September 30, 2013

MEMORANDUM

To: Tom Moore, Western Governors' Association (WGA) (WRAP)

From: Zac Adelman, University of North Carolina/Institute for the Environment
Ralph Morris, ENVIRON International Corporation

Subject: Lessons learned from the WestJumpAQMS and the next steps to improve ammonia emissions estimates in the Western U.S.

INTRODUCTION

ENVIRON International Corporation (ENVIRON), Alpine Geophysics, LLC (Alpine) and the University of North Carolina (UNC) at Chapel Hill Institute for Environment are performing the West-wide Jump Start Air Quality Modeling Study (WestJumpAQMS[1]) managed by the Western Governors' Association (WGA) Air Quality Program. WestJumpAQMS has set up the CAMx photochemical grid model for the 2008 calendar year (plus spin up days for the end of December 2007) on a 36 km CONUS, 12 km WESTUS and several 4 km Inter-Mountain West domains. The WestJumpAQMS Team compiled emissions to be used for the 2008 base case modeling, with the 2008 National Emissions Inventory (NEI) being a major data source. During this process, the WestJumpAQMS team prepared sixteen Technical Memorandums discussing the sources of the 2008 emissions by major source sector. In Memorandum #8, we described the data and modeling approaches used to estimate agricultural ammonia (NH_3) emissions for the WestJumpAQMS[2].

WestJumpAQMS 2008 Ammonia Emissions

Figure 1 displays the annual ammonia emissions by source category for the U.S. 2008 ammonia emissions developed by the WestJumpAQMS. Livestock (58%) and fertilizer (28%) are by far the two biggest source categories making up 86% of the U.S. ammonia emissions. The next largest source category is fires at 5% that is dominated by wildfires that were developed by the DEASCO3[3] project. Although wildfire ammonia emissions rates are uncertain, the locations and temporal variations of the emissions are fairly well characterized. Other area sources (4%) and on-road mobile sources (3%), whose emissions are based on the MOVES model, are the next two largest source categories. Given that livestock and fertilizer application dominate the ammonia emissions

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[1] http://www.wrapair2.org/WestJumpAQMS.aspx
[2] http://www.wrapair2.org/pdf/Memo8_AmmoniaSources_Feb28_2013review_draft.pdf
[3] http://wrapfets.org/deasco3.cfm

inventory, focusing on these two source categories offer the greatest opportunity for improving ammonia emissions for modeling.

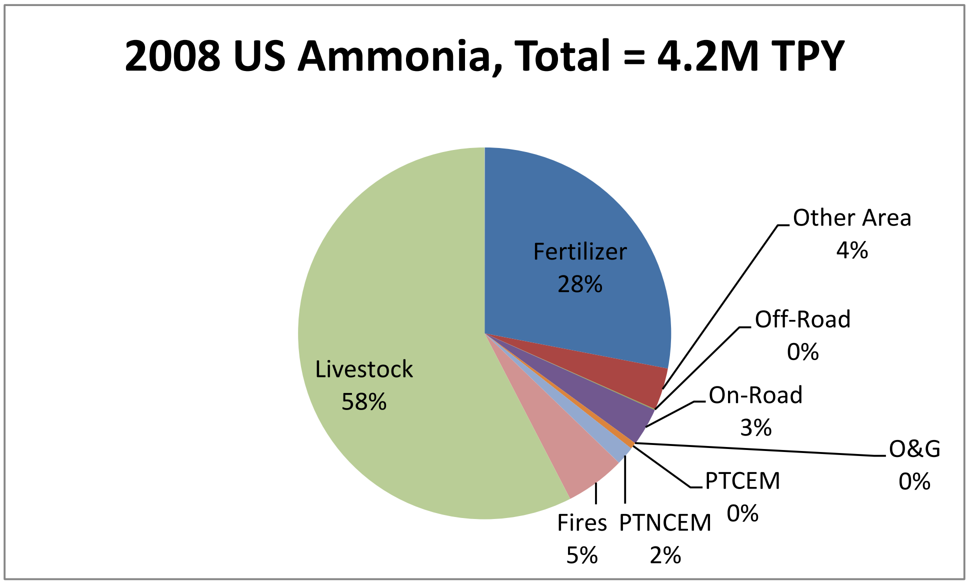

Figure 1. 2008 U.S. ammonia emissions by source category from the WestJumpAQMS.

Purpose

In this memo we discuss the key lessons learned during the collection, preparation, and modeling of the NH_3 data described in Memorandum #8. We highlight the strengths and weaknesses of the data that we used for the WestJumpAQMS and present recommendations for how we can improve the simulation of NH_3 emissions in subsequent modeling studies.

APPROACH

The six major components for simulating NH_3 emissions include:

- Emissions model – a software system that includes algorithms for estimating NH_3 emissions and a framework for input and output of the emissions data
- Emissions factors – estimates of the mass of NH_3 emitted per unit time per animal or amount of nitrogen volatilized as NH_3 per unit time for different types of fertilizer
- Activity – animal population; the number of animals emitting NH_3 per administrative unit (i.e. state or county) or monthly county-level fertilizer consumption
- Spatial allocation – process to convert administrative unit NH_3 emissions estimates to model grid cell estimates
- Temporal allocation – process to convert annual or monthly NH_3 emissions estimates to hourly estimates for input to air quality models

- Air quality model – a software system that combines meteorology, emissions, transport, and chemistry to simulate the sources, transport, and fate of air pollutants in the troposphere

We reviewed each of these components during the WestJumpAQMS project and developed a list of recommendations for each component. The starting point of our review was the release of the Final Ammonia Emissions Technical Memo #8 on February 28, 2013. We convened an NH_3 emissions working group and held calls on April 24, April 29, and May 17, 2013 to review Memo #8 and come up with our list of recommendations. The NH_3 emissions working group included the following people:

- Michael Barna, NPS
- Lisa Clarke, CO APCD
- Curt Taipale, CO APCD
- Daniel Bon, CO APCD
- Kevin Briggs, CO APCD
- Dale Wells, CO APCD
- Jay Ham, Colorado State University
- Tammy Thompson, Colorado State University
- Zac Adelman, University of North Carolina
- Ralph Morris, ENVIRON Intl. Corp.
- Jim Wilkinson, Alpine Geophysics
- Tom Moore, WRAP/WGA

REVIEW AND RECOMMENDATIONS

Results of the WestJumpAQMS NH_3 emissions working group review and recommendations are included below. Table 1 summarizes these results.

Emissions Model

The Carnegie Mellon University (CMU) NH_3 model is sufficient for estimating emissions from agricultural sources of NH_3. It provides a technically sound framework for integrating the parameters for the basic emissions equation used for a bottom-up inventory of county-level agricultural NH_3 sources. The major constraint in the CMU model is the reliability of the input data.

Current air quality modeling research is investigating a bi-directional exchange of NH_3 between the atmosphere and the land surface. The re-emission of surface NH_3 is a missing source that we did not account for in the WestJumpAQMS.

Recommendation: Investigate adding a bi-directional NH_3 exchange model in subsequent modeling studies.

Emissions Factors

As one of the two parameters of the emissions equation, the quality of the emissions factors (EFs) is critical for building reliable estimates of NH_3 emissions. The CMU model supports the application of county-specific EFs by animal type or fertilizer. In cases where county-specific EFs are not available, the model defaults to state or national EFs.

Recommendation: Convene a working group within the WRAP for western states and other agencies to compile updated county-specific EFs. Determine the western states/counties that are receiving default EFs in the CMU model. Compare the EFs currently available in the CMU model (version 3.6) and update them with any new data available from the western states.

Activity

Activity for livestock NH_3 emissions sources refers to county animal populations for different types of livestock. For fertilizer NH_3, activity refers to county-level consumption. As one of the two parameters of the emissions equation, the accuracy of the activity values input to the CMU model are also critical for building reliable NH_3 inventories. The NH_3 inventories used for the WestJumpAQMS came from the NEI08v2. In general, the CMU model simulations for the NEI08v2 used county animal populations from the 2007 Census of Agriculture and fertilizer consumption from the Fertilizer Institute's Commercial Fertilizers 2002 and 2007 reports.

Recommendation: Convene a working group within the WRAP for western states to compile updated county animal populations and fertilizer consumptions for 2008 and 2011. Compare the 2007 activities used for the NEI08v2 with values provided by the states and update the CMU model inputs using the data provided by the western states. If new data are not available from all western states, update the CMU model inputs using 2008 and 2011 Census of Agriculture and Fertilizer Institute Commercial Fertilizer estimates.

Spatial Allocation

County agricultural NH_3 inventories are distributed to model grid cells using spatial surrogates. Spatial surrogates are developed from GIS Shapefiles of agricultural land use categories. For the WestJumpAQMS we used 2002 National Land Cover Database (NCLD) estimates of total agricultural land to allocation both livestock and fertilizer sources to the modeling grid. Better information about the location of agricultural activity is needed to improve the distribution of the county inventories to the model grid cells.

The spatial allocation of livestock sources can be improved through the collection of data on the locations of confined animal feeding operations (CAFOs) within each WRAP state. Latitude/longitude coordinates and the number and types of animals at CAFOs can be used to develop spatial surrogates for distributing the county emissions inventories to a modeling grid. The following CAFO data are required for developing spatial surrogates for livestock sources:

- Latitude
- Longitude
- Current number of animals by species
- Maximum operating capacity (maximum number of animals)

We used CAFO location information in the WestJumpAQMS to develop a surrogate for livestock sources in Colorado. These data were not available for any of the other WRAP states during the WestJumpAQMS.

The spatial allocation of fertilizer sources can be improved with data on the locations of fertilizer application within each WRAP state. Ideally GIS Shapefiles of the application locations for different fertilizer types would allow us to map county fertilizer inventories to the actual application locations. Alternatively, Shapefiles with the locations of field crops and orchards could be used to improve the spatial distribution of fertilizer sources.

Recommendation: Convene a working group within the WRAP for western states to collect CAFO and fertilizer application locations for the years 2008 and 2011. Use these data to develop state-specific spatial surrogates for mapping county agricultural NH_3 inventories to modeling grids.

Temporal Allocation

Under contract with EPA in 2009, ENVIRON reviewed the recent literature regarding approaches and data available for the temporal allocation of livestock and fertilizer NH_3 emissions for the purpose of determining the state of the science for temporal allocation of NH_3 emissions for use in regional-scale air quality modeling. They concluded that the process-based modeling methods of Pinder et al. (2006)[4] and Goebes et al. (2003)[5] and the inverse modeling technique of Gilliland et al. (2006)[6] represent the state-of-the-science with respect to the seasonal and monthly temporal allocation of agricultural NH_3 emissions. We used these monthly data and approaches for the WestJumpAQMS.

Recent work to integrate the influence of meteorology on agricultural NH_3 emissions presents an improved approach to simulate the hourly temporal variability from livestock sources. The SMOKE emissions model includes two algorithms to generate

4 Pinder, R. W., P. J. Adams, S. N. Pandis, and A. B. Gilliland (2006). Temporally resolved ammonia emission inventories: Current estimates, evaluation tools, and measurement needs, J. Geophys. Res., 111, D16310, doi:10.1029/2005JD006603

5 Goebes, M. D., R. Strader, et al. (2003). "An ammonia emission inventory for fertilizer application in the United States." Atmospheric Environment 37(18): 2539-2550

6 Gilliland, A., K., K.Appel, R.W. Pinder, and R.L. Dennis, 2006. Seasonal NH3 emissions for the continental United States: inverse model estimation and evaluation. Atmospheric Environment, 40, pp. 4986-4998

hourly, meteorology-based temporal variability from livestock sources. We did not use meteorology-based temporal allocation in the WestJumpAQMS.

Recommendation: Use the meteorology-based temporal allocation algorithms to estimate hourly temporal variability for livestock NH_3 sources.

Air Quality Model

Air quality modeling simulates the fate and transport of the NH_3 emissions and produces results that can be compared against observations of ambient NH_3 concentrations. For the WestJumpAQMS project we used CAMx to simulate NH_3 concentrations over 36-km, 12-km, and 4-km modeling domains focused on the intermountain-West. Previous modeling studies of the Rocky Mountain region indicate that NH_3 concentrations are underestimated in air quality models and that the diurnal patterns of the NH_3 predictions are anticorrelated with hourly NH_3 observations[7]. The major issues in the air quality model performance for NH_3 include:

- Measured NH_3 peaks during the day contrasting with simulated NH_3 peaks at night
- Overestimation of NH_3 dry deposition
- Underestimation of NH_3 concentrations
- Poor skill in predicting NH_3 invalidates the models for conducting source apportionment studies of NH_3

While comprehensive evaluation of the NH_3 results in the WestJumpAQMS modeling are not yet available, diagnosis of the cause of the poor performance of the air quality models in predicting NH_3 concentrations should be a focus area of subsequent modeling studies. A preliminary analysis of the CAMx model performance suggest that the summer particulate NO3 underestimation may be due to too low NH3 concentrations since total NO3 (NO3+HNO3) performance is much better and wet NH4 deposition is also underestimated. However, whether such NH3 underestimation is due to too low NH3 emissions and/or too high NH3 dry deposition rate could not be determined.

Recommendation: Conduct diagnostic modeling to determine the weaknesses in the ability of air quality models to predict NH_3 concentrations at sites in the intermountain West. Implement improvements to the emissions processing of NH_3 sources and in the air quality modeling of these sources to improve model performance. The implementation of a bi-directional ammonia flux in CAMx, as is done in CMAQ, is also recommended.

[7] Rodriguez, et al., Modeling the fate of atmospheric reduced nitrogen during the Rocky Mountain Atmospheric Nitrogen and Sulfur Study (RoMANS): Performance evaluation and diagnosis using integrated processes rate analysis, *Atm Env* 45(1), 2011, pp. 223-234,

Additional Monitoring and Emissions Data Needed

There is very little monitoring data collected related to ammonia. Outside of routine CSN 24-hour ammonium (NH4) measurements and weekly NADP wet NH4 deposition, most of the ammonia-related measurements have been limited to special field studies. More recently starting in 2011 the AMoN ammonia network has been expanded to include approximately 50 sites across the U.S.[8] AMoN measures two-week ammonia concentrations, so has limited temporal and spatial coverage. But is an improvement over past data availability. Additional ammonia and ammonia-related measurements are needed to more fully evaluate the emission inventories and air quality models. The diurnal variation in ammonia concentrations is important and it is important to have complete information on ammonia and ammonium, as well as NO3 and HNO3 in order to understand the reduced and reactive nitrogen cycle. Addition data on emissions factors and spatial and temporal variability in ammonia emissions is also needed.

[8] http://nadp.isws.illinois.edu/AMoN/

Table 1. Summary of WestJumpAQMS NH_3 emissions modeling components review

Parameter	WestJump Modeling	Evaluation Activities	Recommendation
Emissions Model	CMU model version 3.6 outputs from EPA (NEI2008v1)	Reviewed EPA technical support document	Run the CMU model for WRAP states using updated emissions factors and activities for modeling year; investigate bi-directional flux model
Emissions Factors	Animal-specific County, state, or national level factors from the CMU model version 3.6 (ca. 2002)	Reviewed EPA technical support document	Literature review for updated emissions factors and coordinate with state agriculture divisions for county or state specific factors; use these factors as input to the CMU model
Activity (animal population)	County-level 2007 animal population from Census of Ag.	Reviewed EPA technical support document	Coordinate with state agriculture divisions to receive updated animal numbers by county; use these as input to the CMU model
Spatial Allocation	Total agricultural surrogate from the 2002 NLCD maps county to grid cell; updates for CO CAFOs based on state-provided permits	Qualitative evaluation of emissions locations at large CAFOs in Colorado and Wyoming performed for the 3-State Air Quality Study; RoMANS showed improved NH3 performance following update to CO CAFO locations	Collect state water quality division permitting data for large CAFOs and convert these data into spatial surrogates; collect fertilizer application data from the states and convert these data into spatial surrogates
Temporal Allocation	EPA NEI state-specific monthly profiles based on inverse NH3 modeling	Literature review by ENVIRON for EPA and review of meteorology-based algorithms	Implement meteorology-dependent hourly variability
Air Quality Model	CAMx simulations at 36-km, 12-km, and 4-km grid resolution focused on the intermountain-West	Comprehensive model performance evaluation against surface monitors of meteorology and chemical observations	Conduct detailed evaluation of NH_3 predictions from air quality models to diagnose the cause and improve poor model performance