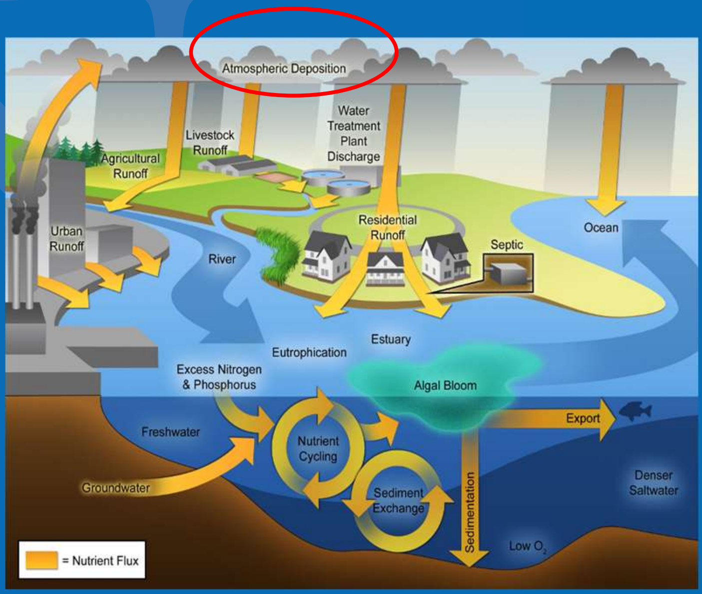
Modeling of Nitrogen and Sulfur Deposition in the Chesapeake Bay Watershed: Trends and Sources

Sarah E. Benish[1], Jesse O. Bash[2], Kristen M. Foley[2], Sergey Napelenok[2], Christian Hogrefe[2], Wyat Appel[2], Lewis Linker[3]

[1]Oak Ridge Institute for Science and Education (ORISE), US Environmental Protection Agency, Research Triangle Park, NC, USA
[2]US Environmental Protection Agency, Research Triangle Park, NC, USA
[3]US Environmental Protection Agency, Annapolis, MD, USA



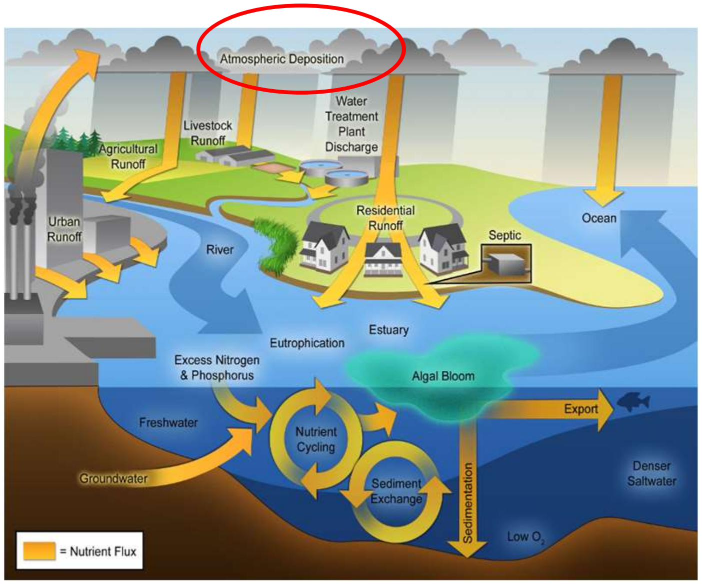
Office of Research and Development
Center for Environmental Measurement and Modeling, Atmospheric and Environmental Systems Modeling Division

CMAS Conference
November 2, 2021

United States Environmental Protection Agency

Motivation

- Consequences of surplus nutrients due to atmospheric nitrogen deposition include stimulated algae growth, costly drinking water treatment, and loss of biodiversity.
- A major pathway of N nutrient loading to the Bay involves the transfer of N-containing compounds from the atmosphere to the surface through scavenging by precipitation (wet deposition) and fallout directly to the surface (dry deposition).
- Use chemical transport models, like CMAQ, to understand atmospheric deposition:



How do new estimates of deposition compare to observations and previous long-term simulations?

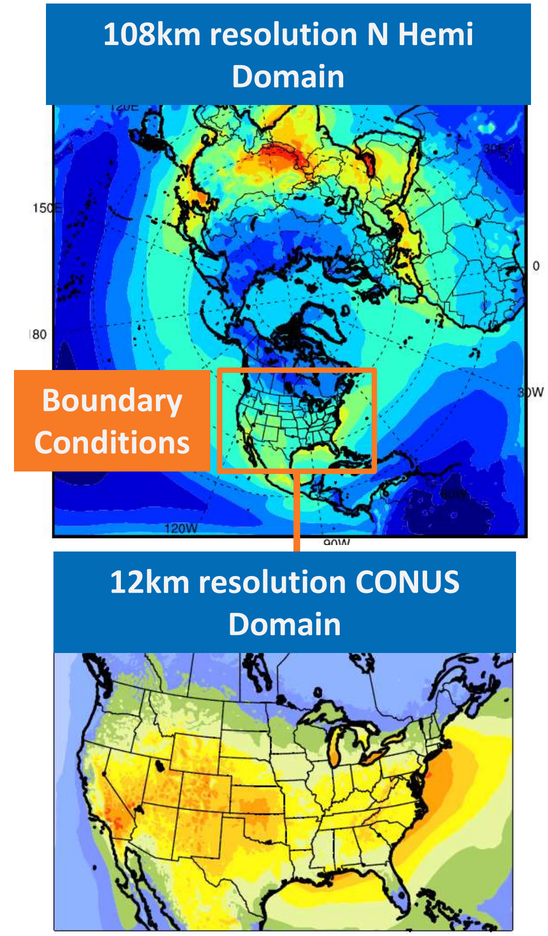
Where and why does deposition change throughout the Chesapeake Bay Watershed?

Which emission sources are contributing to the Bay's high nutrient loading?

EQUATES: EPA's Air QUAlity TimE Series Project

- Temporal coverage: 2002-2017
- Spatial domains: Northern Hemisphere and contiguous US
- Meteorology inputs: New meteorological modeling for both domains using state-of-the-science retrospective simulations
- Emissions inputs: New inventories were developed using EPA's 2017 NEI as the base year with consistent methods used for each sector to avoid artificial step changes
- CMAQ version 5.3.2 (publicly released in October 2020)

EQUATES will supersede previous CMAQ time series and provide a unified set of modeling data across applications



Improvements Over Existing CMAQ Simulations

	ECODEP CMAQv5.0.2 Zhang et al. (2019)	EQUATES CMAQv5.3.2
Model	CMAQv5.0.2 (CB05TUCL-AERO6; w/ bidi NH_3)	**CMAQv5.3.2 (CB6R3-AERO7; w/bidi NH_3)**
Date range	2002 – 2012	**2002 – 2017 (2018 to follow)**
Domain/ Resolution	12km CONUS	**108km N Hemi + 12km CONUS**
Meteorology	WRF3.4	**WRFv4.1.1**
Emissions	Various NEIs / Modeling Platforms	**2017 NEI as primary base year; consistent methods used for each sector (when feasible) to avoid artificial step changes**
Boundary Conditions	GEOS-Chem	**N Hemi CMAQv5.3.2**

CMAQv5.3.2 Updates:

Aerosol and Gas Chemistry

- Improved parameterization of organic nitrates

Deposition

- New land use specific scheme available

Emissions and tools

- New Detailed Emissions Scaling, Isolation, and Diagnostic, **Integrated Source Apportionment method,** pre/post processing tools

Measurement Model Fusion Improvements to Wet Deposition

EQUATES

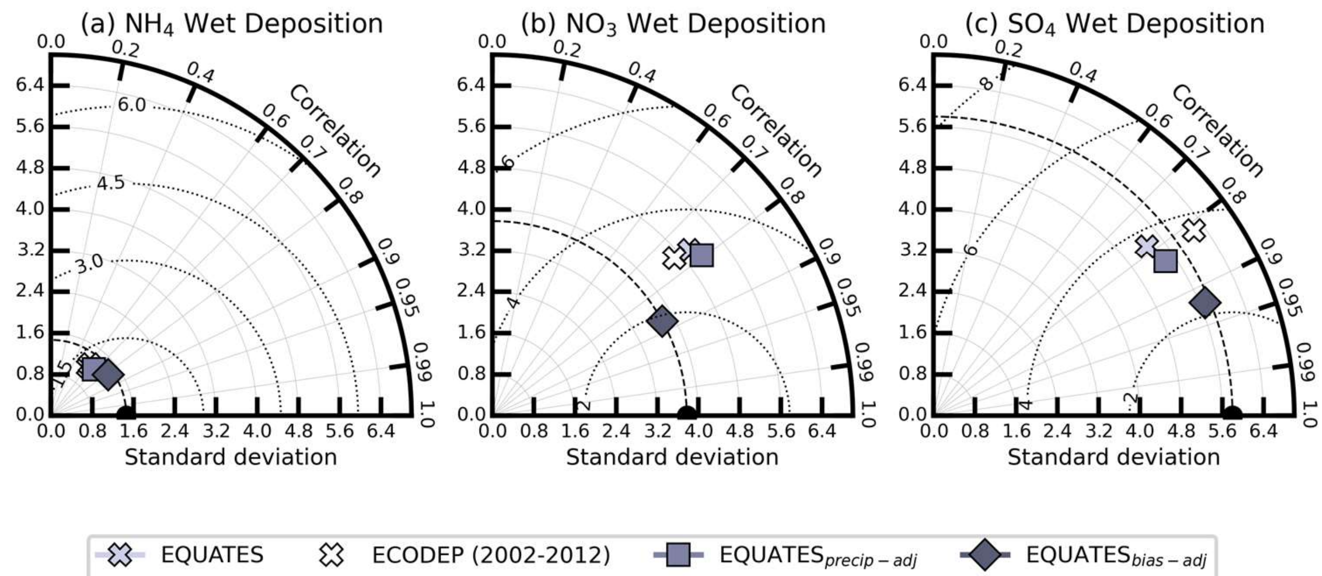
- No correction

$EQUATES_{precip\text{-}adj}$

- Precipitation from PRISM is used to adjust the modeled wet deposition

$EQUATES_{bias\text{-}adj}$

- Universal kriging with exponential covariance structure applied to ratios of measured/modeled wet deposition



For more details on the MMF technique, please see Zhang et al., 2019 (doi: 10.1029/2018JD029051)

EPA United States Environmental Protection Agency

Measurement Model Fusion Improvements to Wet Deposition

EQUATES

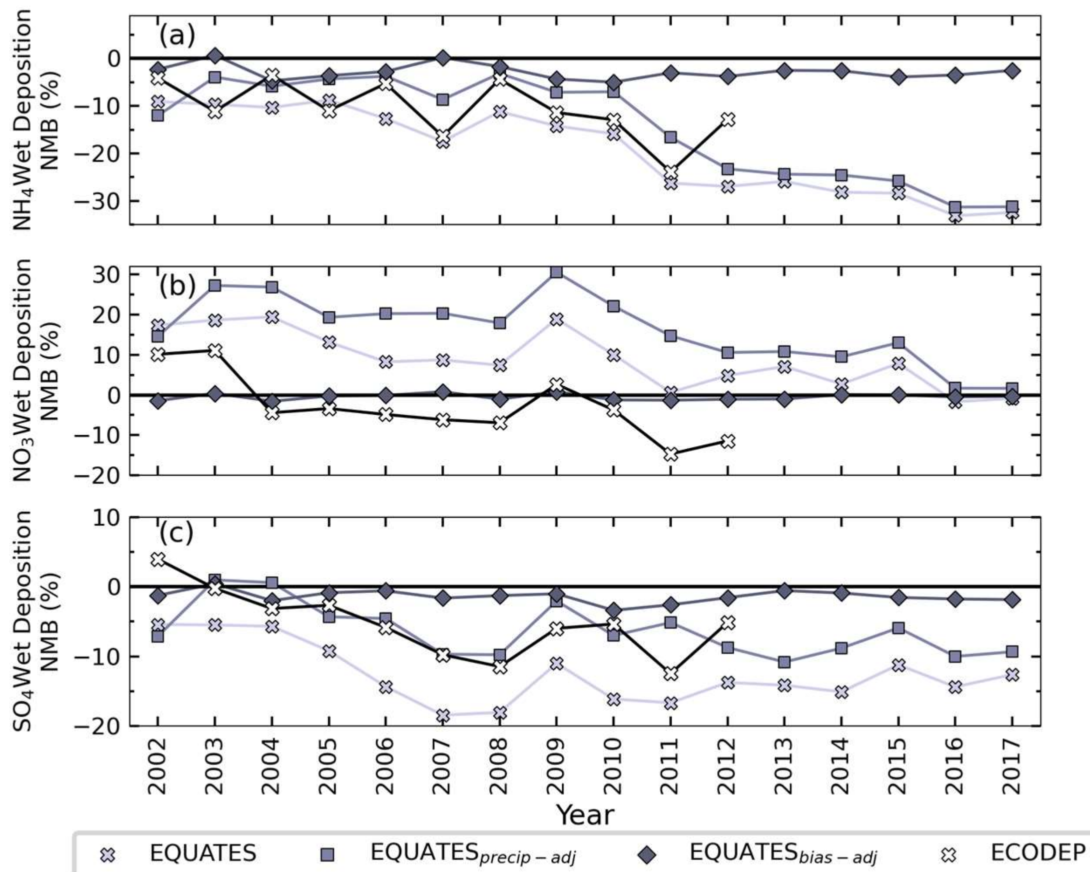
- No correction

EQUATES$_{precip\text{-}adj}$

- Precipitation from PRISM is used to adjust the modeled wet deposition

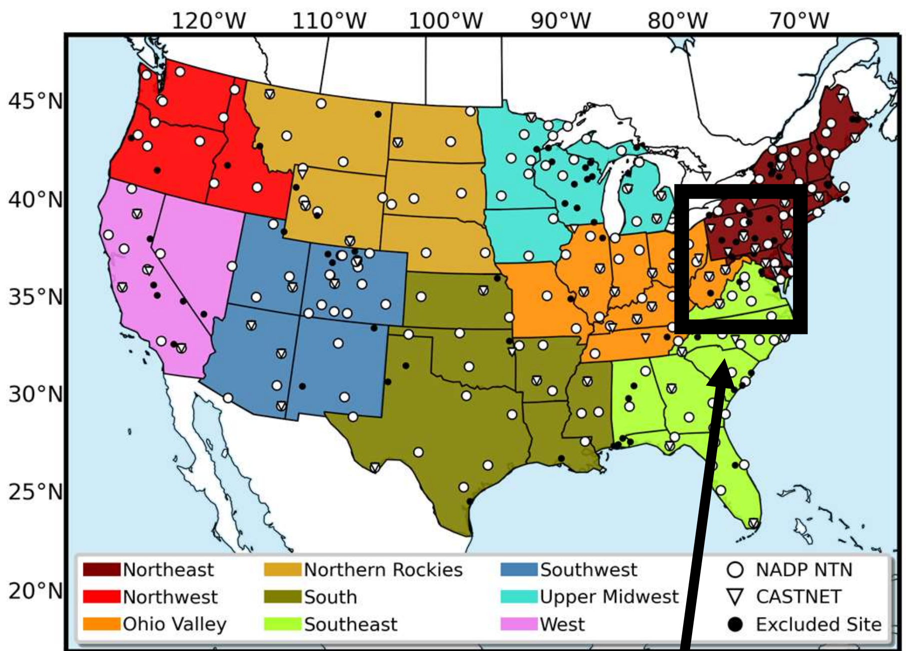
EQUATES$_{bias\text{-}adj}$

- Universal kriging with exponential covariance structure applied to ratios of measured/modeled wet deposition

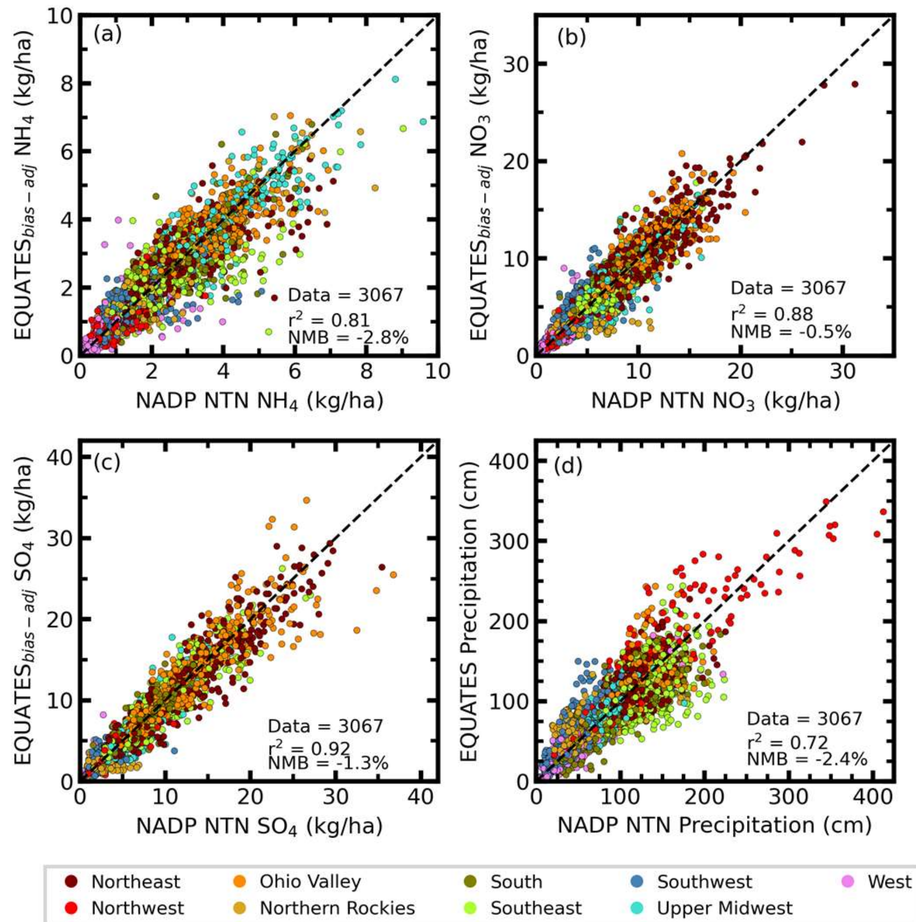


For more details on the MMF technique, please see Zhang et al., 2019 (doi: 10.1029/2018JD029051)

Comparison to NADP Wet Deposition Measurements

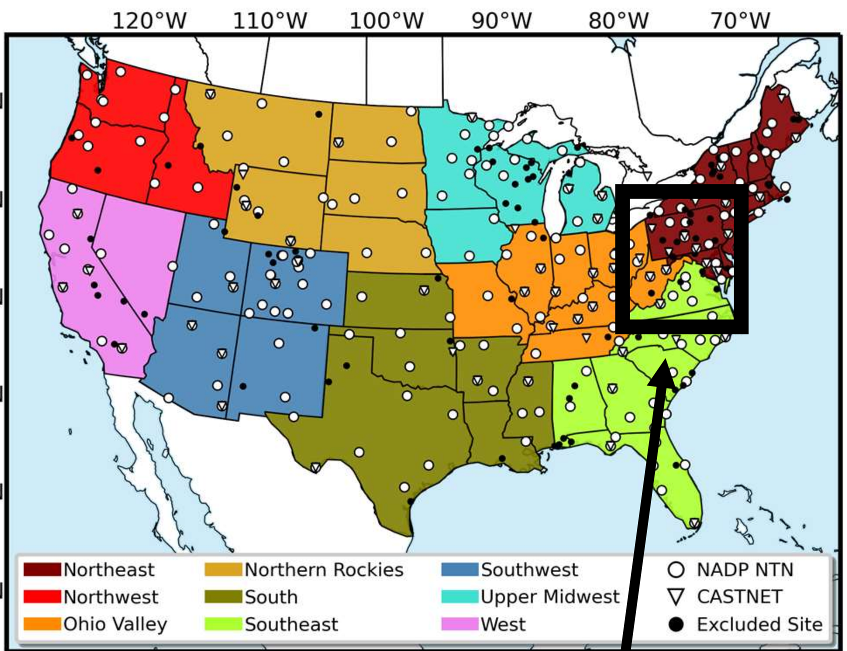


Approximate Boundary of Chesapeake Bay Watershed

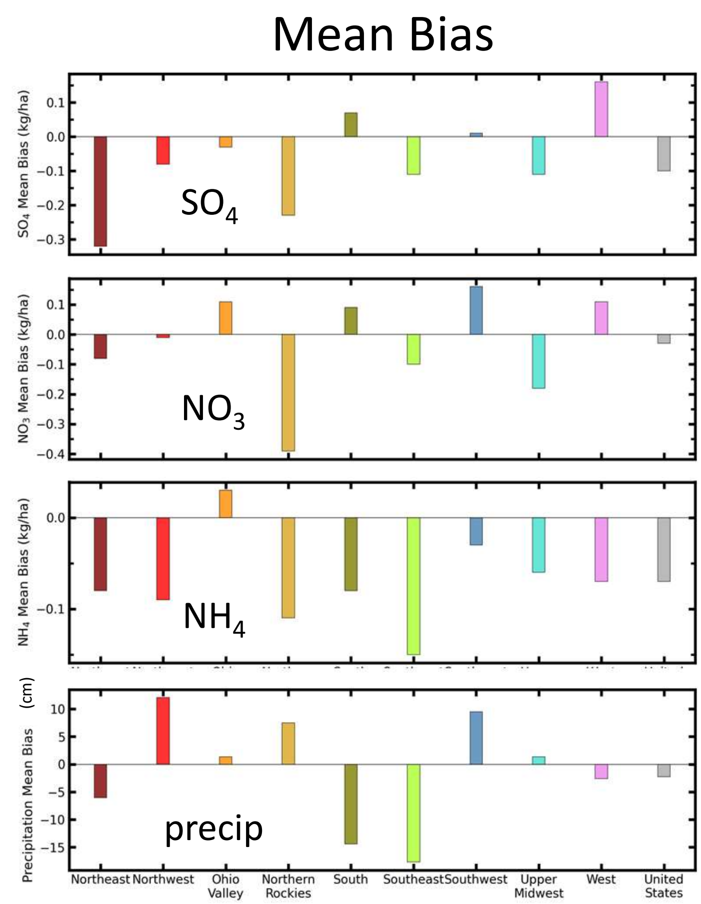


EPA United States Environmental Protection

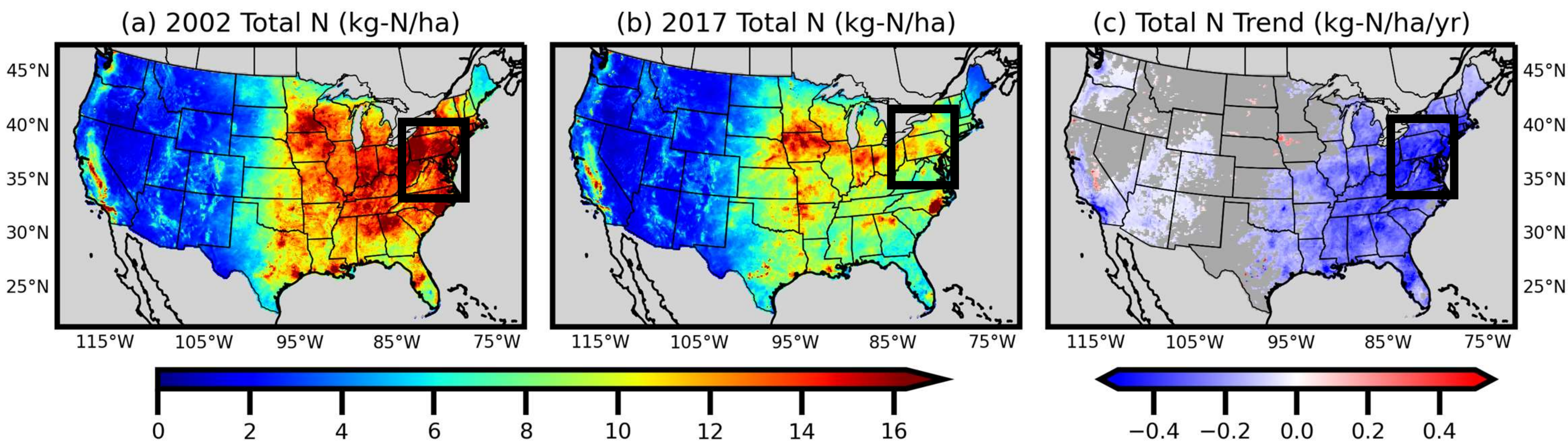
Comparison to NADP Wet Deposition Measurements



Approximate Boundary of Chesapeake Bay Watershed

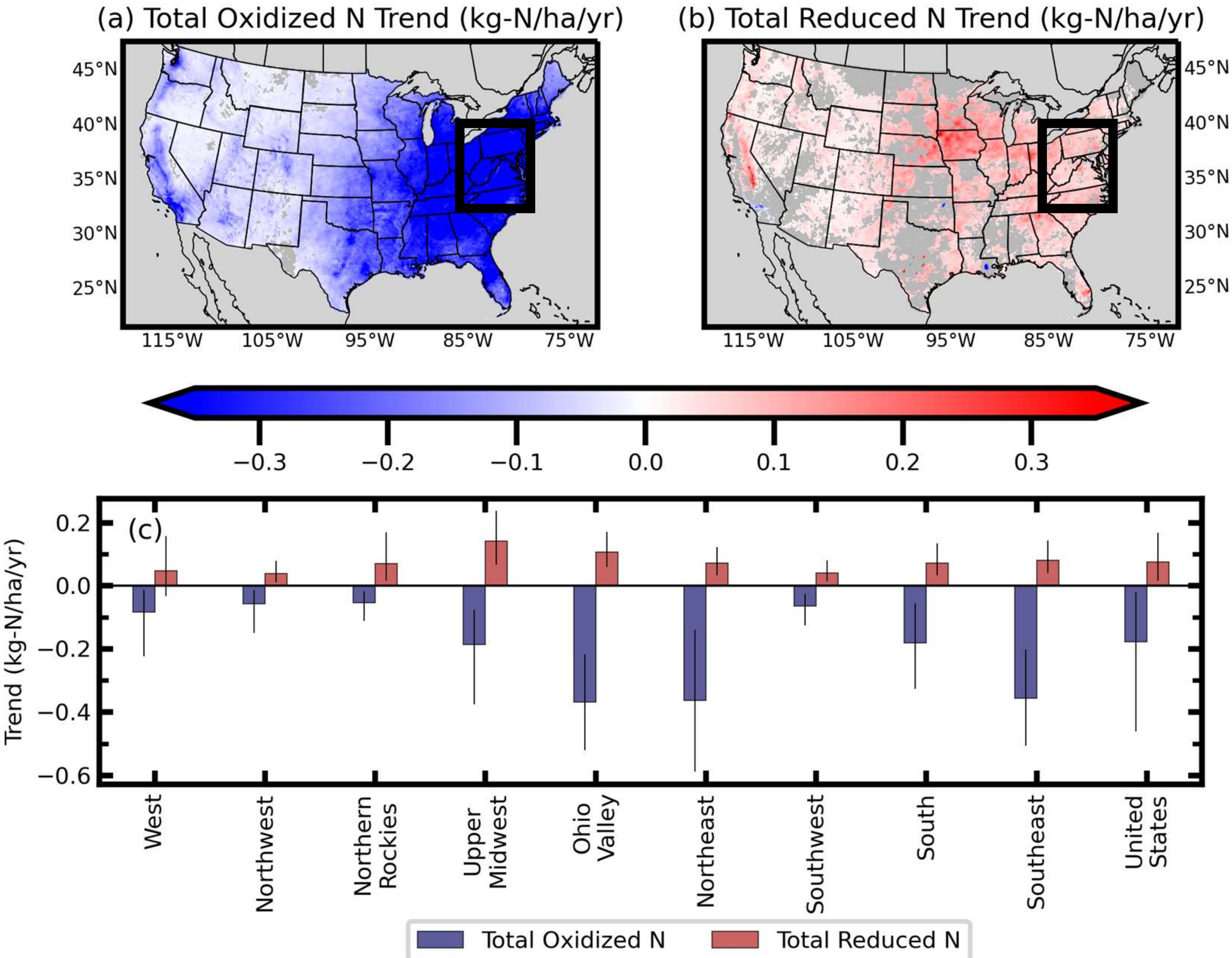


Total (Wet+Dry) Nitrogen Deposition Trend

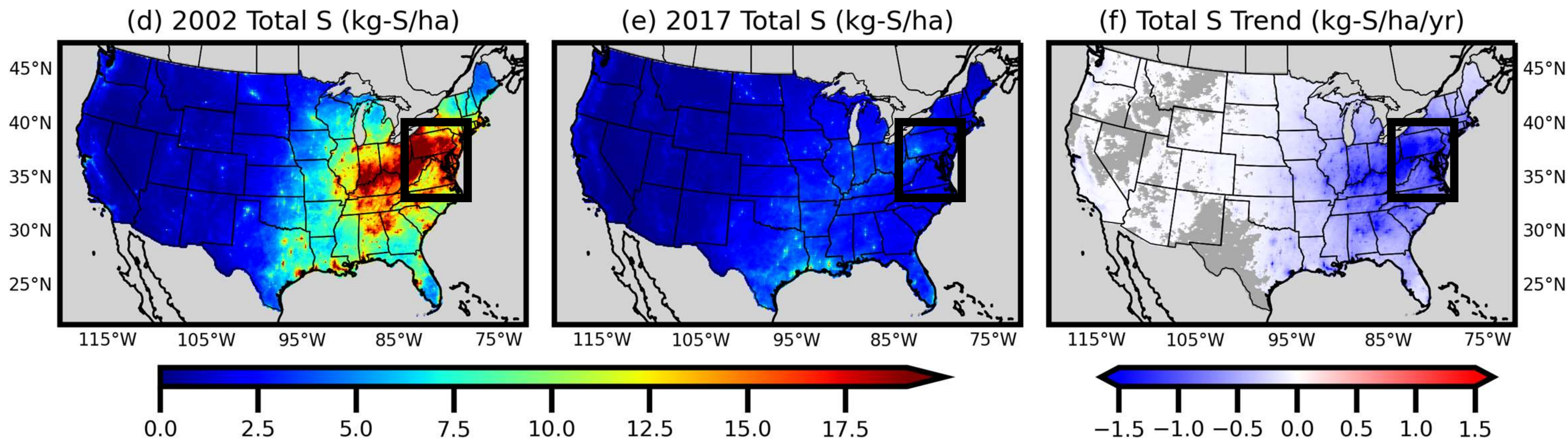


: Approximate Boundary of Chesapeake Bay Watershed

United States Environmental Protection Agency



Total Sulfur Deposition



□ : Approximate Boundary of Chesapeake Bay Watershed

Application: Nitrogen Source Apportionment using ISAM

Quantifies the contributions of various emissions (source sectors and geographic regions) to pollutant levels in the domain, tracking concentration and deposition with near perfect mass closure.

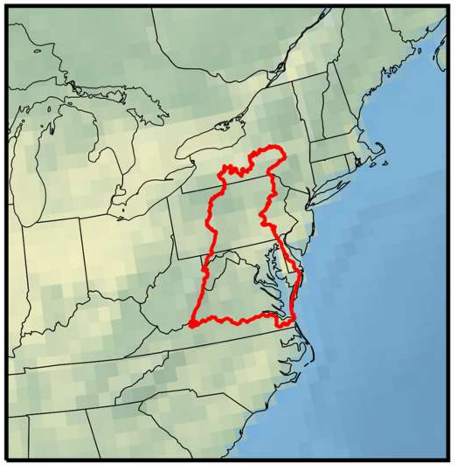
Can calculate source attribution of a large number of sources directly in the model in one simulation.

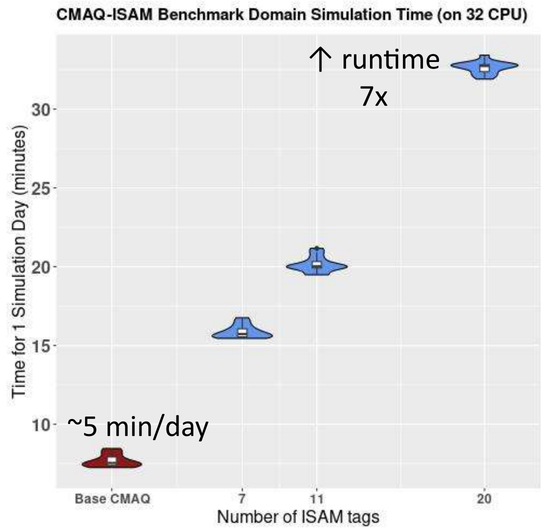
For each species, the production and loss terms from each chemical reaction is tracked (generalized for the available mechanisms) and propagate changes to tags based on stoichiometry and production/loss rates of the precursors.

Model
- CMAQv5.3.2

Time
- January-December 2016

Grid
- 12 km windowed domain



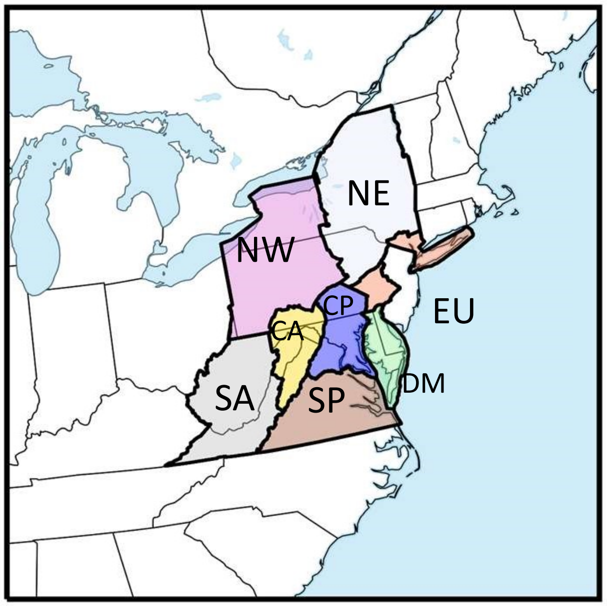


ISAM=Integrated Source Apportionment Method

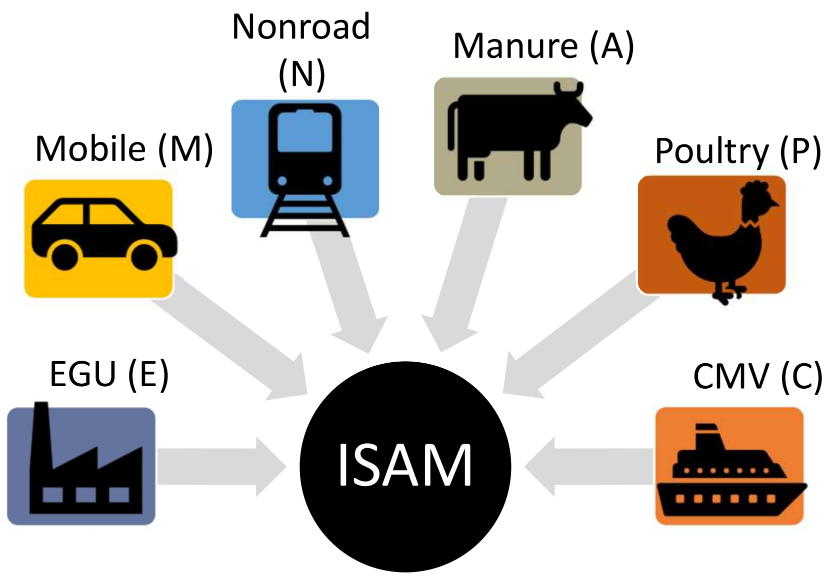
EPA United States Environmental Protection Agency

Model Set Up
Run CMAQ with ISAM options:

1. Geographic regions



2. Emission streams



3. Compounds of interest

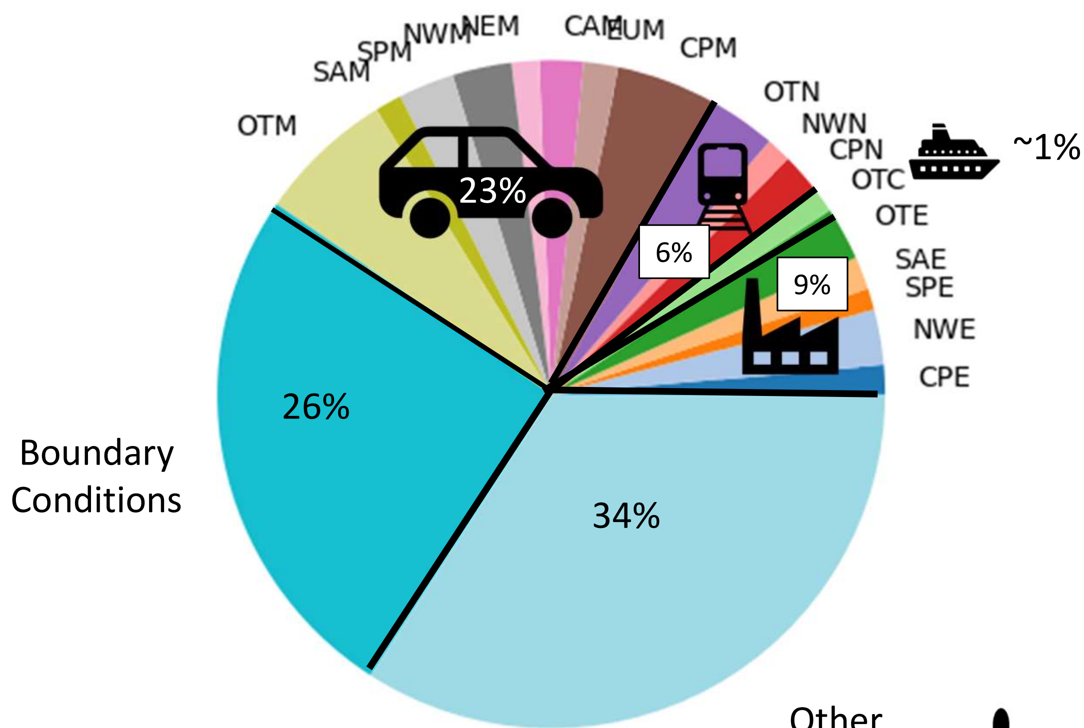
Tag Class	**Model species**
Sulfate	SO_2, H_2SO_4, SO_4^{2-}
Nitrate	HNO_3, HNO_2, NO_3^-, NO_3, NO_2, NO, Organic Nitrates
Ammonium	NH_3, NH_4^+
EC	Elemental Carbon Aerosols
OC	Organic Carbon Aerosols
VOC	Volatile Organic Aerosols
PM25_IONS	Cl, Na, Mg, K, Al, Si, Mn, and other aerosol cations
CO	CO
Ozone	All Nitrate species + all VOC species

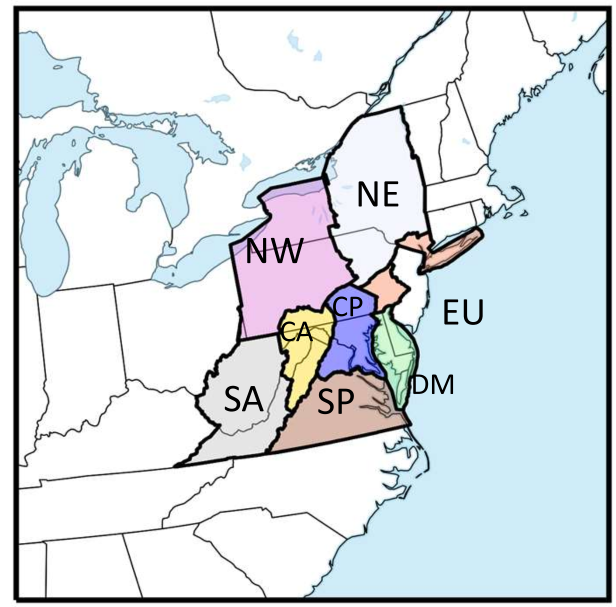
2-letter region identifier + 1-letter emission identifier Appended to each compound

United States Environmental Protection Agency

Nitrogen Deposition in the Chesapeake Bay Watershed

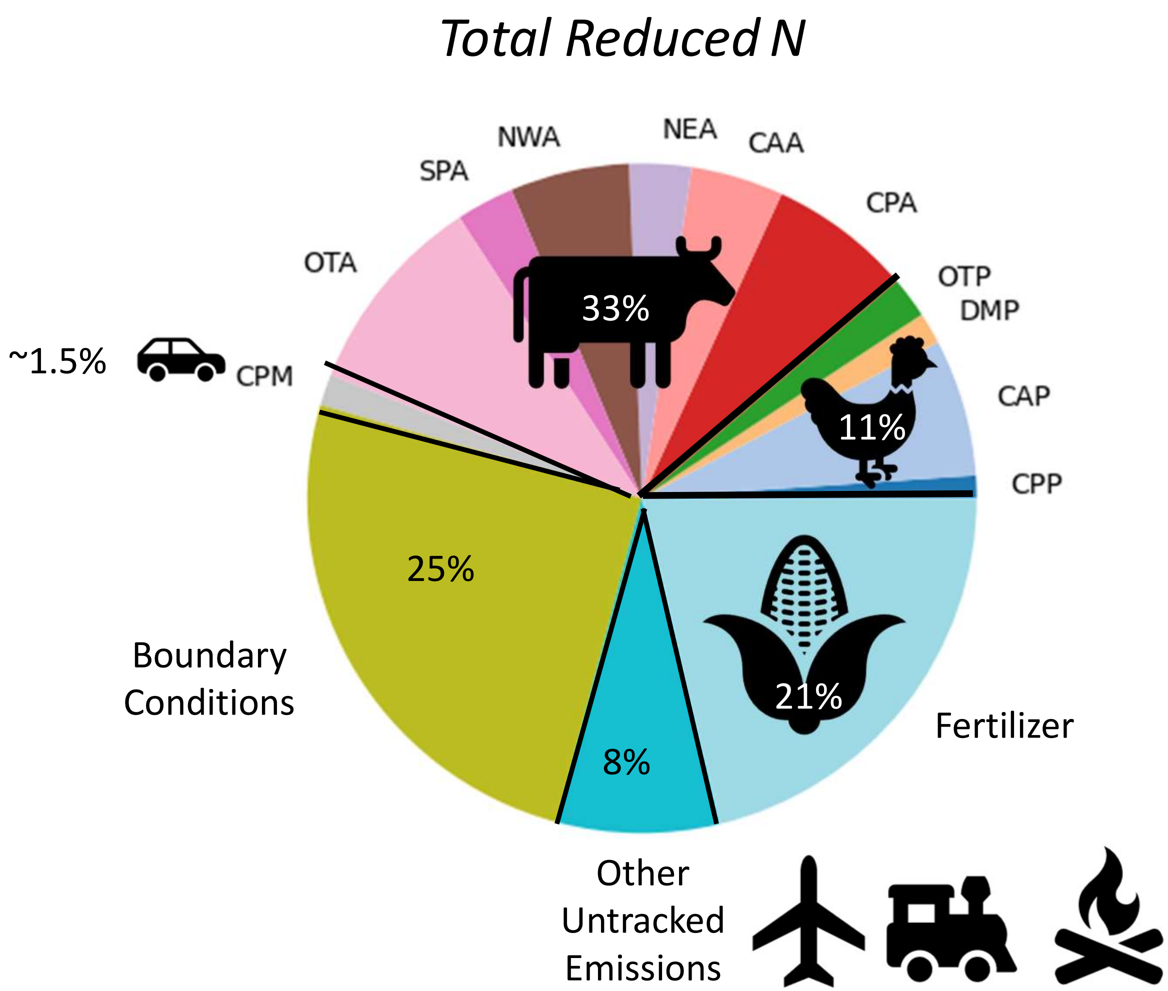
Total Oxidized N

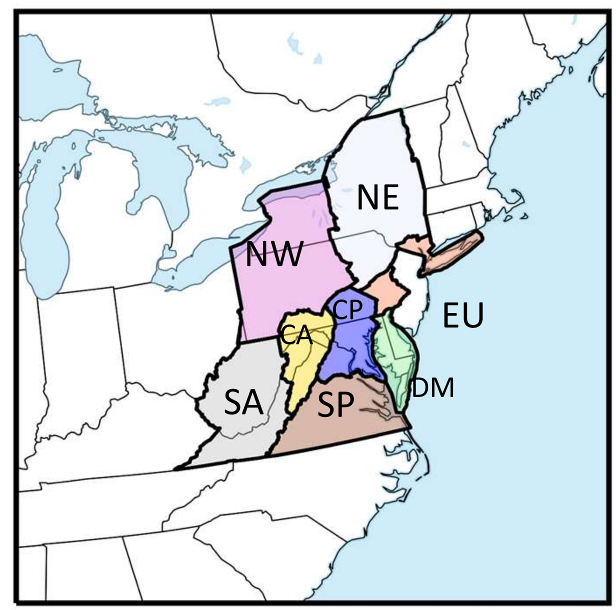




Other Untracked Emissions

Nitrogen Deposition in the Chesapeake Bay Watershed





Summary

How do new estimates of deposition compare to observations and previous long-term simulations?

Where and why does deposition change throughout the Chesapeake Bay Watershed?

Which emission sources are contributing to the Bay's high nutrient loading?

- Precipitation and bias corrections to modeled wet deposition improve agreement with NADP NTN wet deposition measurements
- Adjustment decreases the annual NMB of wet deposition across the US by ~20-30% annually compared to CMAQv5.3.2

- Overall decreasing total N deposition trend of –0.2 kg-N/ha/yr from 2002-2017 is driven by declines in oxidized N deposition due to policies targeting NOx
- Modeled total deposition trends of S decreased across all climate regions, especially in the eastern US

- Boundary conditions and other untracked sources are the largest contributors to N deposition inside the Chesapeake Bay Watershed
- Mobile sources constitute a large amount to total oxidized nitrogen deposition (~25%)
- Non-poultry animal manure is an important source of total reduced nitrogen deposition (~30%)