1

# Advances in Linked Air Quality, Farm Management and Biogeochemistry Models to Address Bidirectional Ammonia Flux in CMAQ

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**Abstract:** Recent increases in anthropogenic inputs of nitrogen to air, land and water media pose a growing threat to human health and ecosystems. Modeling of air-surface N flux is one area in need of improvement. Implementation of a linked air quality and cropland management system is described, and a tool to facilitate estimation of fertilizer input information required by the air quality model is presented. Preliminary evaluation of the coupled system against observations indicates improved wet deposition estimates.

**Keywords:** Linked-Model, Ammonia Emissions, Agricultural Soils

## Introduction:

Recent increases in regional-to-global air, land and water nitrogen (N) inputs pose a growing threat to human health and ecosystem. Policy actions that address this threat demand improved characterization of all aspects of the N-cycle, including air quality. Areas in which improvements are needed include: 1) modeling of N species that exhibit bi-directional surface exchange (e.g., ammonia ($NH_3$)), 2) integration of agricultural practices and meteorologically-driven emissions to reduce $NH_3$ and inorganic fine particulate ($PM_{2.5}$) concentration and deposition uncertainty, and 3) modeling systems that support joint air, land and water environmental options to protect human health and ecosystems. This chapter describes the implementation of linked bi-directional air quality and cropland agricultural management models to improve estimates of $NH_3$ soil flux, total reduced N deposition and ambient $PM_{2.5}$ concentrations.

## Methodology:

The first step towards these improvements is to implement a bi-directional flux approach into the Community Multi-scale Air Quality (CMAQ) model (Byun & Schere, 2006). Figure 1 illustrates this implementation. The primary changes to the standard CMAQ approach include the separate treatment of agricultural cropland from other sources of NH3, input of the rate and depth of fertilizer applications as a driver of cropland emissions, and dynamic tracking of the soil ammonium ($NH_4^+$) pool. Details of the bidirectional flux model in CMAQ (BIDI) is provided in Bash et al., (2013). In BIDI, the emissions inventory for cropland $NH_3$ emissions is replaced by a compensation point approach described in Nemitz, et al., 2001) to allow for bi-directional exchange. The compensation point is a function of temperature and emission potential (Γ). Sensitivity analyses suggest that soil emission potential ($\Gamma_{s)}$ can be a significant contributor to flux uncertainty (Dennis et al., 2013) and so its credible estimation is important.

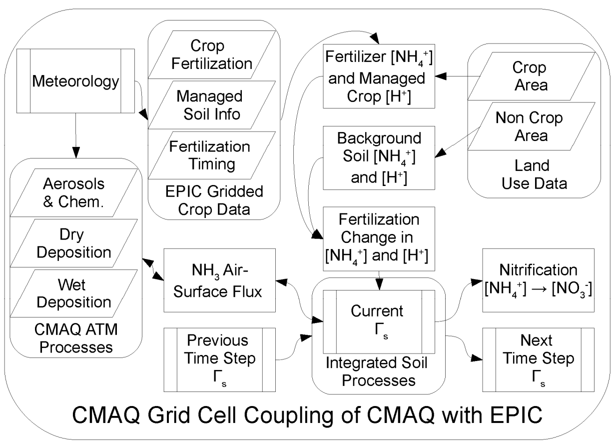


Figure 1. Implementation in bi-directional CMAQ (After Cooter,et al., 2013).

The U.S. Department of Agriculture Environmental Policy Impact Climate (EPIC) model is used to calculate soil nitrogen biogeochemistry leading to $\Gamma_s$ (http://www.epicapex.brc.tamus.edu). The initial implementation for CMAQ is described in Cooter et al., (2012). The system now also includes year-specific gridded modeled hourly meteorology and daily deposition. A user interface, the Fertilizer Emissions Scenario Tool for CMAQ (FEST-C) has been developed to produce EPIC-based, BIDI-ready input files containing initial soil pH and soil $NH_4^+$ in the upper 1cm and underlying soil layers. This is followed by daily simulated fertilizer application rate in each layer. BIDI then uses this information to track the ammonium-N in each layer and to compute $\Gamma_s$, and to determine whether NH3 is emitted or deposited. FEST-C produces this information on any projected or latitude/longitude grid, for any U.S. domain and grid resolution for which gridded meteorology is available (Figure 2).

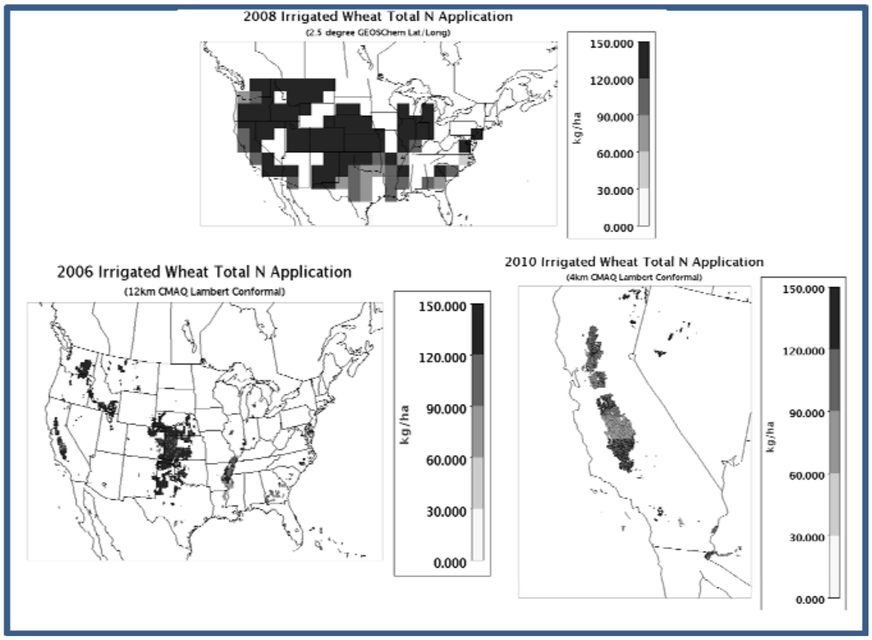


Figure 2. The FEST-C interface supports generation of model-ready daily fertilizer rate and depth for multiple gridded U.S. domains and resolutions (Top, GEOschem 2.5$^{o}$ CONUS; Lower Left, CMAQ 12km CONUS; Lower Right, CMAQ 4km CalNex).

## Results and Discussion:

Evaluation of BIDI system results shows improved CMAQ estimates of annual NHx wet deposition, the bias is reduced from -20% to -4%. Estimates of ambient nitrate aerosol and inorganic $PM_{2.5}$ concentrations inorganic $PM_{2.5}$ improve during the spring and fall seasons (Bash, et al., 2013).

Applications that make use of this linked system include: simulating the air quality response to increased corn production in support of the U.S. Renewable Fuels Standard (RFS); improving our understanding of the seasonal and regional signature of nitrous oxide emissions from intensive agricultural areas; linkage of this system to water quality models to explore the impact of alternative management practices on nutrient loading to estuaries, especially the hypoxic zone in the U.S. Gulf of Mexico; and the exploration of the response of various ecosystem services to future alternative climate and landuse futures.

A linked air quality and farm management system has been implemented to reduce uncertainty in our estimates of $NH_3$ flux from agricultural soils. Support tools have been developed to facilitate use of this linked system by the air quality modeling community. Preliminary evaluations indicate that the system does indeed improve our estimates of regional wet deposition and inorganic $PM_{2.5}$. This flexible system is being used to address a number of questions related to joint air, land and water issues in order to better protect human health and to sustain ecosystems.

## Acknowledgments and Disclaimer

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**Questioner Name:** Clemens Mensink

**Q:** In the bi-directional ammonia flux model, what are the most sensitive input parameters?

**A:** Dennis et al. (2013) address the sensitivity of bi-directional flux estimates in detail. The authors conclude that at the continental scale, $NH_3$ emissions change by 40% with a 50% change in $\Gamma_s$ and by 30% with a 50% change in fertilizer application rate. Continental deposition changes are much smaller because of the dominance of livestock emissions.

**Questioner Name:** Pius Lee

**Q:** Since bi-directional flux of NH3 is very sensitive to soil moisture (e.g. WRF soil moisture nudging), one of the studies in CalNex domain attempted 12km and 4km CMAQ measurements coupled with EPIC. How is the soil moisture (precipitation) accuracy handled across those two horizontal scales?

**A:** Each example case employs, WRF results simulated at the desired air quality model scale, so 2 different WRF simulations are used. EPIC is run at the native scale of the WRF data, e.g., either 12km or 4km. No additional downscaling is performed. EPIC has its own dynamic soil temperature and soil moisture process models that are driven on a daily time scale by the same WRF information that drives CMAQ. In CMAQ, soil layer 2 (the entire soil profile less the topmost 1cm) temperature and soil moisture are nudged. The soil nitrification process (a function of soil moisture and soil temperature) have been added to CMAQ so that the hourly $NH_4^+$ transformation and volatilization processes within CMAQ are driven by consistent meteorology, soil moisture and soil temperature. There are potential differences between CMAQ and EPIC soil moisture and soil temperature estimates that could impact estimates of daily fertilizer demand. A formal evaluation has yet to be completed, but differences appear to be small enough that we do not anticipate this to be a significant source of additional uncertainty.