United States Environmental Protection Agency

Improvements in CMAQ NH_3 Emission and Deposition Processes

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Scope of the Talk

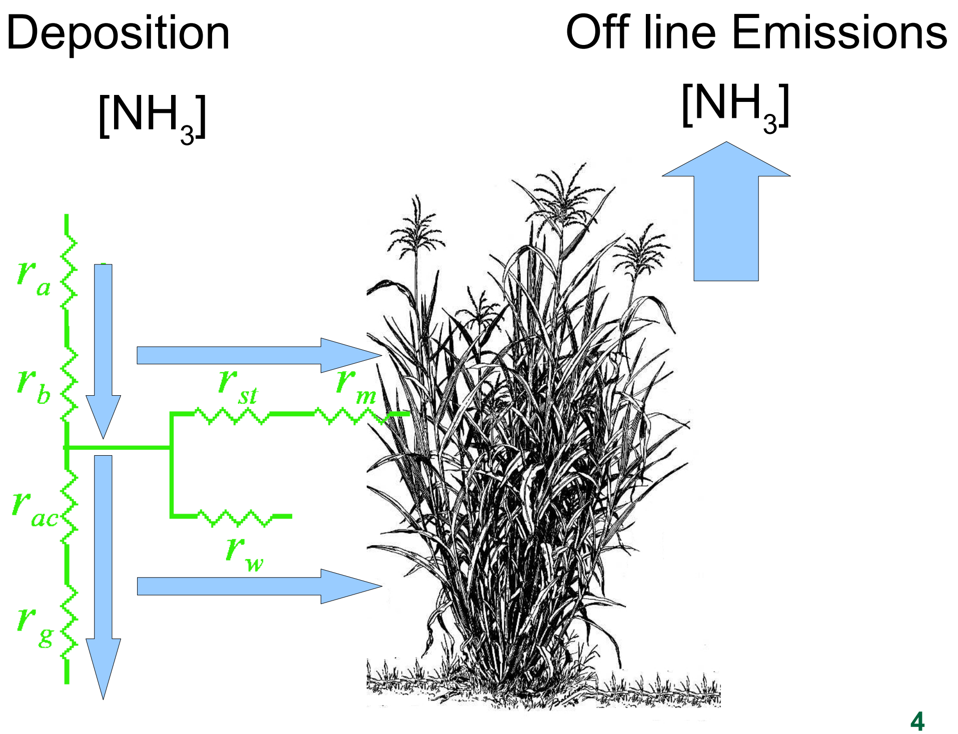
- Motivation
  - What is bidirecitonal NH3 exchange?
  - Why invest the effort?
- NH_3 bidirectional exchange in CMAQ v5.0
    - Coupled Agro-ecosystem model to the chemical transport model
  - Impact on model results
    - Concentration, deposition and emission fields
  - Evaluation against network observations
    - NH_x Wet Deposition, Inorganic aerosol and NH_3 ambient concentrations
  - Chesapeake Bay deposition budget
- Temporal NH_3 CAFO emissions (still in development)
  - Conceptual model and preliminary evaluation
- Next Steps

Reduced N in the environment

- NH_3 is the primary atmospheric base
  - Precursor to atmospheric particulate matter formation
    - Deleterious to human respiratory and cardiovascular systems
    - Short term climate forcer
  - NH_3 + NH_4^+ Deposition accounts for ~35% of the total nitrogen deposition in the U.S. (Dennis et al. In Review)
    - Contributes to excess nitrogen in ecosystems
      - Surface water eutrophication and terrestrial biodiversity loss
    - Contributes to soil and surface water acidification
- NH_3 air-surface exchange is bi-directional
  - NH_3 can be emitted (evasion) or deposited
  - Net evasion or deposition varies spatially and temporally
    - Depends on land use, environmental variables, ambient NH_3 concentration and land management practices
  - Unidirectional dry deposition velocity concept does not represent this dynamic process

NH_3 air surface exchange

- Unidirectional exchange is used by most air-quality models
- Assumes that the subsurface concentration is zero
  - Not applicable to NH_3
  - NH_3 emissions and deposition are typically modeled separately
    - Overestimates deposition in areas where there is a large subsurface NH_3 concentration, e.g. agricultural fields.



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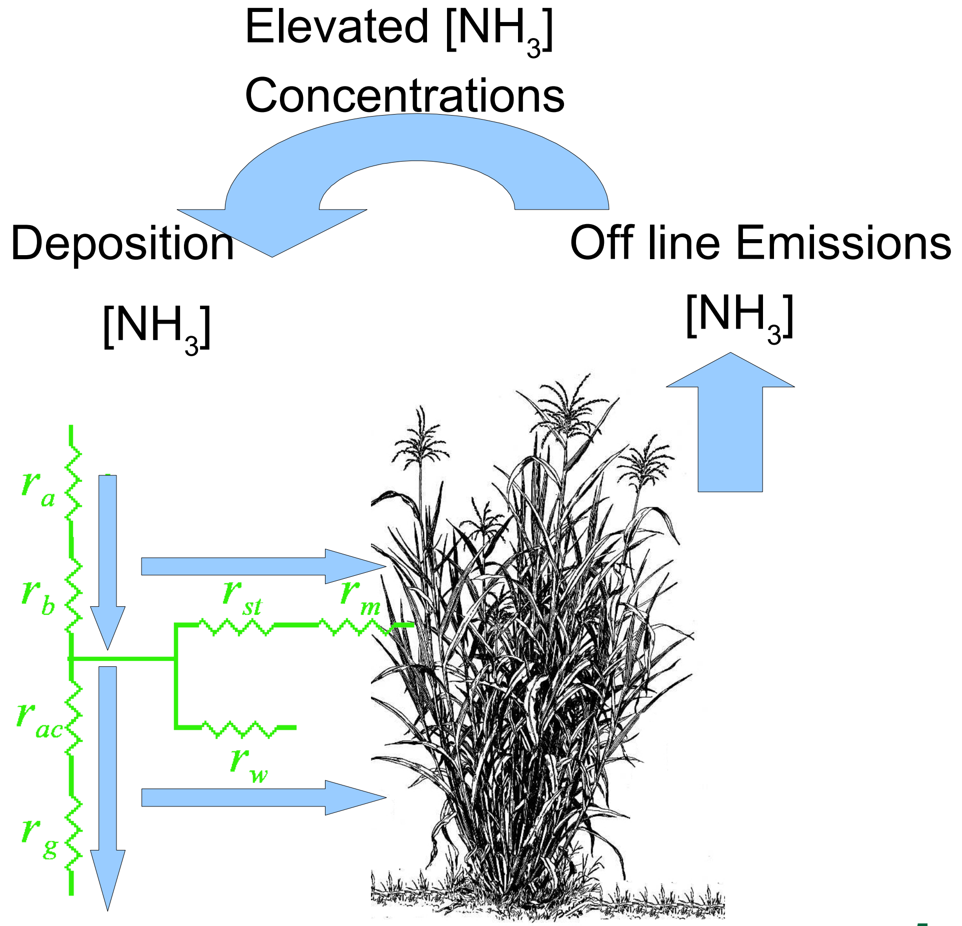
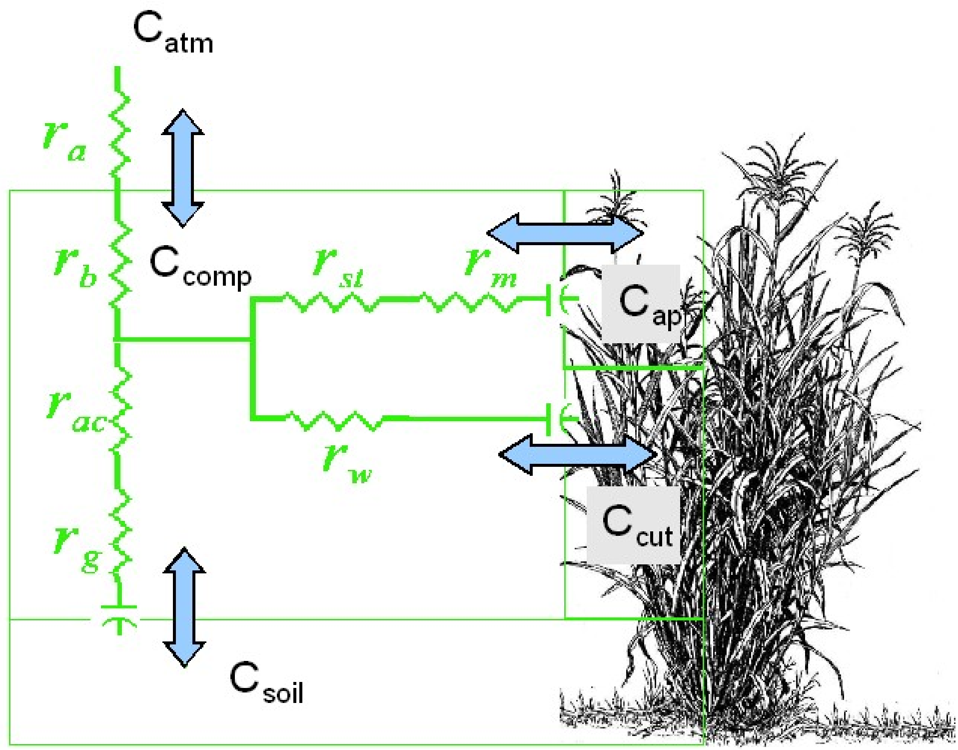


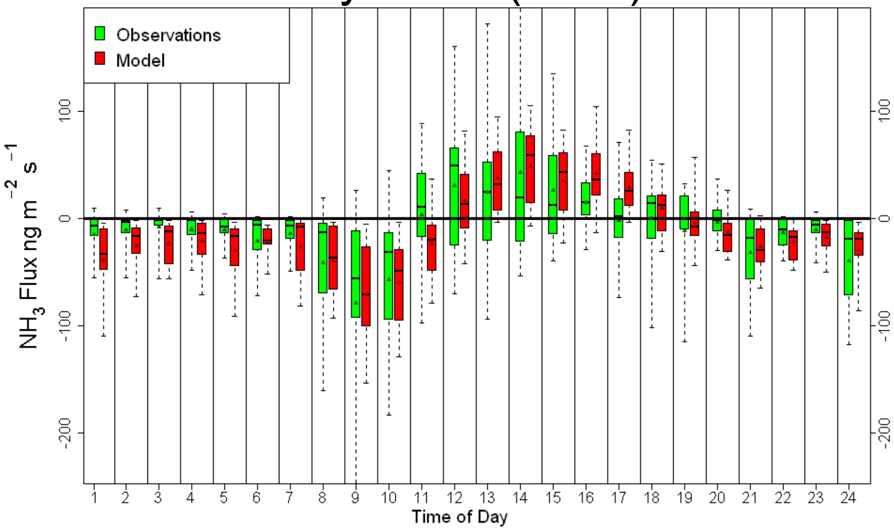
NH_3 air surface exchange

- Regional and global models generally do not parametrize bidirectional NH_3 exchange
- CMAQ Bidirectional exchange model was developed based on field scale models (Bash et al. 2012, Bash et al 2010, Cooter et al. 2010)
  - Estimates a compensation point based on soil water solution and apoplastic NH_4^+ and pH
    - Compensation point is an ambient concentration at which the flux is zero
  - Modeled NH_3 flux evaluated in a collaborative measurement campaign (Pleim et al. in review, Walker et al. 2012)

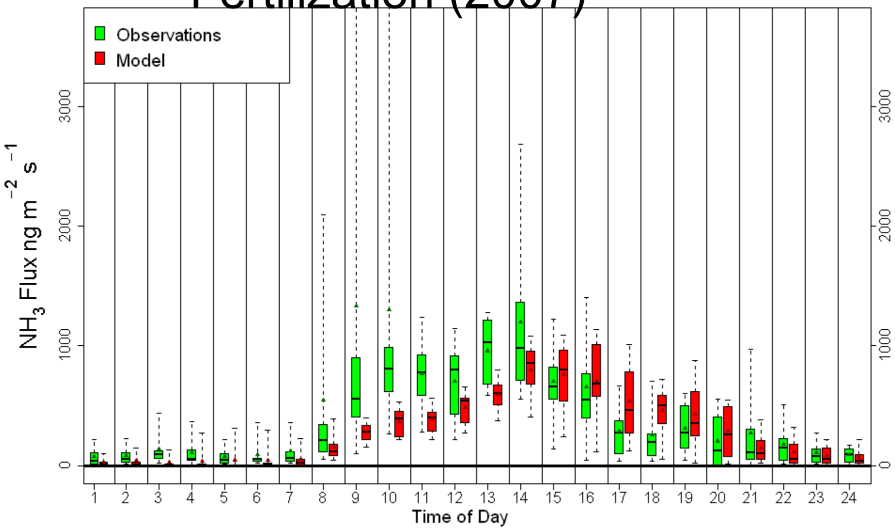


Modeled Bidirectional NH_3 air surface exchange

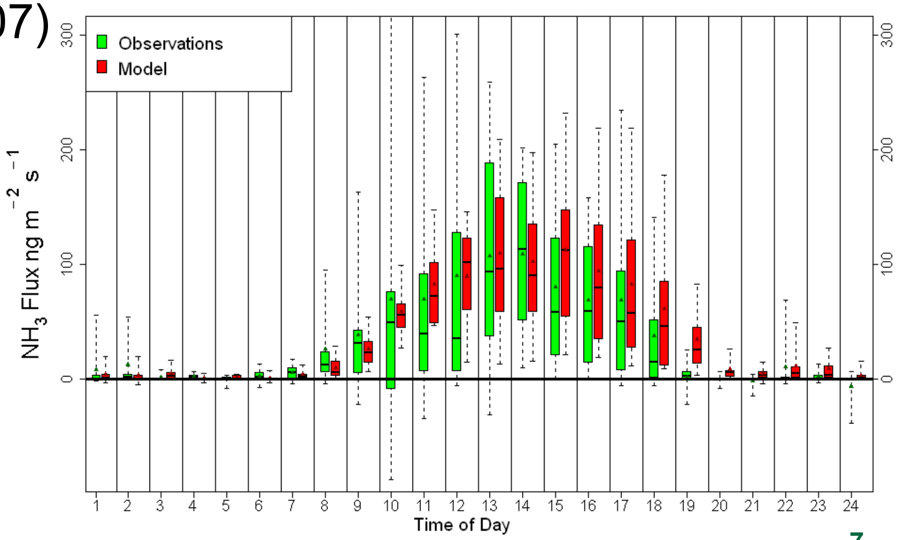
Soybeans (2002)



Corn 1 Week following Fertilization (2007)



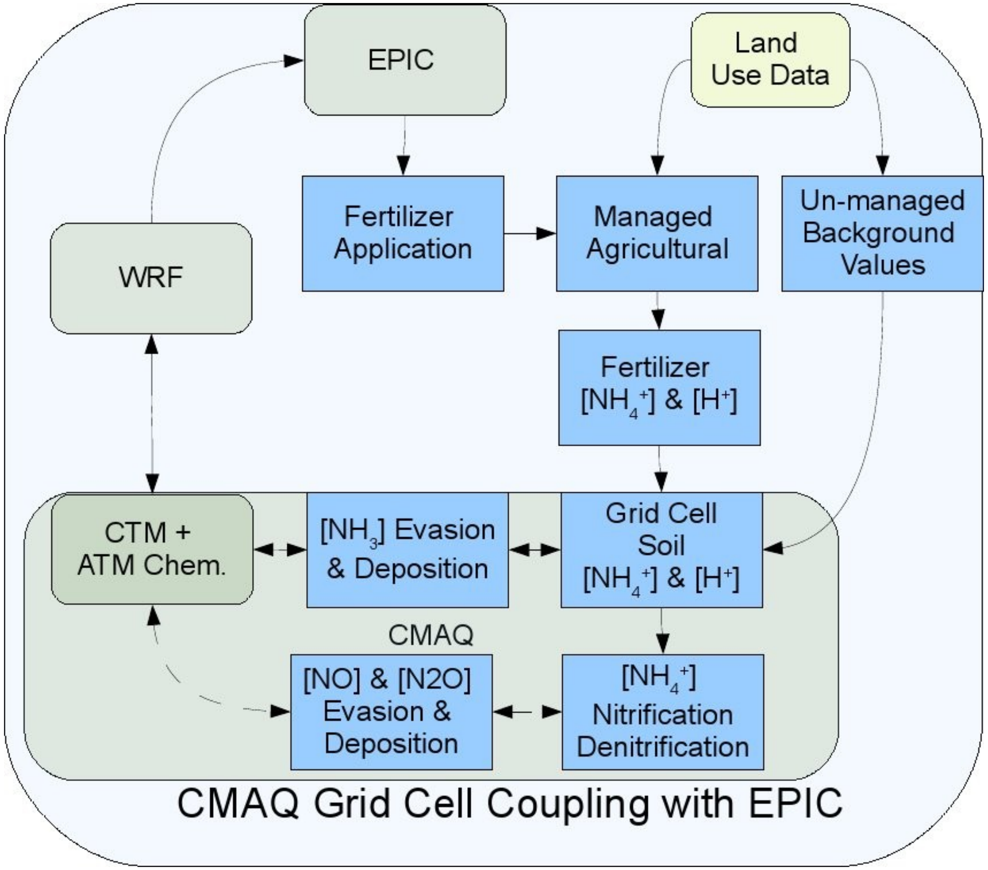
Corn 1 Month following Fertilization (2007)



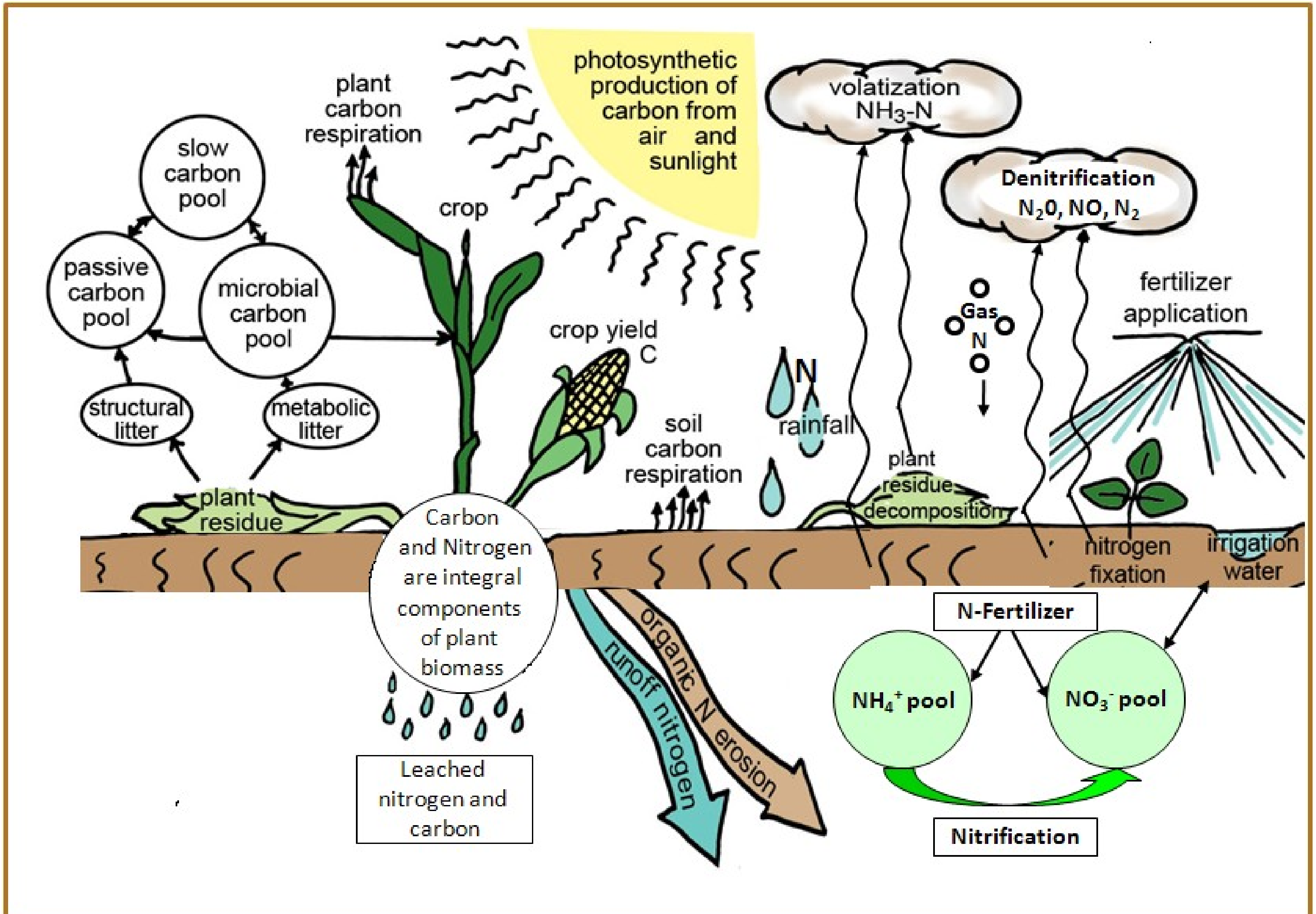
- Direction and magnitude of the flux captured well
- Dynamics following fertilization captured
- Dry deposition of NH_3 is reduced

Regional Scale Application

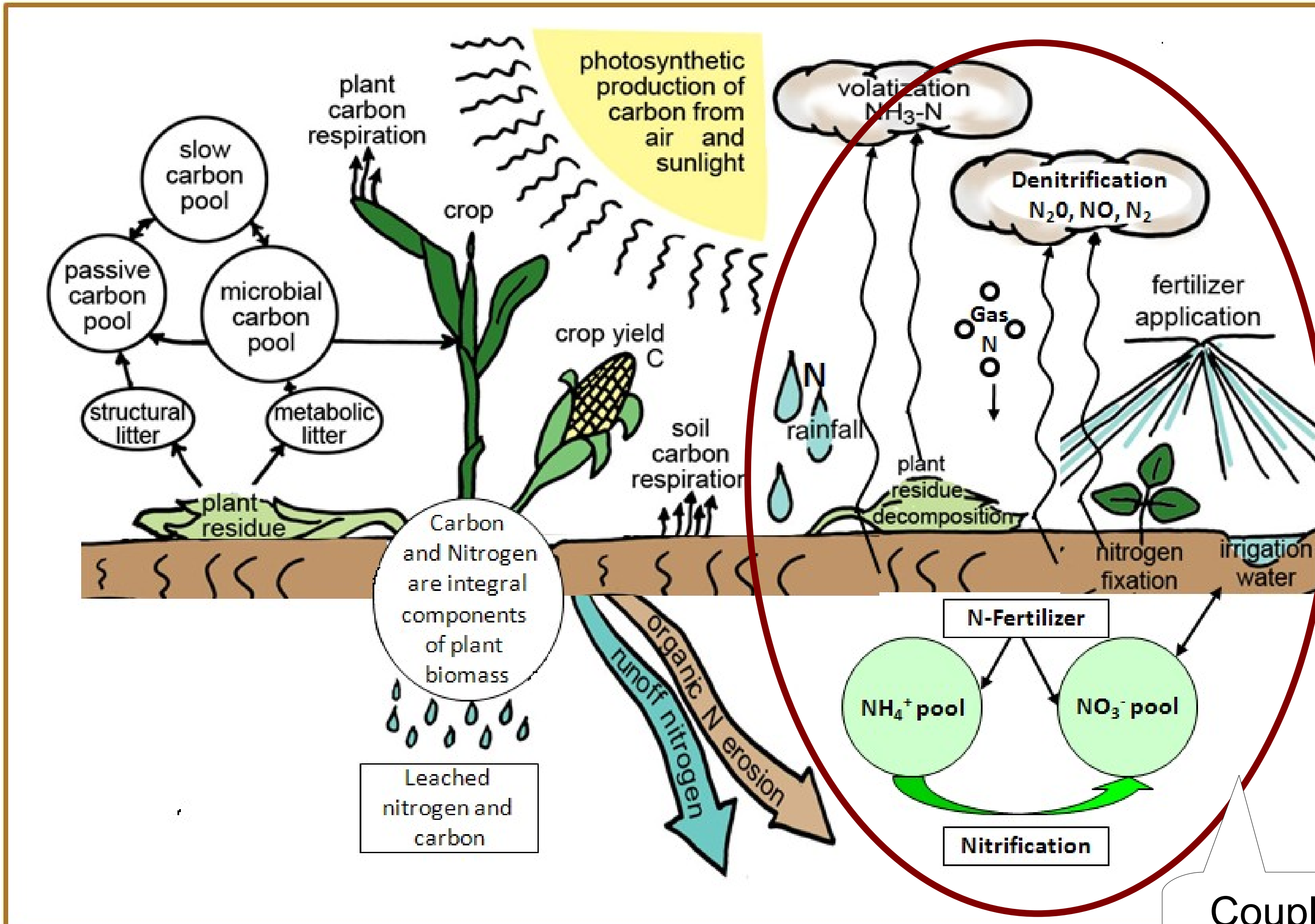
- Agriculture activity data modeled using the USDA's Environmental Policy Integrated Climate model (EPIC) for the Continental US (Cooter et al. 2012)
- Fertilizer NH_4^+ is applied to sub-grid cell agricultural land use soil layers by crop type
- The NH_3 flux is estimated for each sub grid cell land use type
- CMAQ modeled soil NH_4^+ in agricultural soils are updated due to the NH_3 flux and nitrification
- Aggregated fluxes are passed to the CTM



EPIC Processes



EPIC Processes

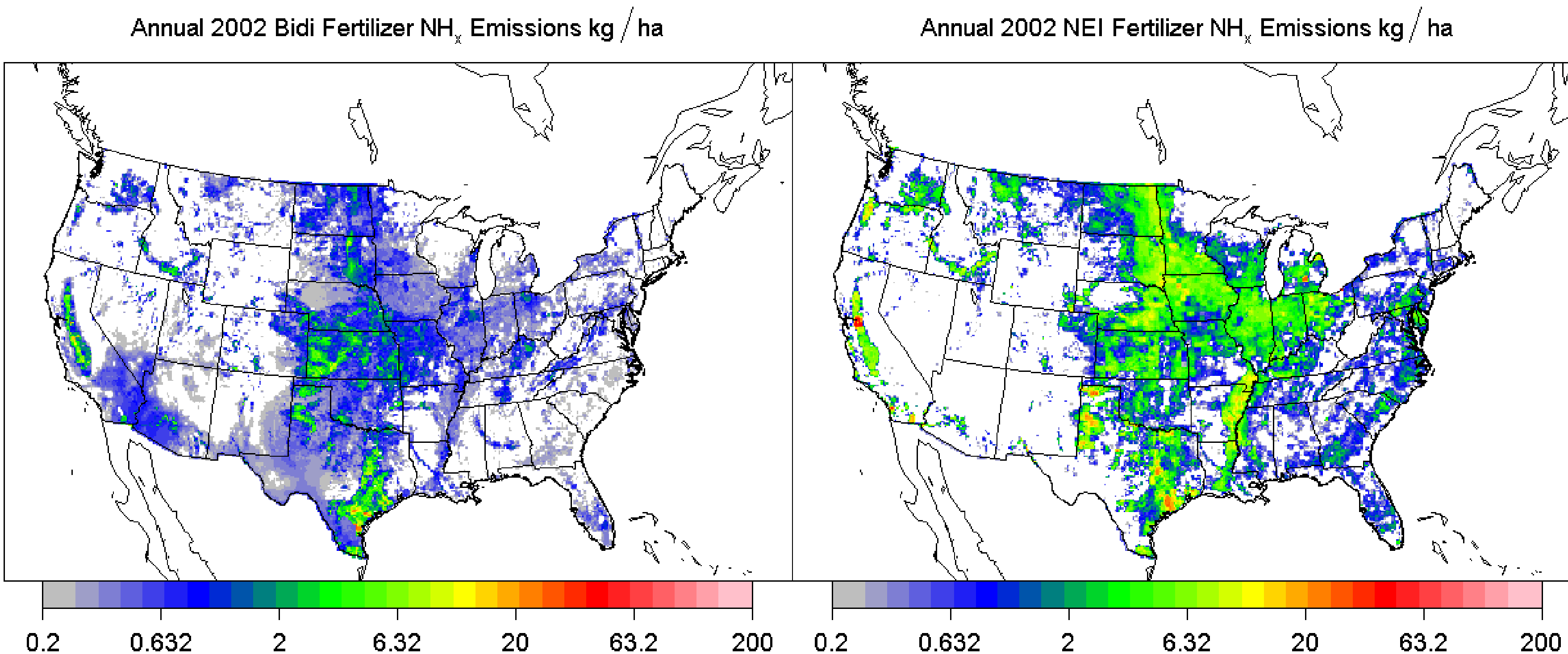


Coupled With CMAQ

Regional Scale Simulations

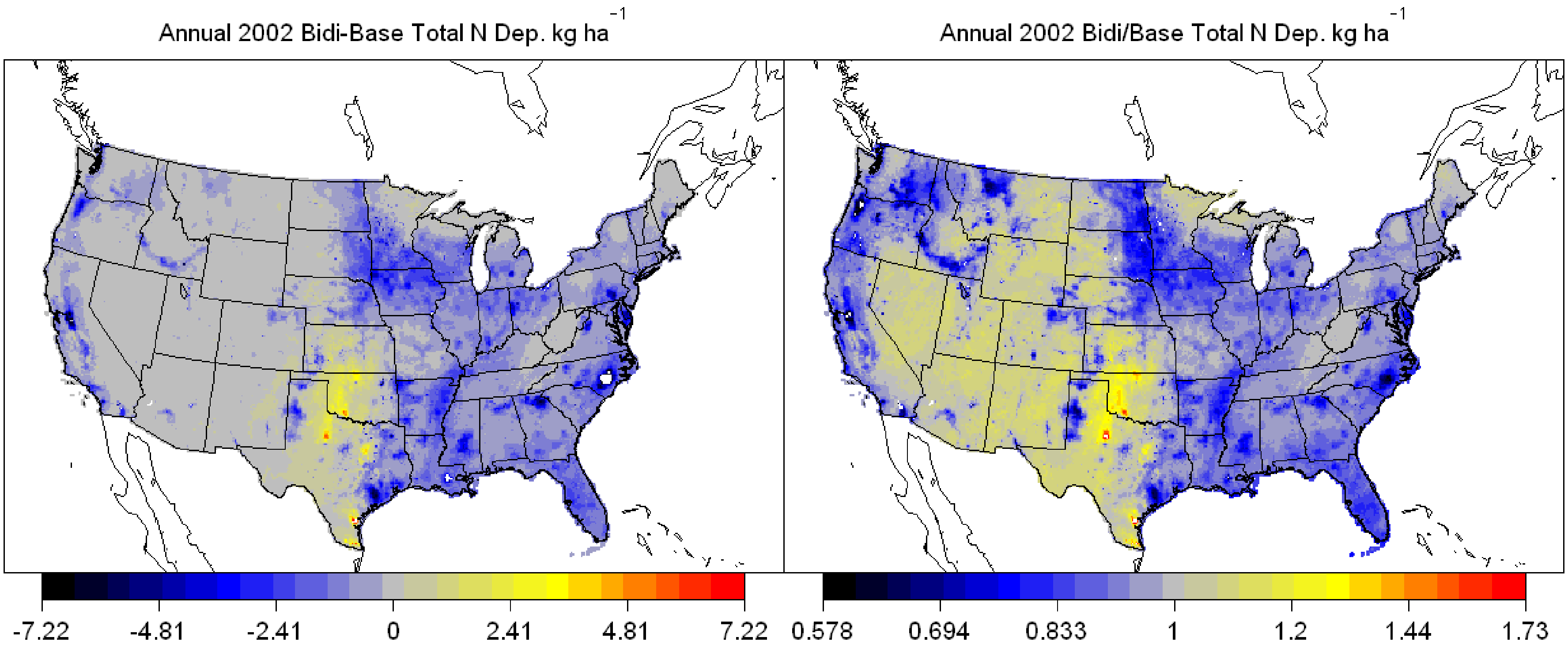
- Simulations using CAMQ v5.0.1
  - 2002 annual run evaluated against network observations
  - July 2007 simulations (Base case only)
    - CAFO diurnal emissions evaluated against NH_3 observations
- Two model cases were simulated
  - Base case:
    - NEI Emissions
    - No bidirectional NH_3 exchange
  - Bidi case:
    - NEI Emissions without NH_3 evasion from agricultural cropping sectors
    - Bidirectional NH_3 exchange
  - Identical model inputs and configurations except for the NH_3 emissions from cropping systems and bidirectional NH_3 exchange

NH_3 emissions



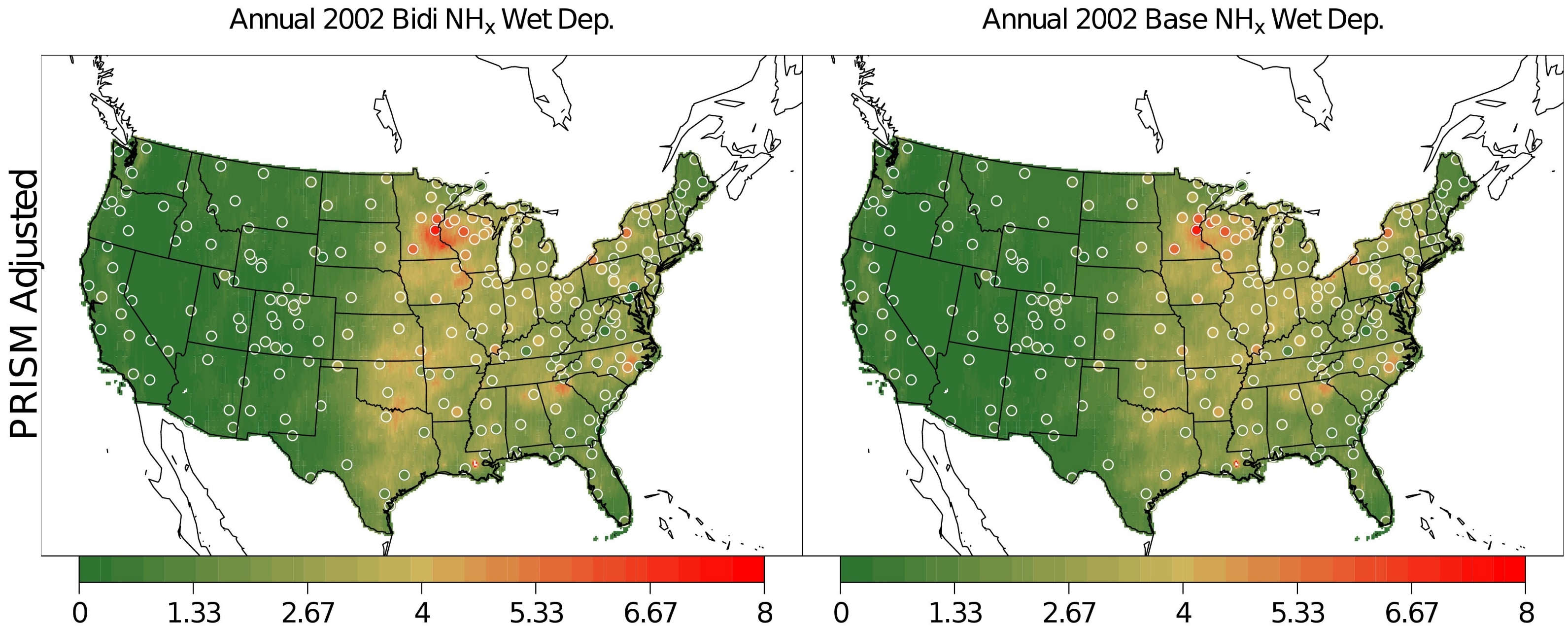
- 66% lower fertilizer emissions (20% total reduction)
  - 30% from fertilizer and 70% from animal operations in CMU
  - 13% from fertilizer and 87% from animal operations in Bidi
    - More in line with other contemporary estimates (Gilliland et al 2006)

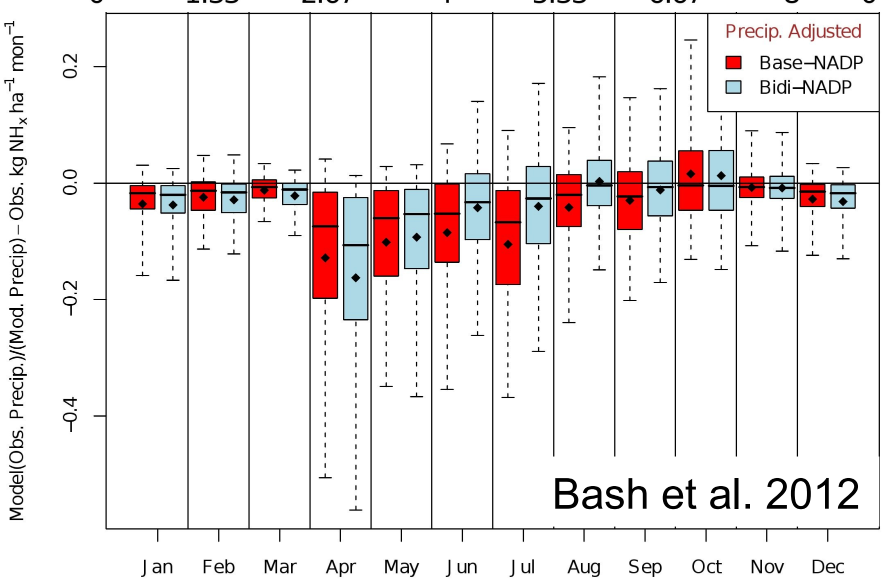
Total N Deposition



- 6.4% lower total N deposition to Continental US
  - Reduced NH_3 dry deposition to agricultural areas
  - Increased NH_x wet deposition in the West and Midwest

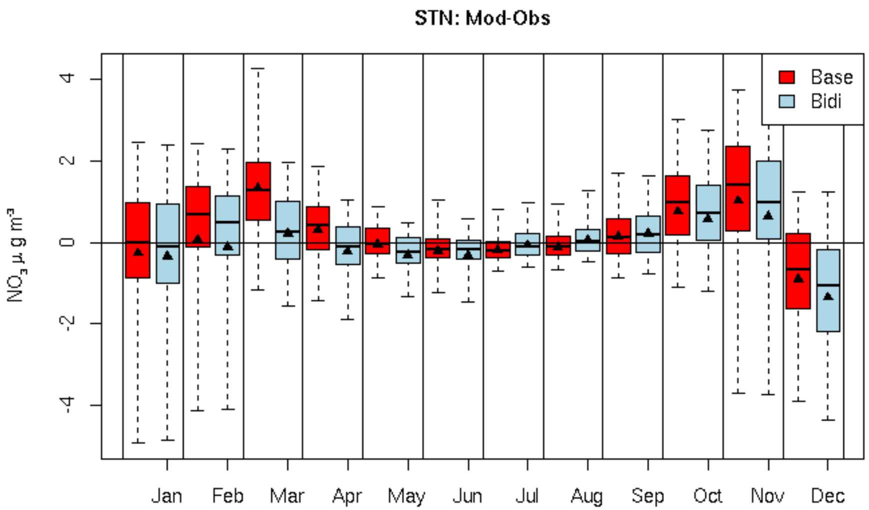
NH_x Wet Deposition

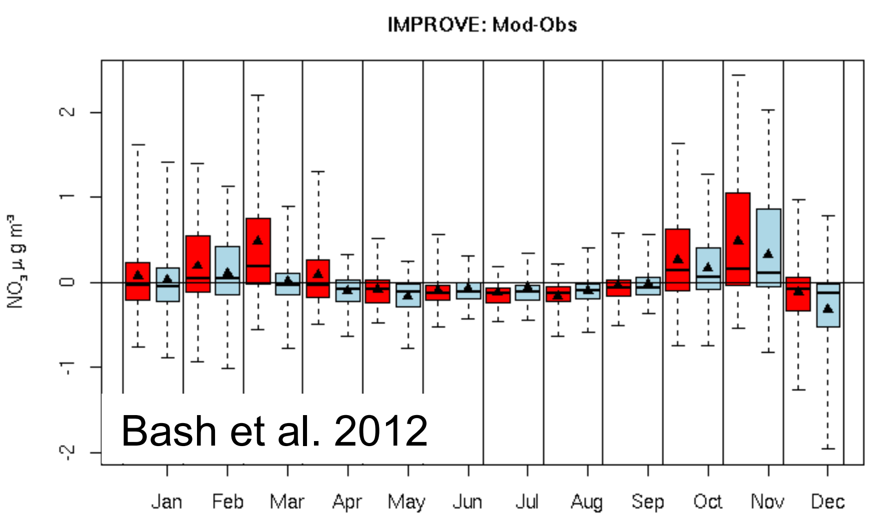




- NHx wet dep. bias and error reduced using bidi NH3 exchange
  - 6.2% reduction in NMB and 2% reduction in NME
  - Regional improvements in the West and Upper Midwest, Degradation in the Southeast
- Accounting for model precip. errors is critical

NO_3 Aerosol Concentrations

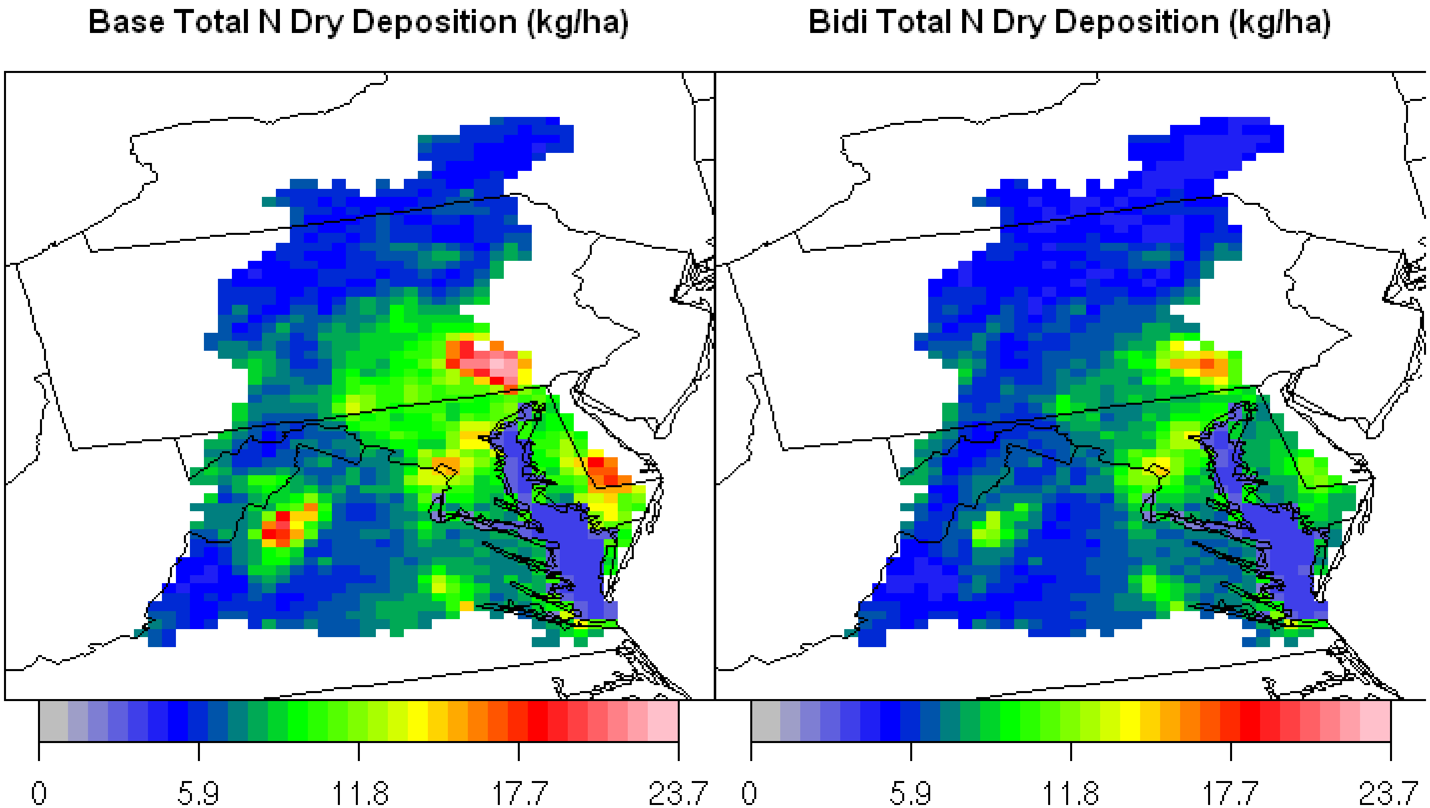




Bash et al. 2012

- Improved annual and seasonal NO_3^- estimates at IMPROVE and STN sites
  - Introduced an annual bias of -11% and increased NMB at STN sites
  - 18% reduction in NMB at IMPROVE sites
- Large reductions in spring and fall over estimates
  - Up to 80% reduction in NMB
  - Due to reduced NH_3 evasion from cool soil surfaces

Chesapeake Bay Total N Dry Deposition



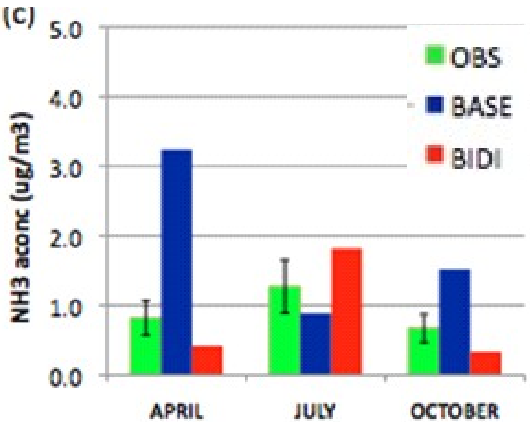
- 16.0% reduction in total N dry deposition
  - 3.3% increase in direct deposition to water bodies
  - 16.1% reduction in deposition to terrestrial land use
    - -19% wetlands, -15.6% developed, -13.8% forested, -20.2% agriculture

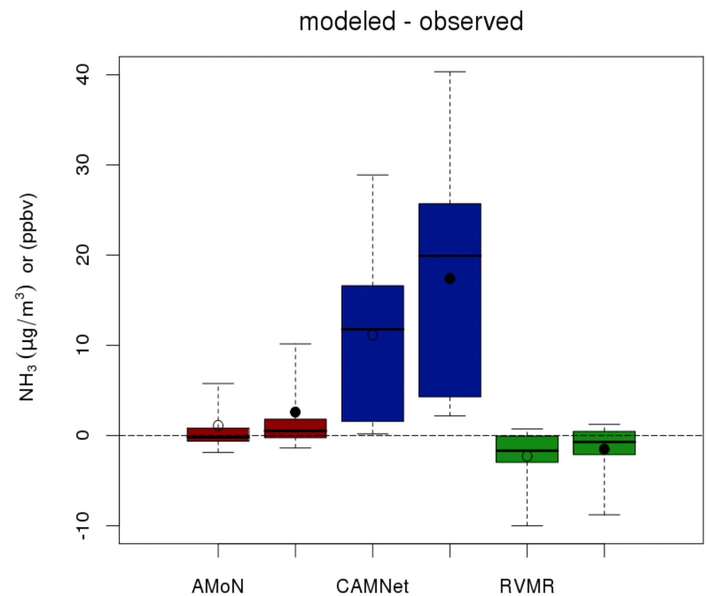
Change in Chesapeake Bay N Deposition

	Dry Deposition			Wet Deposition		
Land Use	Total N	Oxidized N	Reduced N	Total N	Oxidized N	Reduced N
Total	-16.0%	-0.7%	-46.4%	8.7%	0.9%	17.8%
Terrestrial	-16.1%	-0.8%	-46.1%	8.6%	0.8%	17.7%
Water	3.3%	0.1%	12.4	8.7%	0.9%	19.7%
Forest	-13.8%	-0.8%	-46.3%	8.8%	0.8%	18.4%
Developed	-15.6%	-0.6%	-44.3%	8.5%	0.8%	17.2%
Agriculture	-20.2%	-0.6%	-45.5%	8.1%	0.9%	16.3%
Wetlands	-19%	-0.1%	-52.7%	9.0%	0.8%	18%

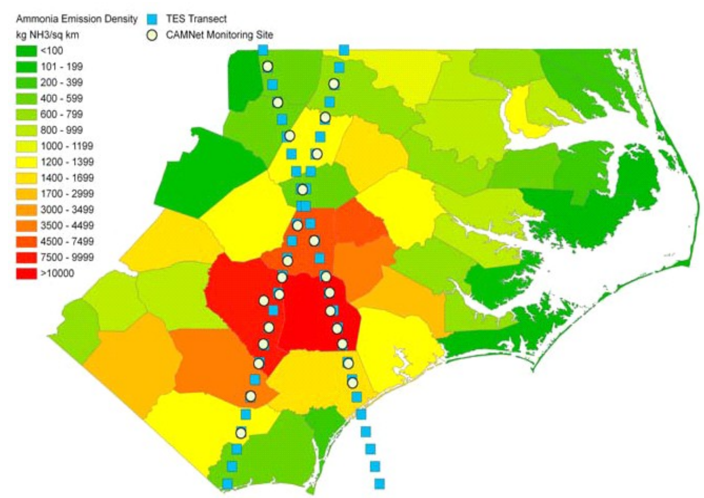
2009 Ambient NH_3 Case Studies

- Fertilizer emission dominated sites
  - Improved seasonal NH_3 estimates





- Animal emission dominated sites
  - Degradation in NH_3 model estimates when using bidirectional exchange
  - Model biased high against two week surface and biased low against mid day satellite observations
  - Model biased 10x high against nighttime and ~50% low against daytime surface observations



Conceptual Mechanistic Model for Animal Emissions

- Use a resistance model approach
- Assume NH_3 at the source is >> that in atmosphere
- Assume NH_3 emissions originate from an aqueous pool
- Key parameters are atmospheric resistance and $NH_4^+{}_{(aq)} \leftrightarrow NH_{3(g)}$ equilibrium

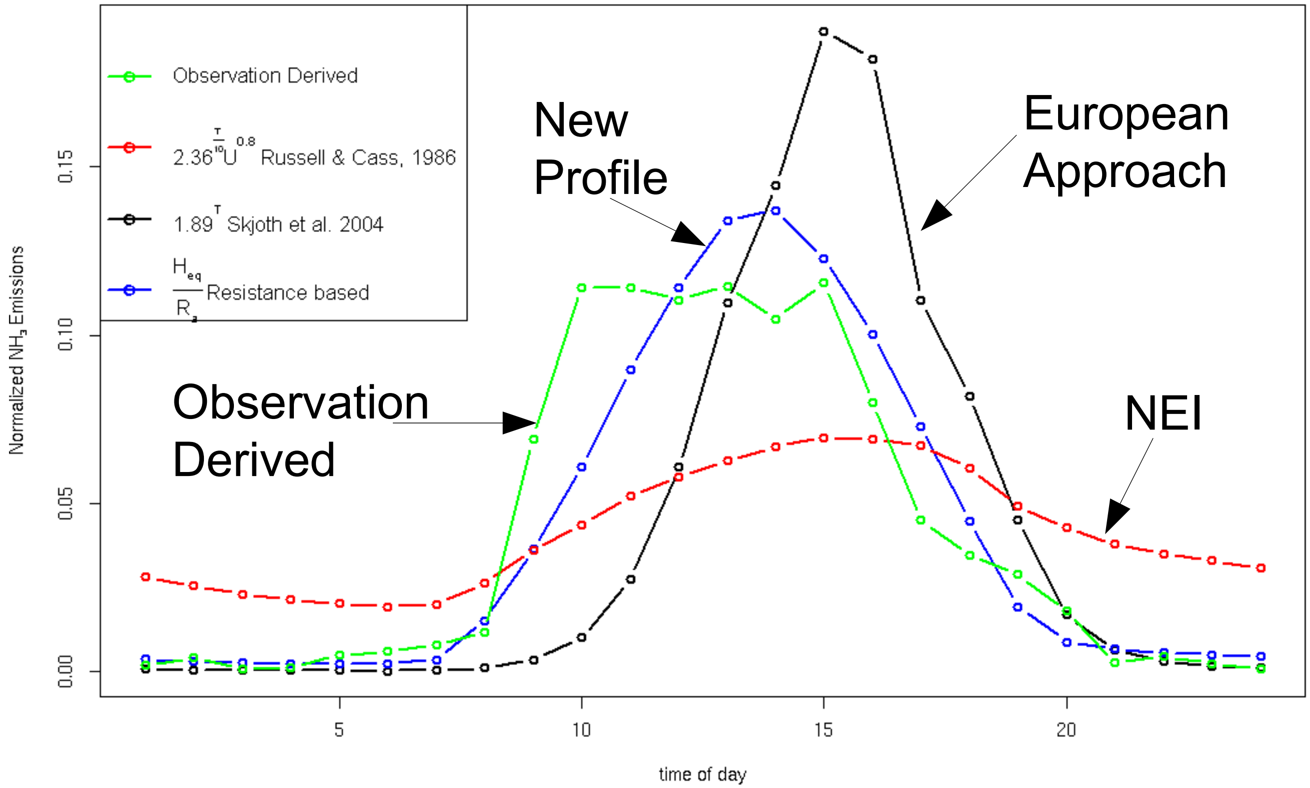
R_a

$R_{management}$


Urea -> $NH_4^+{}_{(aq)}$-> $NH_{3(g)}$

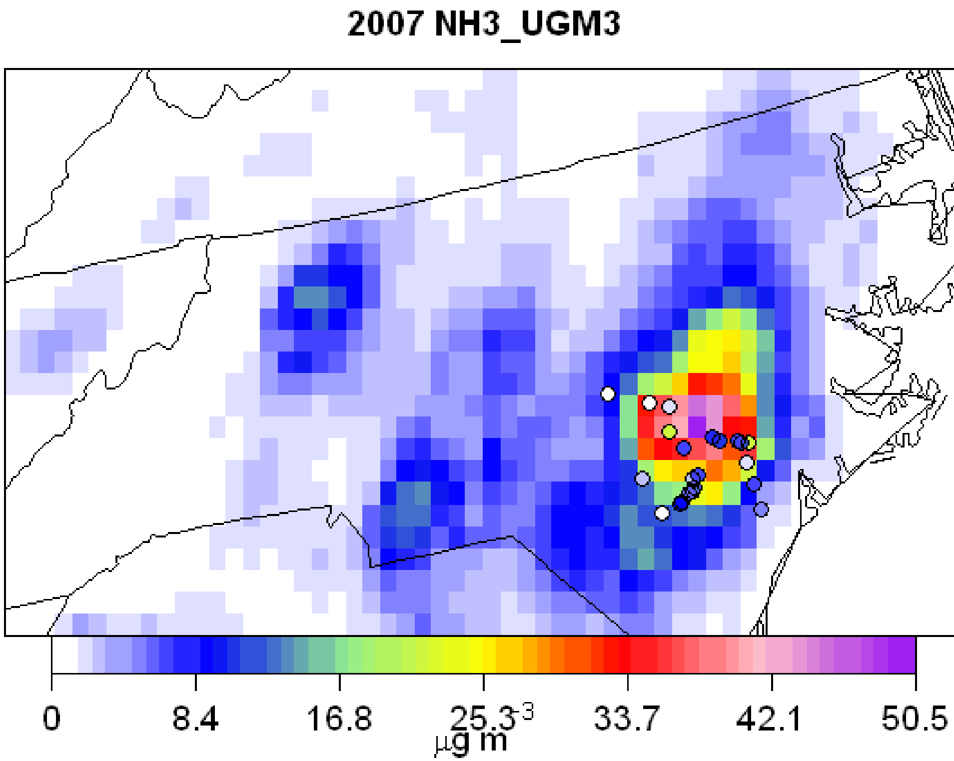
Surface NH_3 pool

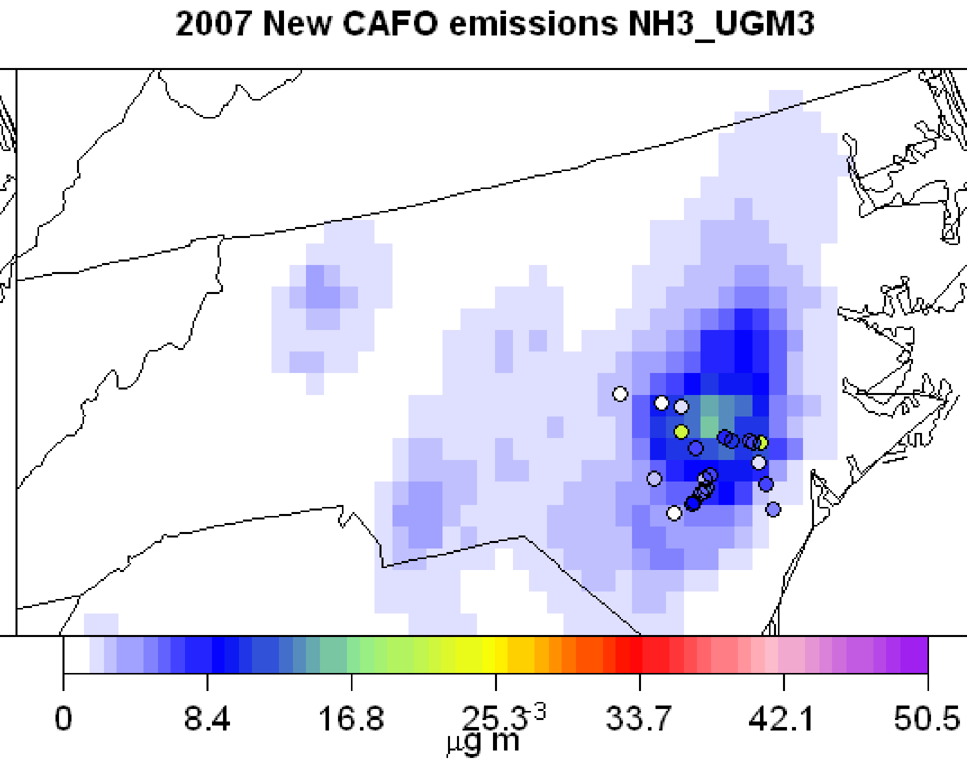
Improved Diurnal NH_3 Profile



- Semi-mechanistic model comprised of Henry's solubility equilibria and aerodynamic resistance
  - Used to temporally reallocate monthly emission totals
- Compares well with observation derived profiles and European emission modeling profiles

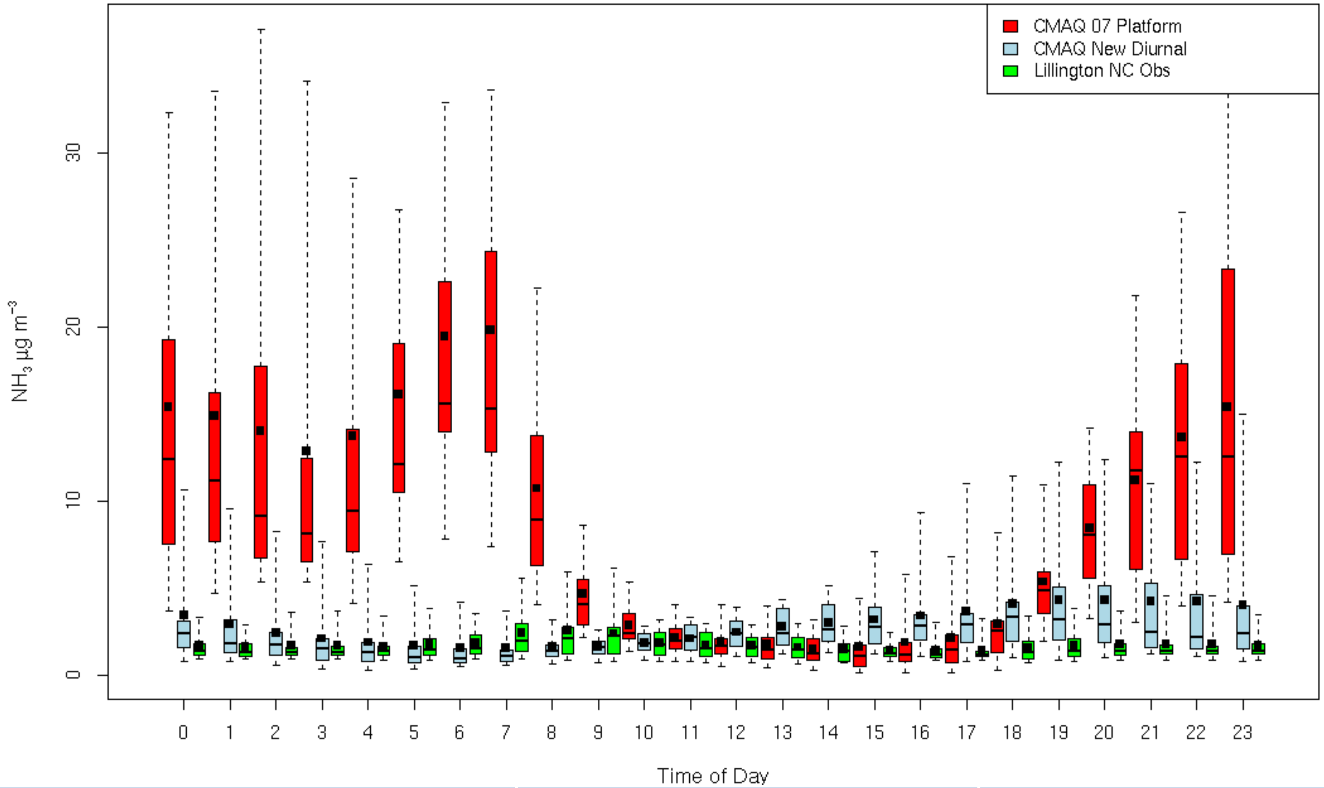
Improved NH_3 Estimates





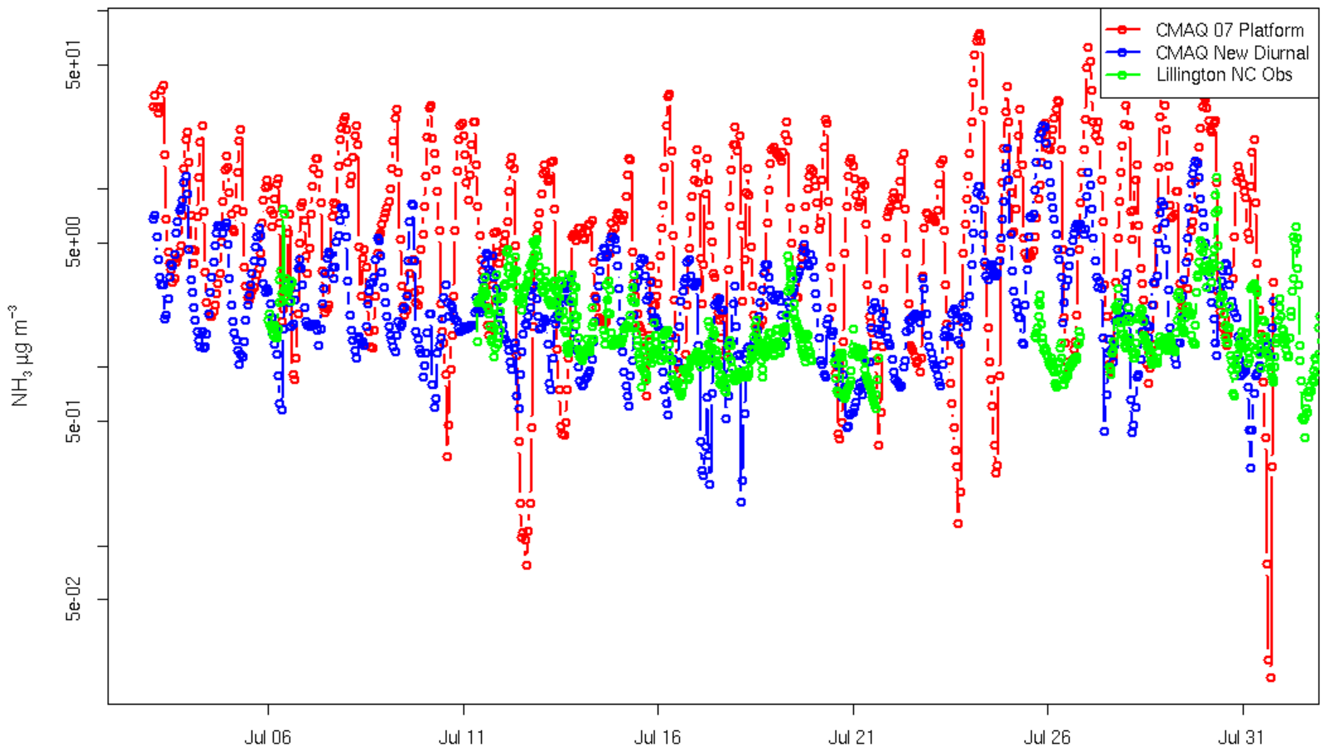
	Mean	NMB
Observations	7.5 µg m^{-3}	-
NEI Profile	25 µg m^{-3}	238%
New Profile	8.1 µg m^{-3}	9%

Model and Observations at Lillington, NC



	Mean	NMB
Observations	1.8 µg m^{-3}	-
Original Profile	9.0 µg m^{-3}	349%
New Profile	2.9 µg m^{-3}	59%

Model and Observations at Lillington, NC



- New emissions profile capture the dynamics and magnitude of emissions better
  - Large disagreements still exist
- Bi-directional NH_3 model will likely better capture the observed variability but increase bias at this site

Current and Future Research

- Field measurements and modeling to better understand soil nitrification processes and N cycling in natural systems
  - Are these processes important to air-quality as well as climate?
  - Expand soil geochemistry to include organic N mineralization and soil nitrification processes
    - Improve geochemistry in natural systems
    - Couple N_2O and NO fluxes with land use management
- Modeling and measurements at animal facilities to develop better mechanistic NH_3 emission estimates
- Compensation points in water bodies
- Couple CMAQ with meteorological, biogeochemical, and hydrological models
  - Develop tools for robust system analysis of future climate/emission scenarios

Conclusions

- CMAQ with bidirectional NH_3 exchange:
  - Represents the state-of-the-science of NH_3 air-surface exchange
  - Improved NH_x wet deposition and NH_4^+ and NO_3^- evaluation
  - Connects land use and agricultural management practices to ambient air-quality and acid and nutrient deposition
  - Reduces N dry deposition to terrestrial land use by ~15%
  - Increased direct N dry deposition to water bodies by ~3%
- Satellite observations, monitoring networks, and intensive NH_3 measurements integrated with modeling is improving process based NH_3 emission estimates
  - Allowed for robust case study evaluations
  - Necessary to identify modeling and measurement needs

Questions?

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