

***Interactive comment on*** “**Evaluation of a regional air-quality model with bi-directional NH<sub>3</sub> exchange coupled to an agro-ecosystem model**” *by*  
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Referee #2 (Comments):

Response to Referee 2:

I greatly appreciate this reviewer’s detailed and constructive comments which have substantially improved the paper. The original reviewers comments are in black and our replies are in blue.

General comments:

1) I have a number of specific comments below, but in general, it is not easy to know

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which parts of this manuscript are describing new developments, and which are repeating material from other papers by this group of authors, for example those of Cooter et al. (2010, 2012) and Walker et al. (2012). The Cooter paper for example also makes use of EPIC, so when this paper says that it is the first study to use an agro-ecosystem model, is it?

Response: This manuscript details the first application of a coupled agro-ecosystem and photochemical air-quality model for continental scale air-quality simulations. This differs from the Cooter et al. (2012) manuscript which details continental scale EPIC model simulations and from Walker et al. (2012) which details the results of a measurement campaign and field scale modeling. This builds upon and expands on the work of both these manuscripts by scaling up the field scale modeling presented in Walker et al. (2012) and coupling CMAQ atmospheric deposition and evasion processes with the soil N geochemistry and nutrient management simulations in Cooter et al. (2012). CMAQ with NH<sub>3</sub> bidirectional exchange only uses the EPIC fertilization estimates and initial soil ammonium content as inputs. Nitrification processes in EPIC have been moved to CMAQ and CMAQ estimated NH<sub>3</sub> deposition and evasion parameterizations have been coupled with the soil ammonium pool to maintain the soil ammonium mass balance in 0.05 m and 1 m soil layers in CMAQ. The sentence beginning on line 13 page 11378 and section 2 have been edited to emphasize this distinction.

1) Also, the writing could be clearer. The authors have a fondness for long sentences, often without the use of commas, and containing more than one subject. The text should be carefully checked, with a view to using clear simple English.

Response: The manuscript was revised for clarity.

Specific comments

1) P.11376, lines 11-14. This paragraph is hard to understand. Clarify.

Response: This paragraph was clarified.

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2) P.11376, line 24. Find a more relevant citation. The Sutton reference does not address health issues in any detail.

Response: A more appropriate reference was found.

3) P.11377, line 7. Here the Sutton reference would fit very well though.

Response: The referee's suggestion was taken.

4) P.11378, lines 1-3. The cited reference (Erisman et al. 2007) cannot logically be used to support a statement, based partly on a 2011 paper, otherwise on two earlier papers that Erisman doesn't cite, that recent changes leave a gap of 30%.

Response: It is not clear what the referee is suggesting. No citation was provided for "a 2011 paper" and Erisman et al. 2007 clearly states; "There is no difference between the measured and modelled trend. . . . However, the absolute systematic difference is still in the order of 30%." in section 5 on page 145.

5) P.11378, line 9. It could be good to give a more recent ref than 1993 also, e.g. Fowler et al., 2009.

Response: The Fowler et al. (2009) reference was added as suggested by the referee.

6) P.11378, line 12. I would say that current AQ models do not generally include a mechanistic description. The study of Wichink-Kruit et al. (2010) did include bi-directional exchange.

Response: Agreed, most air-quality models do not include a mechanistic description of NH<sub>3</sub> bi-directional exchange as stated in the manuscript. The 2010 Wichink-Kruit reference was added as suggested by the referee.

7) P.11378, line 20. plural, alters.

Response: Corrected as suggested by the referee.

8) P.11378, lines 17-21. Long sentence, difficult to follow

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Response: Agreed, this sentence was split and simplified.

8) P.11378, lines 17-21. Long sentence, difficult to follow

Response: Agreed, this sentence was split and simplified.

9) P.11380, Section 2 intro. This text should make it clearer how the current study differs from Cooter et al. (2010) and 2012. The 2010 paper was already using CMAQ, bi-directional exchange, and at least some of EPIC.

Response: Section 2 was edited to distinguish the differences between these complementary papers. Overall this was addressed in the general comments.

10) P.11380, line 23. Which depths do these layers represent?

Response: The depths of the soil layers were added to the Section 2 intro.

11) P.11380, Equation 1. Is the factor  $hm$  really needed? The basic equations should be as simple as possible, and units can as well be per  $m^2$  rather than per ha. If a units term is needed, it is clearer to put it in the numerator than the denominator. Actually why have two denominators in two styles?. (I know Massad had this, but in general it is not good practice. Also the style  $a/bc$  can be misread  $(a/b).c$  or  $a/(b.c)$ , explicit parentheses never harm.

Response: The units of Napp were changed to  $g\ m^{-2}$ , the factor  $hm$  was removed and explicit parentheses were added from equation 1 as suggested by the referee. Note that both Massad et al. 2010 and the unrevised version of this manuscript were missing a conversion factor from kg to g for Napp. This was accounted for in this revision.

12) P.11380, Equation 2. Where is the layer structure in this equation? What happens with diffusion/transport between layers? This looks like the equation for a single layer model to me.

Response: Ammonium is readily absorbed onto soil cation exchange complex and should be immobile, thus infiltration of ammonium is not modeled (Sutton et al., 2011).

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Evasion of  $\text{NH}_3$  from the soil  $\text{NH}_x$  pool in CMAQ is modeled in parallel from both soil pools. This assumes that the rate of gaseous diffusion between soil layers is negligible compared to the evasive and nitrification losses of ammonium from the soil pool. The description of equation two has been edited to clarify this assumption.

13) P.11381, Section 2.2. Again, it is not obvious how much of this is new.

Response: This is the initial application of a two layer compensation point model with a dynamic soil ammonium pool on the regional scale as previously addressed in the referee's general comments. Equations 3 and 4 can be found in the companion papers by Cooter et al. and Walker et al. However, they are part of the methods section in this manuscript and necessary to understand what algorithms were incorporated into a regional scale model.

14) Eqn. (3). Why is the canopy compensation point physically located at 0.5 hc? This is below the aerodynamic displacement height, so not entirely obvious for a big-leaf approach. Between which points is  $R_a$  calculated?

Response: The in-canopy  $\text{NH}_3$  concentration gradient is not constant and  $\text{NH}_3$  can be exchanged between in-canopy air and vegetation surfaces along this gradient (Bash et al. 2010).  $R_{inc}$  was split so that half of the resistance was applied between the soil and canopy compensation point and the other half is applied between the canopy compensation point and the atmosphere above in order to reconcile this with the resistance model framework. Since the fluxes can come from above or below the canopy in a bi-directional model, splitting the in-canopy resistance seems appropriate. Requiring the ground flux to pass through the entire canopy before it can encounter the leaves does not seem reasonable. This is not necessarily 0.5 hc and the manuscript was edited to reflect this.  $R_a$  is estimated for the first model layer which is typically configured to be from the top of the canopy to a height of  $\sim 20\text{m}$  to  $\sim 36\text{m}$ .

15) P.11381, line 12. Again, unnecessary complications with units. Why is  $V_m$  needed? There is nothing in this equation containing liters, and the authors have any-

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way switched units compared to those used by Nemitz et al. (2001). The switch of the meaning of  $\chi$  from volume mixing ratio in previous papers (e.g. Nemitz et al, and even the companion Walker et al. 2012) to the mass concentration used here is also confusing. I would suggest that the authors find a different symbol for the mass-concentrations (C perhaps). Or just re-write in the same units as normally used.

Response: Nemitz et al., (2001) clearly states that all concentrations are in mol l<sup>-1</sup> in equation 7. Mn and Vm were simply added to give the reader a consistent set of units for all the equations in the manuscript.  $\chi$  has been change to C as suggested by the referee to avoid any confusion regarding units.

16) P.11381, line 17. What is a "cropping practice".

Response: This sentence was clarified by changing "agricultural cropping practice" was changed to "fertilizer application due to agricultural management practices".

17) P.11383, Why run such an old year as 2002? Surely the quality and quantity of data has increased since then?

Response: 2002 is a standard evaluation year for CMAQ simulations with numerous sensitivity runs available to help judge the effect and magnitude of the changes introduced with the bi-directional ammonia. WRF meteorology and CMAQ were updated to use 2001 NLCD land use data for 2002 and a complete set of updates to the meteorology using 2006 NLCD for 2006 and later years is not yet available. The NLCD updates are important to a correct delineation of the land area with crops. Importantly, 2002 is the only year currently available with continental US simulations of EPIC fertilizer applications and consistency in year was important to track the effect of EPIC improvements through the development process. Updating the EPIC information to estimate fertilizer application in more recent years is in process and not yet available. There are relatively dense observations for NH<sub>x</sub> wet deposition (N = 243 sites) and nitrate aerosol (N = 364 sites) and the number and quality of these monitoring sites has remained constant over the last couple of decades. Routine network observations of

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ambient ammonia did not begin until 2009, however a fully vetted emissions inventory is not yet available for 2009 and updated meteorology for 2009 with the latest land use information is not yet available.

18) P.11383, line 21. Use SI units.?

Response: The pressure in mb was converted to Pa as suggested by the referee.

19) P.11384, Eqn. (9). Doesn't this bias-adjustment lead to a mass error, since the scaling of deposition fields is done after the model runs are finished? How large were these bias-correction factors, and what were their seasonal variations?

Response: Model precipitation biases will introduce errors in the amount of NH<sub>x</sub> scrubbed from the atmosphere. If we assume that the errors in the precipitation and the wet deposition are linear, then we can correct for precipitation biases in wet deposition. The mass bias introduced by predicted precipitation biases will require improvements in modeled precipitation through inverse modeling or improved algorithms to correct. The magnitude and seasonality of these corrections were added to section 3.2.

20) P.11384, the bias correction of rainfall from WRF is obviously important to this manuscript, and some discussion appears later, but the lines around Eqn. (9) give too little information.

Response: The explanation of the equation 9 was revised and more discussion regarding this correction was added to section 3.2.

21) P.11385, Section 3.1: a Table would help to summarize all the percentage changes discussed here, then the number of significant digits could be reduced in the text. (I get nervous with modelers who can predict changes to 3 significant digits.) Also, since almost no information has been given on the extent of the bias correction (e.g. "may be too high" is a little vague), it is not possible to really understand these paragraphs. This paragraph doesn't read very well anyway. Emissions are for example 'too high' or 'lower', and I can infer that they mean with respect to the base-case, but it should be

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clear.

Response: A table of the domain wide emissions and the change in emissions has been added. Changes in the modeled deposition and emissions are now reported to two significant digits. More information regarding likely errors in the seasonal adjustments in the NEI emissions has been added. The paragraph has also been edited for clarity.

22) P.11386., line 3 biased high or low?

Response: This is a change in the model total N (wet + dry) deposition due to the use of the bi-directional exchange option in CMAQ. A network of total N deposition observations does not exist to evaluate the bias in these model results.

23) P.11387, Sect. 3.3. Are these discussions about total nitrate aerosol, or fine mode? (How important is coarse mode nitrate in these simulations?)

Response: The equipment used in STN and IMPROVE observations have an effective particle size cutoff of 2.5  $\mu\text{m}$ . Thus, modeled PM<sub>2.5</sub> concentrations were used in the NO<sub>3</sub>- aerosol evaluation. The first paragraph of section 3.3 was edited to state this. Modeled coarse PM concentrations were 2% higher in the bi-directional model and the mean coarse mode concentrations were approximately 40% lower than the PM<sub>2.5</sub> concentrations. However, there are not routine observations of coarse PM in the CONUS domain to evaluate the model results.

24) P.11387, Sect. 3.3. The discussion of nitrate biases pre-supposes that the model should get the ammonium-nitrate equilibrium right. There are some recent papers which suggest that the partitioning coefficient used in models is likely different to that found in observations (e.g. Aan de Brugh et al., 2012). How do such considerations affect your discussions?

Response: Recently Aan de Brugh et al (2012) recommended modeling the equilibrium partitioning of nitrate in coarse resolution models by calculating the partitioning using

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the temperature and relative humidity from model layers at a higher altitude to account for observed discrepancies between vertical HNO<sub>3</sub> and PM<sub>10</sub> NO<sub>3</sub> profiles and the equilibrium partitioning coefficient. The application of this correction to account for the dynamics of partitioning to the coarse mode would not likely result in significant changes in the nitrate aerosol estimates because CMAQ does not assume equilibrium partitioning in the coarse mode and models the dynamic transfer of HNO<sub>3</sub>, H<sub>2</sub>SO<sub>4</sub>, HCl and NH<sub>3</sub> between the coarse particle and aerosol phase (Kelly et al., 2010).

25) P.11390, line 1. No need to use the word successfully. Presumably there would not be a paper in any other case.

Response: The reviewer's suggestion was taken.

26) P.11390, why is the last line giving conclusions from another paper. The conclusions should be from this paper, or at least explain why another paper is referred to.

Response: The last sentence of the manuscript was rewritten.

27) Figures: the map-plots should be larger (2 per page), as the contents of the bullets are difficult to see. (Maybe it would be worth zooming in on some interesting areas?)

Response: Two panel high resolution maps were made for all the map plots.

27) Fig. 5. I didn't find this plot very useful, most of the points are buried in the bottom corner, and curved regression lines don't help. Re-plot as log-log, so we can see the full range of concentration changes better.

Response: Fig. 5 was re-plotted using a log-log scale.

References:

Kelly, J.T., Bhave, P.V., Nolte, C.G., Shankar, U., Foley, K.M, Simulating emission and chemical evolution of coarse sea-salt particles in the Community Multiscale Air Quality (CMAQ) model, Geoscientific Model Dev., 2010, 1, 257-273

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