EPA's Air Quality Time Series Project and Source Apportionment Applications to the Chesapeake Bay Watershed

April Modeling Workgroup Quarterly

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EPA United States Environmental Protection Agency

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- 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:
  - Given recent improvements in CMAQ, how do new estimates of deposition compare to observations and previous long-term simulations?
  - For a given emission source in the watershed, what is the fraction deposited to a particular point?

United States Environmental Protection Agency

CMAQv5.3 Updates | EQUATES | Source apportionment in Chesapeake Bay | Progress and Next Steps

Aerosols and Gas Chemistry

- Improved organic aerosol and carbon-nitrogen chemistry estimates (Pye et al. 2015 ES&T, Xu et al. 2018 ACP, Pye et al. 2017 ACP)
- Updates to chemistry: Improved parameterization of organic nitrates
- Updated full halogen chemistry and added dimethyl sulfide (DMS) chemistry – included in optional detailed mechanism (Sarwar et al., Atmospheric Environment, 2019)

Deposition

New Land Use Specific scheme available

Emissions

New Detailed Emissions Scaling, Isolation, and Diagnostic

Instrumented models

The Integrated Source Apportionment Method (ISAM) has been updated to greatly improve efficiency and runtime

Updated CMAQ tools

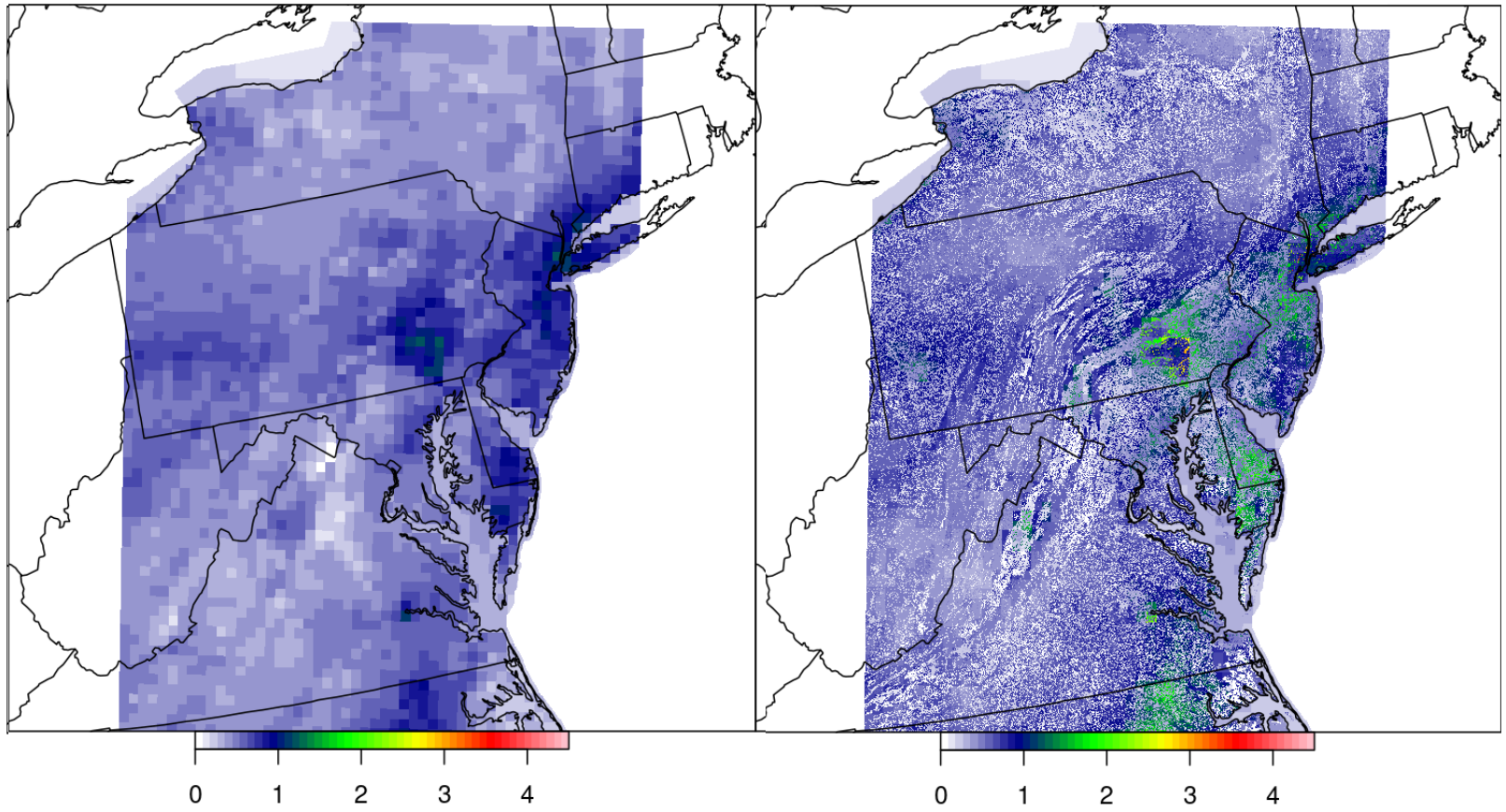
Updated pre and post processing tools

ISAM=Integrated Source Apportionment Method

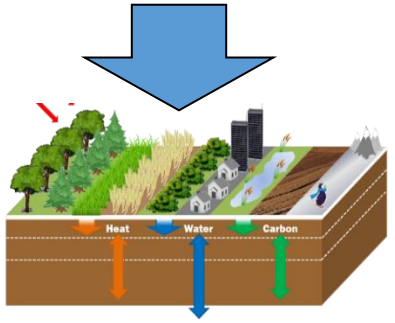
Land Use Specific Deposition in CMAQv5.3

CMAQ 12 km Grid Cell Average Deposition

CMAQ 12 km Land Use Specific Deposition

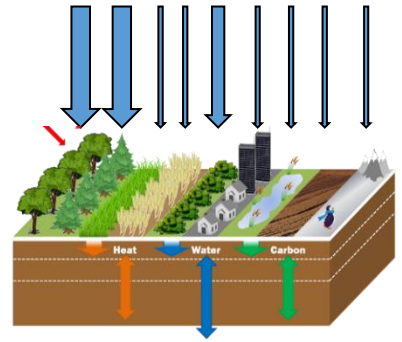


Grid Cell Average Dry Deposition



Earlier versions of CMAQ

LU Specific Dry Deposition

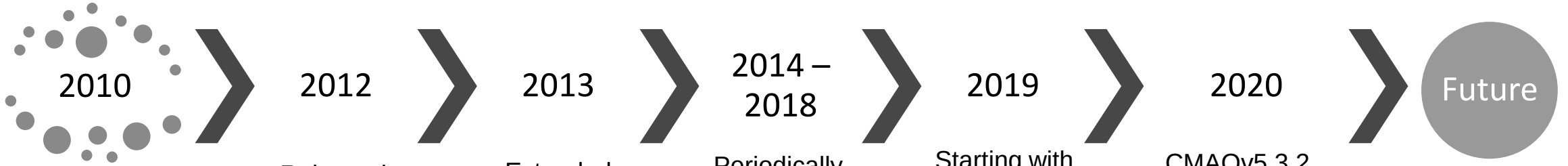


CMAQ v5.3+ With STAGE deposition option

Slide courtesy of Jesse Bash

Photochemical models (like CMAQ) are tools for estimating the pollutant concentrations/depositions that would result from given emissions, meteorology, and other specified conditions.

- Various tools have been developed over the years to provide these responses
- For policy applications and general scientific understanding, it is often the responses of model predictions to emission changes that inform decision making.
- ISAM now included as part of the base CMAQ model and is a build option



2010: Collaboration between EPA-OAQPS and EPA-ORD was established to explore implementing source apportionment in CMAQ.

2012: Released ISAM for PM species in CMAQ v4.7.1 (lagged after the base model, and with its own code base).

2013: Extended ISAM to Ozone (NOx, VOCs, etc.)

2014 – 2018: Periodically updated ISAM after CMAQ releases primarily with the help of post-docs.

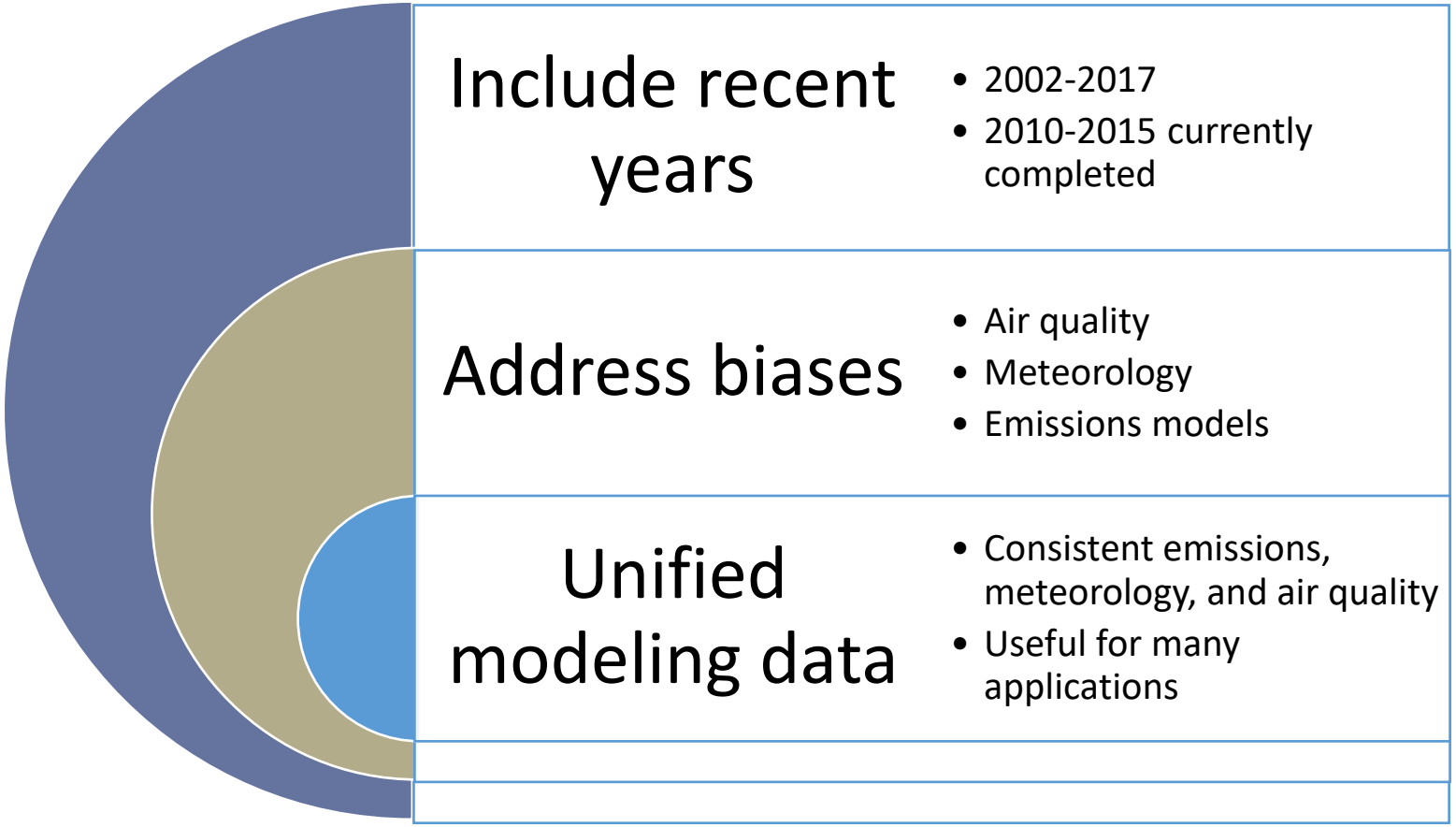
2019: Starting with CMAQv5.3, ISAM release was integrated with the base model release. Completely reformulated the ISAM chemistry module, sped up code.

2020: CMAQv5.3.2, major improvements in ISAM predictions for ozone and other secondary gas-phase species and dry deposition

New ISAM release much faster than previous version!

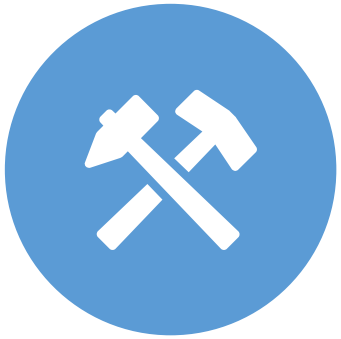
Future: Continue improving and refining CMAQ-ISAM, extending to other species (SOA), and look for feedback from the users.

ISAM=Integrated Source Apportionment Method



EQUATES: EPA's Air QUAlity TimE Series Project

Applications of Mulityear CMAQ Simulations

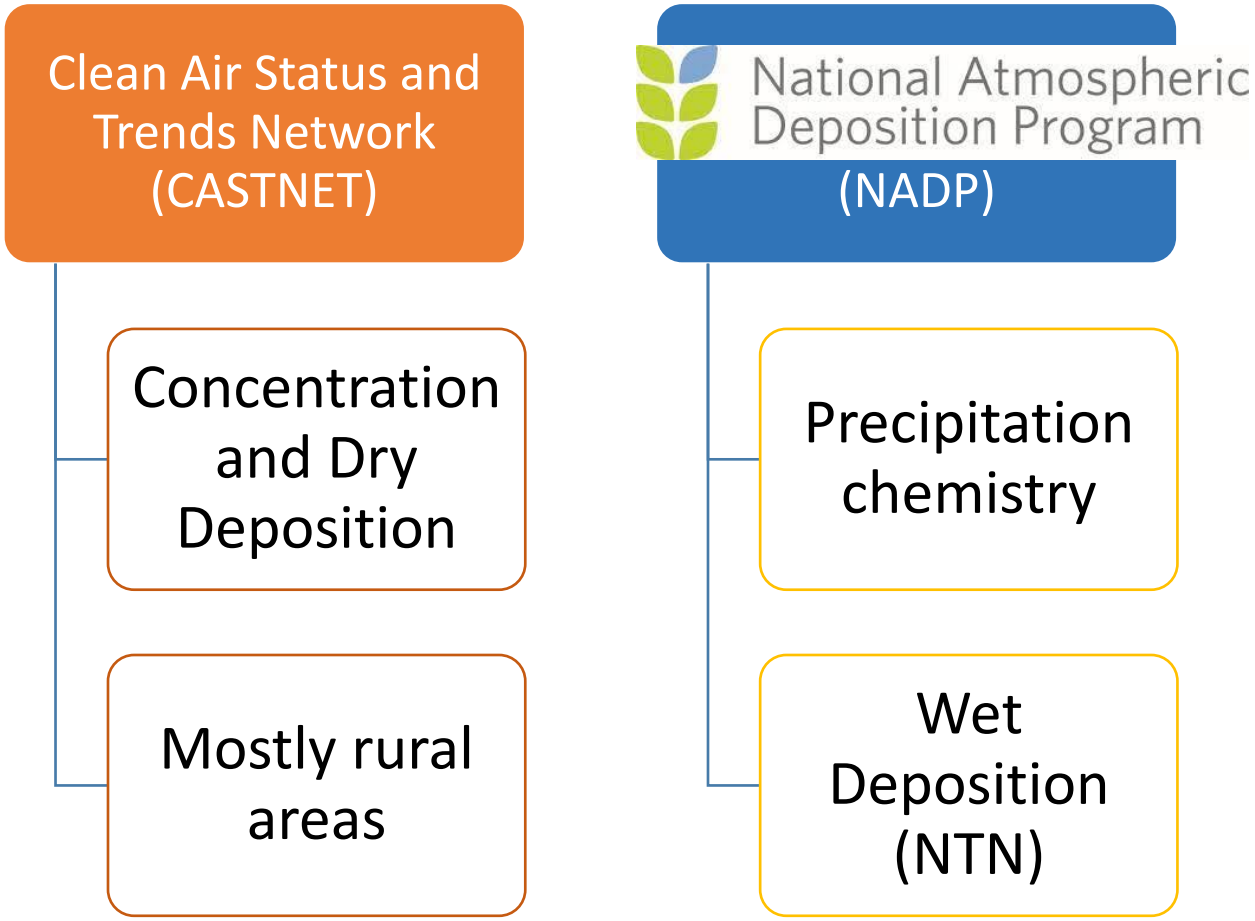


Decadal and multidecadal simulations used for a variety of applications

Annual deposition estimates 2002-2012 used by TDEP, CASTNET, EnvrioAtlas, Critical Loads Mapper, and to support nutrient assessments

Model/observation fused O_3 and $PM_{2.5}$ surfaces used for epidemiological and ecological studies

Dynamic Evaluation



Network	Measurement Method	Compounds of interest	N of Sites	Length of record (years)
CASTNET	Weekly filter pack	Particles (SO4, NH4, NO3); Gases (SO2, HNO3)	94	45
NADP (NTN)	Weekly precipitation collector +rain gage	SO4, NH4, NO3, precipitation amount	258	43
NADP (AMoN)	Biweekly passive sampler	NH3	101	14

Table from CASTNET 2021 Fact Sheet

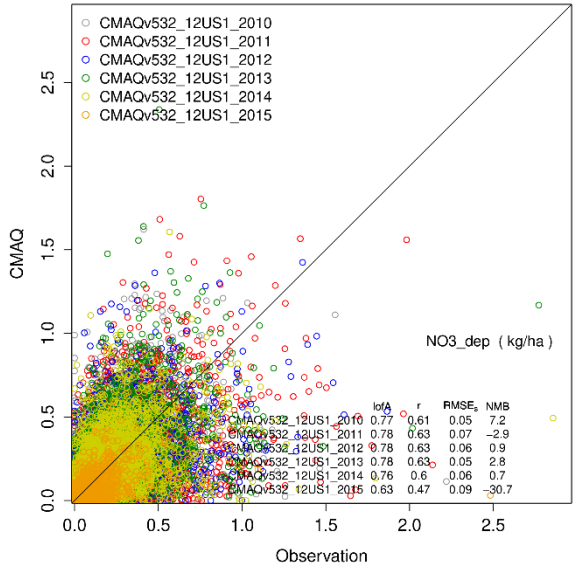
United States Environmental Protection Agency

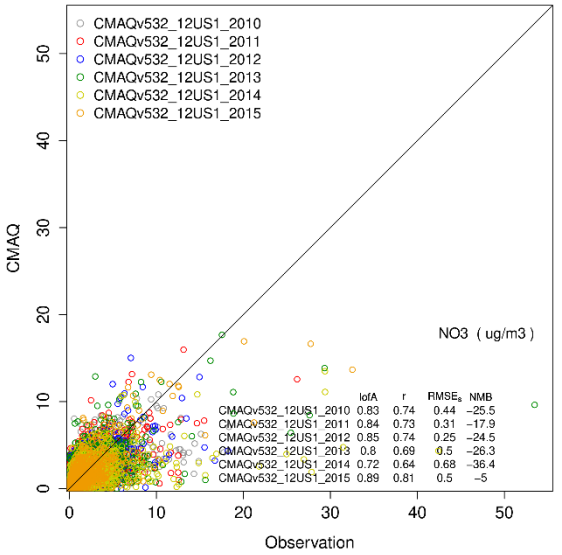
Wet Deposition

Concentration

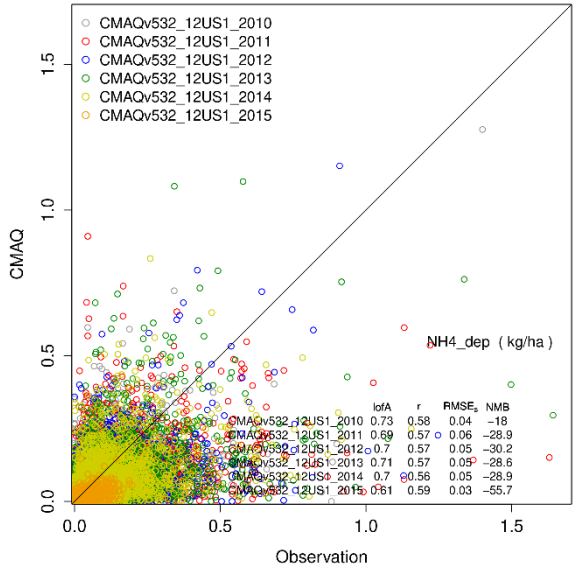
Precipitation

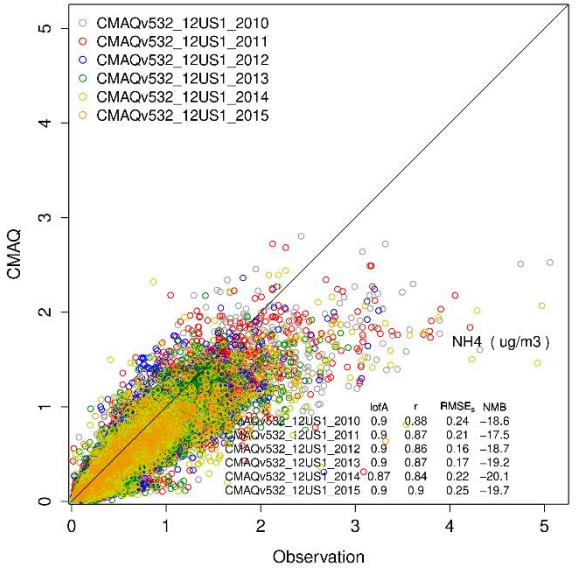
NO3

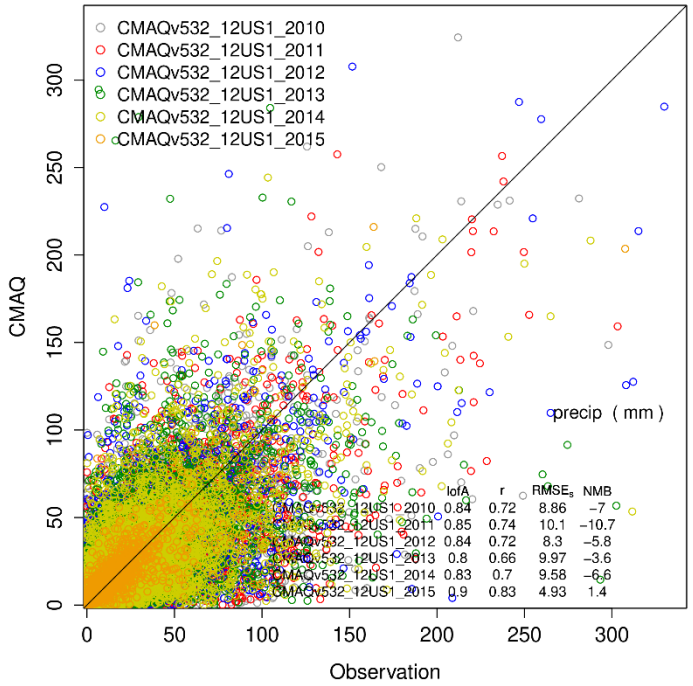




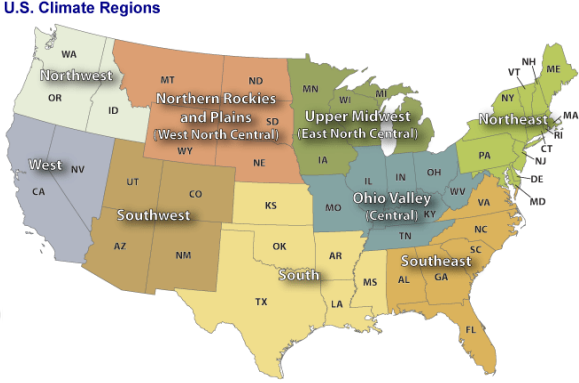
NH4



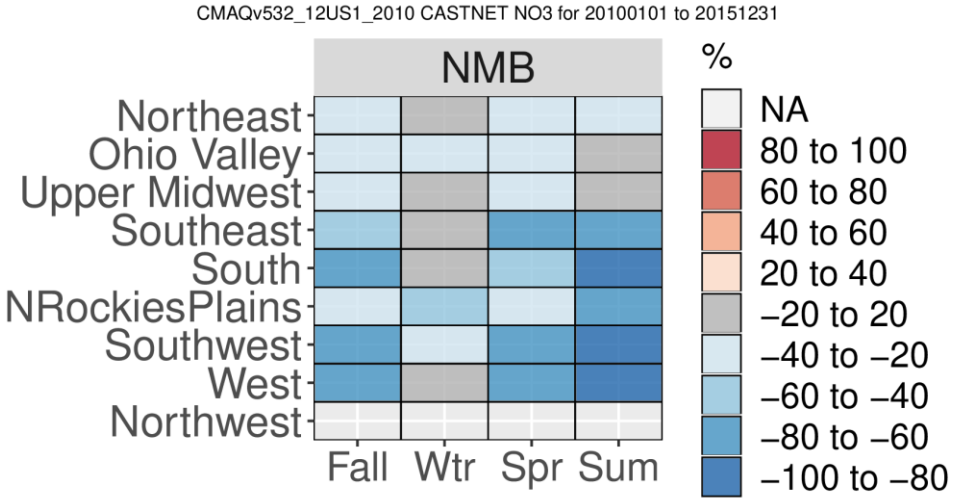


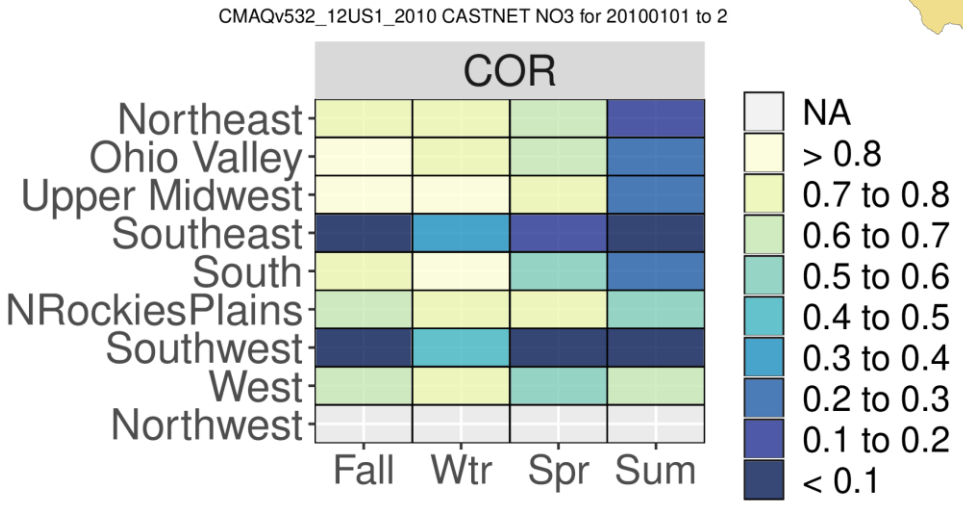


NO3 and NH4 Concentration

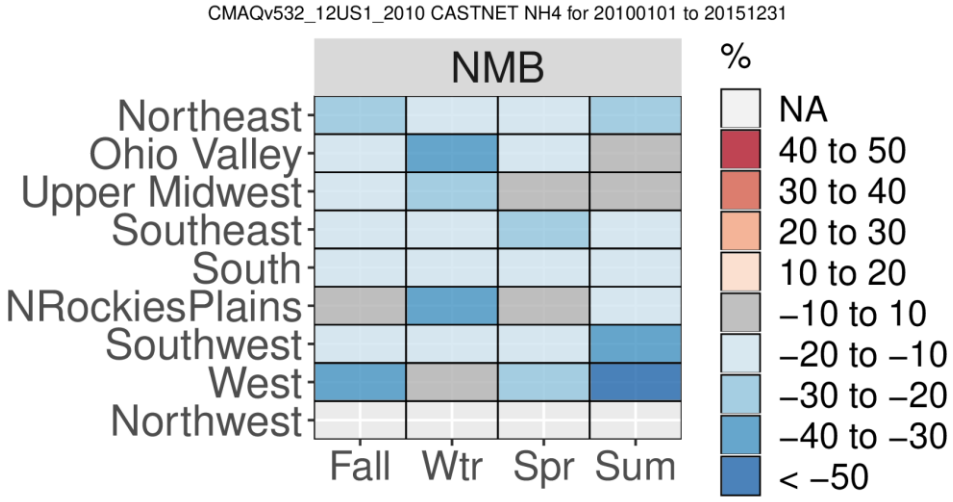


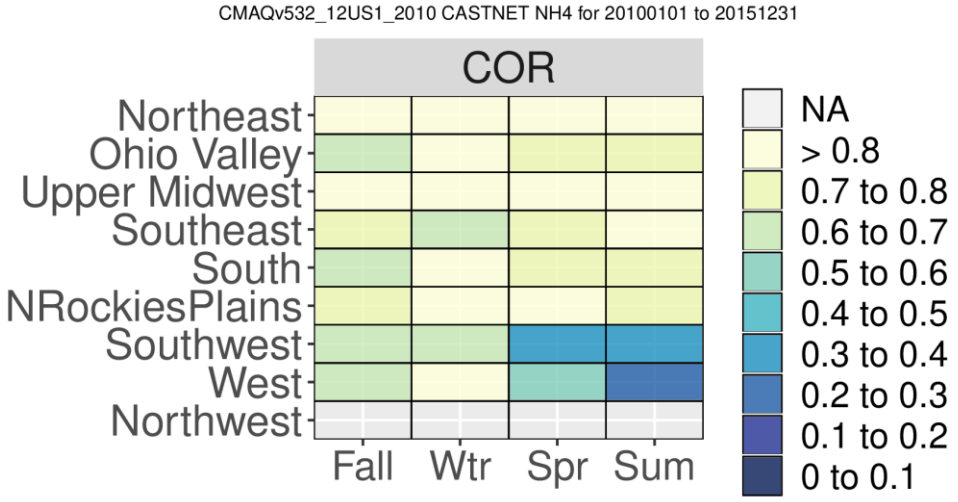
NO3





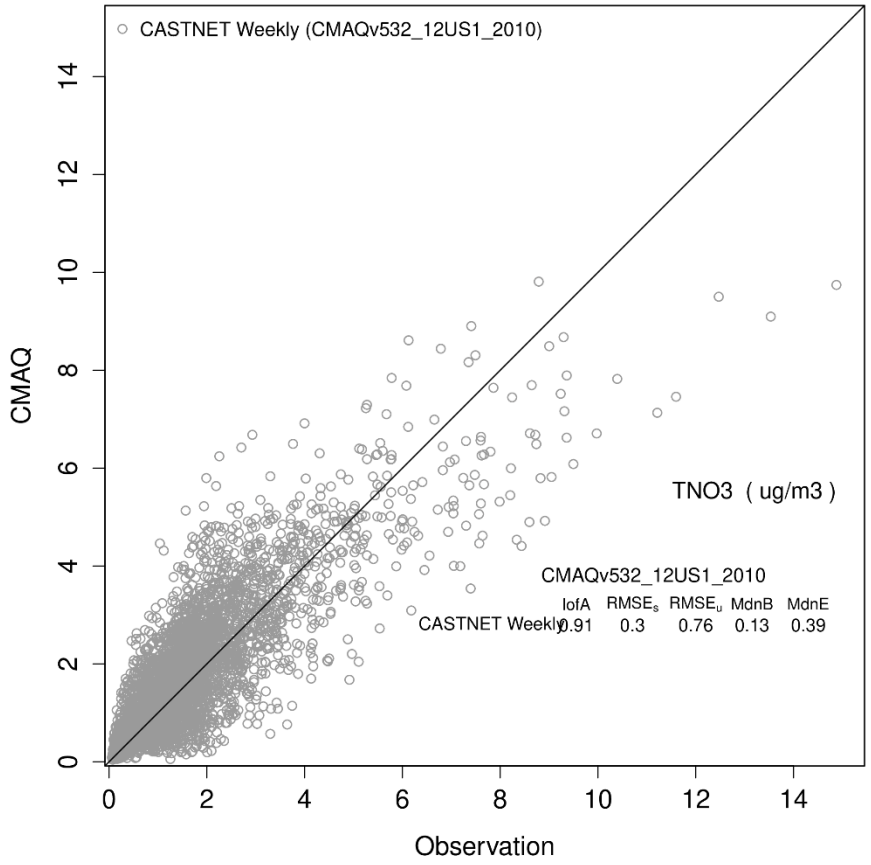
NH4

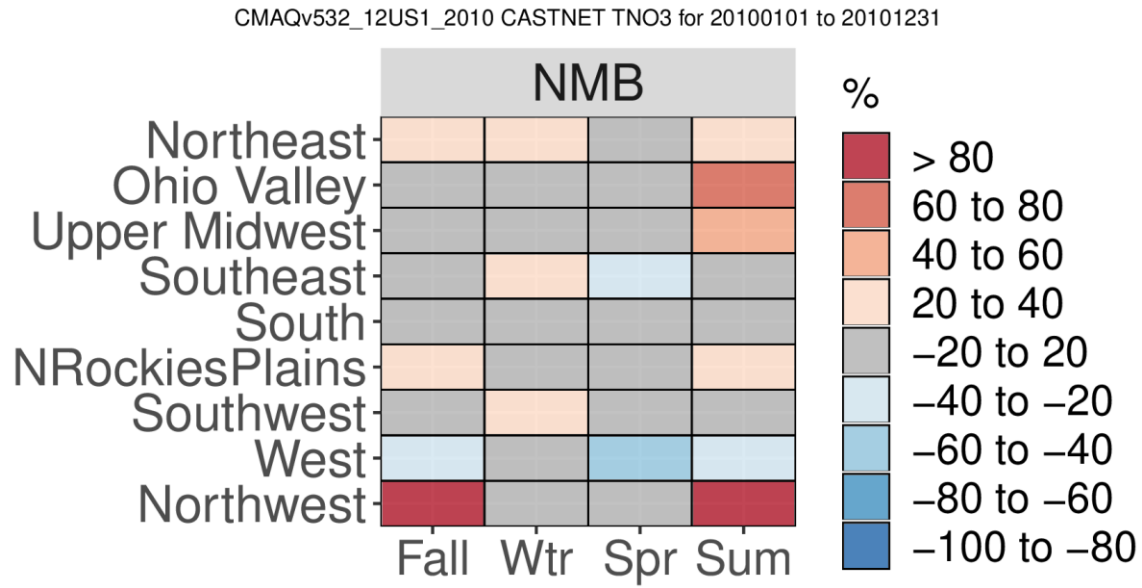


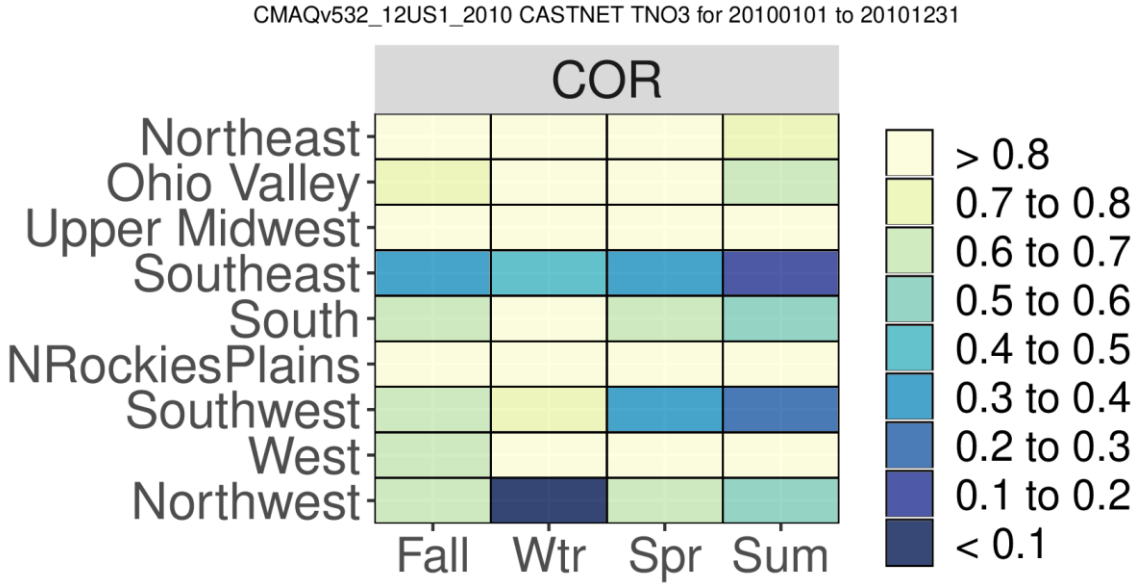


2010 EQUATES TNO3:

Concentration



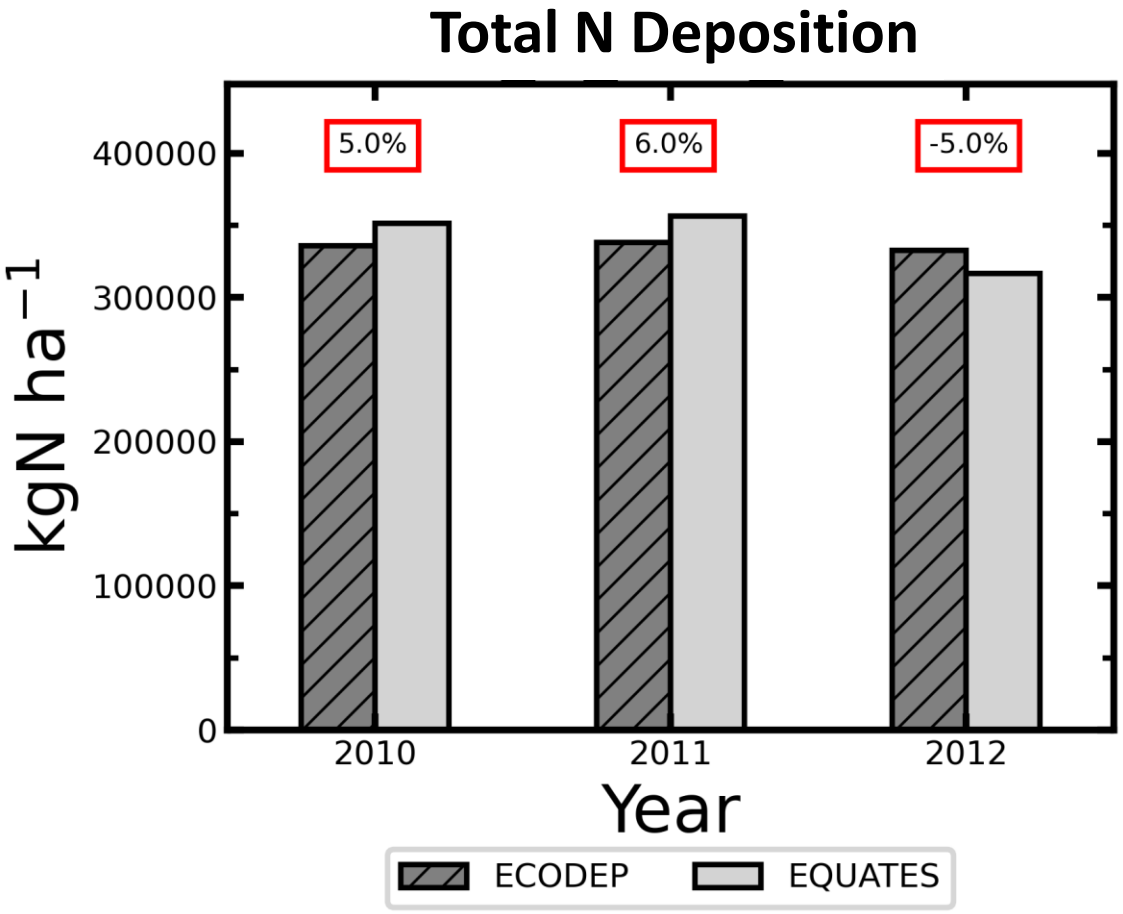


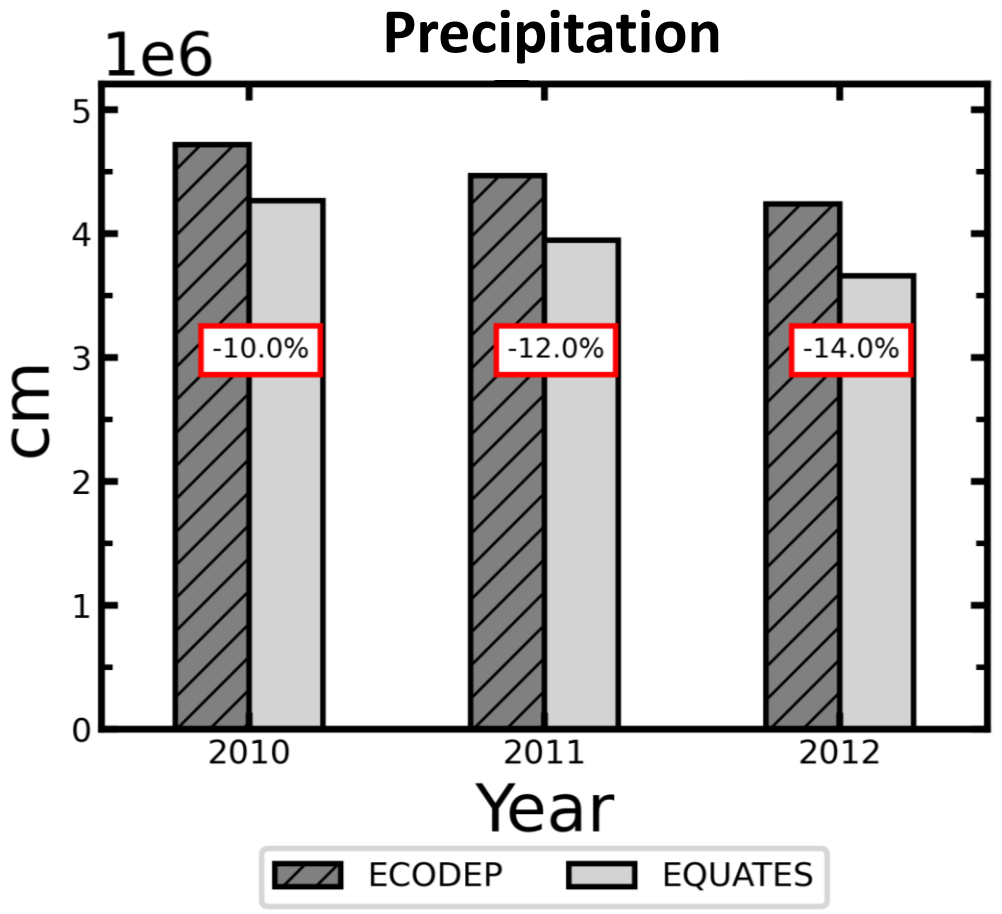


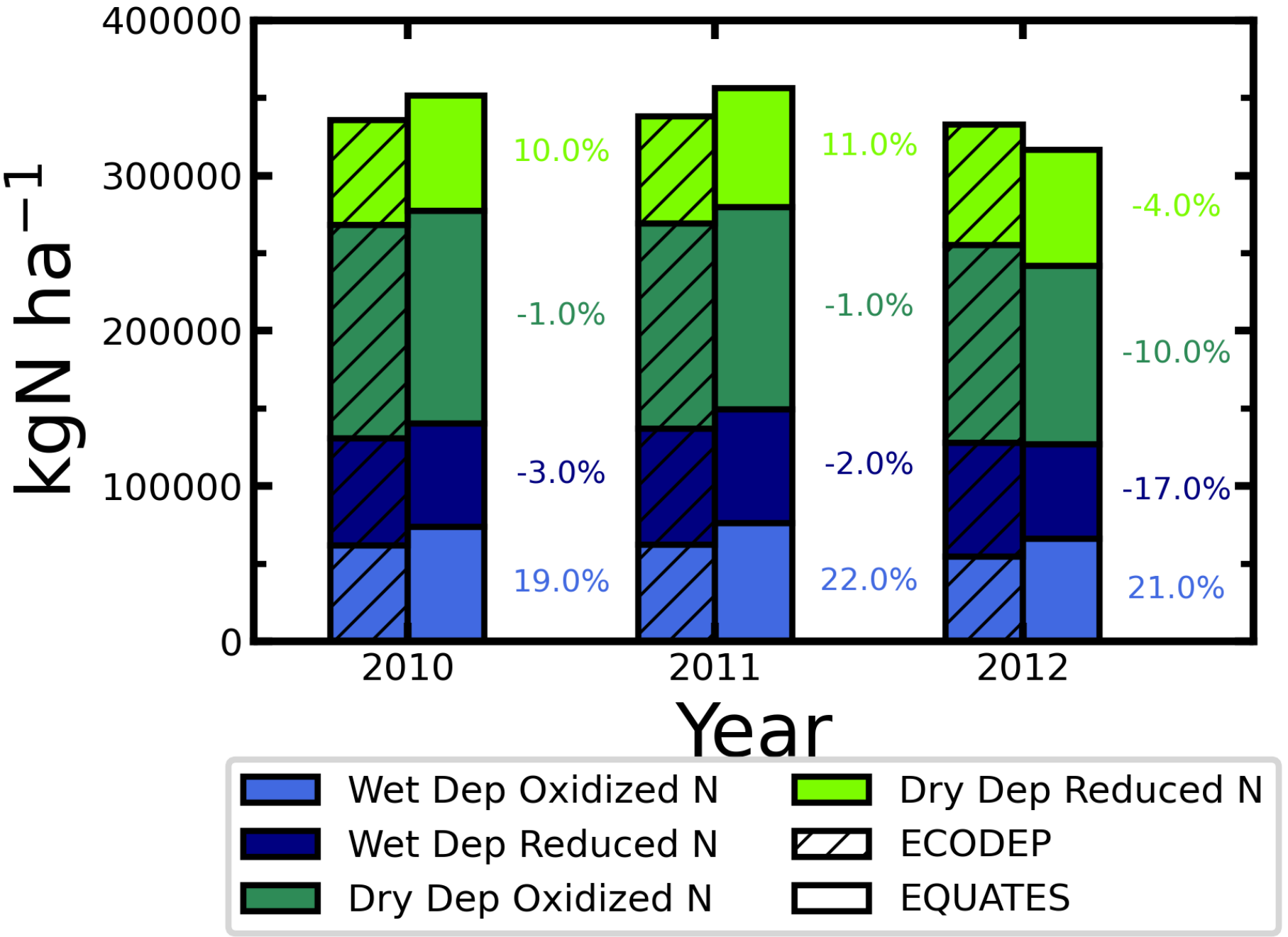
Comparison to ECODEP (atmospheric deposition inputs for Phase 6 of the Chesapeake Bay Model)

	ECODEP	EQUATES
Model	CMAQv5.0.2	CMAQv5.3.2
Date Range	2002-2012	2002-2017*
Domain/Resolution	12 km CONUS	108 km N Hemisphere+ 12 km CONUS
Meteorology	WRFv3.4	WRFv4.1.1
Emissions	Various NEIs/Modeling platforms	2017 NEI as primary base year; consistent methods used for each sector to avoid artificial step changes
Boundary Conditions	GEOS-Chem	N Hemisphere CMAQv5.3.2

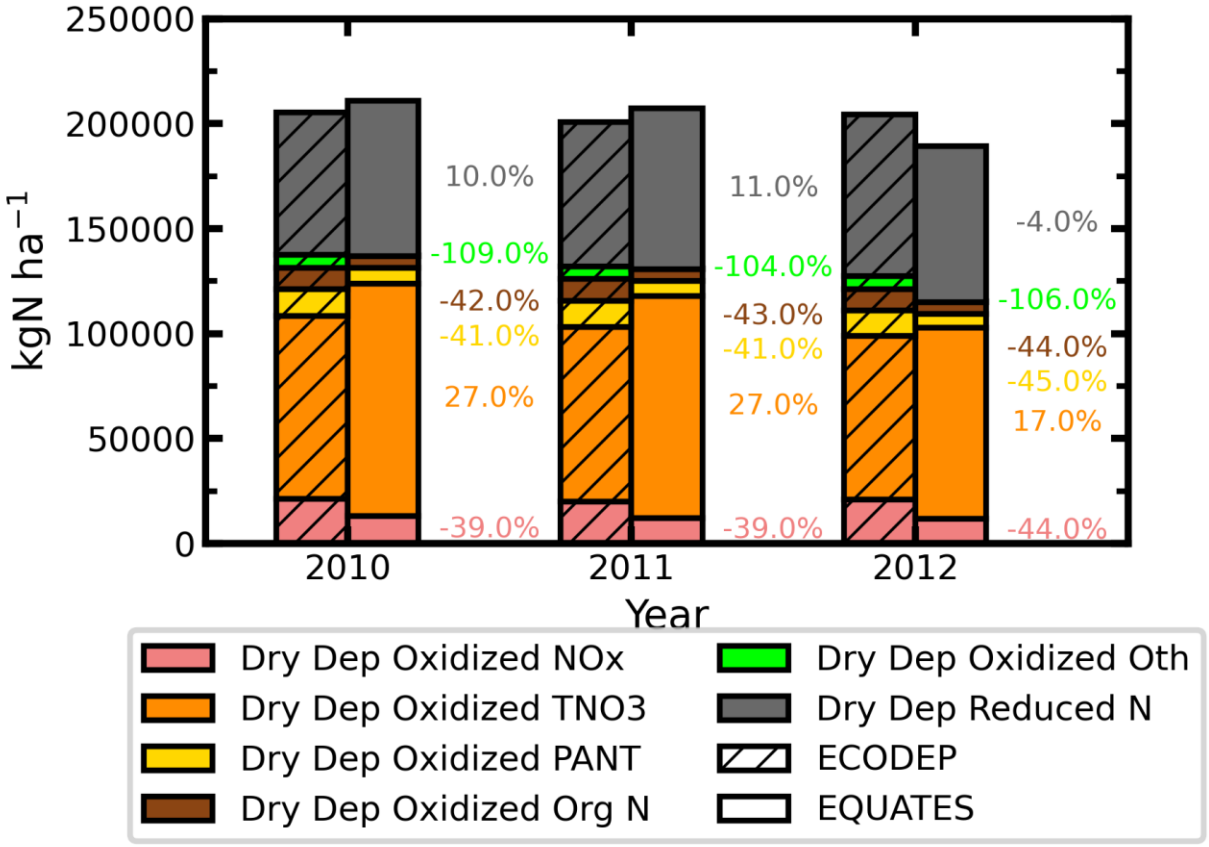
Changes in Total (Wet+Dry) N Deposition



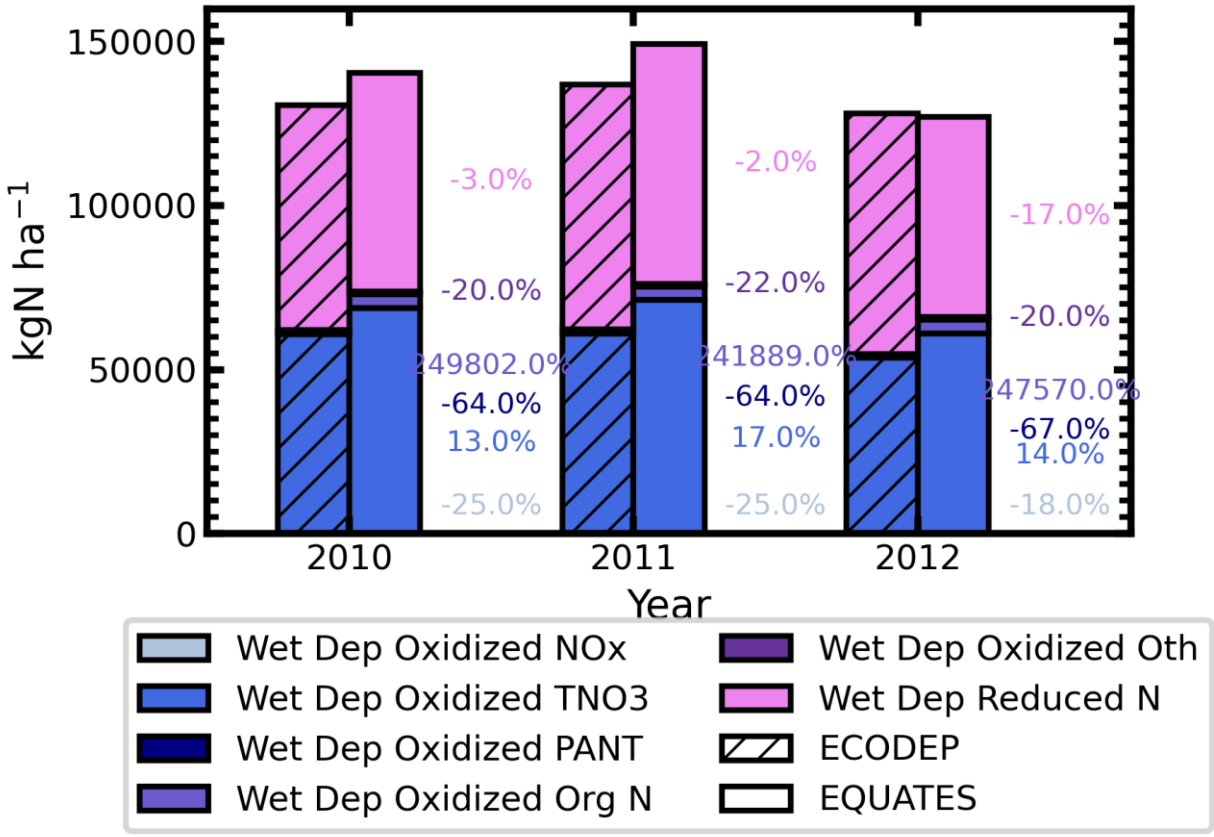



400000
300000
200000
100000
0
kgN ha−1
10.0%
-1.0%
-3.0%
19.0%
11.0%
-1.0%
-2.0%
22.0%
-4.0%
-10.0%
-17.0%
21.0%
2010
2011
2012
Year
Wet Dep Oxidized N
Wet Dep Reduced N
Dry Dep Oxidized N
Dry Dep Reduced N
ECODEP
EQUATES

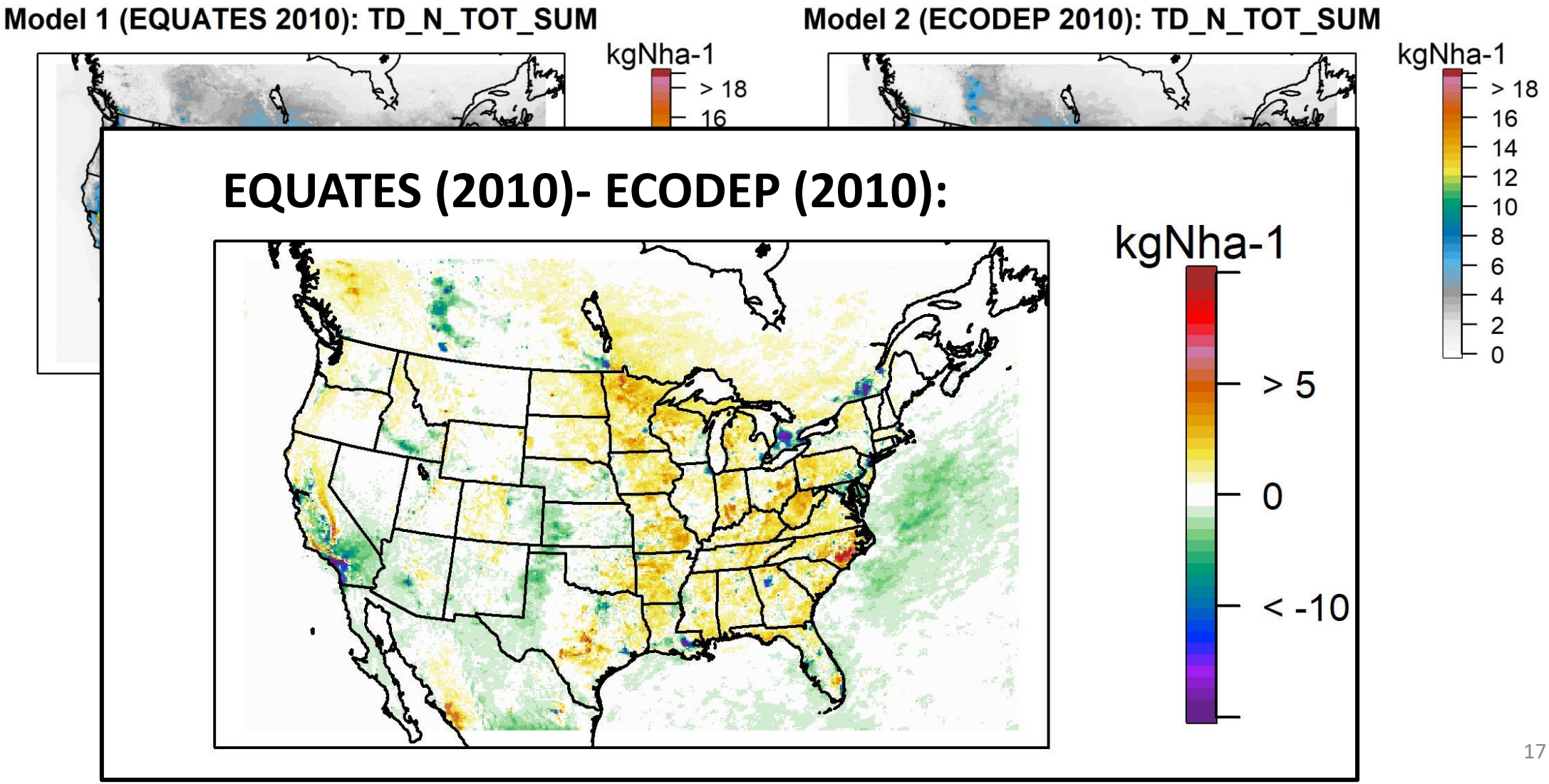
Dry Nitrogen Deposition



Wet Nitrogen Deposition



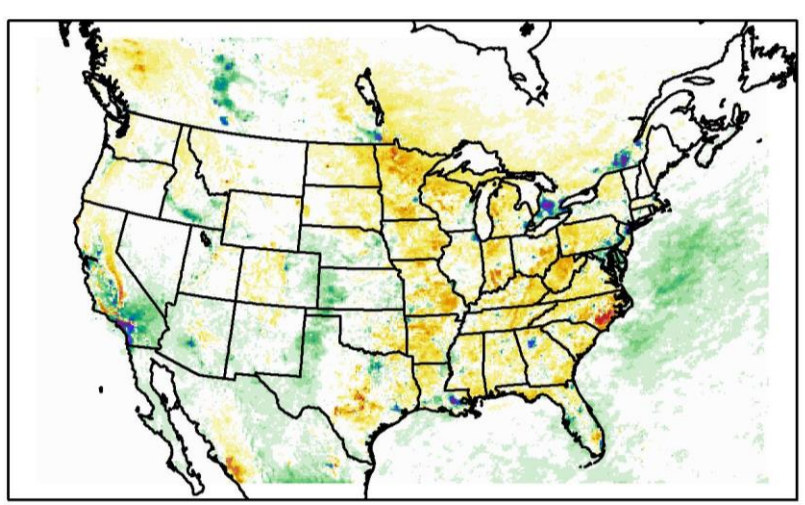
2010 Changes in Total (Wet+Dry) N Deposition



United States Environmental Protection Agency

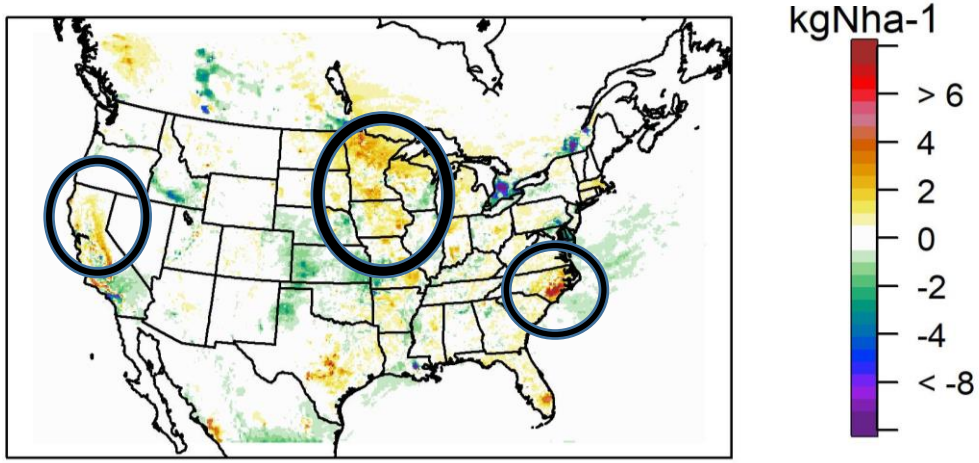
More reduced N in agricultural regions of NC, Midwest, CA

EQUATES(2010)-ECODEP(2010): Total Nitrogen

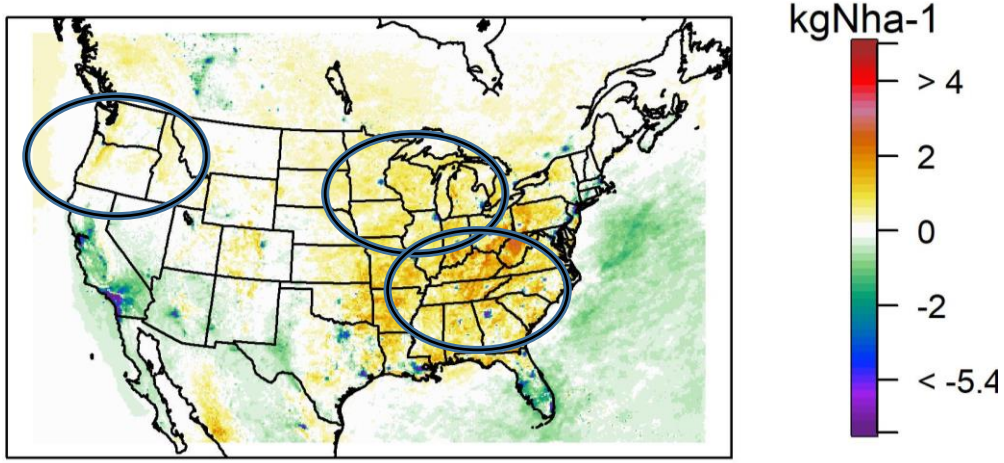


More oxidized N in EQUATES than ECODEP in rural areas; less in urban centers

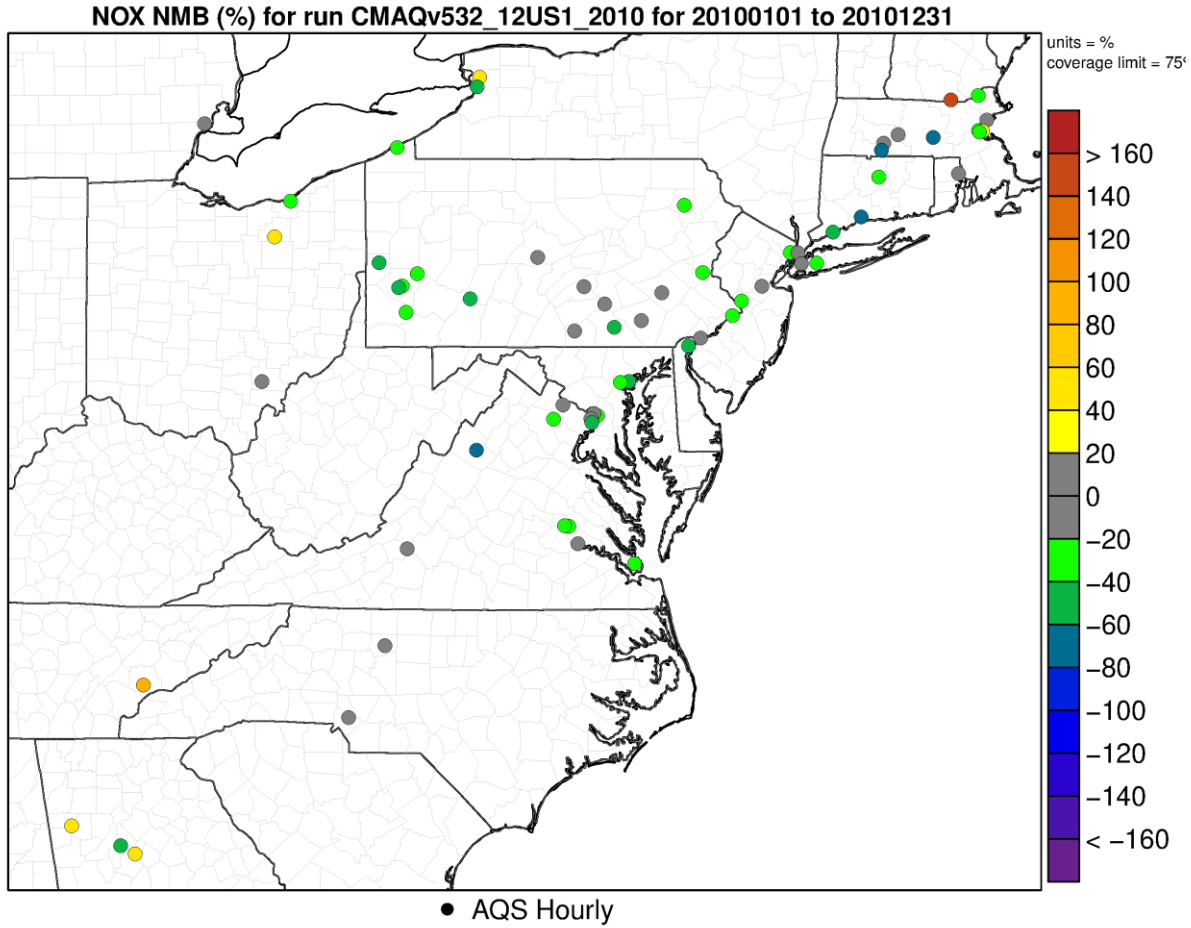
EQUATES(2010)-ECODEP(2010): Reduced Nitrogen

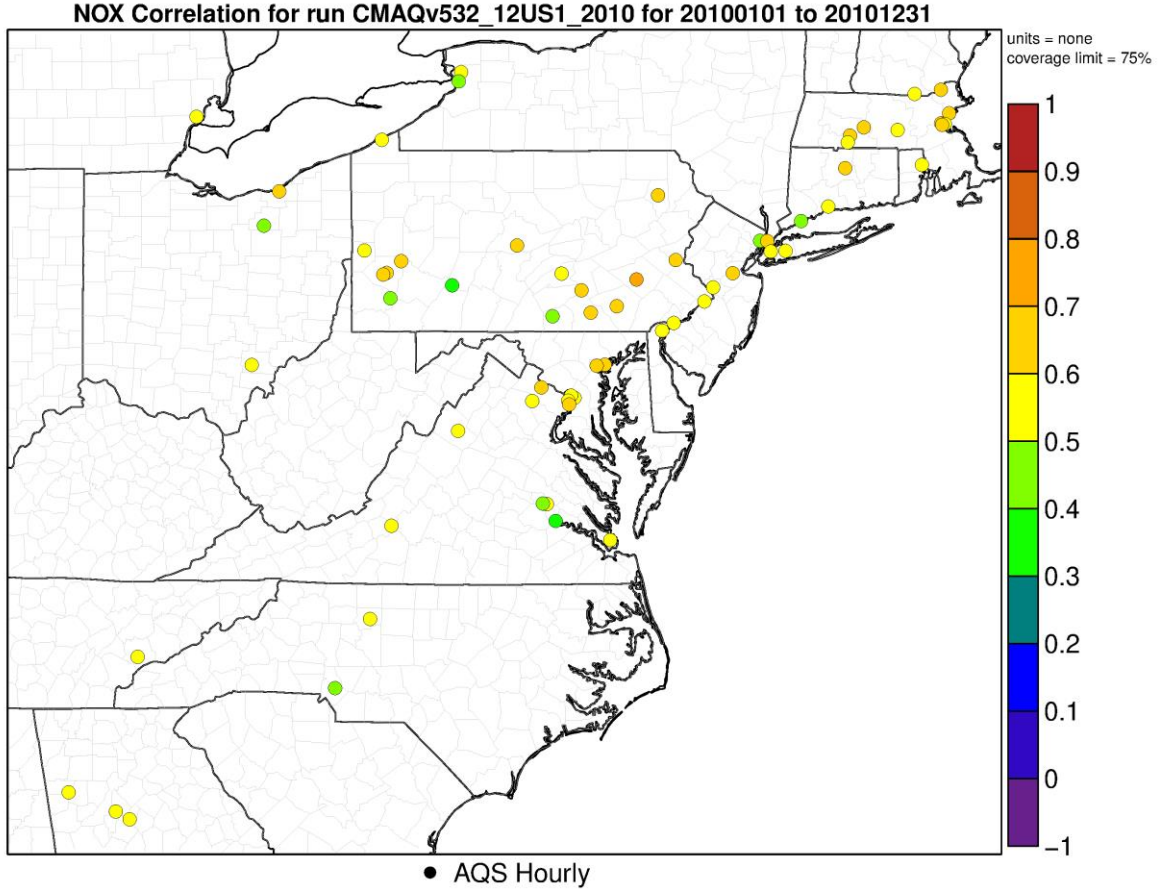


EQUATES(2010)-ECODEP(2010): Oxidized Nitrogen



2010 EQUATES NOx vs AQS





AQS=Air Quality System

United States Environmental Protection Agency

CMAQv5.3 Updates → EQUATES → **Source apportionment in Chesapeake Bay** → Progress and Next Steps

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.

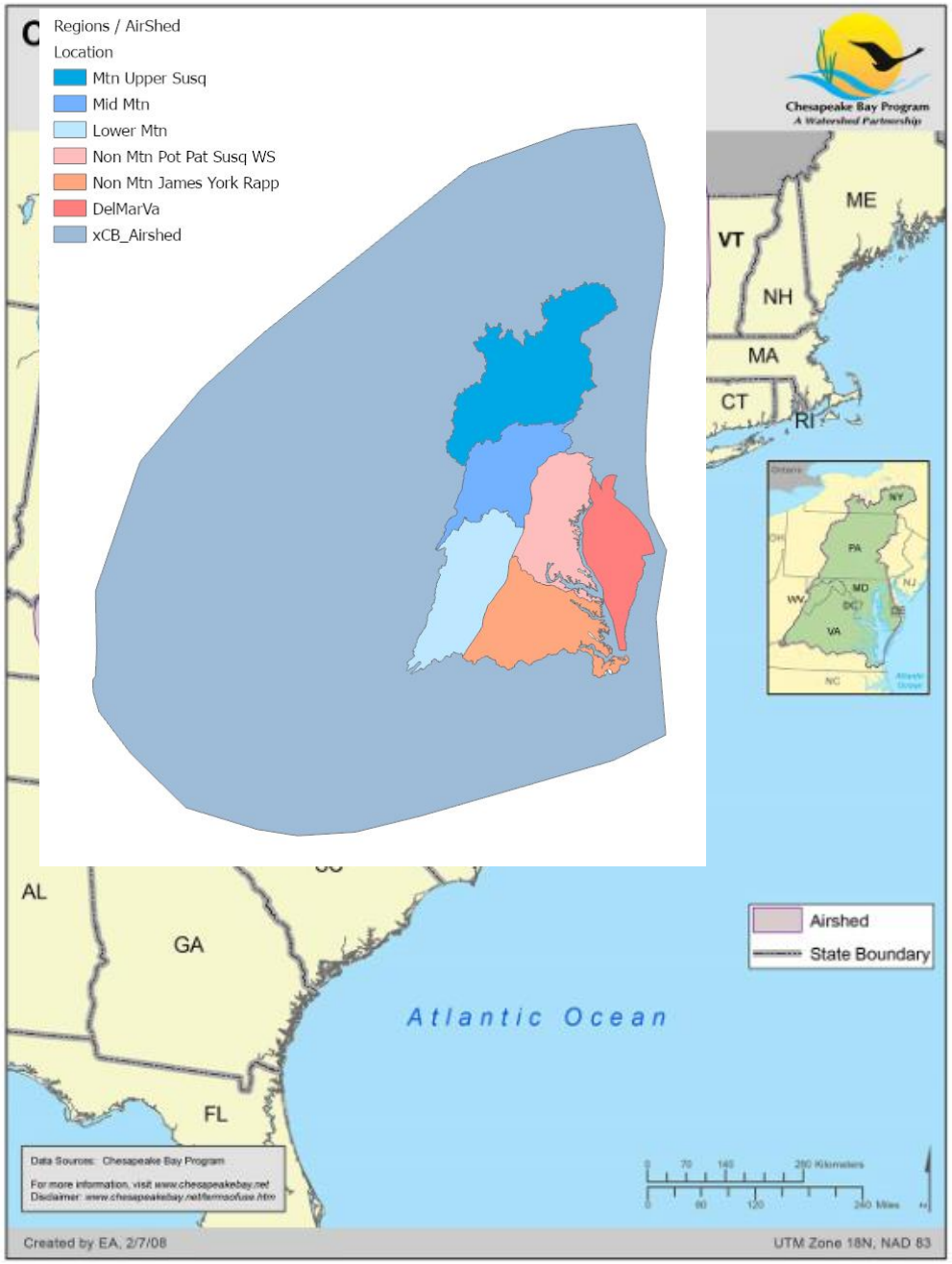
For each species, the production and loss terms from each chemical reaction is tracked (generalized for the available mechanisms) and propagate changes to tags based on stoichiometry and production/loss rates of the precursors.

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

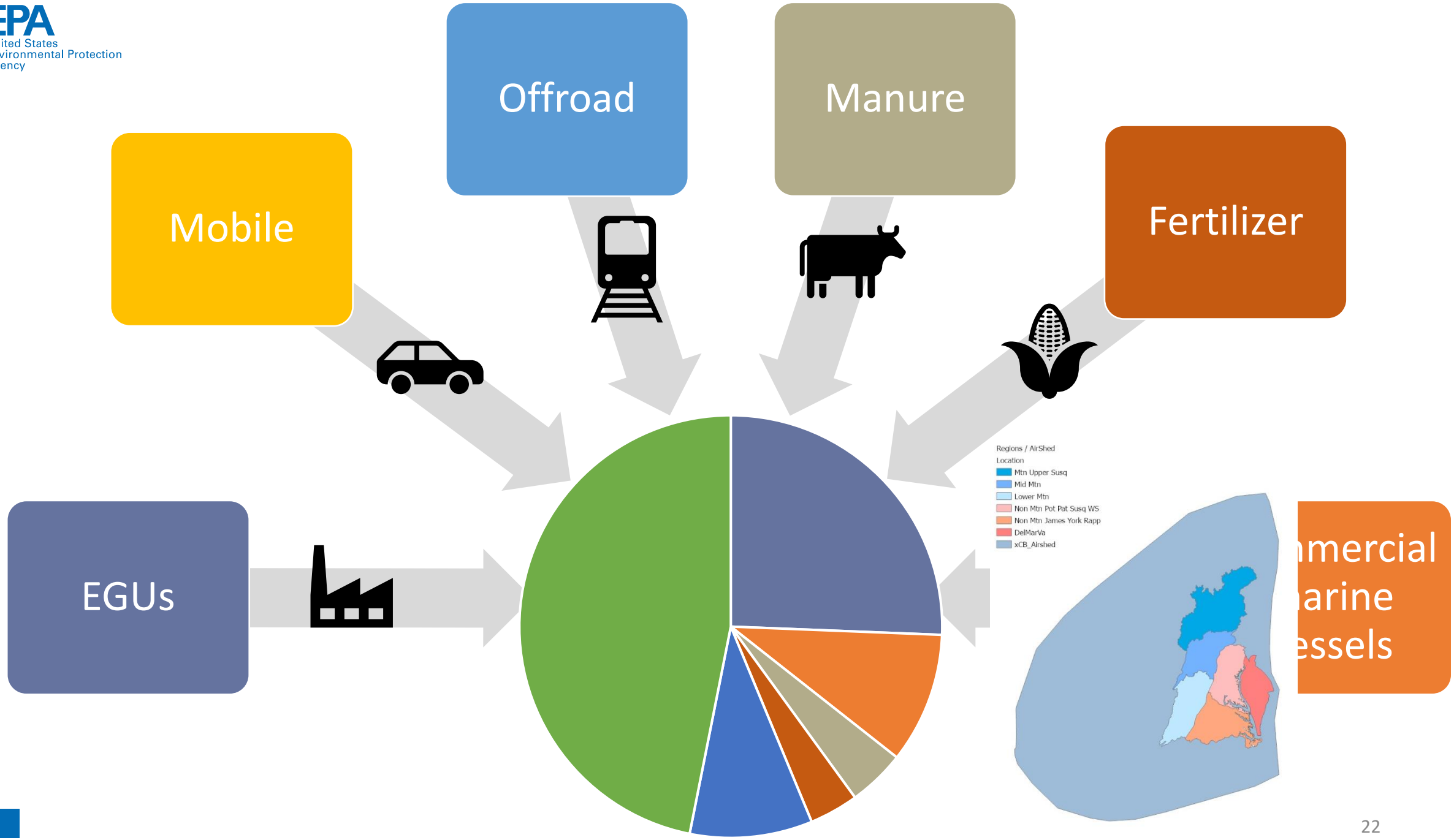
ISAM=Integrated Source Apportionment Method

Chesapeake Bay ISAM

- Atmospheric deposition to the Chesapeake Bay Watershed is among the largest sources of its nutrient loadings.
- The Chesapeake Bay Watershed has one of the largest land-to-water ratios of any coastal water bodies in the world, is home to more than 18 million residents, and contains several heavily polluted urban areas.
- Previous studies have estimated nearly 75% of the airborne nitrogen arriving to the Bay is generated by sources within the Bay's airshed.
- State and local policymakers are interested in using modeling platforms to better understand the connection between atmospheric emissions from controllable sectors and the subsequent nutrient deposition.
- One of the first applications of the revised ISAM.



ISAM=Integrated Source Apportionment Method



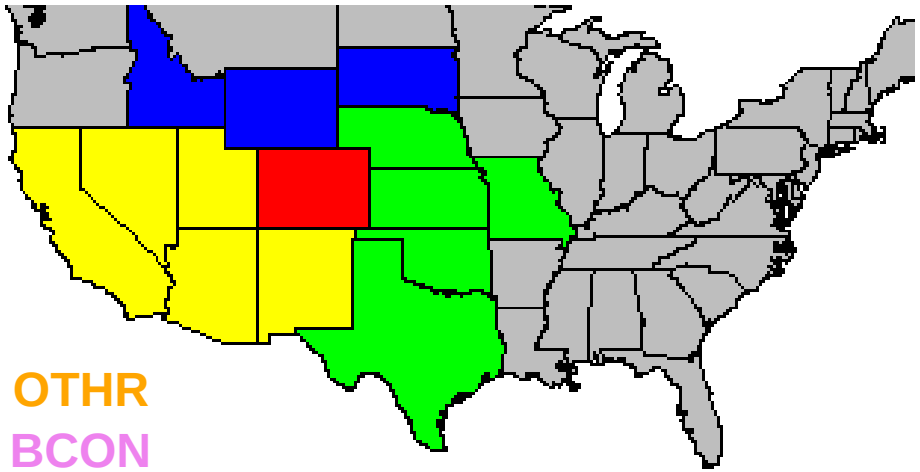
ISAM=Integrated Source Apportionment Method

Rocky Mountain National Park, CO ISAM Application

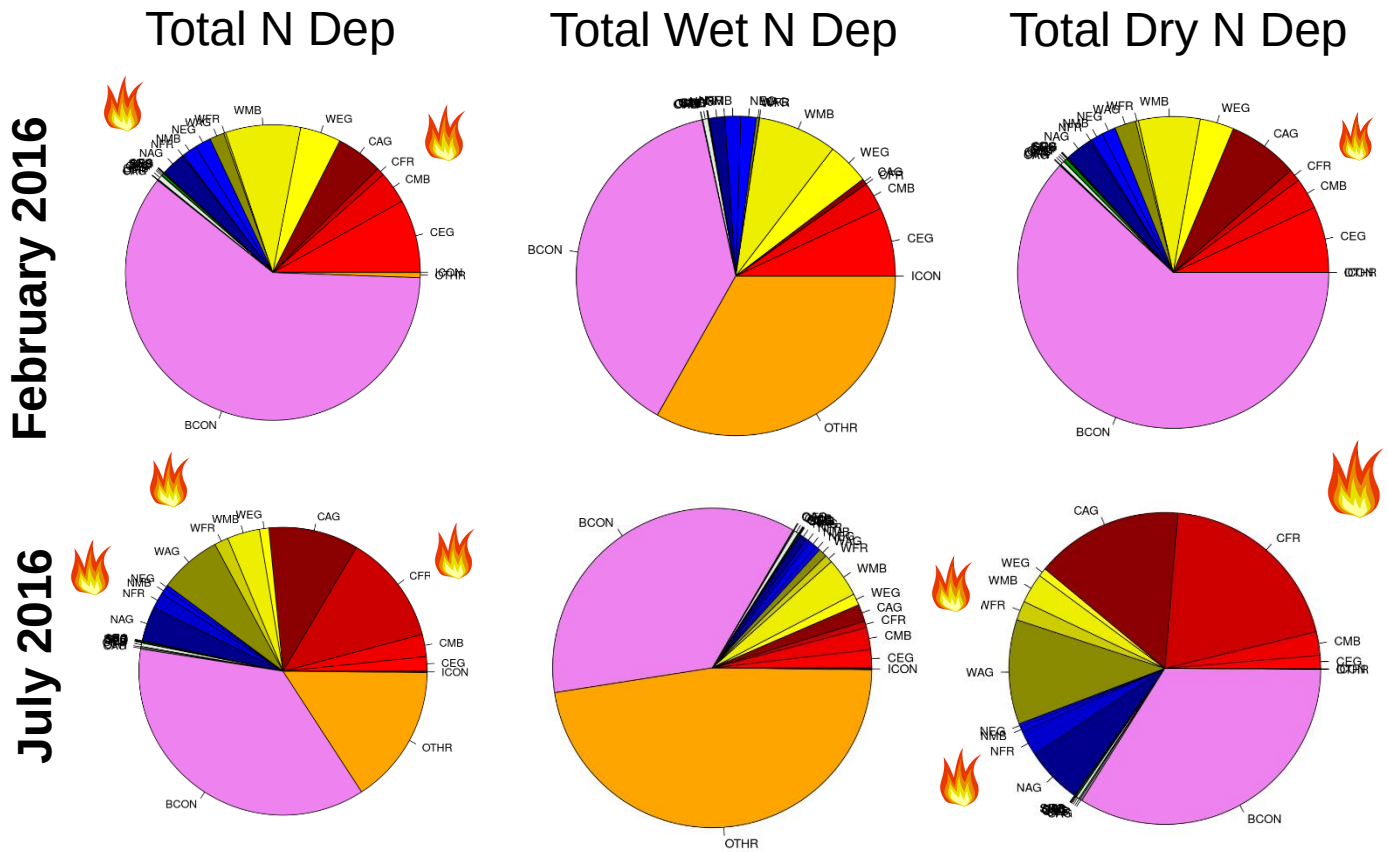
REGIONS
- C=COLORADO
- W =WEST = CA, NV, AZ, UT, NM
- N=NORTH = ID, WY, SD
- S=SOUTH = NE, KS, OK, TX, MO
- OTHER = Rest of the domain, BCs, ICs

EMIS STREAMS
- EG = EGU's
- MB = Onroad + nonroad (mobile sources)
- FR = Fires (Agricultural, Wildland, etc)
- AG = Livestock and fertilizer

Individual species aggregated to total, oxidized, reduced, wet ,dry deposition



Courtesy of Donna Schwede, EPA



- Source contribution varies seasonally
- BCON, OTHR major contributors
- Fires are important contribution to total and dry N deposition

ISAM=Integrated Source Apportionment Method

- CMAQv5.3 new developments:
  - Many improvements in chemistry: improved treatment of organic aerosols, updated marine chemistry, expanded representation of secondary pollutant formation
  - New land-use specific deposition model
  - Incorporated ISAM into base model build
- EQUATES progress:
  - Preliminary results for 2010-2012 show overall total N deposition changed little between EQUATES and ECODEP, but precipitation decreased ~10%
  - Fall 2020: Finish CMAQ simulations; 2021: data post-processed to meet collaborator needs and shared across platforms
- Source apportionment in the Chesapeake Bay:
  - Simulations for 2016 will begin soon
  - First application of revised ISAM tool

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Questions?

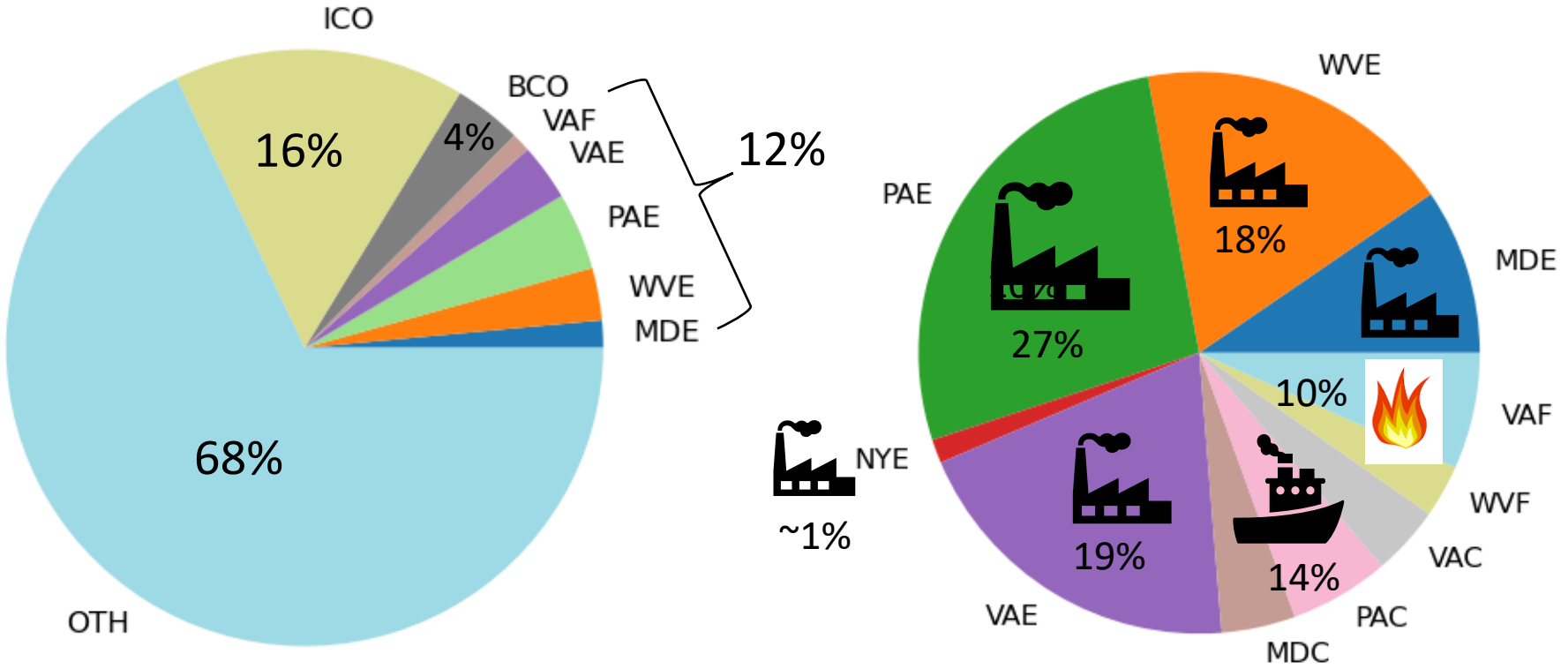
Chesapeake Bay Watershed Preliminary Results

REGIONS

- Maryland (MD)
- West Virginia (WV)
- Pennsylvania (PA)
- New York (NY)
- Virginia (VA)
- Washington, D.C. (DC)

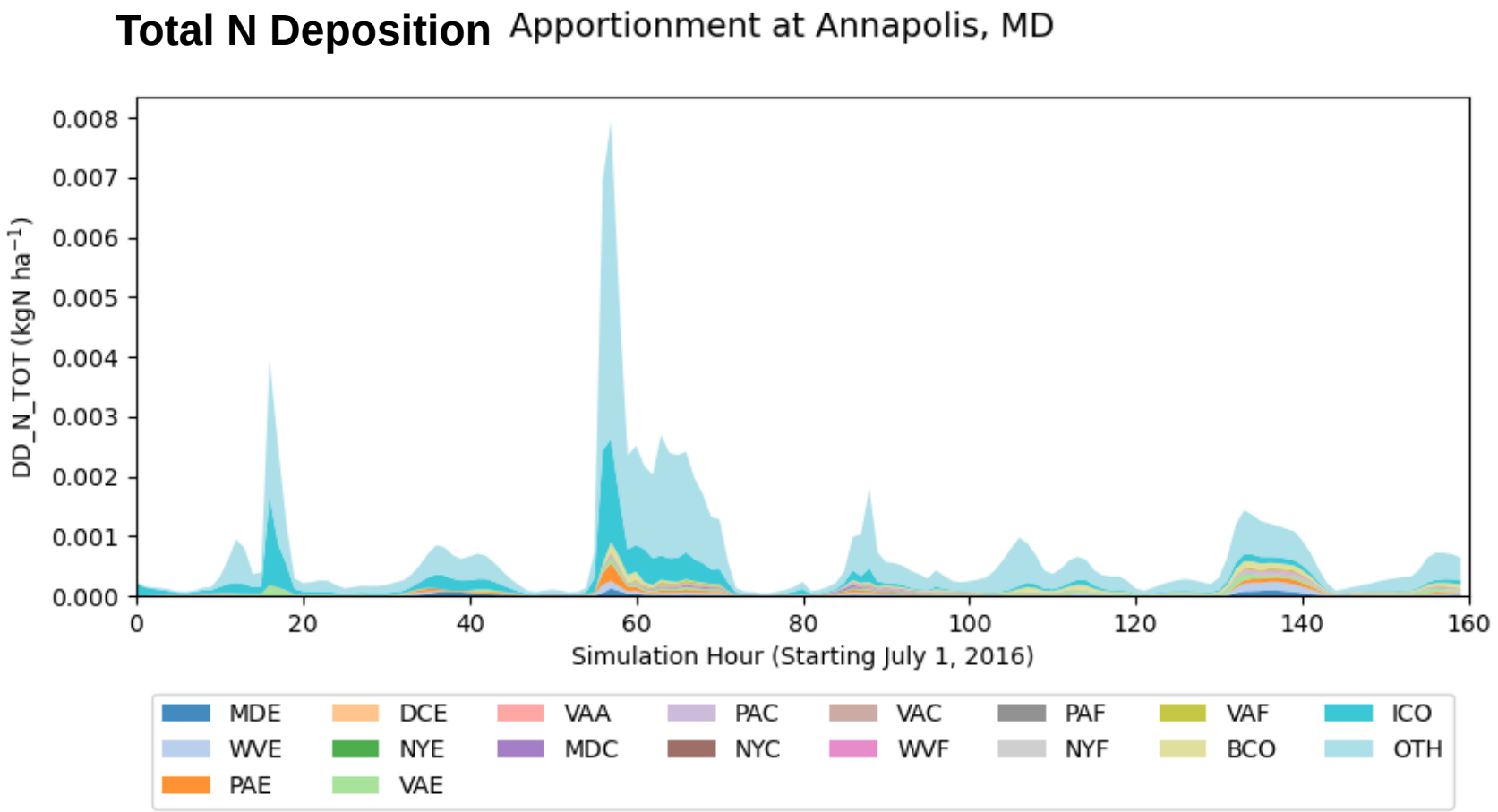
EMIS STREAMS

- EGUs (E)
- Agricultural fires (A)
- Commercial marine vessels (C)
- Fires (F)



- Large contributions from initial and boundary conditions
- EGUs in PA, WV, VA, and MD are influential
- Smaller contribution from fires, CMV

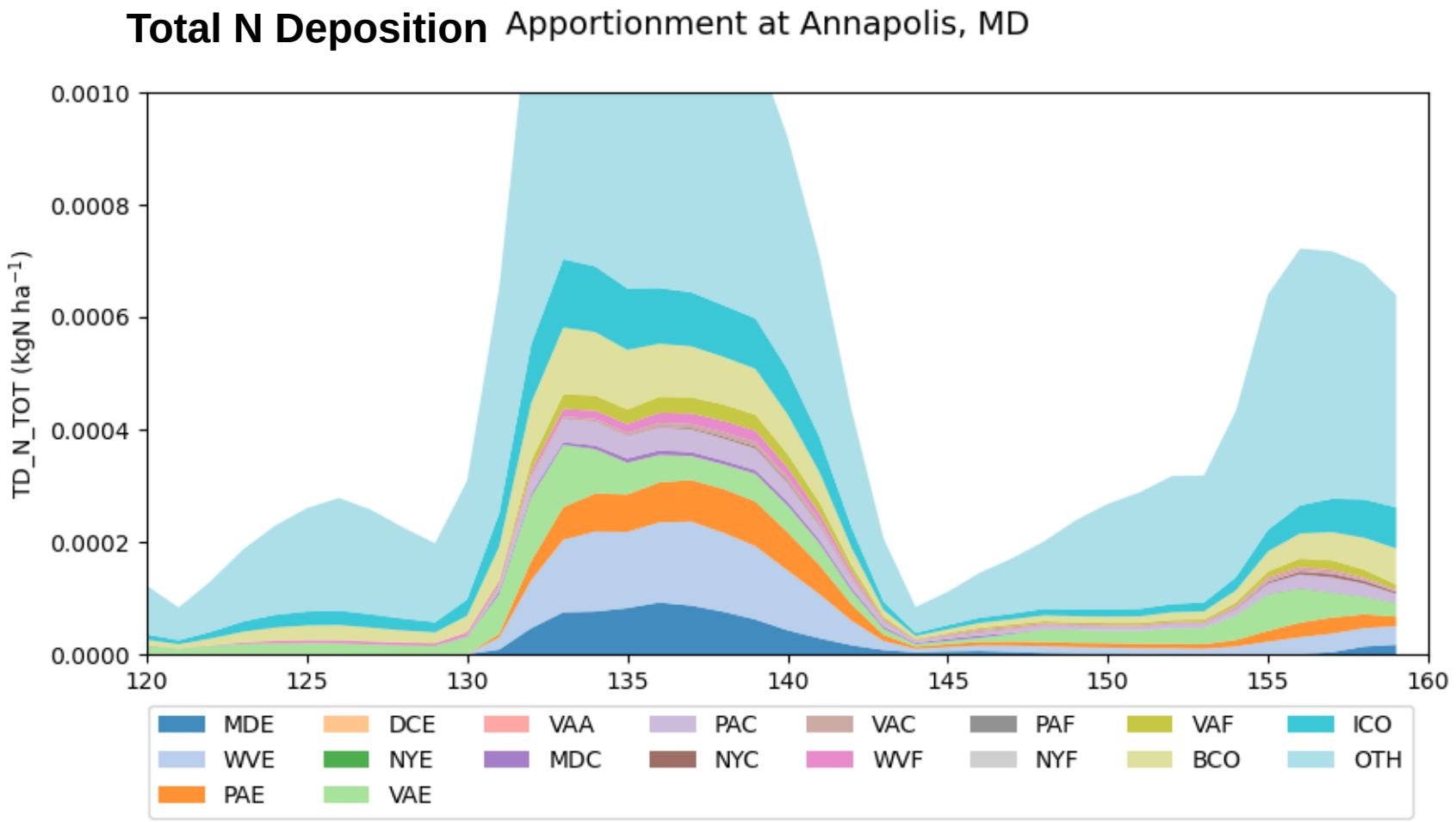
Chesapeake Bay Preliminary Results



TAG ID:
1st two letters: State abbreviation
Last letter:
E=EGU
A=Agricultural fires
C= Commercial marine vessels
F= Fires
BCO=Boundary Conditions
ICO=Initial Conditions
OTH=Other

ICO, OTH dominating total N deposition, especially toward the beginning of the simulation

Chesapeake Bay Preliminary Results



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E=EGU
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OTH=Other

At the end of the simulation, still see large contribution from OTH, BCO, and ICO, but also from EGUs in MD, WV, PA, and VA

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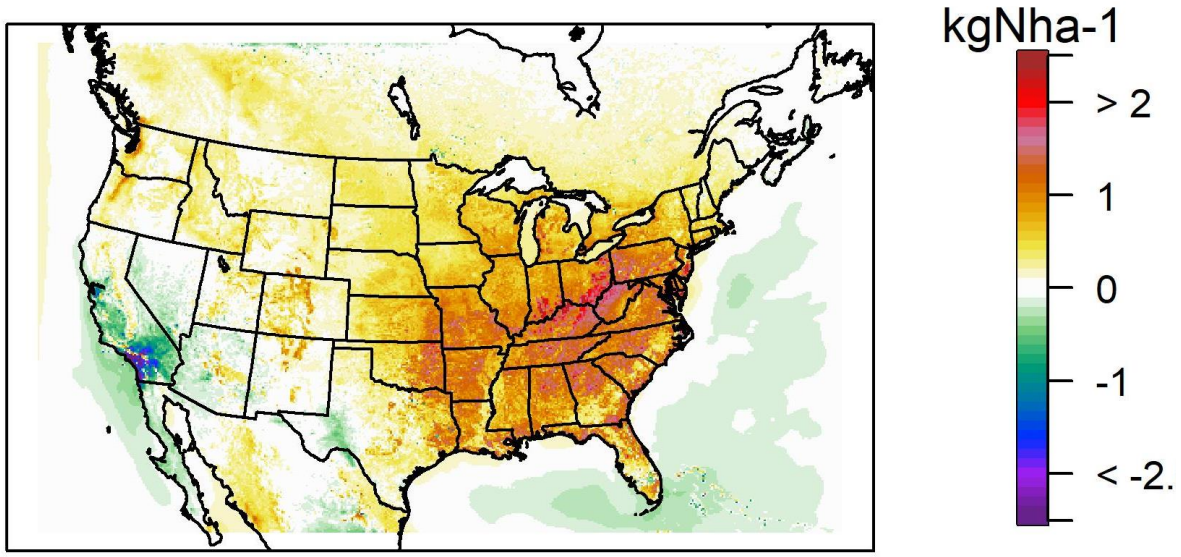
EQUATES(2010)-ECODEP(2010): Dry Deposition of TNO3



EQUATES(2010)-ECODEP(2010): Wet Deposition of TNO3