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Evaluation of bidirectional NH3 exchange in CMAQ 5.0 against network observations and CMAQ 4.7.1

Jesse O. Bash[1]; Jon Pleim[1]; John T. Walker[2]; Robin Dennis[1]; Ellen J. Cooter[1]; Kristen Foley[1]

1 U.S. EPA National Exposure Research Laboratory

2 U.S. EPA National Risk Management Research Laboratory

bash.jesse@epa.gov

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Outline

- Overview of bidirectional exchange
  - General framework in CMAQ
- Mercury
  - Changes from 4.7.1
- Ammonia
  - Flux experiments and model evaluation
  - Application in CMAQ v5.0
  - Impact on NHx wet deposition
  - Evaluation against aerosol observations
- Conclusions and next steps

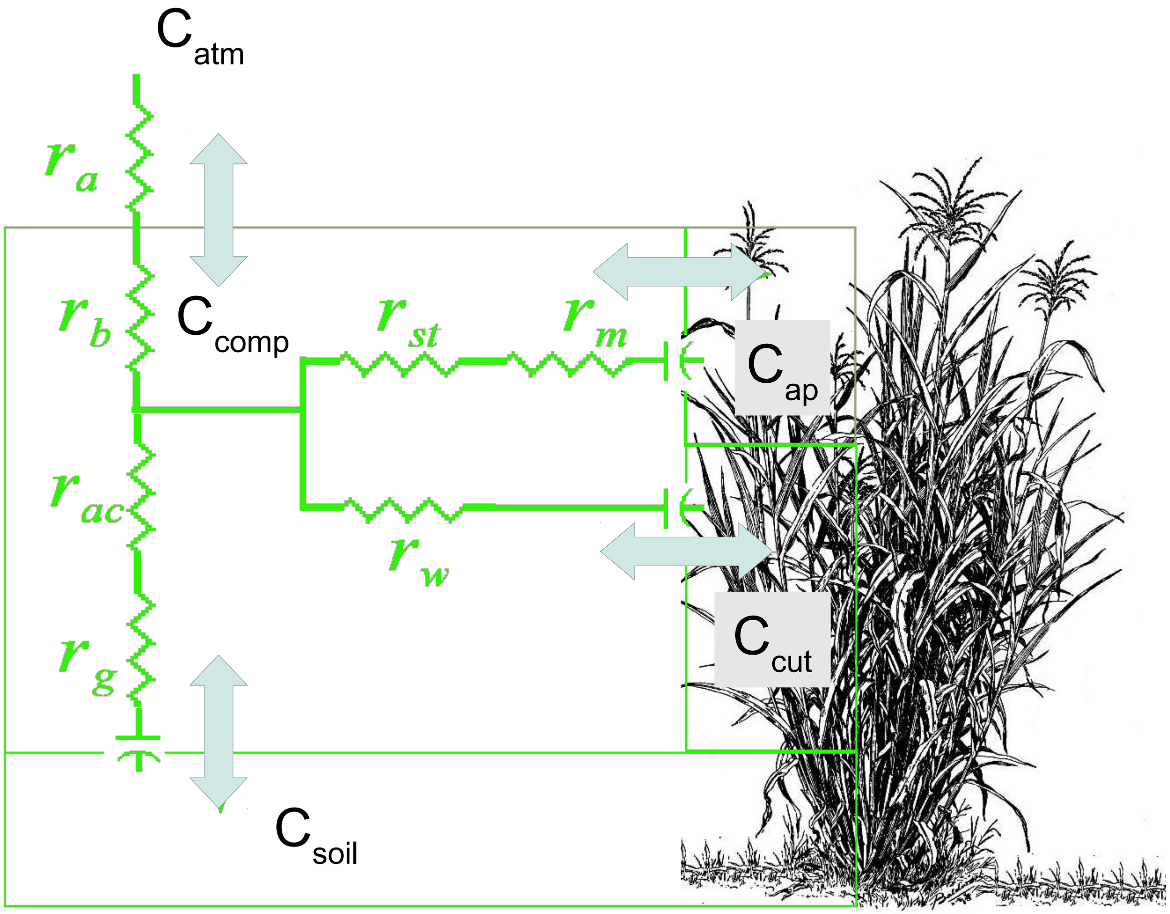
Motivation

- Once in soils or the water column Hg can be transformed into organic Hg compounds
  - Potent neurotoxins
- NH_3 is the primary atmospheric base
  - Contributes to PM formation
    - Deleterious to human health
- Net acidification impact on soil and contributes to surface water eutrophication
  - Contributes to decline in species biodiversity and ecosystem services
- Objectives
  - Develop a mechanistic model for agricultural cropping NH_3 emissions coupled to the bidirectional NH_3 exchange model
  - Develop a mechanistic model for Hg re-emissions
  - Reduce uncertainty in NH_3 and Hg emissions and transport
    - More correct parameterization to provide better top down NH_3 emissions estimates
  - Better characterization of atmospheric sinks and sources of Hg and NH_3

Bidirectional Exchange

- Air surface exchange of NH_3 and Hg^0 is bidirectional
- Regional and global models not parameterized for bidirectional exchange
- CMAQ bidirectional model was developed based on field scale models
  - Uses a compensation point parametrization
    - Compensation point is an ambient concentration at which the flux is zero
  - NH_3 evaluated in a collaborative measurement campaign
  - Hg^0 constrained by published observations
- Scaled to regional applications using land use data

Bidirectional Exchange



- Estimates a net flux
  - Emissions and deposition
- Consistent set of assumptions regarding emission and deposition
- Developed from field studies
- Multiple source/sink system
  - Soil and vegetation interior and surface fluxes

Hg Bidirectional Exchange

- Better representation of the state-of-the-science of Hg air-surface exchange
- Small changes in wet deposition and ambient concentrations
  - Larger changes expected in hemispheric or global simulations
- Simplifies Hg emission processing
- Now a run time options and supports MODIS, NLCD and USGS land use data
- Details in Bash 2010 JGR

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NH3 Air-Surface Exchange Development

- Collaboration between EPA, NOAA ARL, and UK CEH in 2007 field campaign
  - Fertilized corn field in Lillington, NC
- Measured air-surface exchange fluxes above the canopy and in-canopy sources and sinks
- Measured vegetation and soil ammonium and hydrogen ion concentrations
- Used USDA EPIC model processes to simulate soil nitrogen geochemistry following fertilization
  - Model vegetation uptake and nitrification losses of soil NH_4^+

Bash et al 2010 ES&T
Cooter et al 2010 Atmos Environ

NH3 Air-Surface Exchange Application

- Used EPIC to simulate national agricultural management practices for 42 major crops
  - Estimates initial soil ammonium content, managed pH, fertilizer application rates, timing, and method
- Added and coupled EPIC soil ammonium evasion and nitrification routines to CMAQ
- Requires land use and agricultural management files
  - BELD4, national Soil pH by crop, and national fertilizer application date, rate and method by crop
- Connects agricultural management practices more directly with NH_3 emissions and air quality.

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Appel et al 2011 Geosci. Model Dev.

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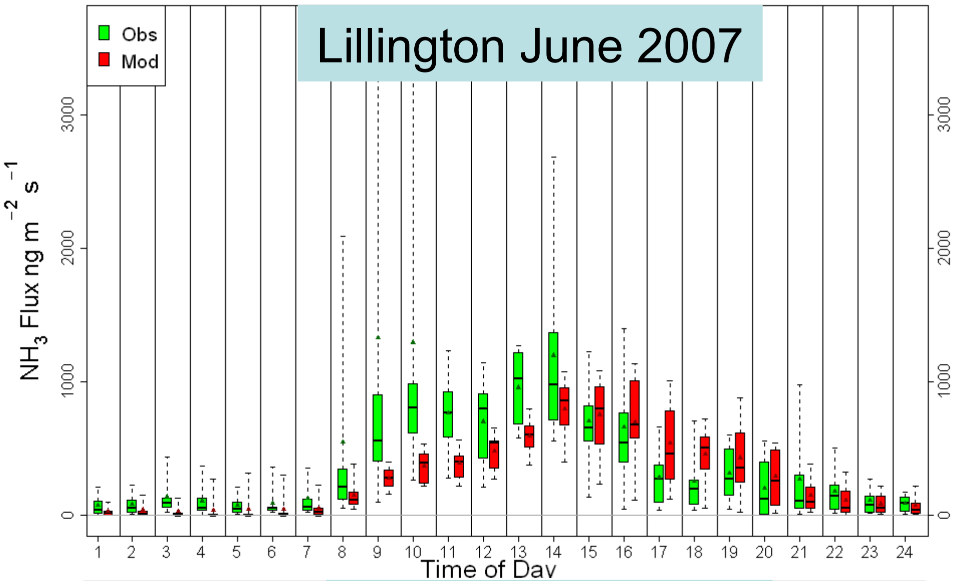
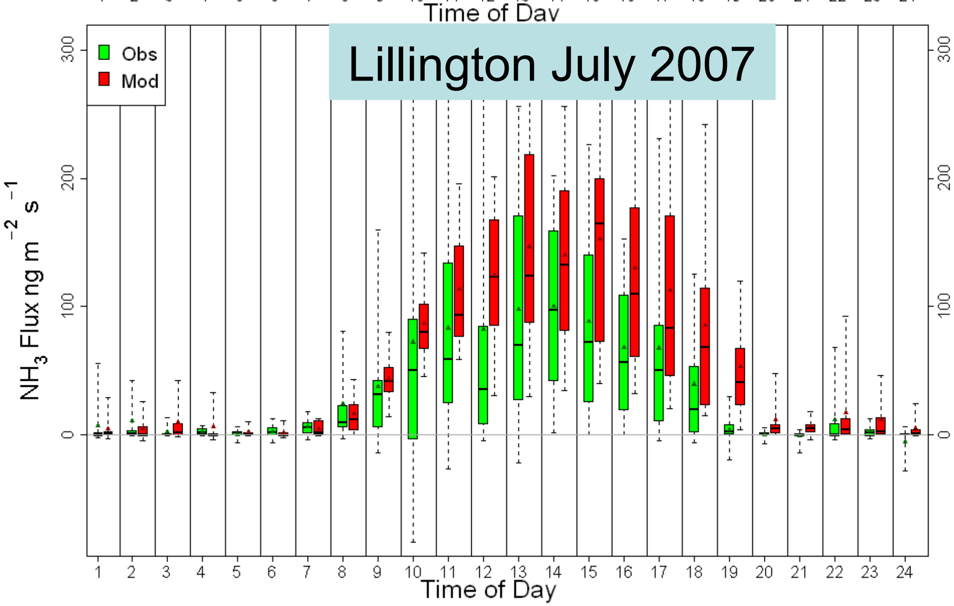
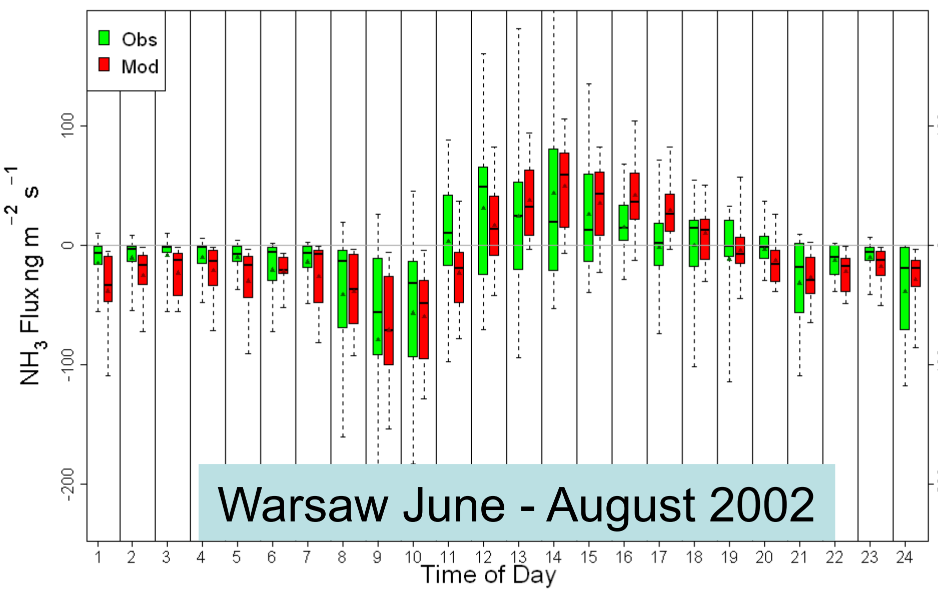
Evaluation Against Flux Observations



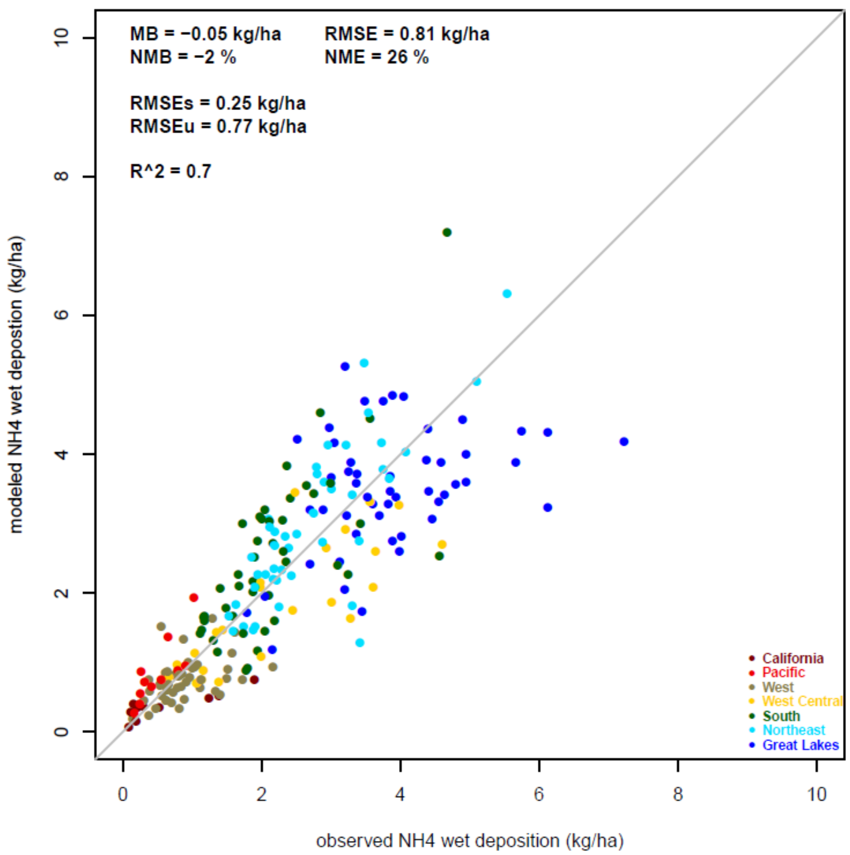
- Box model estimates were within measurement uncertainty with field experiments under high and low fertilizer conditions ($p < 0.001$, bias < 20% or 3 ng m-2 s-1)
- Model canopy uptake agreed with observations



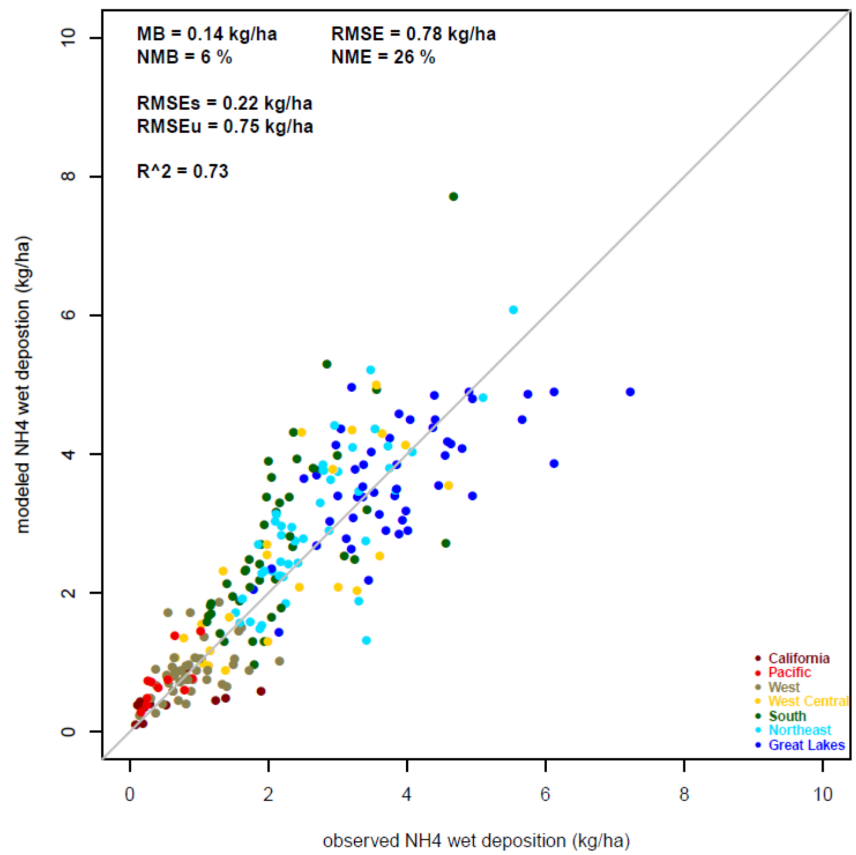


Regional Scale Evaluation

V4.7.1



V5.0



Eval against NADP NHx wet dep

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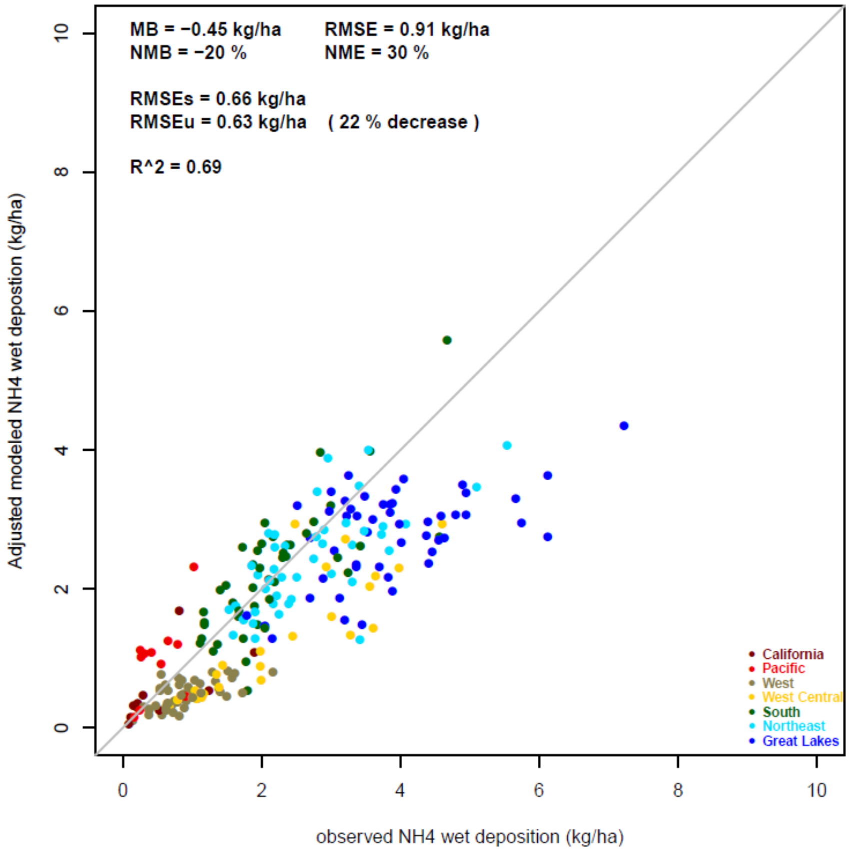
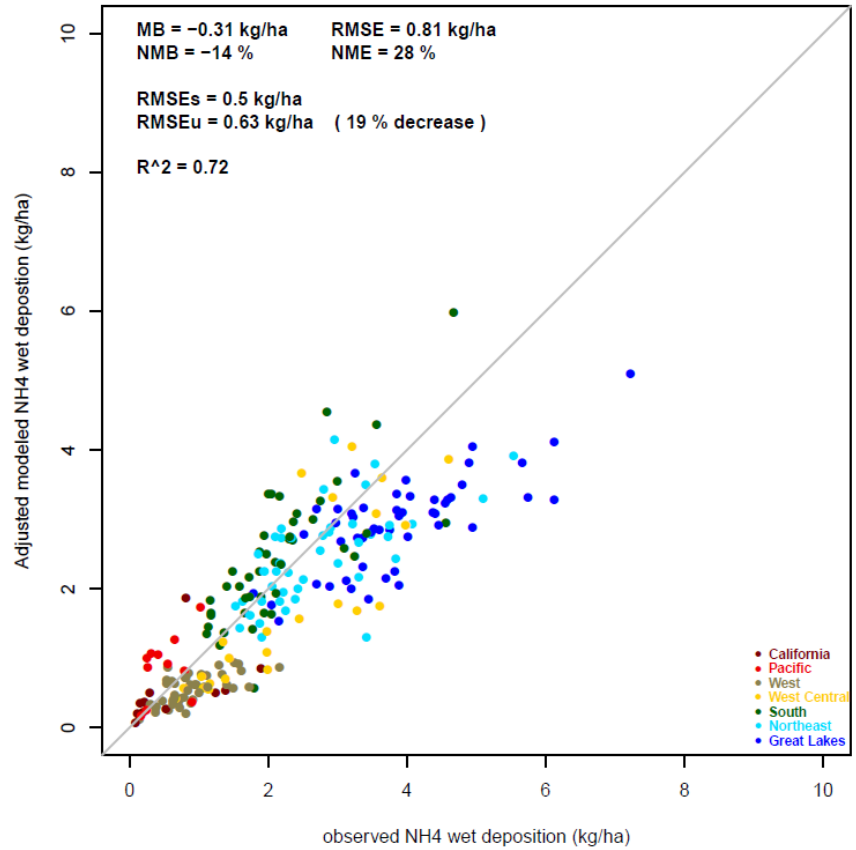
Regional Scale Evaluation

V4.7.1



V5.0



Eval against NADP NHx wet dep with Precip adjustment

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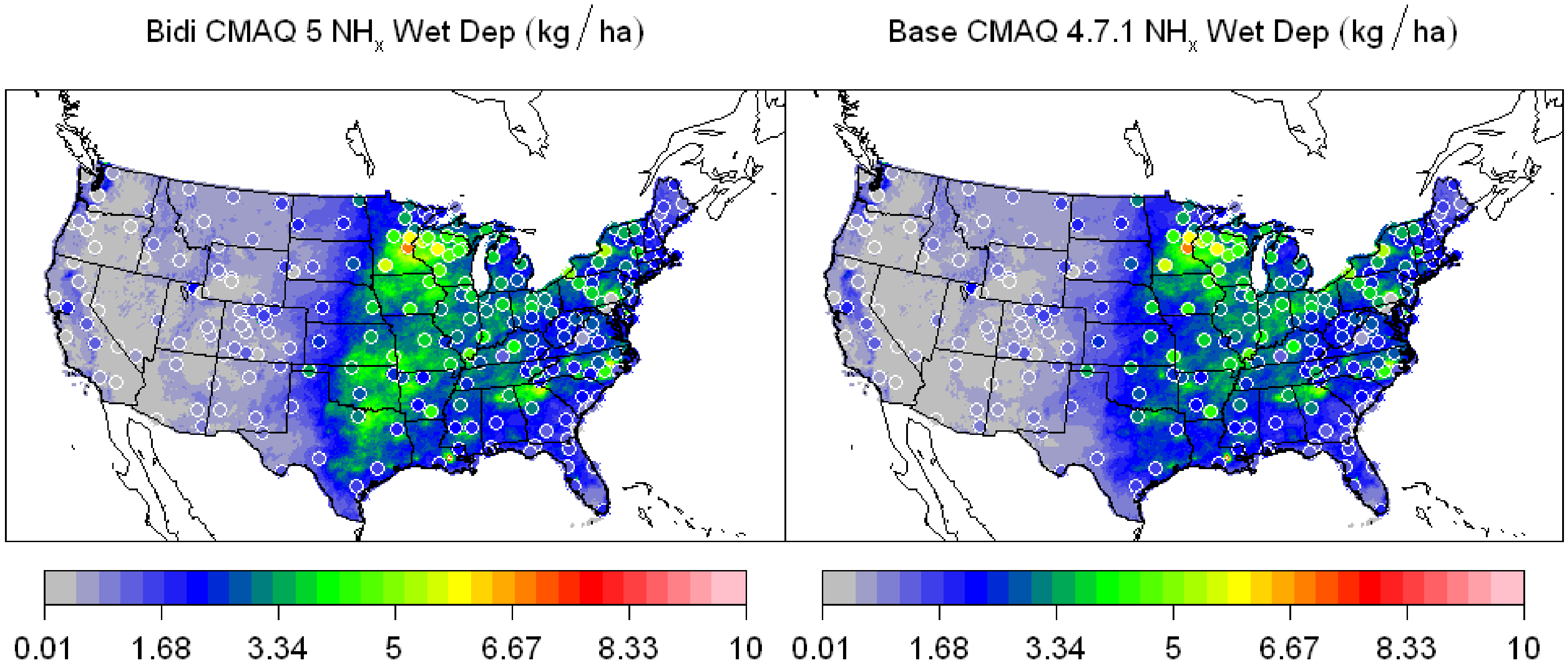
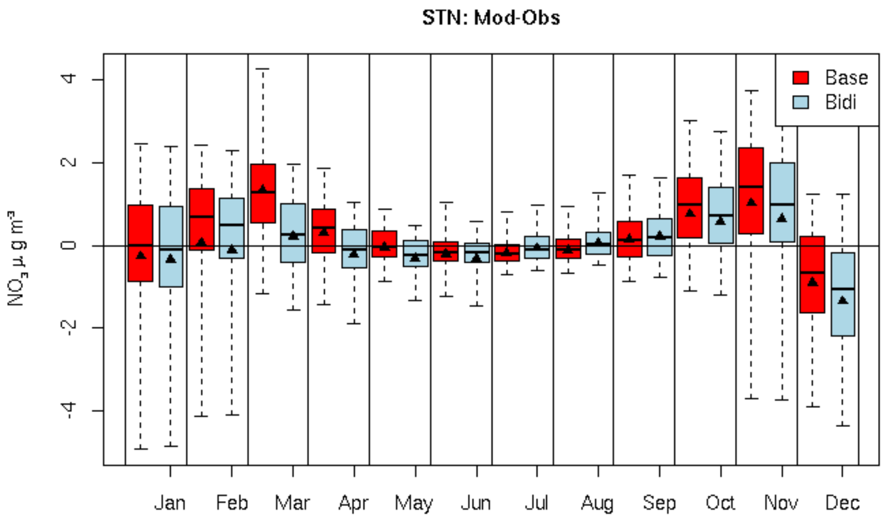
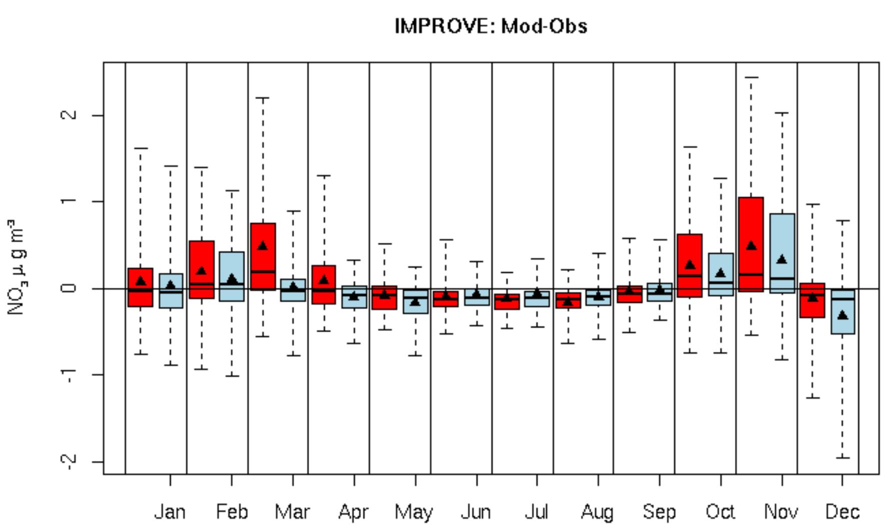
Regional Scale Evaluation



- Ratio of modeled NHx wet deposition field and interpolated observations
- Significant reduction in NHx wet deposition bias in most of the modeling domain

Regional Scale Evaluation





- Improvements in NO_3^- aerosol concentrations at both urban and rural sites
- Reduction in annual bias and error
  - 3% and 4% reduction in NMB and NME at STN sites
  - 10% reduction in both NMB and NME at IMPROVE sites
- Bidirectional NH_3 captured seasonal trends at both sites better
- Still a problem with December

NH3 Bidirectional Exchange

- Better representation of the state-of-the-science of NH_3 air-surface exchange
- Connects agricultural management practices with NH_3 emissions, NHx deposition, and ambient aerosol concentrations.
- Improved temporal and spatial representations of NH_3 emissions
- Significant improvements in NHx wet deposition and NO_3^- aerosol estimates

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Next Steps

- Revised EPIC input files for 2002
  - Year specific using WRF meteorology and Canada EPIC agricultural management simulations
- 2002 and 2006 annual simulations with CMAQ 5.0
- Inverse modeling of 2009 CAFO emissions and bidirectional sensitivity analysis
- Separate flux into emissions and deposition estimates in Hg bidi
- Manuscripts in preparation

Pleim et al – Bidi field scale eval and development

Bash et al – Bidi pilot evaluation

Jeong et al – Bidi evaluation and inverse modeling of emissions

Cooter et al – National scale EPIC simulations and CMAQ inputs

Gore et al – Bidi pilot N budget

Dennis et al – Uncertainties in Bidi parameterizations on N deposition budget