United States Environmental Protection Agency

CMAQ NH_3 Bidirectional Model Pilot Study Evaluation

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2010 CMAS Conference, October 12th
Chapel Hill, NC

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National Exposure Research Laboratory | Atmospheric Modeling and Analysis Division |
Atmospheric Exposure Integration Branch

Outline

- Objectives and Background
- CMAQ bidirectional NH_3 pilot study
- CMAQ Model simulations
  - Bidirectional and Base model configurations
- Results and Evaluation
  - Bidi and Base model nitrogen budget (Gore et al. 4:10 PM Poster session)
  - NH_x wet deposition evaluation
  - NH_4 ambient concentration evaluation
- Conclusions

Reduced Nitrogen in the Environment

- 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
- NH_3 emissions remain uncertain
  - Complex multimedia air-surface exchange processes
  - Difficult to measure fluxes
- Objectives:
  - Develop a mechanistic model for agricultural cropping NH_3 emissions coupled to the bidirectional NH_3 exchange model

NH_3 air-surface exchange

- Air-surface exchange of NH_3 is bidirectional
- Regional and global models parametrized using the deposition velocity concept
  - A unidirectional approach
- Bidirectional exchange models have been developed and evaluated for field scale applications
- The CMAQ bidirectional NH_3 air-surface exchange model was parametrized using data from a collaborative measurement campaign
  - Evaluated at the field scale
  - Do these processes scale to regional applications?
- NH_3 bidirectional model requires more input parameters
  - Provided by a soil nitrogen model (Cooter et al, 4:10 PM Poster Session)

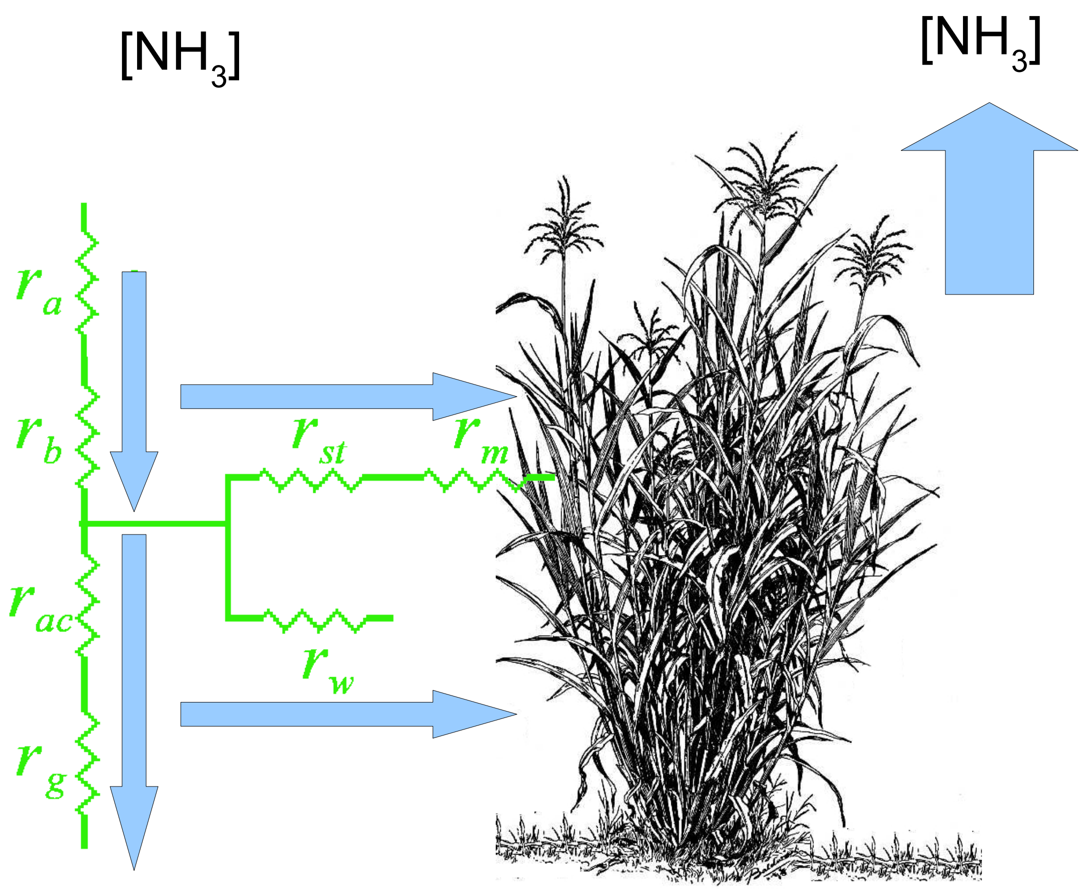
The NH_3 Compensation Point

- Compensation point is an ambient concentration at which the flux is zero
  - Air-surface system is in equilibrium
- CMAQ NH_3 bidi model has soil and vegetation compensation points
  - Based on the thermodynamic equilibrium of NH_4^+ and H^+ in aqueous solutions in soil and vegetation
    - Non-agriculture land cover based on mean observed values
    - Agriculture land cover based on geochemical cycling model estimates
- Soil and vegetation compensation points and resistance model used to define a canopy compensation point

Unidirectional Exchange

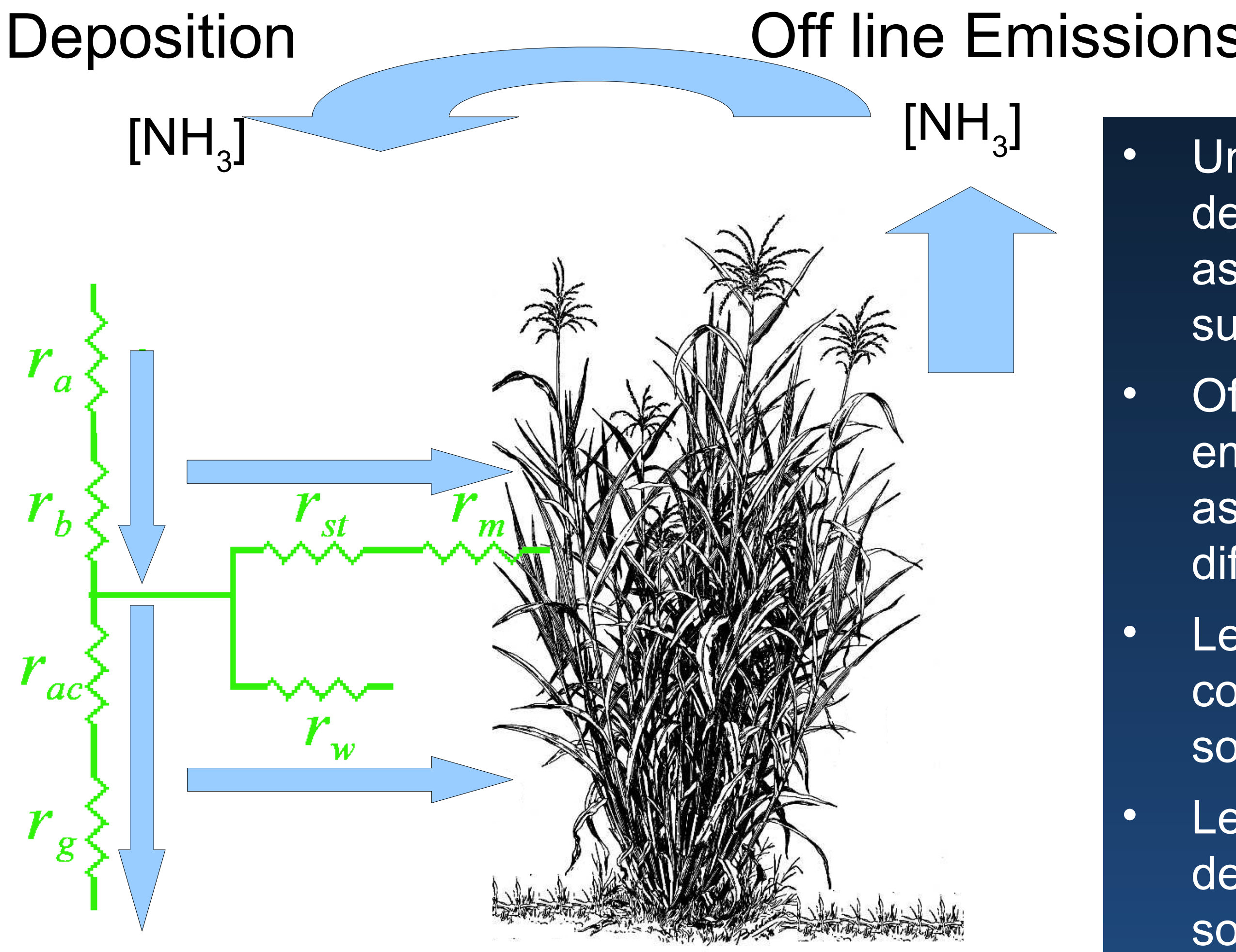
Deposition

Off line Emissions



- Unidirectional dry deposition velocity assumes the surface is a sink
- Off line emission emissions model assumptions may differ
- Leads to high concentrations over sources
- Leads to high deposition over sources

Unidirectional Exchange



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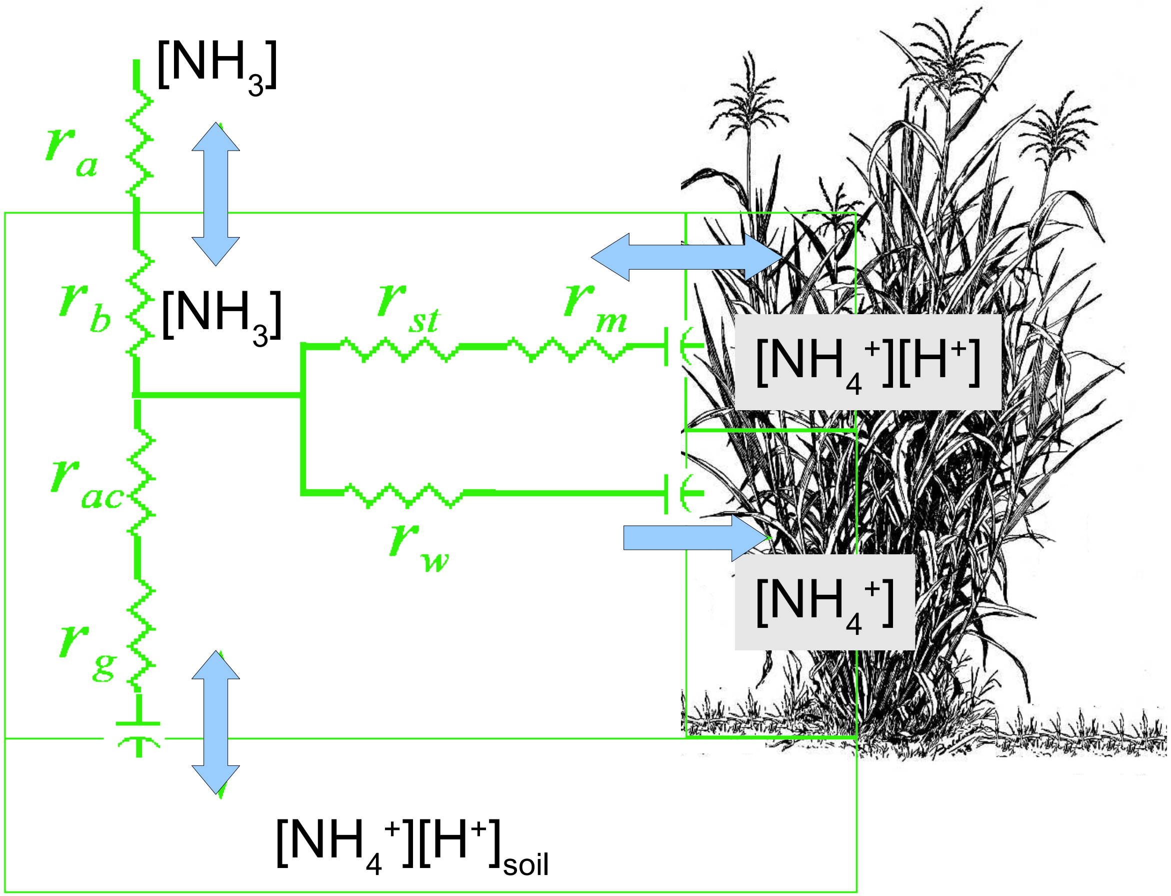
Bidirectional Exchange

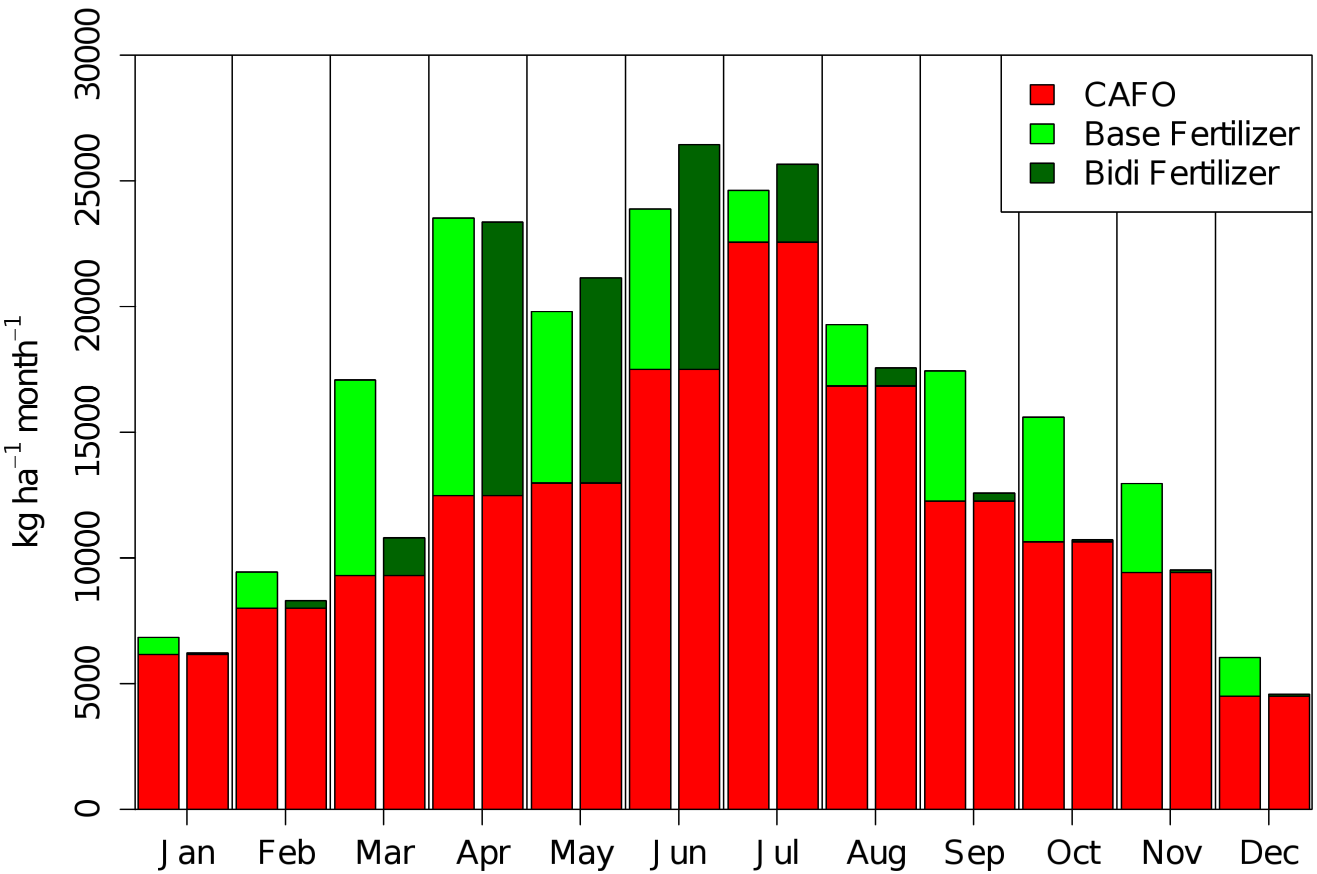


- Parametrizes a net flux over sources and sinks
- Consistent set of assumptions
- Parametrized from field studies
- Multiple source/sink system
  - Component fluxes contribute to net flux

Model Simulations

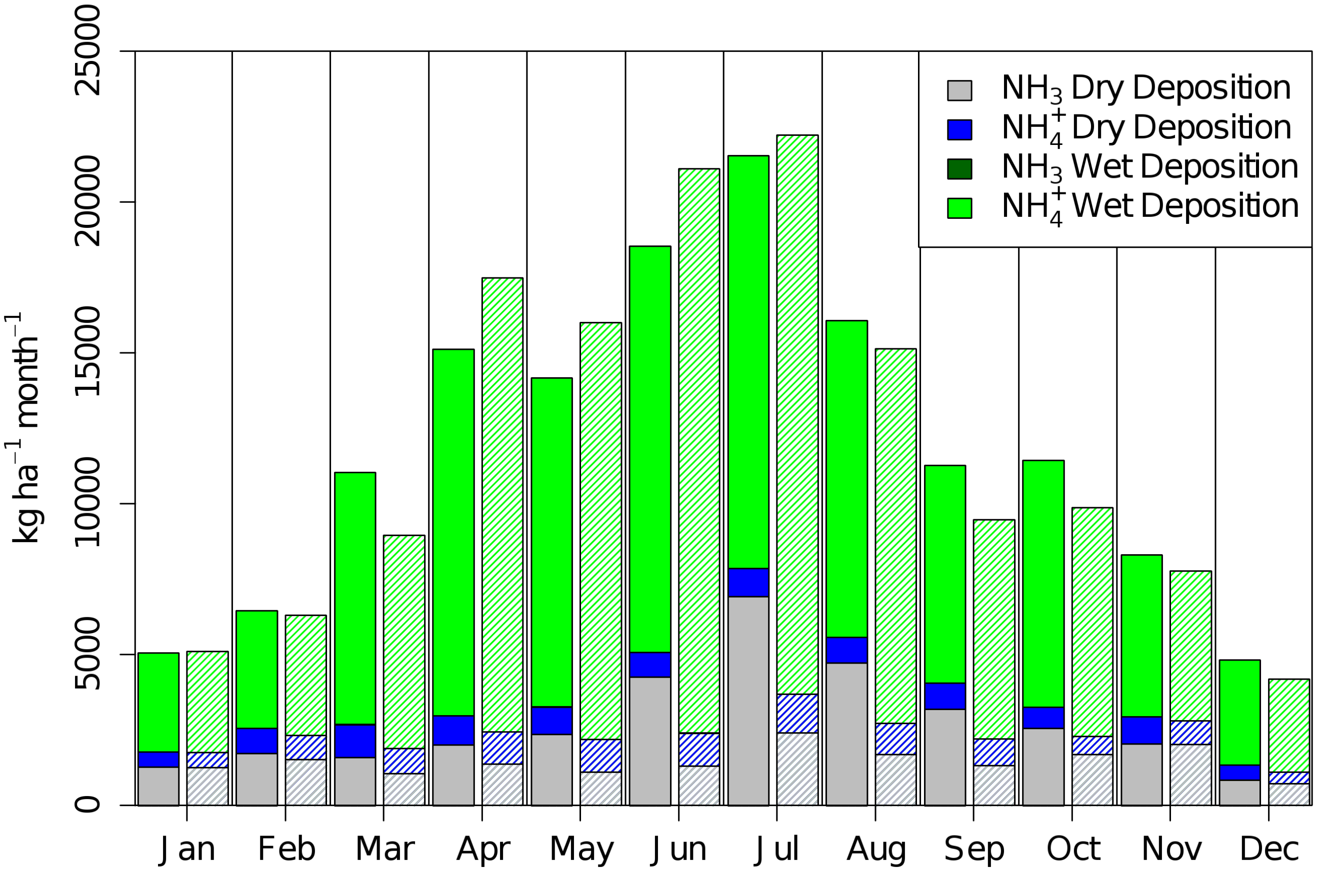
- 2002 annual simulations
- Base Case
  - CMAQ 4.7.1
  - 2002af NEI emissions
  - Based on CMU estimates of fertilizer NH_3 emissions
- Bidi Case
  - CMAQ 4.7.1 with bidirectional NH_3 exchange
  - 2002af NEI emissions without fertilizer emissions
  - Agricultural soil NH_4^+ and H^+ based on parametrizations of soil nitrification and acidification processes
    - Land use and crop information based on USDA farm-level survey information

Annual Emissions



- Base fertilizer emissions 34% of total NH_3 emissions
- Bidi fertilizer emissions 31% of total NH_3 emissions
- 11% reduction in emissions in Bidi model
- Bidi changes the deposition of NH_3

Annual Deposition (Non agriculture land use)

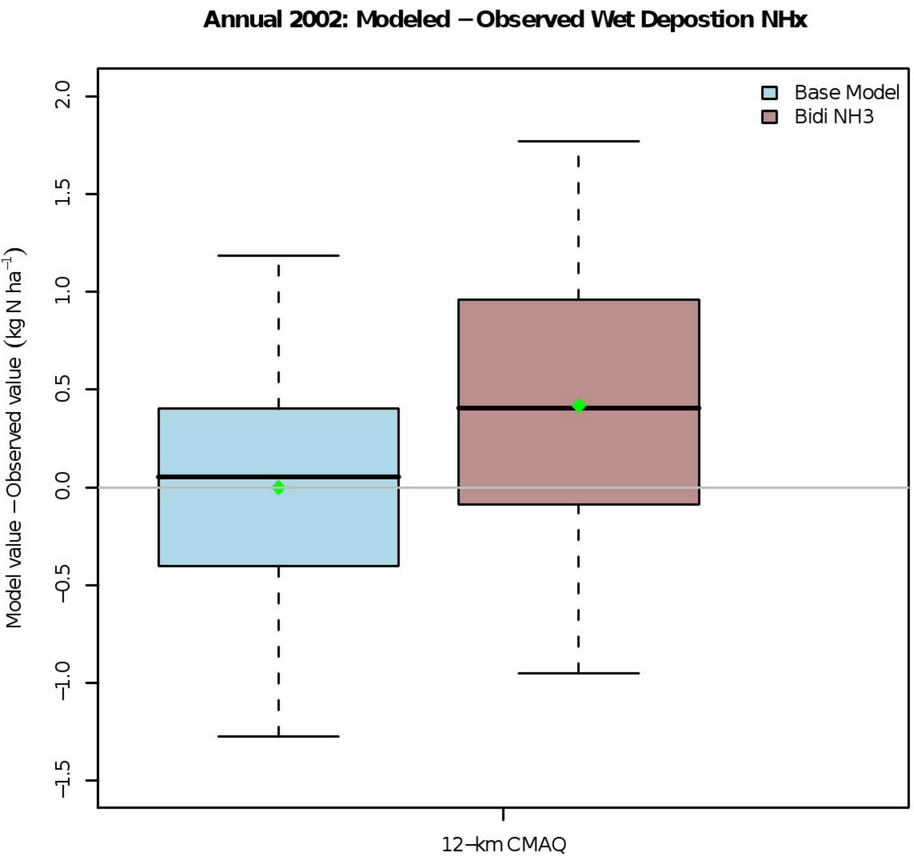


Fraction of Total Deposition

	Base	Bidi
NH_3 dry	23%	12%
NH_4^+ dry	7%	7%
NH_3 wet	0%	0%
NH_4^+ wet	70%	81%

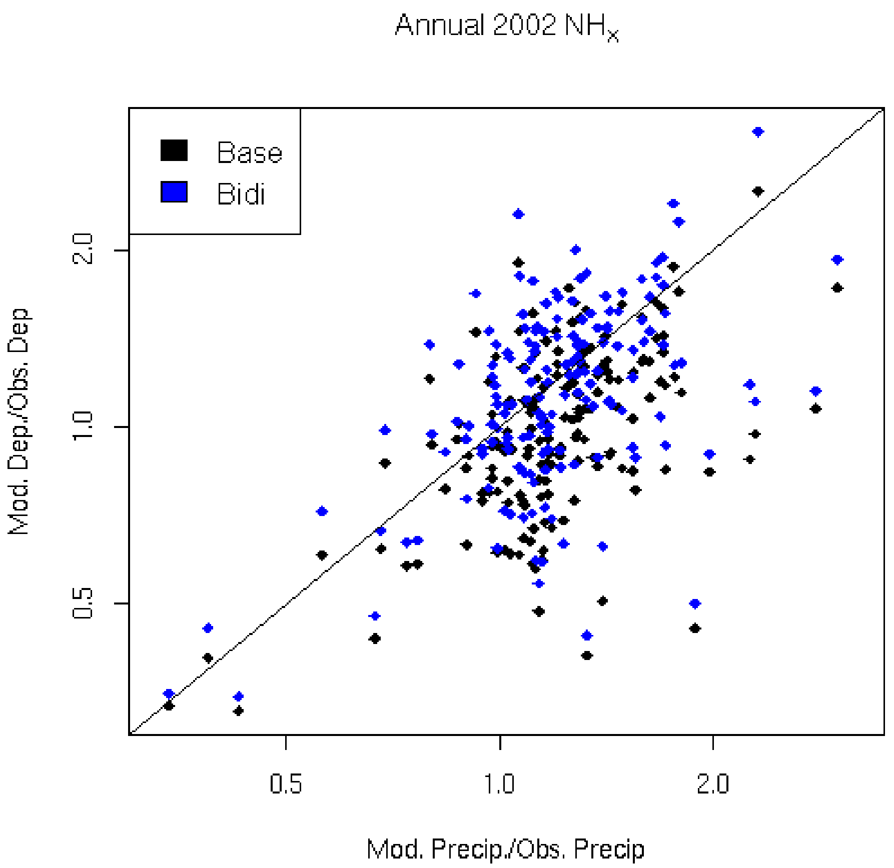
Evaluation against NADP NH_x Wet Deposition

Annual NH_x deposition biases



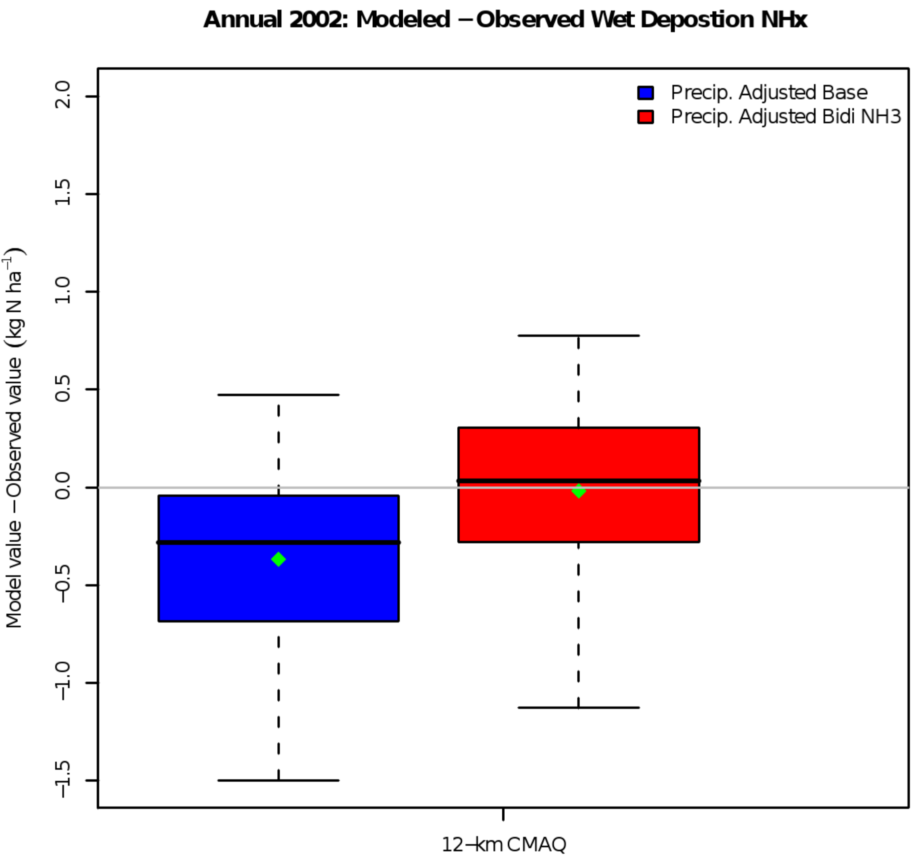
	r	NMB	NME
Base	0.730	0%	19%
Bidi	0.740	14%	24%

Precipitation Correction



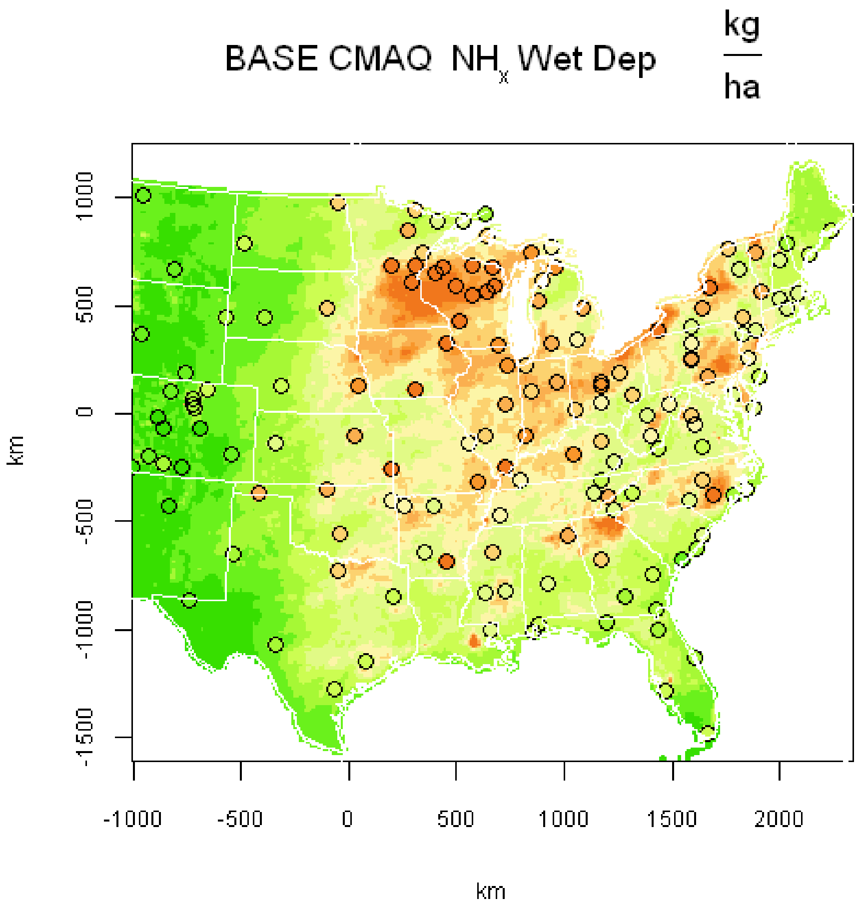
- Modeled annual precipitation biases introduce biases in wet deposition estimates
- Precipitation and deposition biases significantly ($p<0.001$) correlated
- Better correlation regionally
- Wet deposition results linearly adjusted to correct for precipitation biases
- For more details see Foley et al. at the 4:00 poster session

Annual NH_x deposition biases

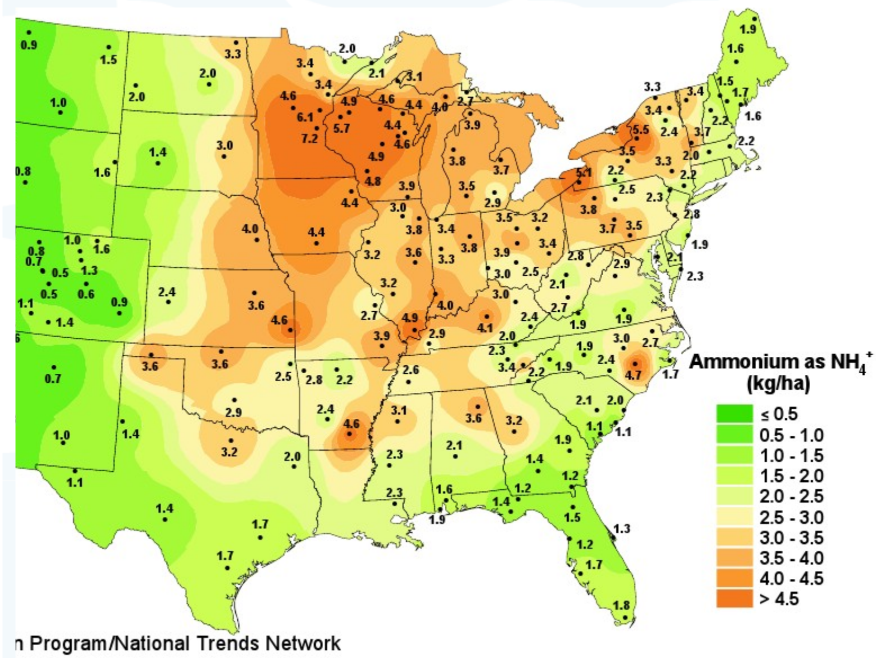


	r	NMB	NME
Precip. Adj. Base	0.794	-13%	17%
Precip. Adj. Bidi	0.807	1%	14%

Annual NH_x Wet Deposition

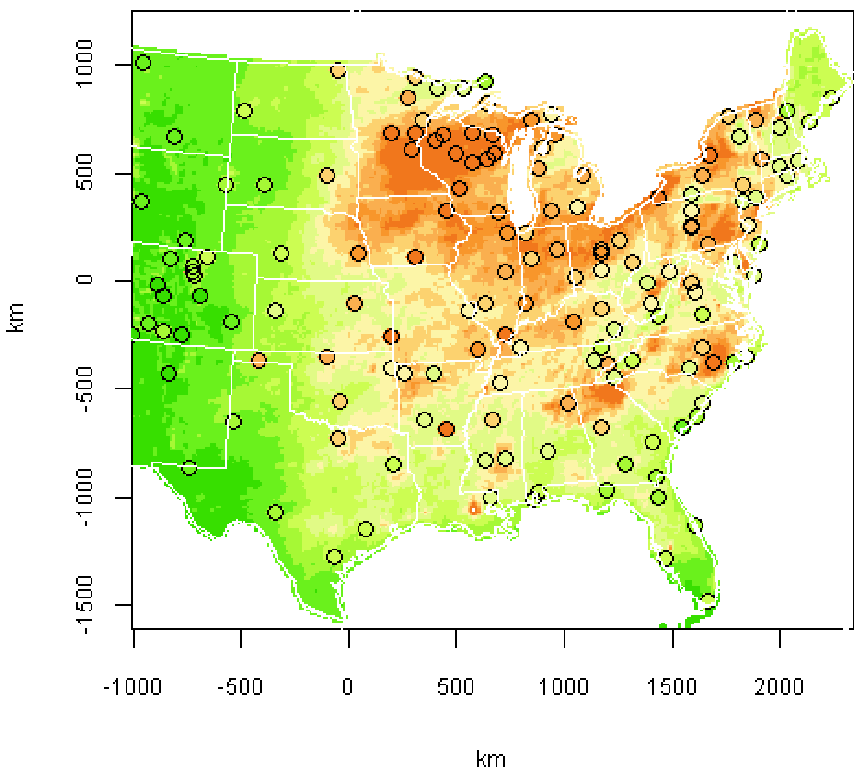


NADP Interpolated Map

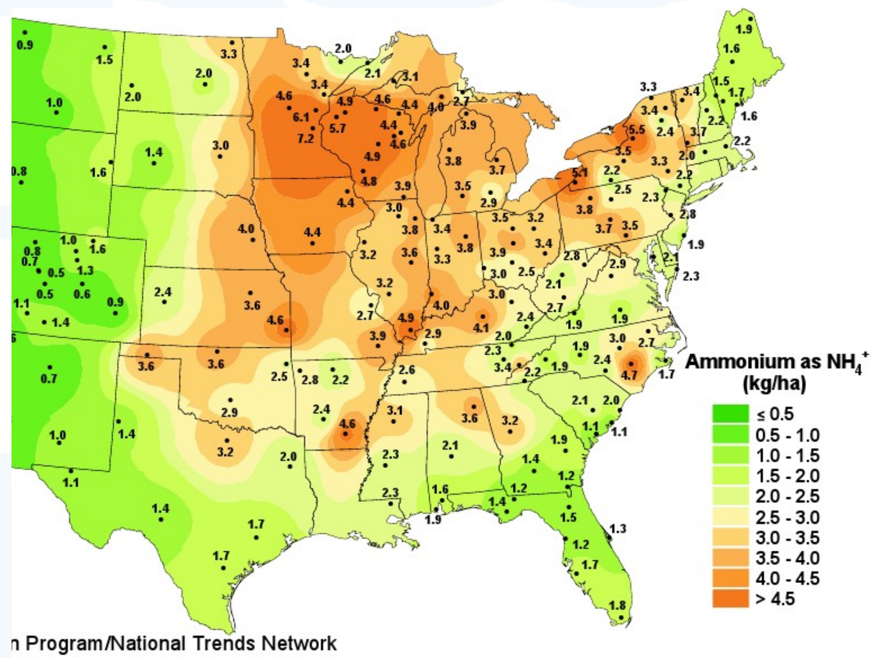


Annual NH_x Wet Deposition

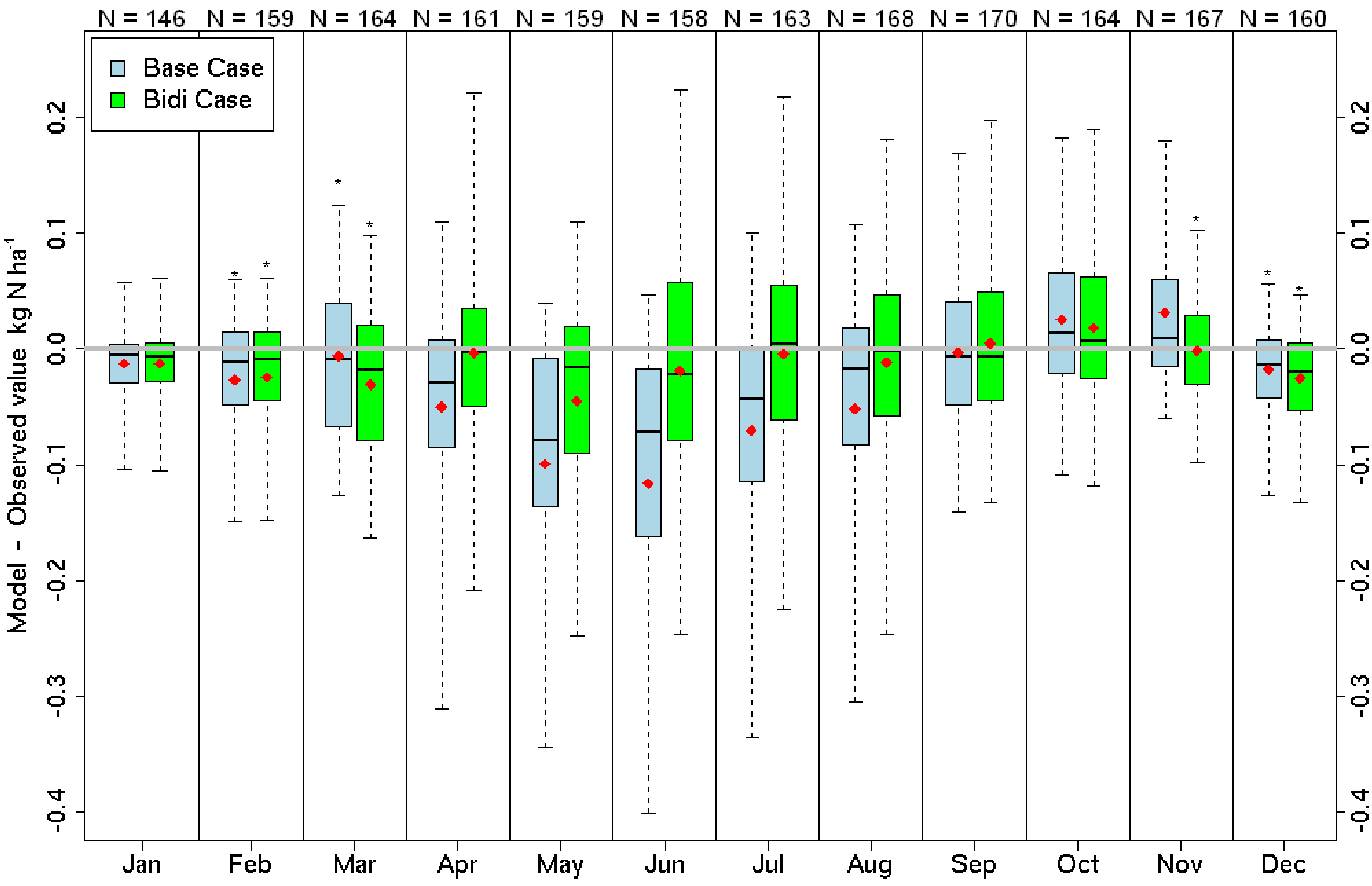
BIDI CMAQ NH_x Wet Dep $\frac{kg}{ha}$



NADP Interpolated Map

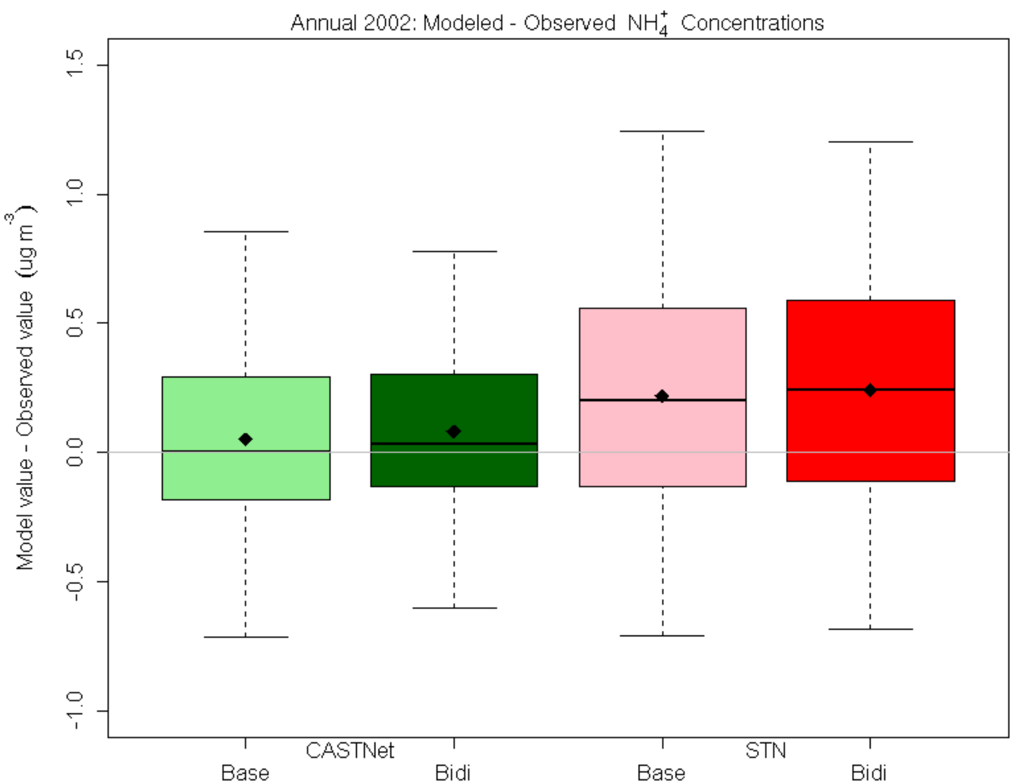


Seasonal NH_x Wet Deposition



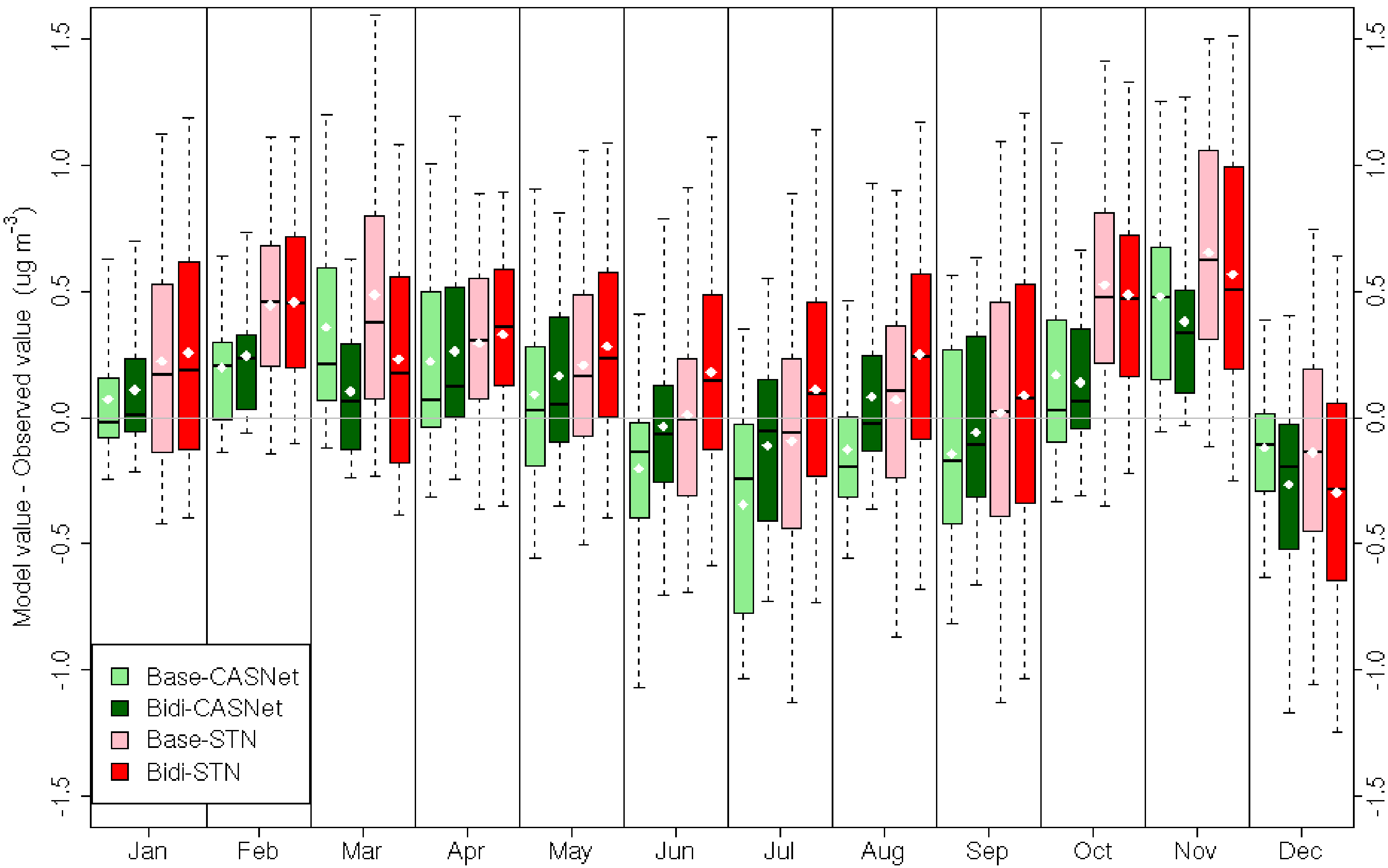
Evaluation against ambient NH_4 observations

Annual ambient NH_4^+ concentration

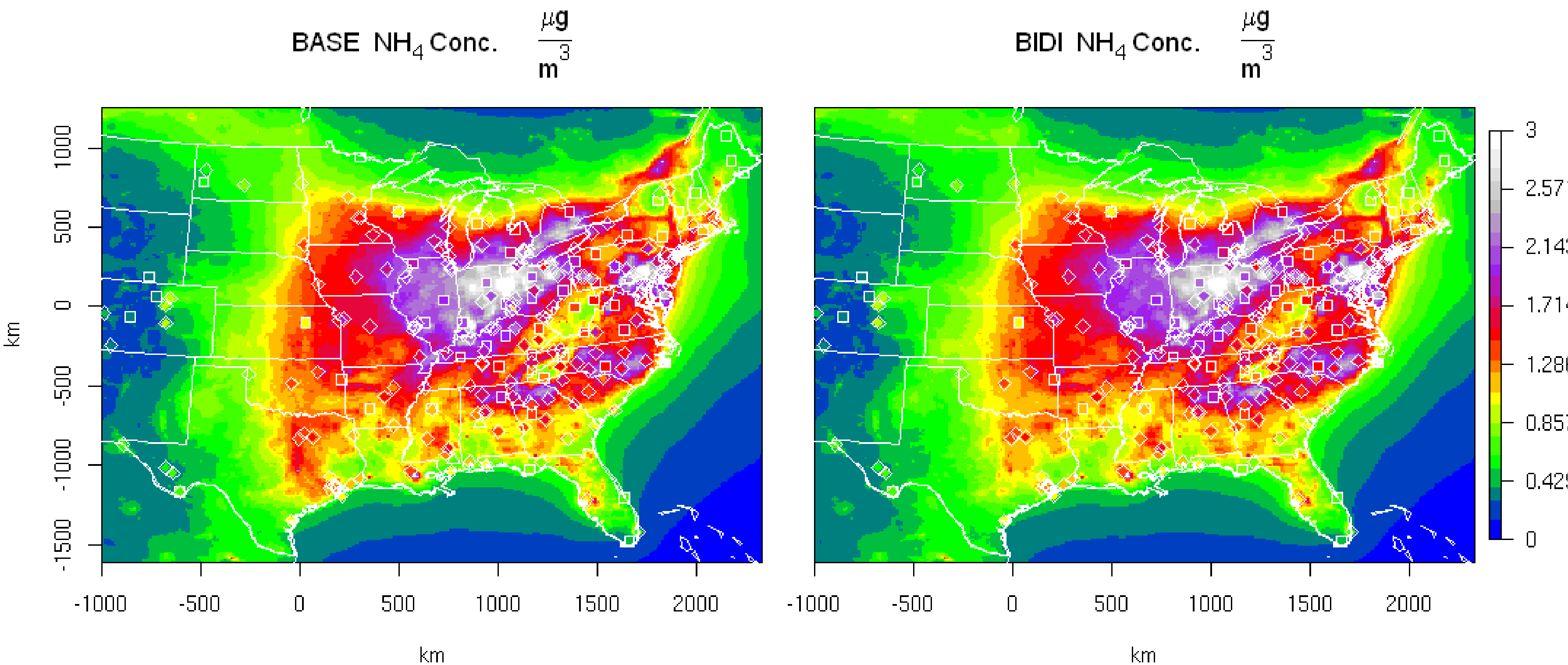


	r	NMB	NME
Base CASTNet	0.793	4%	26%
Bidi CASTNet	0.833	6%	24%
Base STN	0.672	14%	32%
Bidi STN	0.692	16%	32%

Seasonal ambient NH_4^+ concentrations



Annual ambient NH_4^+ concentrations



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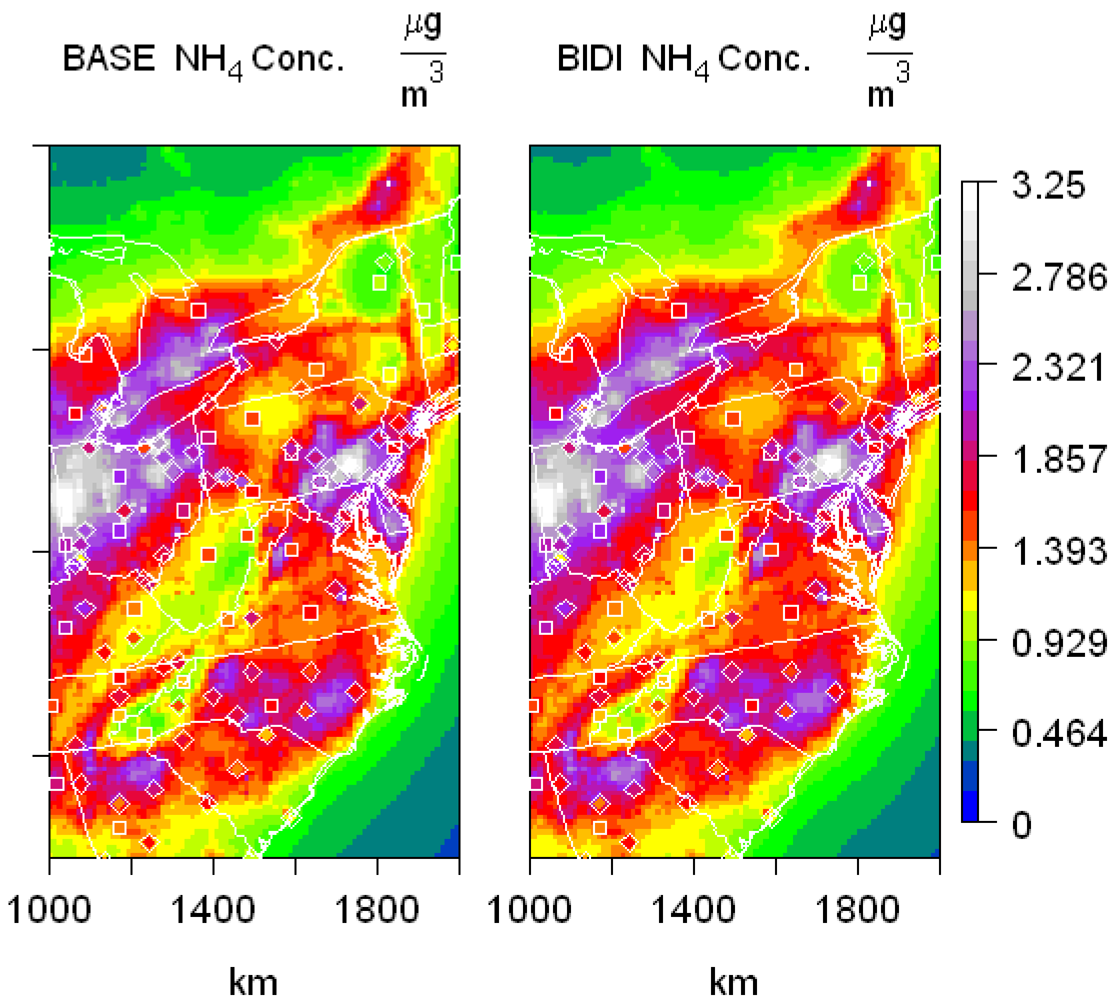
Regional Improvements in NH_4^+



- Annual bias at CASTNet sites reduced from -12% to -4%
- NH_3 emissions in the region changes less than 5%
- Increase in concentrations was due to changes in dry deposition
  - ↓ NH_3 Dry deposition
  - ↑ NH_4 Concentrations
  - ↑ NH_4 Dry Deposition
  - ↑ NH_x Wet Deposition

Conclusions

- CMAQ with Bidi NH_3 was coupled to an agricultural soil nitrogen cycle model
- Reduced dry deposition
  - By a factor of 2 at background sites
  - By a factor of 3 for the model domain
- Increased partitioning to the aerosol phase and wet deposition
- Increased transport of reduced N out of the modeling domain by ~10%
- Improvements in precipitation corrected wet deposition and ambient aerosol estimates support these changes in the NH_3 emissions and fate

Caveats and Future Research

- Ambient NH_3 measurements needed for a more robust model evaluation
  - Ambient surface observations from AmoN and TES satellite derived observations are becoming available
  - Need 2009 meteorology and emissions for CMAQ
- Need to revisit CAFO NH_3 emissions
  - Were developed using inverse modeling techniques on a previous version of CMAQ
    - Will improvements in modeling science and inverse modeling techniques improve these estimates?
- Beta version of an in-line fertilizer scenario application tool are in development for the next release of CMAQ

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Questions?

Thanks to John Walker, Robert Pinder, Kristen Foley, and Wyat Appel