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Atmospheric Chemistry and Physics Discussions

Interactive comment on "Simulations of Sulfate-Nitrate-Ammonium (SNA) aerosols during the extreme haze events over Northern China in October 2014" *by* D. Chen et al.

Anonymous Referee #1

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The manuscript by Chen et al. considers factors that may help explain deficiencies in WRF-Chem simulations of secondary inorganic aerosol in extreme haze events in China. Following studies with other models, they consider additional heterogenous reactions, and perform sensitivity studies to evaluate the impacts of these reactions as well as uncertainties in emissions. The topic is timely and of importance / relevance for ACP. The paper is generally well written, despite some grammatical issues. More quantitative comparison could be made to recent papers that have evaluated SO2 and NO2 trends in this region, or that have estimated the contribution of different aerosol precursor emissions to PM2.5 in Beijing. The final model performance is indeed much better, although there is still room for improvement in the model and in our understand-

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Discussion paper

ing of these haze events. I recommend publication following revisions to address the comments below.

Comments:

General: This work seems to still be missing a key reaction, which is aqueous-phase oxidation of S(IV) (the sum of dissolved SO2, HSO3−, and SO32−) by dissolved nitrogen dioxide (NO2) that has been documented in the literature (Lee and Schwartz 1983, Clifton et al 1988, Sarwar et al 2013). As shown in Zhang 2015b, this made a substantial improvement to GEOS-Chem (in ways which would likely similarly improve the WRF-Chem) beyond the heterogenous reactions that are considered here. Thus, I would also suggest the authors include this reaction in their analysis as an additional sensitivity calculations.

3.5: There are several recent papers on SO2 and NO2 trends, for example Krotkov et al., ACP, 2015, see Fig 8, or Cui et al., ACP, 2016. The former would be useful to compare to when considering the SO2 and NO2 emissions trends projected in this paper.

3.11: GEOS-Chem was also used to specifically quantified the role of NH3 in Zhang et al. 2015b.

3.6: Not clear what is meant by “published paper”. Perhaps official report? Or bottom up inventory?

p4/Table 1: What scheme is used for calculating gas-aerosol partitioning of HNO3/NO3 and NH3/NH4?

5.8: One would reach the same conclusion in this particular case, but more rigorously the moles of NH3 should be compared to the moles of 2 x SO2 + NOx.

5.13: Recent Nature Geo paper (McLinden et al., 2016) highlights missing SO2 sources in this (or similar) inventory.

8.20: Could some comparison to other studies / domains / models be referenced here, in terms of substantiating what it to be considered a “reasonable” accuracy for this type of model? At present, that word is used rather loosely.

10.15: Well, that would depend on the NOx/VOC regime, which the authors could easily check from their modeling results.

10.17: This could also instead indicate that SO2 oxidation is too weak / slow in the model.

Section 4: It wasn’t clear to me why the detailed speciated analysis was limited to only a few days. Why was this not performed for the entire month? Were the observations just not available? The peak PM2.5 concentrations earlier in the month, Oct 7 - 10, were the largest of the month, and at a time when RH was well simulated in the model. Seems like this would be a good target to include in the analysis.

11.24: The average magnitude is improved, the the temporal correlation is not likely improved. Can the authors provide a table, or perhaps just write directly on these plots, what the statistics such as Rˆ2 and NMB are for these results?

Fig 7: In terms of comparing the observed to modeled % contributions from sulfate/ammonium/nitrate, it would easier to evaluate visually if the plots were of just these 3 species. At the very least, they could remove CL from the obs, so make a more direct comparison.

12.27: This could be understood more quantitatively by considering results from Zhang 2015b.

General: Did the authors try increasing the RH as a sensitivity test?

Corrections: General: I didn’t type up all of the grammatical corrections; please have Jerome do a final proof-read of the article prior to resubmission.

abstract, last line: situations âĂŤ> concentrations 2.4: exceeding the WHO standard

tenfold 2.15: PM2.5, the formation 3.1: 2014 may not be reflected (or are not reflected) 3.15: WRF-Chem and 3.16: conducted simulations . . . To our best knowledge 3.17: WRF/Chem model. âĂŤ> WRF-Chem. 3.18: using available 3.22: analysis for 3.28: missing comma 3.35: et al., 4.19: nonvolatile, the 5.14: from two other aspects 5.36: fall into 6.8: respectively, 6.17: include equation number, comma goes directly after the equation on the same line, and then “Where” is not capitalized. 6.21: units of surface area per unit volume of air seem incorrect. 7.8: we first 7.10: simulations; we then tested. . .

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