

## Referee #1

We are grateful to Dr. Song for his time reviewing this manuscript, and for the valuable comments. Below we present our detailed responses to Dr. Song's comments with the comments in italic and our response in normal font.

- *Geoscientific Model Development Discussions: "On the simulations of aerosol pH in China using WRF-Chem (v4.0): sensitivities of aerosol pH and its temporal variations in haze episodes". Ruan et al. investigates the aerosol pH simulations in WRF-Chem model focusing on haze episodes in Beijing. Overall, the paper is scientifically sound, clearly written and easy-to-follow. I only have a few minor comments:*

- *Line204: WRF-Chem*

**Response:** Thank you for pointing out this typo. It has been corrected.

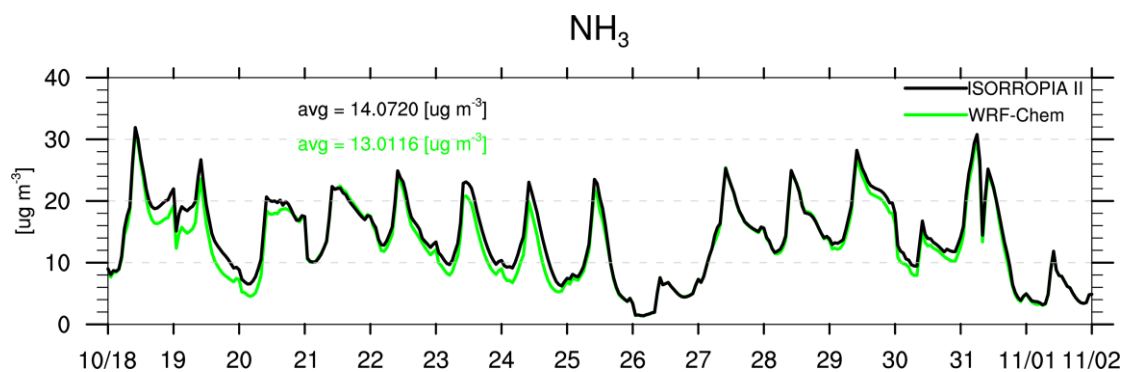
- *Section4.1.1: I think the minimal response to elevated NVCs in the nearly neutral cases may be related to the role of carbonate. At least in E-AIM and ISORROPIA, the aerosol pH cannot get very high (8 or 10) because of the buffer role of carbonate.*

**Response:** We thank the reviewer for pointing out this. In the revised manuscript the role of carbonate was added in the revised text as "[Further, carbonate could play a buffer role in keeping aerosol pH values from getting too high.](#)"

- *Section4.3: It is interesting to see a systematic difference between ISORROPIA and MOSAIC even when the model inputs are the same. The authors list several possible contributing factors including AWC, phase-partitioning method, activity coefficients and solution method. I suggest the authors to investigate this issue further: (1) is there any difference in the predicted gas-phase ammonia concentrations between the two models? This can give some clues on the contribution of phase partitioning method; (2) the authors note the large difference in AWC in the paper. It seems that both ISORROPIA and MOSAIC use the ZSR method. ISORROPIA uses a look-up table for hygroscopic curves of different electrolytes. One possible way to further examine the role of AWC calculation method is to replace the hygroscopic curves in ISORROPIA by the ones from WRF-Chem.*

**Response:** We think these are very good suggestions so we compared the predicted NH<sub>3</sub> concentrations between the two models and the results are shown in Figure R1 as attached. As we can see, there are negligible difference in predicted NH<sub>3</sub>, suggesting that phase-partitioning method may not contribute to the pH difference. Therefore, in the revised manuscript we deleted the statements on phase-partitioning.

Regarding the second point, we agree with the reviewer that it is interesting to investigate the exact factors contributing to the systematic pH difference calculated by the two models. However, it requires substantial efforts to review the details of ISORROPIA code and seems out of scope of this study. In addition, ISORROPIA and MOSAIC differs in many ways and a comprehensive comparison could be the focus of future work. Note in the revised manuscript this section is moved to the supporting material as Text S1 follow the suggestion of reviewer#2 since more comprehensive comparisons between the two models' pH outputs has been done by Pye et al. (2020).



**Figure R1.** Time series of  $\text{NH}_3$  concentrations predicted by WRF-Chem (CTL3meta, green line) and ISORROPIA II (black line) at the surface in Beijing. ISORROPIA II (“forward” mode, assuming metastable) was run with WRF-Chem simulated hourly chemical concentrations along with T and RH.

- *Figure5&6: it is good to show the different subplots in the same vertical scale or write a note to remind the different scales.*

**Response:** Thanks for the suggestion. For Fig. 5, in view of the large differences in y-axis values in different subplots, we kept the different scales and wrote a note as “Different scales are used.” For Fig. 6 (now Fig. 8), we have made the vertical scales the same in each subplots.

## Reference

Pye, H. O. T., Nenes, A., Alexander, B., Ault, A. P., Barth, M. C., Clegg, S. L., Collett, J. L., Fahey, K. M., Hennigan, C. J., Herrmann, H., Kanakidou, M., Kelly, J. T., Ku, I. T., McNeill, V. F., Riemer, N., Schaefer, T., Shi, G. L., Tilgner, A., Walker, J. T., Wang, T., Weber, R., Xing, J., Zaveri, R. A., and Zuend, A.: The acidity of atmospheric particles and clouds, *Atmos. Chem. Phys.*, 20, 4809-4888, <https://doi.org/10.5194/acp-20-4809-2020>, 2020.