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Interactive comment on "Modeling the Diurnal Variability of Agricultural Ammonia in Bakersfield, California during CalNex" *by* C. R. Lonsdale et al.

Anonymous Referee #1

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General comments: The authors present a NH3 modelling study based on a variety of ammonia measurements (surface, flight, satellite) performed during the CalNex measurement campaign. The focus lies on determining possible causes for the discrepancies in the diurnal variation between the modelled and observed concentrations. The paper further describes a few possible adjustments by applying a more representative temporal allocation of the NH3 emissions and the application of a bi-directional NH3 flux scheme.

An interesting study is presented, comparing modelled concentrations with NH3 observations covering a range of the vertical and spatial distribution of ammonia concentrations. Potentially this could be a really useful and informative publication, as almost no model studies using this range of observations are available, but some work will be needed to improve it before final publication.

In particular, I found that with the wealth of data and observations available more could be done, specifically on the presentation of the results and a systematic (final) discussion which is more or less missing. The setup of the paper is done rather well, describing the observations used as well as the applied models etc. The results & discussion/conclusion section however will need some work. As an example the last section feels a bit rushed. In the first paragraph of the results the comparison is described in a systematic fashion, while for the final version of the model only a short description is given, lacking any final conclusions, which leaves the reader without any sense of improvement/idea that the final version of the model improved much but the bias(a bit).

Specific comments:

I am missing an overall figure with the observed and modelled concentrations for the Bakersfield concentrations. The authors do show the diurnal cycles and a boxplot for the individual hours but this does not give a feel of the possible events and variability between the days which can occur during the measurement interval. A simple plot with the time series would bring some clarity. One could also add the observed TES observations as a second Y-axis. Another idea would be to add temperature/wind speeds to explain the variation of the concentrations(as emissions from fields for example are related to both).

2. On the measurements itself: Surface: If the instruments used have an inlet with some piping etc, this could cause artifacts in the observed NH3 concentrations in the early morning. Some words on this and other possible artifacts would be helpful.

Only seven days of the observations are used and compared with the model, is this the entire measurement period? If not why are only 7 days of the measurements used?

Satellite: I am not convinced by the model vs satellite comparison. Especially the comparison for the observations near Bakersfield look rather poor. Some words on the quality of the TES data? Also by using the RVMR on has to know for certain the vertical

is described well in the model. The RVMR is only 20%-60% of the surface value, and depending on the NH3 profile doesn't have to be in relation to the surface. Some words on any effects caused by the RVMR and maybe a comparison on the profile of TES and the model? Similar to the study by shephard et al?: Shephard, M. W., McLinden, C. A., Cady-Pereira, K. E., Luo, M., Moussa, S. G., Leithead, A., Liggio, J., Staebler, R. M., Akingunola, A., Makar, P., Lehr, P., Zhang, J., Henze, D. K., Millet, D. B., Bash, J. O., Zhu, L., Wells, K. C., Capps, S. L., Chaliyakunnel, S., Gordon, M., Hayden, K., Brook, J. R., Wolde, M., and Li, S.-M.: Tropospheric Emission Spectrometer (TES) satellite observations of ammonia, methanol, formic acid, and carbon monoxide over the Canadian oil sands: validation and model evaluation, Atmos. Meas. Tech., 8, 5189-5211, doi:10.5194/amt-8-5189-2015, 2015.

Also the observed concentrations near Bakersfield seem to be quite low at time. Any effects due to the sensitivity/retrieval of TES for these low retrieved concentrations? You could add a figure with the observed and modelled profiles and the AVK of the satellite observations to show the difference in the vertical (and yes the DOF are low but the profiles are still used for the RVMR). Aircraft observations: Possible artifacts? Include the uncertainties in the discussion of the results / conclusions.

2. Model: Some discussion on performance of the model for the vertical distribution of NH3 would be helpful. Also include some words on the performance for species like HNO3 and sulfates as these are probably causes for any discrepancies in the diurnal cycle.

2.3. PBL: Figure 7. shows the performance of the WRF PBL when compared to the HSRL observations. The authors conclude that the deviations are not a probably cause for any faults in the diurnal cycle of NH3. I do not agree with this conclusion. From the plot one can conclude that for small PBL heights there are large deviations up to a factor 2 when compared to the modelled WRF PBL. You can convince me by showing a figure of the diurnal cycle of the PBL for both HSRL and WRF? And/or the normalized version of the cycle? By adding a diurnal cycle figure you also strengthen

C3

any comments and conclusions in the paper that the errors in the PBL have no effect.

2.x Emissions: Can you add a table or a short paragraph on the emissions sources and their relative totals?

3.3 Hysplit, I think this section can be removed as in the remainder of the paper only 3 sentences are dedicated to the results.

4. Results: A bit of extra structure and discussion in the results will greatly improve the manuscript. The authors have a wealth of data available but only scarcely use it. The flight data is only used for the basic version of the model, and not discussed in the latter parts of the manuscript, while the variation in the emissions will also affect the vertical distribution of the NH3 concentrations. The systematic discussion of possible causes for the discrepancies between the modelled and measured concentrations as given in 4.2 should be added for the other versions of the model. Each version should rule out one or more of the possible causes, which will add to the overall discussion of the state of the model (and not just this model, but the overall performance of most CTMs). Adding a table with the airborne observations vs each of the modelled versions would help.

Table 2. add some correlations and statistics similar to table 1. A figure or table in which you split the statistics per hour of the day will give some further insight on the performance of the model for each part of the day. Partially this is done already in figure 4, but some correlations / bias plot could be added for more information. In this figure/table one can then easily point out the improvements in the later model versions similar to figure 8.

5. Conclusion / Discussion:

I am missing a final discussion on how one would improve the model in the future or what kind of measurements would be needed (does not have to be long). A few points for a start of the overall discussion and state of CMAQ/NH3 modelling (bit broad):

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- What kind of measurements would the authors perform to further understand the model and reasons for discrepancies between modelled and observed concentrations
- Discuss point by point what this study improved, for now I can only see a small improvement to the bias. - -

Final words:

I recommend rewriting some parts of the manuscript following a few of the stated highlights to improve the overall quality of the paper. When rewritten this paper can be a great start for future model (improvement) studies.

C5