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Atmospheric Chemistry and Physics Discussions

Interactive comment on "High resolution modeling of gaseous methylamines over a polluted region in China: Source-dependent emissions and implications to spatial variations" *by* Jingbo Mao et al.

Anonymous Referee #2

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Gas-phase amines can influence the new particle formation and growth in the atmosphere. Although their concentrations in the ambient air are clearly lower than ammonia they play an important role in the particle formation and growth due to higher reactivity compared ammonia. Largely due to the lower concentrations and higher reactivity they will only affect the processes near the source regions.

Due to lack measurements of amines previously the emissions of amines have been modelled using fixed ratios (FR) between ammonia and amines. This paper presents a simulation study over the Yangtze River Delta Region to produce and test source

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dependent amine-to-ammonia ratios (SDR) in order to improve future model simulations of amines in the atmosphere. The idea is worthy and can produce a significant contribution to the field. However, there several things that need to be improved before publication. In the following I detail the changes by sections that are needed before publication:

Methods

- please state the emission frequency (daily, hourly, more frequent?), what is available in the dataset and what is used in this study.
- Is the emission data available online, and/or how to get it?

- What is the reasoning behind the emission sectors?
- In Zheng et al. (2015) and current study, the times for observations are different, why? I don't see any other than "other industry" sector in Zheng et al. (2015), where are the other emission factors coming? The numbers do not match with Zheng et al. (e.g. 31.8. [C1/NOx]/[NH3/NOx]:0.000076/0.037=0.0021 and current works states 0.0032) or am I missunderstanding something? And please describe the calculation in the text.
- SDR is based on NUIST, but main study on Fudan, why not do two simulations with the finest resolution for both stations?

- Model description must be improved, now the authors only say they follow Yu & Luo (2014), but this is the first time of implementing amine compounds in WRF-Chem, it needs to be explained in detail

Absolutely necessary information:
- What is the particle uptake mechanism for amines?
- What are the oxidation coefficients? and which oxidants?

- other removal mechanisms? wet depostion for example?

Results

- NMBs in Table 4 are not correct, it looks like that they are only bias of the total mean ($\frac{(\overline{C_m}-\overline{C_o})}{\overline{C_o}}$). Correct way to calculate NMB is $\frac{\sum_{i=1}^{N}(C_m-C_o)}{\sum_{i=1}^{N}C_o}$, check Boylan & Russell (2006) for more information. As it is now, it can give a wrong impression of model ability to reproduce observations.

- It would be reasonable to focus on NUIST since the emission (SDR) factors are based on this station, so could you make run with the domain4 also for NUIST
- Please add domain 3 for Fudan in Table 5 also, to facilitate comparing to NUIST site
- Please analyse the discrepancy between model and observations more carefully, now the reasons for discrepancies are vague
- in addition to separating Fudan by agricultural/residential sector, add separation by land/sea also. This would allow evaluating non-pollution sector concentrations.
- The sensitivity test is doubling/halving SDRs only. Can you use the uncertainty from observations to create uncertainty range in SDR and do sensitivity test with max/min range for that, could you do different particle uptake coefficients, this would be interesting. This way we could have an idea to which of the uncertainties are in most urgent need of new research

- Authors refer to short lifetime for amine many times without a reference or calculation of lifetime of amines, please add reference and/or calculation from your model
- Can you compare the particle size distributions with observations to evaluate the particle sink for amine?

Boylan, J.W., Russell, A.G., 2006. PM and light extinction model performance metrics, goals, and criteria for three- dimensional air quality models. Atmospheric Environment 40, 4946-4959.

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