

Interactive comment on "Estimating NH₃ emissions from agricultural fertilizer application in China using the bi-directional CMAQ model coupled to an agro-ecosystem model" by X. Fu et al.

Anonymous Referee #2

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General comments

This manuscript "Estimating NH3 emissions from agricultural fertilizer application in China using the bi-directional CMAQ model coupled to an agro-ecosystem model" applies a recently developed modeling system to estimate NH3 emissions from fertilizer applications in China. The model system consists of three parts: a semi-empirical agroecosystem model, a meso-scale meteorology model, and an air quality model quipped with a bi-directional ammonia flux module. National datasets are used to derive the

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model inputs. This model system is used to estimate ammonia emissions from agricultural fertilizer application in China for 2011. Estimated emissions are compared to other published results. Simulated aerosol nitrate is compared to limited observations at three sites to assess model performance.

Accurate ammonia emissions are crucial for correctly simulating aerosol concentrations and in developing aerosol control strategies using regional air quality models. Developing and evaluating models to estimate ammonia emissions falls within the scope of ACP and is of interest to the readers. However, this manuscript is lacking in two areas. First, there is insufficient observational data available to evaluate the developed model system. Second, the comparison with previously published studies seems tenuous since different years are being compared without some type of normalization. Is one year higher then another simply because more fertilizer was applied? What role do economic factors play in determining amount of fertilizer applied and techniques used? Without some way of normalizing between years, evaluating models by comparing total estimated ammonia emissions for different years is difficult. Similarly, lack of independent observational data to evaluate any of the models, makes it very difficult to conclude any one model better represents the actual ammonia emissions. Obviously, further observations are beyond the scope of this manuscript. However, the authors may consider running this model system using input data from one of the years previously reported to make a more valid comparison on the two models. Nevertheless, the manuscript represents an advancement in modeling agricultural emissions and could be published in ACP after minor changes and more explicitly addressing the need for more thorough model evaluation with observational data.

Methodology and inputs

In section 2.2.2 Soil Information, both the China Soil Scientific Database and the US soil profile data are used. Given the different agricultural practices and history of each country, the authors should address the appropriateness of combine the two databases when calculating soil pH. How does each compare with actually soil pH measurements

in the respective countries?

The terms basal and topdressing fertilizer should be defined and explained in section 2.2.4. What is the differences between the two? For example, is one applied before the other, type of fertilizer used, method of application?

The term bi-directional is not defined or explained anywhere in the text. It should be further explained in section 2.3 and why it could be important to include in estimating ammonia emissions.

Results and Discussion

Two conditions are necessary for the formation of ammonium nitrate particles (NH4NO3). First, there has to be enough gas phase ammonia to partition to the particle phase and neutralize all the sulfate before it can react with nitrate. Second, the partial pressure product of gas phase ammonia and nitric acid has to be sufficient to create thermodynamically favor conditions for NH4NO3 formation. Since the molar ratio of NH3:HNO3 in ammonium nitrate is 1:1, it is not necessarily true that aerosol nitrate is only sensitive to gas phase ammonia. Even in agricultural areas with high ammonia emissions, aerosol nitrate could be low if there is no source of nitric acid. Using CMAQ modeled aerosol nitrate to evaluate the ammonia emissions assumes that CMAQ is correctly modeling gas phase nitric acid. How valid is this assumption? Does CMAQ simulate nitric acid correctly? What is the uncertainty of CMAQ modeled photochemical oxidation products, such as nitric acid? Also, what other aerosol components were measured with the IC system? Was the observed sulfate neutralized? Was there evidence of any other cations indicating the presence of other nitrates in the aerosol? Further and more comprehensive field measurements are necessary to fully evaluate this model system.

The authors pass on including or performing any uncertainty analysis. This is disappointing. While it may be difficult to estimate the uncertainty in some of the model input parameters, what uncertainty analysis has been done for previous CMAQ model stud-

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ies? What is the uncertainty of the bi-directional ammonia flux module? In the end it is difficult for the reader to determine whether the differences between the observations and the two model runs or the differences between the two model runs are significant. From Table 4, it is not clear to me that the coupled modeling system improved the nitrate aerosol simulation at a significant level in all cases. For example, in June the bias in the bidi case is larger than the base case for all three stations.

Specific comments

Page 747, line 4 add "husbandry" or "production" after "livestock"

Page 747, line 20 add space before "Compared" and change "researches" to research

Page 748, lines4 and 5 This sentence is awkward and incorrect. NH3 does not partition to nitric acid.

Page 748, line 12 NH3 was previously defined as ammonia in line.

Page 750, lines 9, 14, 24 change "agriculture" to "agricultural"

Page 750, line 21 remove "36 km"

Page 751, line 2 change "it's" to "it is"

Page 751, line 5 add "section" after "next"

Page 753, line 4 change "accurate" to "accurately"

Page 754, line 3 add space between "Nemitz" and "et"

Page 756, line 19 change "consumption" to "usage"

Figure 2. Add the locations of the nitrate observations to the map.

Figure 3. What does the small insert represent?

Figure 4. Again, what are the small inserts on the left for?

Figure 5. Use month name on the x-axis instead of number

Figure 6. As with Figs. 3 and 4, what is shown in the small insert?

Figure 7. Change the y-axis units to Tg or kg for consistency with other tables. Use the month name on the x-axis.

Figure 8. What are the small inserts for? This is a difficult figure to read because the panels are so small. Consider putting each months map into paper supplemental

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Interactive comment on Atmos. Chem. Phys. Discuss., 15, 745, 2015.