line 407, which reads as follows “.....*MOZ_ddOff and RACM_ddOff simulations will be discussed in the following analyses and the simulations will be referred to as **MOZ17** and **RACM17** respectively.*”

8. **Reviewer Comment:** Line 209: Was a spin-up period considered and if so how long?

Author Response: The model was run for 4 days, and the results are generally consistent across all days. The only caveat is the overestimation of O₃ on the first day, which may be related to the model spinup time. However, given the model simulations are longer than this, we are confident the results for the later days are robust.

9. **Reviewer Comment:** Line 310: Is the model able to represent the diurnal variability and day-to-day variations? Is there a significant difference between daytime and nighttime performance?

Author Response: On line 352, a statement has been added that reads “*An analysis of the diurnal variability of winds showed good qualitative agreement between the model and observations in terms of the timing of increasing and decreasing wind speeds each day (Figure not shown).*” The time series for observed and modeled wind speed is shown in Figure 1 in this document, but is not shown in the manuscript.

10. **Reviewer Comment:** Line 321: I suggest replacing “accurately” with adequately given that the model has clear shortcomings in representing observed conditions

Author Response: Suggested change has been made on line 356, which now reads as follows: “*Given the aforementioned ability of the model to adequately simulate the key meteorological...*”

11. **Reviewer Comment:** Line 339: I suggest to also define an acronym for the RACM simulation without dry deposition, e.g. RACM17_noddep to be consistent with the naming of the other simulations

Author Response: Several acronyms are introduced in the paragraph starting on line 389. The MOZART and RACM simulations including dry deposition of gas species are defined as MOZ_ddOn and RACM_ddOn, and those that do not include dry deposition as MOZ_ddOff and RACM_ddOff, respectively.

12. **Reviewer Comment:** Line 374: I suggest a phrasing of “... do not show a strong sensitivity ...”

Author Response: Reworded as suggested on line 417 as follows: “*The simulated concentrations of NO_X seems less sensitive to the different chemical mechanisms,....*”

13. **Reviewer Comment:** Line 376: I would say that despite missing data there seems to be a clear overprediction in modeled NO_x. Have the authors looked at whether the type of mapping the model 4km data to the site location could explain some of the differences between measured and modeled concentrations?

Author Response: The statement regarding the overestimation of NO_x at Daniel South was misleading. Both simulations predict same NO_x concentration at the station. However, due to missing data points, it is not a good comparison. Hence, the statement regarding the overestimation of the NO_x concentration at Daniel South has been reworded on line 419 as follows: “*The NO_x mixing ratios are underestimated by both simulations even during the high O₃ events. Although the simulated NO_x concentrations at Daniel South is higher compared to other stations, the observed data are missing.*”

14. **Reviewer Comment:** Line 377: I suggest changing “removed” to “further away”

Author Response: Suggested rewording has been done on line 421, which now reads as follows “*.... emphasizing that this station is further from the oil and gas production region*”

15. **Reviewer Comment:** Line 379: Is this a boundary layer issue or an issue in the diurnal cycle of the emissions or is there any other reason?

Author Response: The misleading statement has been reworded on line 419 as follows: “*The NO_x mixing ratios are underestimated by both simulations even during the high O₃ events. Although the simulated NO_x concentrations at Daniel South is higher compared to other stations, the observed data are missing. The observed and simulated NO_x concentrations at South Pass are low and show little variability, emphasizing that this station is further from the oil and gas production region. Overall, the simulations underestimate*”

the observed NO_x concentrations to varying degrees depending on the location and do not capture the diurnal cycle well.”

16. **Reviewer Comment:** Line 381ff: Have you looked whether model grids surrounding the Boulder site have higher NMHC mixing ratios? More information is also needed on how the intercomparison was done and how it was ensured that the modeled total NMHC indeed reflect the same type of information as the measured NMHC (i.e. that it really is an apple to apple comparison)

Author Response: We have looked at the model grid points surrounding the Boulder station and the NMHC mixing ratios are higher but not as high as the observations. In the revised manuscript, we compare the values of speciated VOCs with those from the model and adjust the emissions based on the factors calculated using these values. The detailed process of the calculation is discussed in Section 2.7, line 270.

17. **Reviewer Comment:** Line 388: What is the statement about NMHC removal based on?

Author Response: Both MOZART and RACM simulations have similar NMHC mixing ratios. In order to understand how these chemical mechanisms lead to similar O₃ levels even with low mixing ratios of precursors, we performed VOC and NO_x sensitivity simulations. As mentioned in previous comment #16, the detailed process is discussed in Section 2.7, and the analysis is presented in Section 4 . The major finding from this sensitivity study is mentioned on line 498, which states the following: *“These model runs strongly suggest that ozone formation in the basin is predominantly limited by the NO_x available rather than being controlled mainly by VOC concentrations.*

18. **Reviewer Comment:** Figures 9-14: It is really hard to see any details in the NO_x and VOC graphs, maybe a different color range could help? The paper also first discusses the ozone plots from Figure 12 and then looks into the NO_x graphs. You might want to consider swapping the order of the Figures.

Author Response: The color scheme and color range for Figures 9-14 (spatial plots for O₃, NO_x and VOC for both MOZART and RACM simulations) have been updated.

References

Emmons, L. K., Schwantes, R. H., Orlando, J. J., Tyndall, G., Kinnison, D., Lamarque, J.-F., Marsh, D., Mills, M. J., Tilmes, S., Bardeen, C., Buchholz, R. R., Conley, A., Gettelman, A., Garcia, R., Simpson, I., Blake, D. R., Meinardi, S., and Pétron, G.: The Chemistry Mechanism in the Community Earth System Model Version 2 (CESM2), *Journal of Advances in Modeling Earth Systems*, 12, e2019MS001882, <https://doi.org/10.1029/2019MS001882>, URL <https://agupubs.onlinelibrary.wiley.com/doi/abs/10.1029/2019MS001882>, e2019MS001882 2019MS001882, 2020.

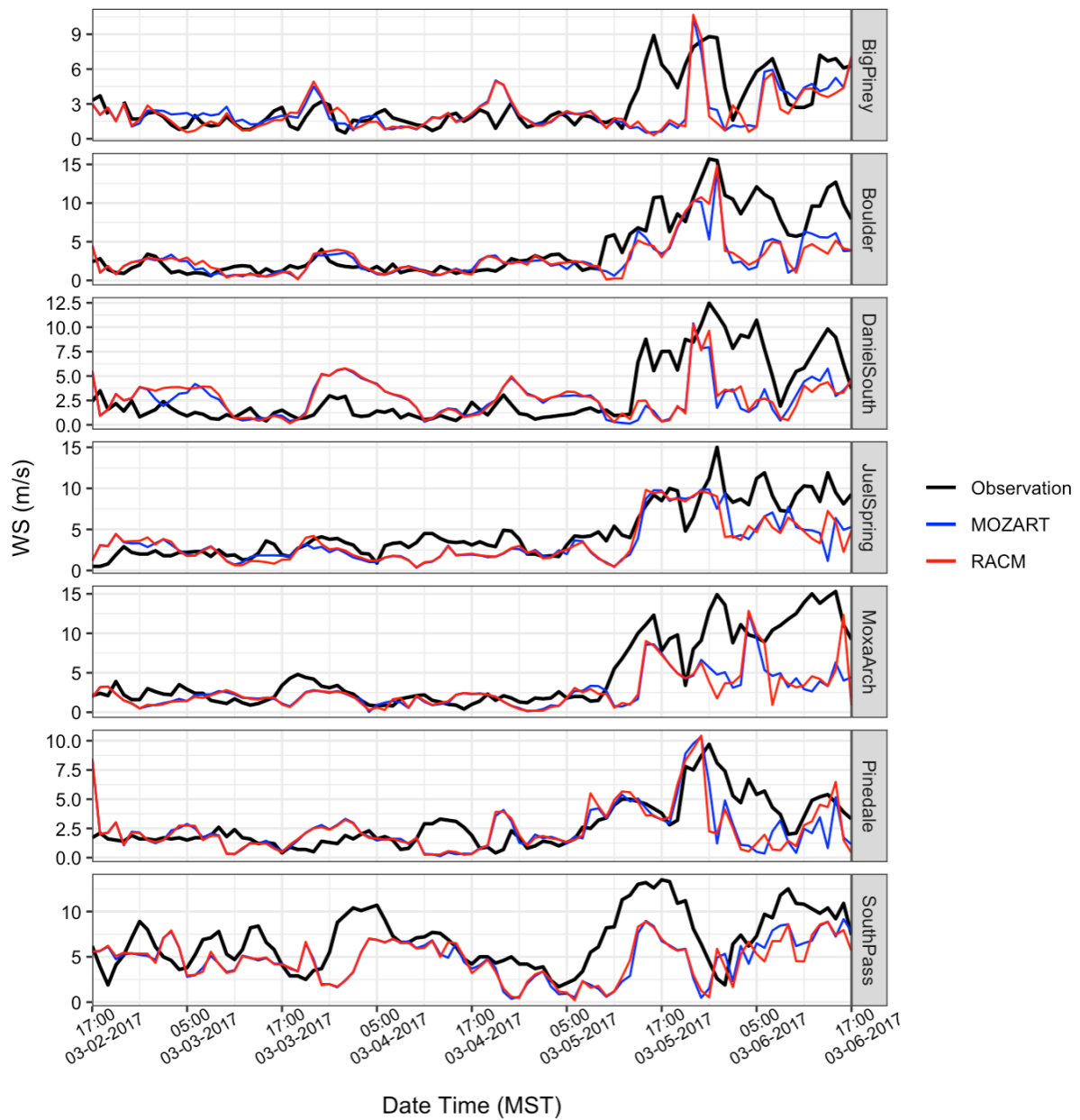


Figure 1: Time Series of observed and simulated Wind Speed (m/s) at seven monitoring stations.
 NOTE: this figure is not included in the manuscript