Development of an Agricultural Fertilizer Modeling System for Bi-directional Ammonia Fluxes in the Community Multiscale Air Quality (CMAQ) Model

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Abstract Atmospheric ammonia (NH_3) plays an important role in fine-mode aerosol formation. Accurate estimates of ammonia from both human and natural emissions can reduce uncertainties in air quality modeling. The majority of ammonia anthropogenic emissions come from the agricultural practices, such as animal operations and fertilizer applications. The current emission estimates at the U.S. Environmental Protection Agency (U.S. EPA) are based on the annual National Emission Inventory (NEI). However, accurate estimation of ammonia emissions in space and time has been a challenge. For instance, fertilizer applications vary in the date of application and amount by crop types and geographical area. With the support of the U.S EPA, we have responded by an agricultural fertilizer modeling system for use with a newly developed ammonia bi-directional flux algorithm in the CMAQ model. This modeling system will simulate NH_3 emissions from fertilizer applications on agricultural lands rather than from emission estimates based on pre-defined emission factors. The goal for this paper is to demonstrate how this agricultural fertilizer modeling system is developed for a continental U.S. CMAQ 12-km modeling domain and the tools we developed in this system.

1. Introduction

Human activities have significantly altered the nitrogen cycle (Galloway et al., 2004). The majority of ammonia anthropogenic emissions come from agricultural

practices, about 51% from animal husbandry and about 28% from agricultural fertilizer applications based on the 2002 NEI. Atmospheric ammonia (NH_3) is a precursor for ammonium nitrate, ammonium sulfate, and ammonium bisulfate aerosol formation. Nitrogen aerosols have significant and deleterious impacts on human health (e.g. Wolfe and Patz, 2002). In addition, deposition of excess N in the form of ammonia and ammonium can have serious impacts on aquatic and terrestrial ecosystems (e.g. Smith et al., 1998; Lovett et al., 2009). Therefore, accurately estimating ammonia from both anthropogenic and biogenic emissions is important not only for air quality studies but also for ecosystem N deposition impact assessments. Currently, NH_3 emissions from fertilizer applications are estimated using the Carnegie Mellon University (CMU) Ammonia Model version 3.6 which relies on county-level fertilizer sales data or estimates Application timing is based on state-level climatological averages that are constant in time. Fertilizer applications are distributed monthly to agriculture land area estimated from satellite land cover data representing the early 1990's. Emissions are then estimated as a function of these estimates and a set of fixed emission factors. Thus, current methods do not account for more recent land use changes or variations in the dates and amounts of fertilizer applications by crop types and geographical area.

The study by Cooter et al. (2010) demonstrated that bi-directional NH_3 flux from managed agricultural soils can be reasonably estimated through integration of the resistance-based flux model of Nemitz et al. (2001) and CMAQ deposition (Pleim et al., 2001; Byun and Schere, 2006) with components of the Environmental Policy Integrated Climate (EPIC) model (Williams, 1995). The results of Cooter et al. (2010) showed good temporal (daily) and accumulated monthly NH_3 estimates and provided a sound foundation for building an agricultural fertilizer modeling system at the regional scale for use with a newly developed ammonia bi-directional flux algorithm in the CMAQ model (Pleim et al., 2010). This modeling system has a mechanistic description of the fertilizer application method, timing, amount, and rate for specific pastures and crops. This is different from previous emission estimates because it can be used to simulate scenarios with different agricultural operation and management techniques. Thus, future scenarios, such as increased bio-fuel production that may impact fertilizer use, can be simulated to assess their impacts on air quality. The purpose of this paper is to describe how this agricultural fertilizer modeling system is developed for a continental U.S. 12km grid-resolution CMAQ modeling domain.

2. Agricultural Fertilizer Modeling System

The agricultural fertilizer modeling system contains three main components within the dash line box in Fig. 1: 1) the EPIC model, 2) tools in the Spatial Allocator to convert mesoscale meteorology Weather Research and Forecasting (WRF) model

data and CMAQ N deposition data for EPIC fertilizer modeling and to convert EPIC fertilizer output for CMAQ air quality modeling, and 3) a simple Java-based interface which air quality modelers can use to generate and visualize fertilizer application data for different modeling scenarios. In this modeling system with WRF and CMAQ, accurate and consistent land use information is important for agricultural fertilizer application modeling, meteorological land surface processes, biogenic emissions, and chemical surface fluxes. Land use data (called BELD4), computed from the most recent 2001 National Land Cover Data (NLCD) products at 30m cell resolution for the U.S., Moderate Resolution Imaging Spectroradiometer (MODIS) for areas outside the U.S., and U.S. Department of Agriculture (USDA) Forest Inventory and Analysis (FIA) tree species and National Agricultural Statistics Service (NASS) pasture/crop categories at county level will be used in this modeling system. The gridded NLCD/MODIS land cover data has been applied in the PX land surface model for WRF/CMAQ modeling (Ran et al. 2010). The tool to generate the BELD4 data is under the development with the support from the US EPA.
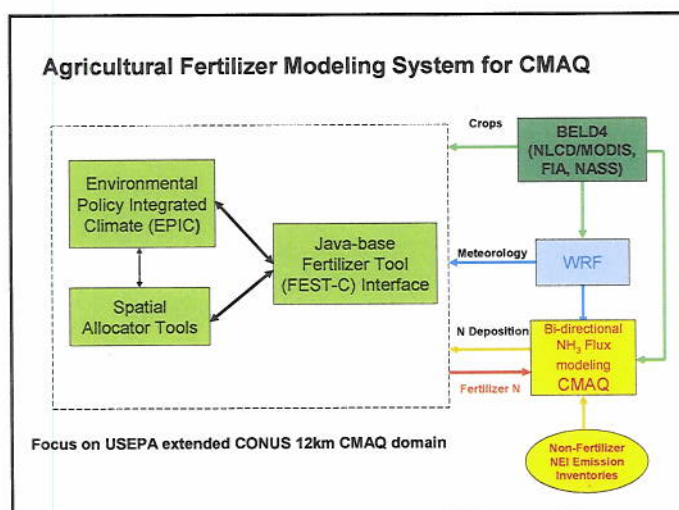

Fig. 1. The agricultural fertilizer modeling system for the CMAQ

EPIC Modeling: The EPIC model is a cropping simulation system developed during the 1980's and is being continuously enhanced (Gassman et al. 2010). It simulates drainage areas that are characterized by homogeneous weather, soil, landscape, crop rotation, and management conditions at field/site scale on a daily time step. It has been used by the USDA and researchers around the world from field to national scale to simulate crop growth, fertilization, erosion, water quality, climate change, and carbon/nitrogen cycling. The development of the EPIC modeling data files is displayed in Fig. 2. We have developed programs to build EPIC

soil and site crop management data sets at the 8-digit hydrologic cataloging unit (HUC) level. The programs use a combination expert knowledge and data compiled for the USDA CRP Evaluation, USDA Conservation Technical Assistance Evaluation, and soil and management data compiled for future USDA and FAPRI analyses. Initially, the system is built for the 8-digit HUC geographic level; however, 12 km grid elevation, slope, land use, and weather data are used to modify the site and heat unit scheduled management to incorporate some attributes of each 12 km grid cell. After the evaluation and analysis of the generated EPIC data files at the 8-digit HUC level, we developed programs to create EPIC site data files for the continental CMAQ 12km grid-resolution domain. Only grid cells with NLCD/MODIS agricultural pasture or crop lands will be used in EPIC modeling. We have completed the development of the EPIC data files for thirty eight NASS irrigated and rainfed pasture and crops in the CMAQ grids over the U.S. Currently, we are evaluating 20-year biogeochemical spin-up runs for all pasture and crops for evaluation and modification.
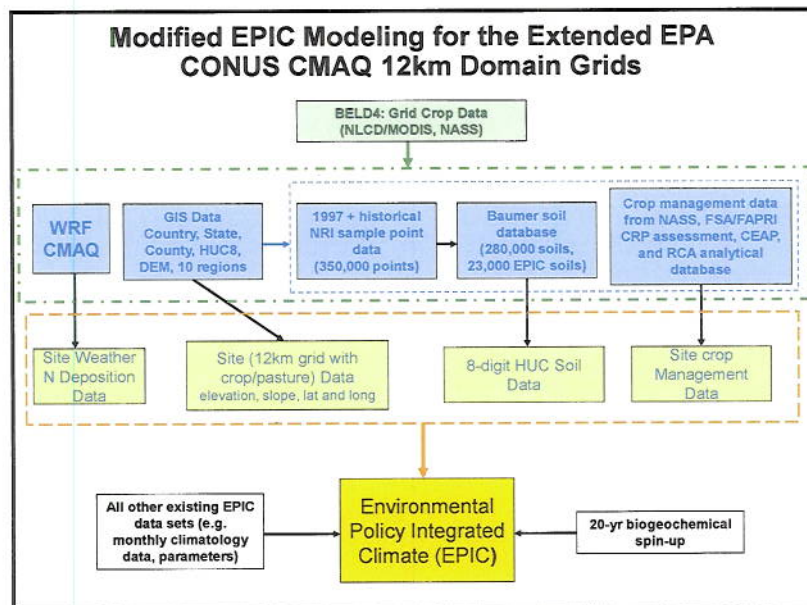

Fig. 2. Modified EPIC modeling for the continental CMAQ 12km domain grids

Tools to Connect EPIC and CMAQ: The tools to connect EPIC and WRF/CMAQ were developed in the Spatial Allocator Raster Tools system (http://www.ie.unc.edu/cempd/projects/mims/spatial/). The WRF/CMAQ-to-EPIC tool extracts weather and N deposition data needed for EPIC modeling from the WRF and CMAQ modeling output. The EPIC model requires as input daily weather data on radiation, maximum temperature, minimum temperature, rain,

relative humidity, and wind speed. The EPIC model is to be modified to take into consideration CMAQ dry and wet N deposition estimates during the fertilizer demand estimation process. The EPIC-to-CMAQ tool extracts EPIC output files at each grid cell to generate NetCDF files containing information on soil conditions, daily or monthly time step EPIC output, and fertilizer applications. Thus, CMAQ can obtain each crop N application data from the NetCDF files and aggregate total applied N in each grid for all crops based on grid BELD4 NASS crop fractions for the bi-directional NH_3 flux modeling.

Fertilizer Emission Scenario Tool for CMAQ (FEST-C) Interface: The Java-based FEST-C interface provides integrated capabilities of running the EPIC model, Spatial Allocator Raster Tools, and VERDI visualization for input and output NetCDF files. The interface contains five components: 1) process WRF weather and CMAQ N deposition data for EPIC modeling, 2) modify management scenario and EPIC run files, 3) run the EPIC model, 4) process EPIC output data into the CMAQ ready format, and 5) visualize input and output data using VERDI. The interface can be launched from a local machine or remote Linux server where the EPIC model and Spatial Allocator Tools are located.

3. Future Work

We are working to complete the EPIC modeling data files for grids outside the U.S. Then, the complete EPIC model will be tested on a Linux server for whole system evaluation. The FEST-C interface components 2 and 3 are fully implemented. We will modify and enhance site, soil, and crop management programs to build EPIC site, soil, and management data files for other domains with different grid resolutions. We will develop and model crop rotation and biofuel scenarios for air quality impact assessment. In addition, we will prepare for climate change applications (e.g., multi-year time slices) and integrate with the coupled WRF-CMAQ for climate, air quality, and agricultural productivity studies.

References

Byun, D.W., Schere, K. L., 2006. Review of the governing equations, computational algorithms, and other components of the Models-3 Community Multiscale Air Quality (CMAQ) modeling system. Appl. Mech. Rev. 59: 51-77.

Cooter, E.J., Bash, J.O., Walker, J.T., Jones, M.R., Robarge, W., 2010. Estimation of NH_3 bi-directional flux over managed agricultural soils. Atmos. Environ. 44: 2107-2115.

Galloway, J. N. and others, 2004. Nitrogen cycles: past, present, and future. Biogeochemistry 70: 153–226.

Gassman, P.W., Williams, J. R., Wang, S., Saleh, A., Osei, E., Hauck, L., Izaurralde, C., Flowers J., 2010. The Agricultural Policy/Environmental Extender (APEX) model: An emerging tool for landscape and watershed environmental analyses. Trans. of the American Society of Agricultural and Biological Engineers (Invited Paper Series) 53(3): 711-740.

Lovett, G.M., Tear, T.H., Evers, D. C., Findlay, S. E. G., Cosby, B. J., Dunscomb, J. K., Driscoll, C. T., Weathers, K. C., 2009. Effects of Air Pollution on Ecosystems and Biological Diversity in the Eastern United States. Year in Ecology and Conservation Biology1162: 99-135.

Nemitz, E., Milford, C., Sutton, M.A., 2001. A two-layer canopy compensation point model for describing bi-directional biosphere-atmosphere exchange of ammonia Q. J. R. Meteorol. Soc. 127: 815-833.

Pleim, J.E., Xiu, A., Finkelstein, P. L., Otte, T.L., 2001. A coupled land-surface and dry deposition model and comparison to field measurements of surface heat, moisture, and ozone fluxes. Water, Air, and Soil Pollution: Focus 1: 243-252.

Pleim, J. E., J. Walker, J. Bash, and E. Cooter, 2010, Development and Evaluation of an Ammonia Bi-Directional Flux Model for Air Quality Models, Air Pollution Modeling and Its Application XXI, Springer, this volume.

Ran, L., Pleim, J., Gilliam, A. R., 2010. Impact of High Resolution Land-Use Data in Meteorology and Air Quality Modeling Systems, Air Pollution Modeling and Its Application XX, Springer, The Netherlands: 3-7.

Smith V. H., Tilman G. D., Nekola J. C., 1998. Eutrophication: Impacts of excess nutrient inputs on freshwater, marine, and terrestrial ecosystems. Environmental Pollution 100 (1-3): 179-196.

Williams J. R., 1995. The EPIC model. In: Singh VP (ed) Computer models in watershed hydrology. Water Resources Publications, Highlands Ranch: 909–1000.

Wolfe, A. H., Patz, J. A., 2002. Reactive nitrogen and human health: acute and long-term implications. Ambio 31: 120–25.

4. Questions and Answers

Dr. B. Fisher: Does the EPIC model include the runoff of nitrogen after heavy precipitation. This is another pathway for the transfer of nitrogen (to be compared with the atmospheric pathway in CMAQ)?

Answer: EPIC does simulate the complete N cycle in soils and N loss from surface runoff and subsurface flow. However, since the model is at single field level, it does not have information about N flow from other EPIC modeling sites. If you want to know N flow information from multiple fields or within a watershed, you may use APEX or SWAT models. For emissions-driven air quality analyses, knowledge regarding field-scale fertilizer applications for 12km grids is sufficient.

Dr. Mohamed Salem: What are the sources of organic phosphorus fertilizers you use in your study?

Answer: Organic phosphorus is based on soil organic matter (carbon) initially and then organic phosphorus is added from plant residues or manure. Grazing is set up to apply the manure excreted daily by livestock. Manure can be applied as fertilizer. We don't have it yet for our pasture, but we may have it in the future.