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

Jesse O. Bash\textsuperscript{1}; Jon Pleim\textsuperscript{1}; John T. Walker\textsuperscript{2}; Robin Dennis\textsuperscript{1}; Ellen J. Cooter\textsuperscript{1}; Kristen Foley\textsuperscript{1}

\textsuperscript{1} U.S. EPA National Exposure Research Laboratory
\textsuperscript{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

• $\text{NH}_3$ 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 $\text{NH}_3$ emissions coupled to the bidirectional $\text{NH}_3$ exchange model
  _ Develop a mechanistic model for Hg re-emissions
  _ Reduce uncertainty in $\text{NH}_3$ and Hg emissions and transport
    • More correct parameterization to provide better top down $\text{NH}_3$ emissions estimates
  _ Better characterization of atmospheric sinks and sources of Hg and $\text{NH}_3$
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
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 $\text{NH}_4^+$

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.

Appel et al 2011 Geosci. Model Dev.
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

Warsaw June - August 2002

Lillington June 2007

Lillington July 2007
Regional Scale Evaluation

V4.7.1

V5.0

Eval against NADP NHx wet dep
Regional Scale Evaluation

V4.7.1

- MB = -0.45 kg/ha
- RMSE = 0.91 kg/ha
- NMB = -20%
- NME = 30%
- RMSEs = 0.66 kg/ha
- RMSEu = 0.63 kg/ha (22% decrease)
- R^2 = 0.69

V5.0

- MB = -0.31 kg/ha
- RMSE = 0.81 kg/ha
- NMB = -14%
- NME = 28%
- RMSEs = 0.6 kg/ha
- RMSEu = 0.63 kg/ha (19% decrease)
- R^2 = 0.72

Eval against NADP NHx wet dep with Precip adjustment
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\textsubscript{3}\textsuperscript{-} 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\textsubscript{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
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