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Atmospheric Chemistry and Physics Discussions

# *Interactive comment on* "Modeling diurnal variation of surface $PM_{2.5}$ concentration over East China with WRF-Chem: Impacts from boundary layer mixing and anthropogenic emission" *by* Qiuyan Du et al.

**Anonymous Referee #2**

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This study is focused on one of the key uncertainties in modeling and forecasting of air pollution, the parameterization of turbulent mixing of chemical species and its impact on hourly variability of the modeled concentrations of fine particulate matter (PM2.5). The sensitivity of the PM2.5 simulations to the diurnal cycle and vertical distribution of the anthropogenic emissions is analyzed here as well. The modeling study deploys one of the widely used atmospheric chemistry models - WRF-CHEM. A number of WRF-CHEM model simulations are conducted over East China for all the seasons, year of 2018.



Accurate simulation of diurnal variability of the ground level PM2.5 is crucial for air quality forecasting applications. It is great to see that this topic is addressed by such rigorous modeling study. This study deserves a publication, but I have reservations on the interpretation of some of the results and conclusions presented here. I suggest addressing the following comments before a final publication in ACP.

Major comments:

- The authors show that setting a minimum exchange coefficient for chemicals in WRF-CHEM improves the simulation results, especially in winter. Actually the WRF-CHEM model has already included this feature for many years. In the community version of the model the exchange coefficients (ECs) that are used for mixing of the chemical species are modified based on the anthropogenic CO and primary PM2.5 emissions. This simple parameterization isn't perfect, but it was designed to help with the strong accumulation of air pollutants near surface, when the modeled boundary layers are too shallow. Why didn't the authors use the existing parameterization in WRF-CHEM? Instead they set the lower limit of the ECs everywhere in the model grid.

- There are discussions of the mismatch between the diagnosed planetary boundary layer (PBL) heights and ECs in WRF-CHEM. I want to remind that both the YSU and MYNN PBL schemes are non-local schemes. The non-local mixing is omitted in vertical mixing of chemicals as ECs from the PBL schemes are only used in the chemical mixing part of WRF-CHEM. Therefore, the vertical mixing of the chemicals isn't always consistent with the parameterization of PBLs in the WRF part of the model.

- Another uncertainty in the PBL parameterization is that the PBL height is diagnosed differently in the individual PBL schemes of WRF. For consistency I suggest using the same diagnostics (e.g. based on bulk Richardson number) to determine the PBL height from the model cases with the YSU and MYNN schemes.

- The sensitivity of the diurnal variation of the simulated PM2.5 to the model vertical resolution is presented here. The horizontal resolution of the nested model grid is 15km.

This is quite coarse resolution, which makes harder to capture the effects of the urban island effect, inversions in the valleys, cold pool events and so forth. The authors are trying to improve the simulation of the PBL structure by refining the vertical resolution, while the horizontal grid remains the same. This shortcoming of the horizontal model grid needs to be discussed. I suggest moving the sensitivity case with the modified vertical resolution into SI.

- The authors consider the injection height of the anthropogenic emissions from the point sources in the model domain. This is advantageous as in many models (especially most of the global atmospheric chemistry models) all the anthropogenic emissions are released in the first model layer. However, it isn't clear how the injection heights for the emissions in East China are estimated in the study. Do the injection heights vary by weather and/or season? This will have a significant impact on the sulfate simulations, for example.

- 3.1. Why the model results are sampled on 3 hourly intervals, when the observations are available every hour?

- The uncertainties related to simulation of the biogenic VOC emissions aren't discussed in the paper. The modeled fluxes of the BVOC species will vary depending on the PBL scheme and model grid.

- How are the biomass burning emissions vertically distributed in the model? What diurnal cycle is applied to them?

- The importance of accurate SOA simulations during summertime is discussed in the Summary. The simulation of the SOA contribution to the total PM2.5 concentrations can help to capture the daytime maxima of the PM2.5 concentrations in summer. This point has to be made clear in the main text, not in Summary. Why the authors didn't include the simulations with the SOA scheme in the main text?

Minor comments:



Line 140: For WRF and WRF-Chem you can also cite this paper: Powers, J. G., et al. (2017), THE WEATHER RESEARCH AND FORECASTING MODEL Overview, System Efforts, and Future Directions, Bull. Amer. Meteorol. Soc., 98(8), 1717-1737, doi:10.1175/bams-d-15-00308.1.

Throughout the text "s" is omitted in plural words: e.g. lines 386, 399, 419. There are other spelling errors as well.

Line 199: I believe this reference is wrong: Lacono et al.. . .

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