



Nitrogen Source Apportionment in the Chesapeake Bay Watershed

July Modeling Workgroup Quarterly

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Objectives

CMAQ Simulation Set Up

Preliminary Results Future Simulations and Summary

- Atmospheric deposition is important nitrogen source to the Chesapeake Bay watershed and was dominant source from about 1960 to 2000.
- Despite declines in deposition due to air quality regulations, atmospheric nitrogen deposition still contributes ~25% of the annual nitrogen load to the Chesapeake Bay watershed (Burns et al., 2021).
- Chemical transport models, like CMAQ, can extend deposition estimates from limited ground networks to understand atmospheric deposition:
 - Given recent improvements in CMAQ, how do new estimates of deposition compare to observations and previous long-term simulations?
 - What are the important emission sources and source regions contributing to nitrogen deposition in the Chesapeake Bay watershed?
 - The analysis centers on the question, "For a nitrogen emission source from different regions in the Chesapeake watershed, what is the fraction that is deposited to a particular region or point?"



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Preliminary Results Future Simulations and Summary

Model

• CMAQv5.3.2

Time Period January-December 2016*

Grid

• 12 km windowed domain

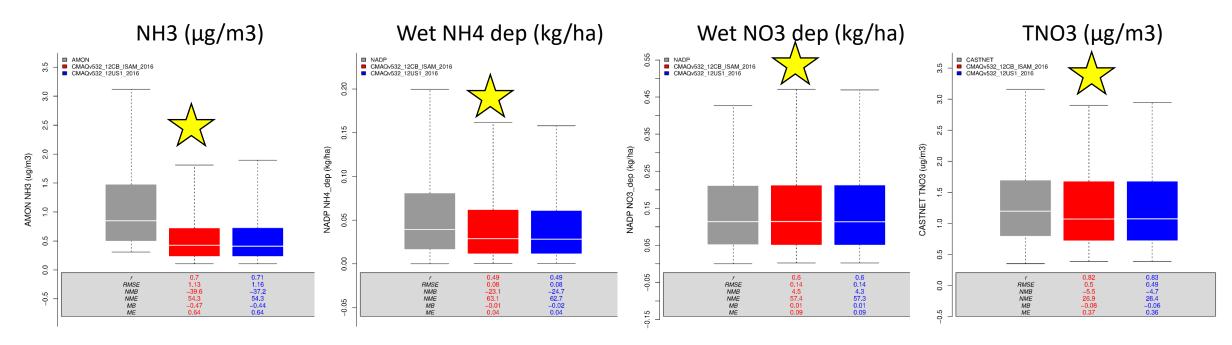




	12US1_2016 (EQUATES)	12CB_2016
Domain	Full Domain	Windowed
Model	CMAQv5.3.2	CMAQv5.3.2
Date Range	2016 (2002-2017 also available)	2016
Resolution	108 km N Hemisphere+ 12 km CONUS	12 km Windowed domain over the Chesapeake Bay Watershed
Meteorology	WRFv4.1.1	WRFv4.1.1
Emissions	2017 NEI as primary base year; consistent methods used for each sector to avoid artificial step changes	Same
Boundary Conditions	N Hemisphere CMAQv5.3.2	Combination of 12 km EQUATES and 108 km N Hemisphere



Windowed Versus Full Domain Results



- Annual 12CB domain simulation was completed to evaluate potential evaluation differences
- NH₃ and TNO₃ ambient concentrations and NH₄ and NO₃ wet deposition totals are largely similar
- Model to model evaluations of dry and wet deposition of N species were compared and the differences were on the same order as the evaluation against observations
- Model differences due to the windowing of the domain are on the order of 1-2% and are consistent with EQUATES simulation results



Source Apportionment: 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.

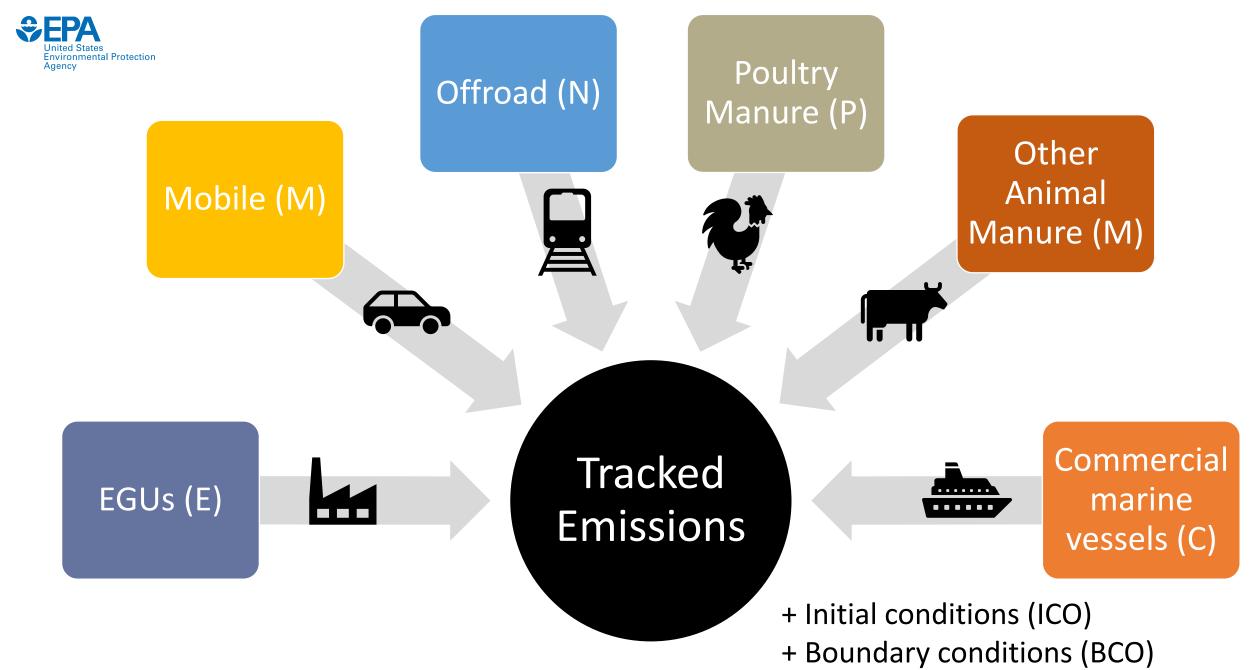
Tag Class	Model species
Sulfate	SO ₂ , H ₂ SO ₄ , SO ₄ ²⁻
Nitrate	HNO ₃ , HNO ₂ , NO ₃ -, NO ₃ , NO ₂ , NO, Organic Nitrates
Ammonium	NH ₃ , NH ₄ ⁺
EC	Elemental Carbon Aerosols
OC	Organic Carbon Aerosols
VOC	Volatile Organic Aerosols
PM25_IONS	CI, Na, Mg, K, AI, Si, Mn, and other aerosol cations
CO	CO
Ozone	All Nitrate species + all VOC species



Source Regions

Tag	Strawman Name
СР	Central Coastal Plain and Piedmont Region
EU	Eastern Urban Region
CA	Central Appalachian-Ridge and Valley Region
DM	Delmarva Coastal Plain Region
NE	Northeast Appalachian Highland Region
NW	Northwest Appalachian Highland Region
SP	South Coastal Plain and Piedmont Region
SA	Southwest Appalachian Region
ОТ	All other locations



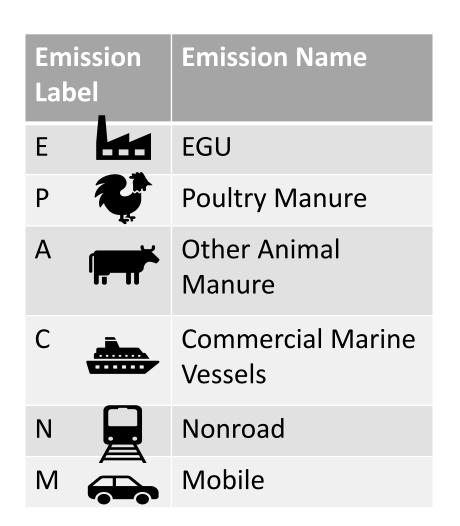


+ Other (OTH-all other emissions)



Tag Name=2 letter Region Label+1 letter Emission Label





BCO=Boundary Conditions
OTH=Other



Objectives

CMAQ Simulation Set Up

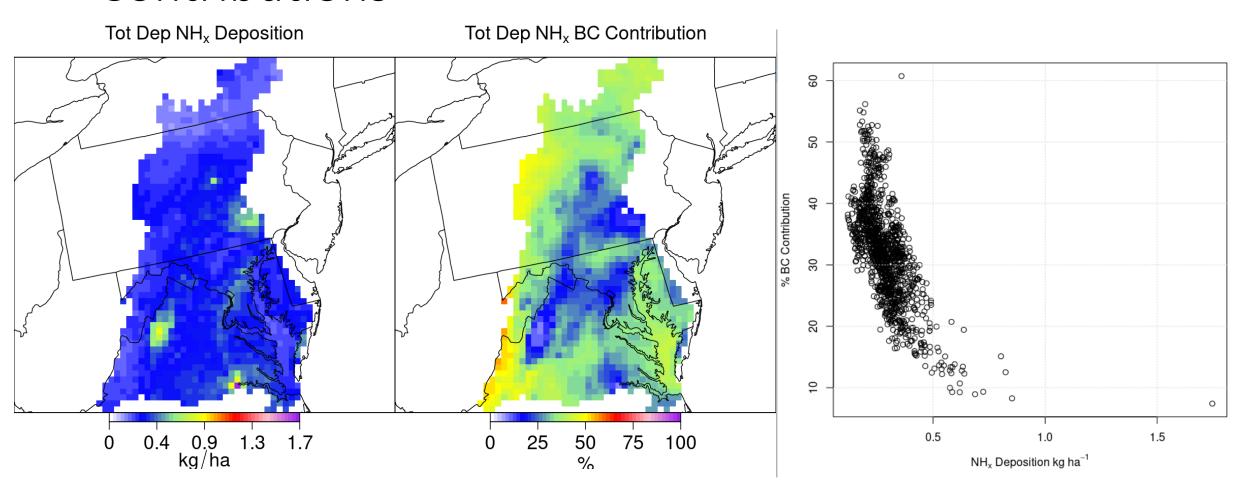
Preliminary Results Future Simulations and Summary

- Model is still running!
- Preliminary Results from January through March 2016 only
- Time of year when deposition is usually the lowest
- Some minor species are not tracked in ISAM
 - Coarse mode aerosol deposition and some organic nitrates
 - Minor components, typically less than 1% of NO_y, total oxidized N, deposition





NH_x Total Deposition: Boundary Condition Contributions

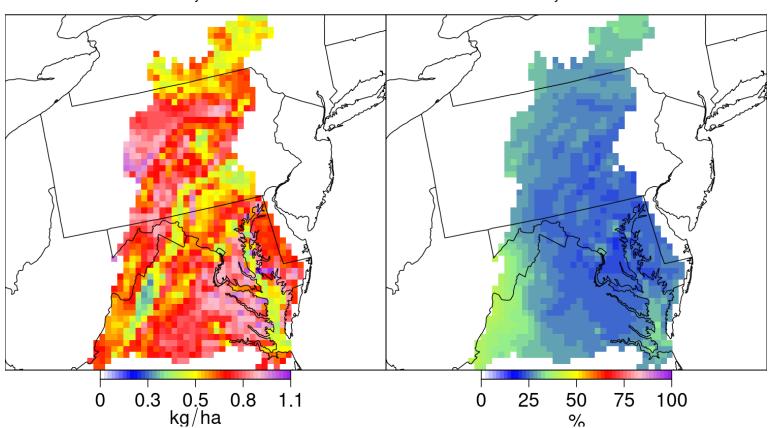




NO_y Total Deposition: Boundary Condition Contributions

Tot Dep NO_v Deposition

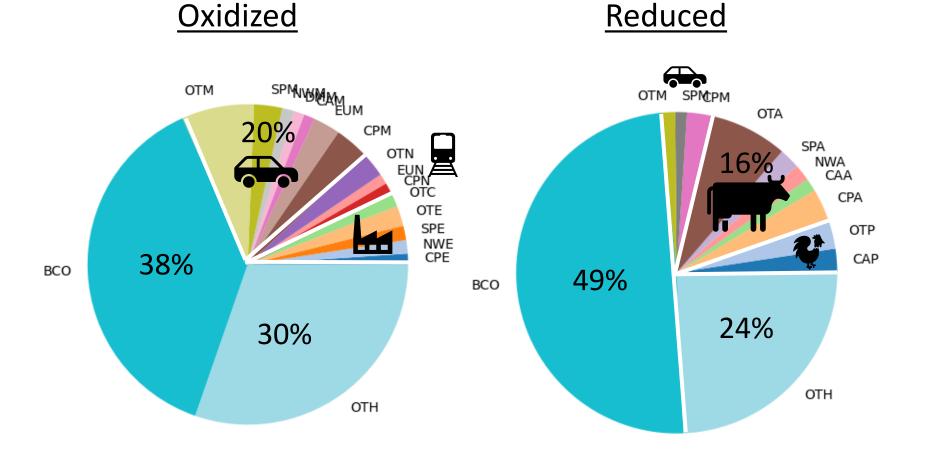


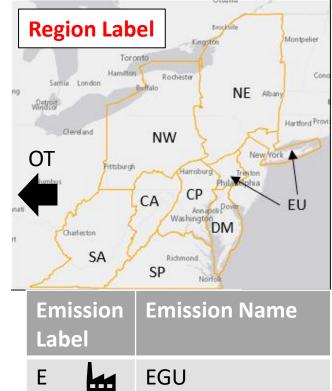


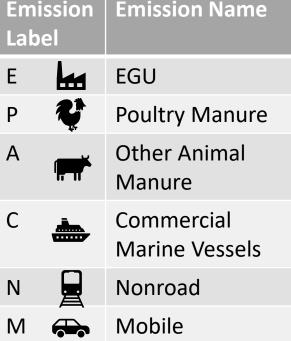
- Boundary conditions contributed to 30% of NH_x and 27% of NOy total deposition
- Areas of high NH_x deposition had low boundary conditions contributions
 - High NH_x deposition is estimated to be from local sources and likely dominated by NH₃
- NO_y boundary condition contributions are more uniform
 - Likely due to the secondary atmospheric formation of major deposition species, e.g. HNO₃.



Wet N Deposition (Jan-March)







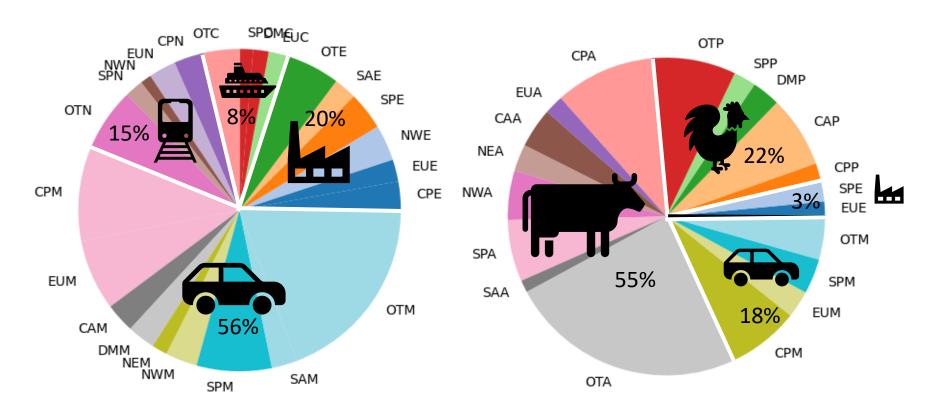
BCO=Boundary Conditions
OTH=Other



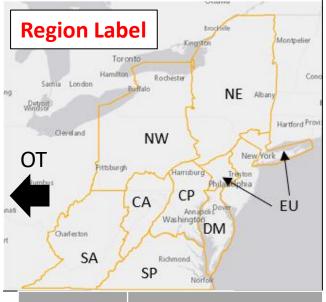
Wet N Deposition (Jan-March)

Oxidized

Reduced



Tag Name=2 letter Region Label+1 letter Emission Label



Emission Label		Emission Name	
Е	44	EGU	
Р	Ų,	Poultry Manure	
Α		Other Animal Manure	
С		Commercial Marine Vessels	
N		Nonroad	
M		Mobile	

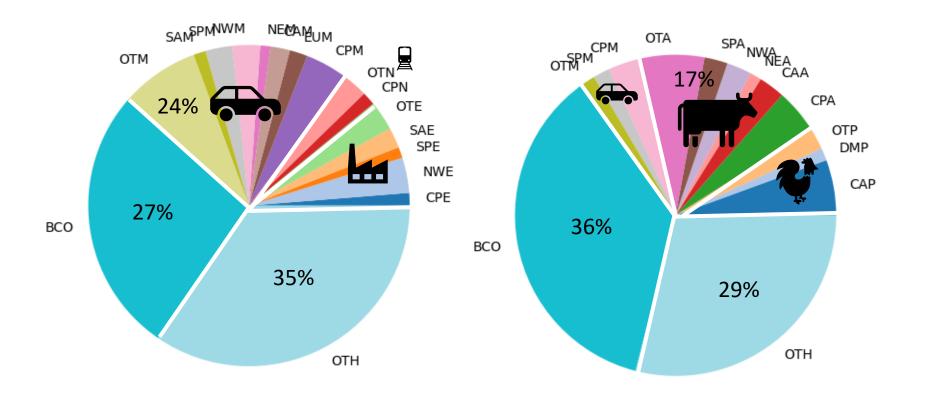
BCO=Boundary Conditions OTH=Other

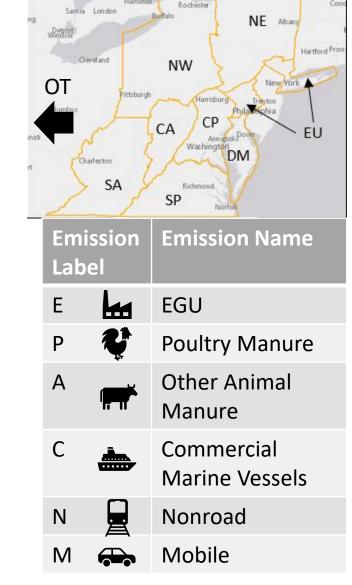


Total N Deposition (Jan-March)

Oxidized

Reduced





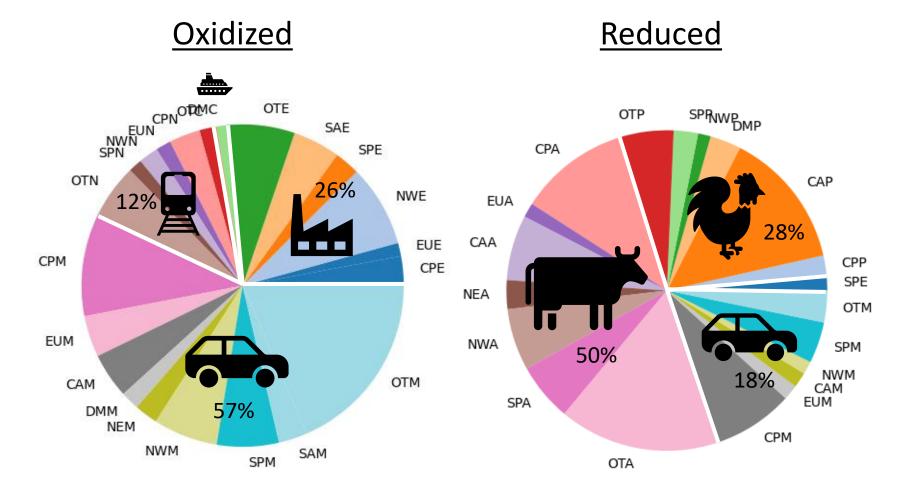
Montpelier

Region Label

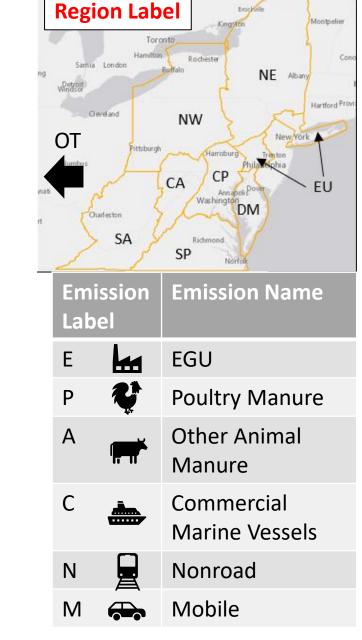
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Total N Deposition (Jan-March)



Tag Name=2 letter Region Label+1 letter Emission Label



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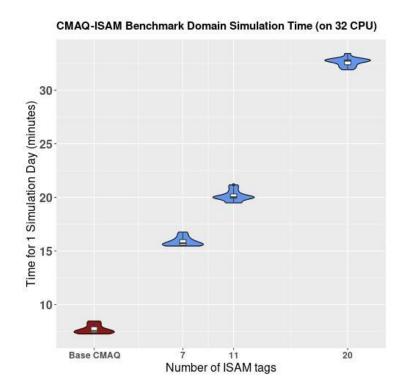


Objectives

CMAQ Simulation Set Up

Preliminary Results Future
Simulations
and Summary

- Assess annual, seasonal source apportionment to Chesapeake Bay Watershed when model is finished running.
- Future simulations will estimate reductions of nitrogen deposition to the Chesapeake watershed and tidal Bay under future conditions of greater penetration of electric vehicles into the existing fleet, greater wind and solar electric generation, and other types of future economic conditions.
 - The next release of CMAQv5.3.3 (release date Fall 2021) with new emissions scaling tools is required to conduct these simulations.





Summary

- Model differences due to the windowing of the domain are on the order of 1-2% and are consistent with EQUATES simulation results.
- The model simulations with ISAM are still running and we expect the full year to be completed in a few days.
- Preliminary results over Jan-March 2016 in the Chesapeake Bay Watershed show:
 - Mobile sources are a large contributor to total oxidized nitrogen deposition (~24% of total);
 - Non-poultry animal manure is an important source of total reduced nitrogen deposition (~17%);
 - Regions outside the Watershed are responsible for ~13% of the total oxidized nitrogen deposition, followed by the Northwest Appalachia and Central Coastal Plain (~7% each);
 - The Other and Central Appalachia regions are responsible for ~9% each of the total reduced nitrogen deposition.



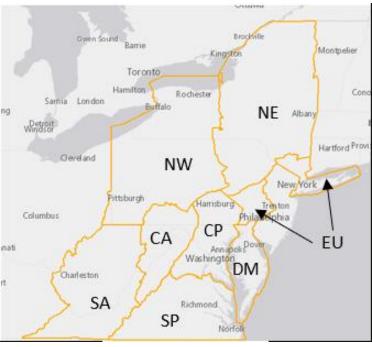
Questions?





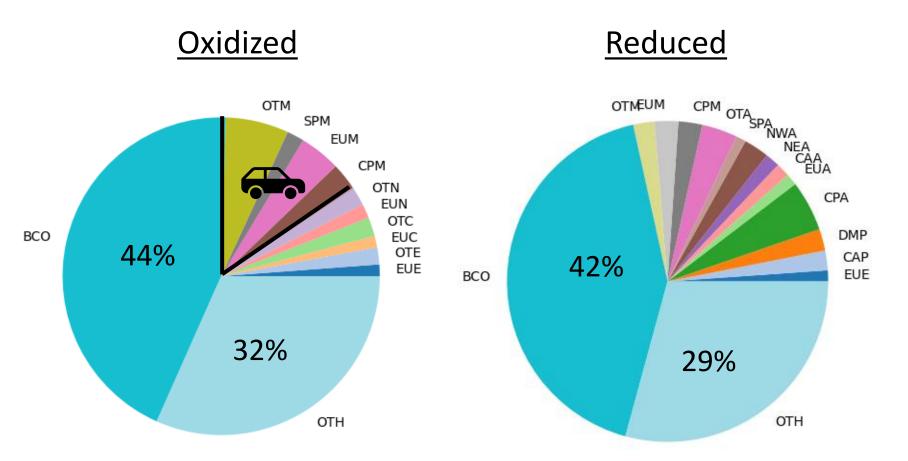
Fraction of Emissions Reaching Chesapeake Bay Watershed

Source Region	EGU	Mobile	Onroad	Poultry Manure	Other Animal Manure	Commercial Marine Vessels	
Central Coastal Plain and Piedmont (CP)							ņ
E Urban (EU)							
Central Appalachian- Ridge and Valley (CA)							
Delmarva Coastal Plain (DM)							_
NE Appalachian Highland (NE)							
NE Appalachian Highland (NW)							
S Coastal Plain and Piedmont (SP)							
SW Appalachian (SA)							





January Wet Deposition



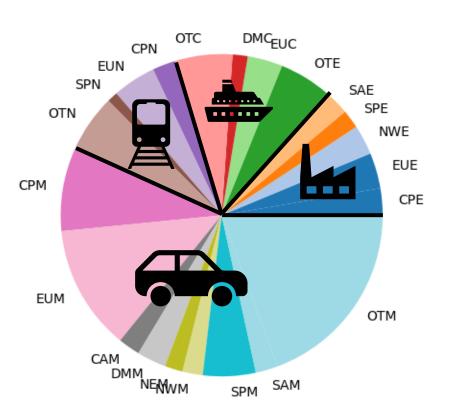


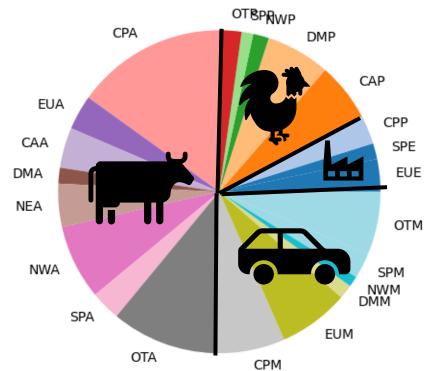
Name
EGU
Poultry Manure
Other Animal Manure
Commercial Marine Vessels
Nonroad
Mobile



January Wet Deposition

Oxidized Reduced



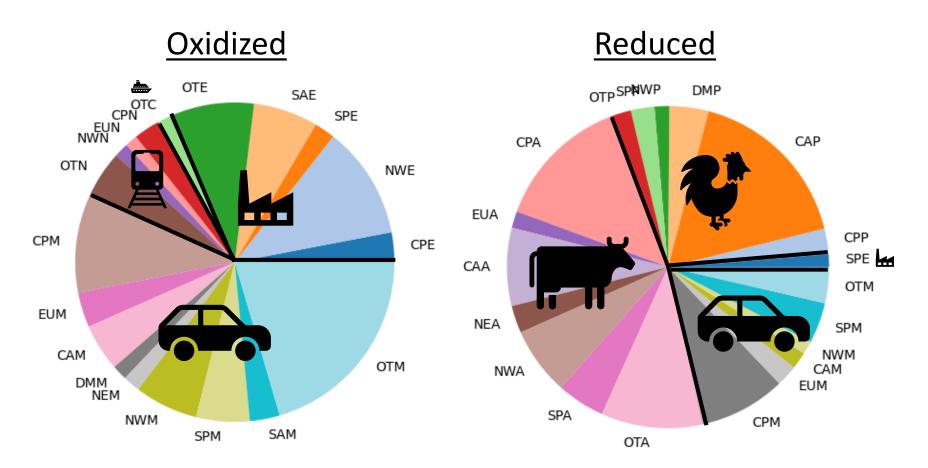




Tag	Name
Е	EGU
P	Poultry Manure
Α	Other Animal Manure
С	Commercial Marine Vessels
N	Nonroad
M	Mobile



January Total Nitrogen Deposition





Tag	Name
Е	EGU
Р	Poultry Manure
Α	Other Animal Manure
С	Commercial Marine Vessels
N	Nonroad
M	Mobile



Chesapeake Bay Watershed Preliminary Results

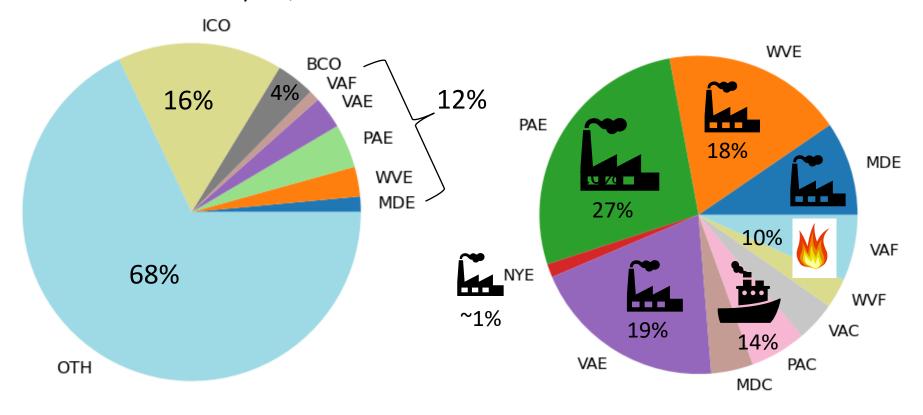
Chesapeake Bay Watershed July 1-7, 2016

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)

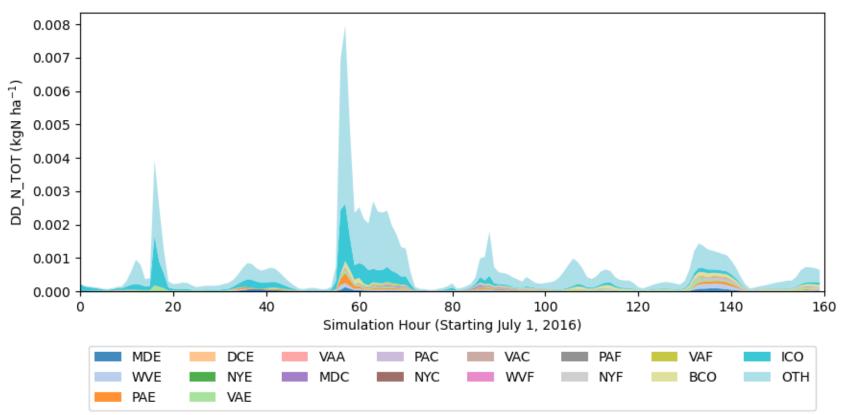


- Large contributions from initial and boundary conditions
- EGUs in PA, WV, VA, and MD are influential
- Smaller contribution from fires, CMV



Chesapeake Bay Preliminary Results

Total N Deposition Apportionment at Annapolis, MD



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

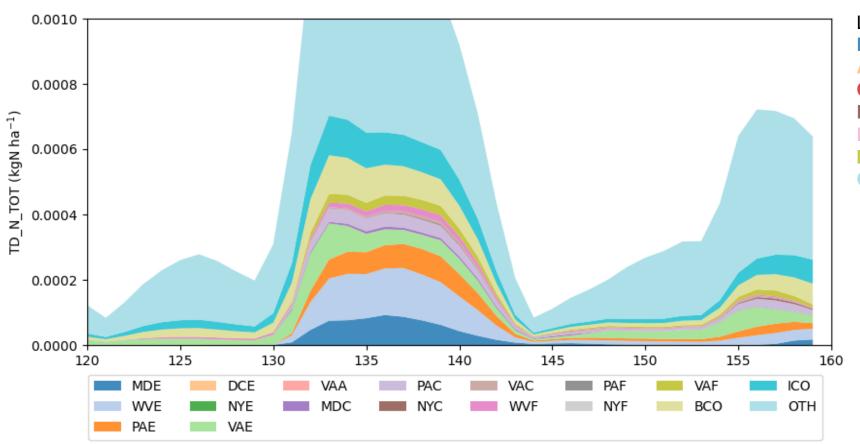
OTH=Other

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



Chesapeake Bay Preliminary Results

Total N Deposition Apportionment at Annapolis, MD



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

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