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**Interactive
comment**

Interactive comment on "Evaluating the sensitivity of fine particulate matter (PM$_{2.5}$) simulations to chemical mechanism in Delhi" *by* Chinmay Jena et al.

Anonymous Referee #2

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In this paper, the authors report WRF-Chem simulations for the Indo-Gangetic Plan region of India, by focusing on Delhi for the Winter Fog Experiment during winter 2017-2018. The authors conducted coupled meteorology-chemistry simulations by deploying the state-of-the-art atmospheric chemistry model WRF-Chem. Three chemistry mechanisms with different levels of complexity were tested. All the simulations are evaluated by comparing the model output with the in-situ measurements of various meteorological parameters and chemical species, and the satellite AOD data. I have reservations with respect to the design of the numerical experiments and the interpretation of the model results.

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Discussion paper

Also, there are a number of operational global chemical weather models simulating air quality on a comparable spatial resolution (∼10km). Given the relatively poor performance of the regional model simulations in this study, it isn't clear what advantages can the presented model configurations offer over the existing global air quality forecast models. Therefore, the paper cannot be published in the present form due to the shortcomings that are discussed below. I encourage the authors to substantially improve the quality of the model simulations and analysis of the results for future publications.

Model configuration: The lines 185-187 are confusing. Was the model simulated without reinitialization for a time period of a month? Since meteorological data assimilation or nudging isn't used here, monthly reinitialization would lead to a strong deviation of the model from the real weather.

I find the discussion of the meteorological evaluation insufficient. According to Table 1, the mean bias for the relative humidity is about -36%. This is a huge underestimate of the humidity, which also indicates that the model wasn't able to capture the fog events. For instance, this is necessary to simulate the sulfate formation in the cloud phase. Figure 6 shows that all the simulation cases overestimate the SO2 mixing ratios. On the other hand, the sulfate concentrations are underestimated at the Delhi airport site, indicating insufficient SO2 to sulfate production in the model.

Moreover, the RMSE for the RH and T2 are too high, while the correlations for all the meteorological parameters are very poor ($R^2 < 0.1$). Another impact of the poor meteorological simulations is the simulated fluxes of the biogenic VOCs. The VOC simulations aren't evaluated here, so it's hard to make firm conclusions.

The caption of Table 1 says "planetary boundary layer height", but there aren't any statistics provided for the PBLH in the Table. I assume the model overestimates the mixing height for the wintertime period presented here.

Anthropogenic emissions: Another weakness of the study is the lack of the diurnal cycle of the anthropogenic emissions ingested into the model. For a megapolis like Delhi,

the hourly variability of the anthropogenic emissions (especially the on-road component) is extremely important. The authors evaluate the simulated hourly PM2.5 mass concentrations by comparing them against the PM2.5 measurements. However, the ingested anthropogenic emissions don't have any hourly variability. While I understand that the EDGAR/HTAP emissions don't provide information about the hourly variability of the emissions, the authors could easily impose such variability in the emissions based on the traffic and other bottom-up information.

Another shortcoming of the anthropogenic emissions used in this study is the lack of day-to-day variability, e.g. weekdays vs. weekends. I assume the day-to-day variability of the emissions for Delhi is significant. The lack of both hourly and daily variabilities of the anthropogenic emissions can explain the large biases for most of the chemical species reported in the paper.

I assume all the anthropogenic emissions are added to the first model level. Therefore, the emissions from the power plants and other point sources aren't adequately included in the model, especially when the boundary layers are shallow. The implications of this approximation need to be discussed.

Photolysis: It isn't clear which photolysis schemes are used for the MOZART and CB-05 gas chemistry schemes. Some of the differences in the simulations of the secondary chemical species are caused by the differences in the photolysis schemes and also how they handle the cloud and aerosol feedback on the photolysis fluxes. The significant dry bias in the model can have a profound impact on the simulations of the photochemistry in the model.

Aerosol feedback: Aerosol feedback on the meteorology is included in all the model simulations. However, the discussion of such important processes in the model is very limited. It isn't clear how the different feedback processes (direct and indirect) are parameterized in the presented WRF-Chem simulations. Table 1 shows the temperature bias is quite different between the GOCART and the other two more advanced aerosol

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schemes. I assume it's caused by the aerosol direct feedback. It'd greatly help to add a model case that doesn't include the aerosol feedback on the meteorology as a base case. It isn't clear how much the model performance improves by simulating the coupled meteorology-chemistry model over the model case without aerosol feedback. How about the aerosol indirect feedback? Its implications for simulating the fog events and so forth.

Fires: The role of the trash burning emissions in the urban areas are highlighted here. However, the FINN inventory doesn't include those emissions. This isn't discussed in the paper.

Lines 259-262: Are the observed spikes in the PM2.5 concentrations caused by shallow PBLH or an increase in the emissions compared to other days?

AOD evaluations: The dust species are included in the model simulations. There's a serious bug related to the dust AOD calculation code in WRF-Chem, which might explain the AOD underestimation due to the dust aerosols. It's reported in this publication: https://gmd.copernicus.org/preprints/gmd-2020-92/

I suggest adding a discussion about how the AOD is calculated in the model and potential uncertainties associated with this parameterization.

The primary goal of the paper is the selection of the optimal chemical mechanism for the Delhi region. As I noted above by improving the meteorological simulations, anthropogenic emission datasets and other components of the modeling system the air quality forecasting capabilities can be improved significantly regardless of the chemistry mechanism. Second, this study is limited to wintertime. These chemical mechanisms need to be tested for summertime also to select the optimal model configuration of WRF-Chem for the region.

Minor comments:

Include the domain plot with the terrain height.

The name "MADE/SORGAM" is wrong. The SORGAM is a very old secondary organic aerosol scheme, whereas the chemistry scheme used here is based on the newer volatility basis set approach to simulate the SOA formation.

Figure 2-3: It's hard to distinguish different model cases in the time series plots.

Figure 4: What is the maximum MODIS AOD over the domain? It seems the AOD values >1 in some parts of the domain.

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