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Recent Enhancements to the Community Multiscale Air Quality (CMAQ) Modeling System

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US EPA Office of Research and Development

EPA Tools and Resources Webinar
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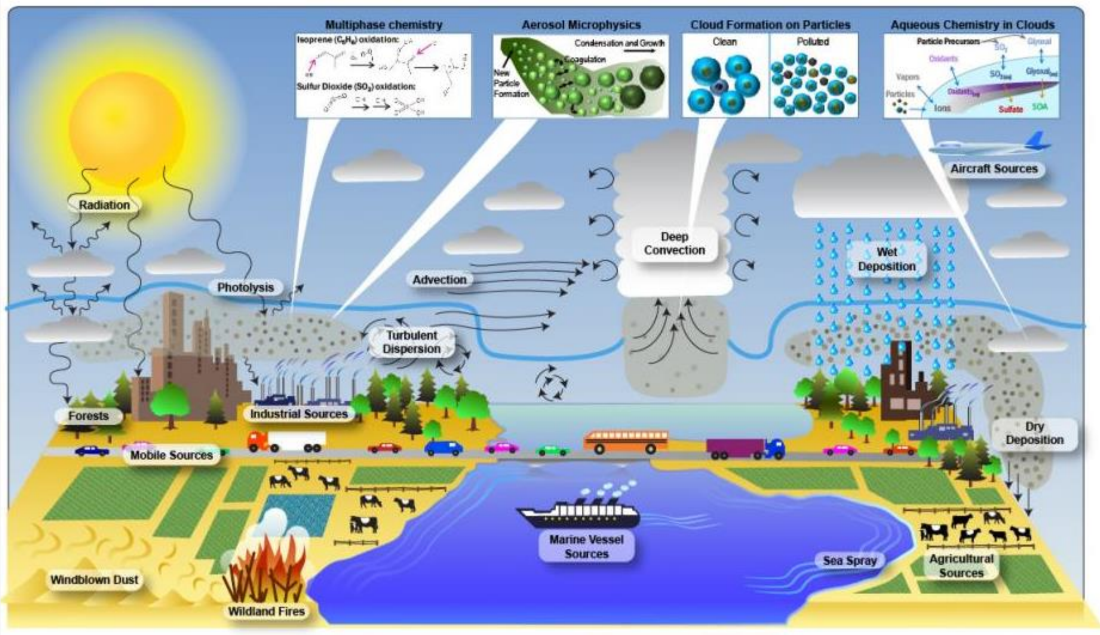
United States Environmental Protection Agency

Why do we need atmospheric models?

Problem

- The **complexity of physical and chemical atmospheric processes**, combined with the **enormity of the atmosphere**, make results obtained from laboratory and field experiments difficult to interpret without a **clear conceptual model of the workings of the atmosphere**, e.g.:
  - Extrapolation of results to other geographic areas
  - Assessing atmospheric chemical state in response to emission perturbations
- Because an understanding of individual processes may not necessarily imply an understanding of the overall system, measurements alone cannot be used to
  - Explore the future state of the atmosphere
  - Formulate effective abatement strategies



Managing air quality requires an understanding of complex phenomena, interactions and emission sources

— Comprehensive models serve as "*numerical laboratories*" to quantify these interactions and source-receptor relationships

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EPA's Air Quality Models:

Vital for implementing the Clean Air Act

Evolution of models guided by increasingly complex application & assessment needs

Problem

Regulatory & Assessment Needs

-Standards
-Assessments

-PSD
-New Source Permitting

NAPAP

1-hr O3
SIP

NAAQS
8-hr O_3
PM 2.5

O3, PM attainment demonstrations
Regional Haze

Nat. Air Toxics Assessment
&
Air Quality Forecasting

- Hg
-Toxics

Meteorology - Air Quality Interactions

Exposure

Background air pollution

Met-AQ Interactions

Exposure & Health

Multimedia

1970 — **2019**

AQDM

UNAMAP

Regional Acid Deposition Model –
Regional Oxidant Model
Eulerian Grid Models
- Acid Deposition
- Ozone

MODELS3

CMAQ
For PM

Neighborhood Scale CMAQ
- CFD

NAM-CMAQ

Multi-pollutant CMAQ

Coupled WRF-CMAQ

CMAQv5.3

CMAQ NextGen

Single Pollutant
Non-reactive
Gaussian Dispersion
Local/urban Scales

Single Pollutant
Reactive
Eulerian Grid
Regional/urban Scales

Multi-pollutant
Multi-scale
Reactive
Eulerian Grid
Regional/urban Scales

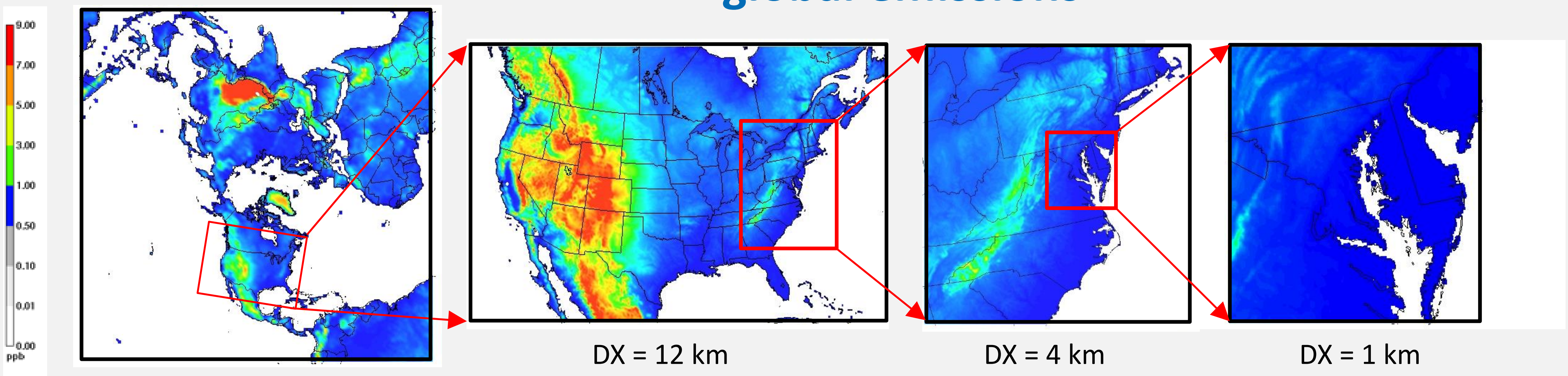
Multi-pollutant
Multi-scale (***local to hemispheric***)
Interactions with Climate forcing and Air Quality changes
Eulerian Grid

Multi-pollutant
Near-source to Global
Reactive
Multimedia: Atmospheric-Hydrologic

Model Development & Applications

Problem

Air pollution must be examined in the context of changing global emissions



DX = 108 km

DX = 12 km

DX = 4 km

DX = 1 km

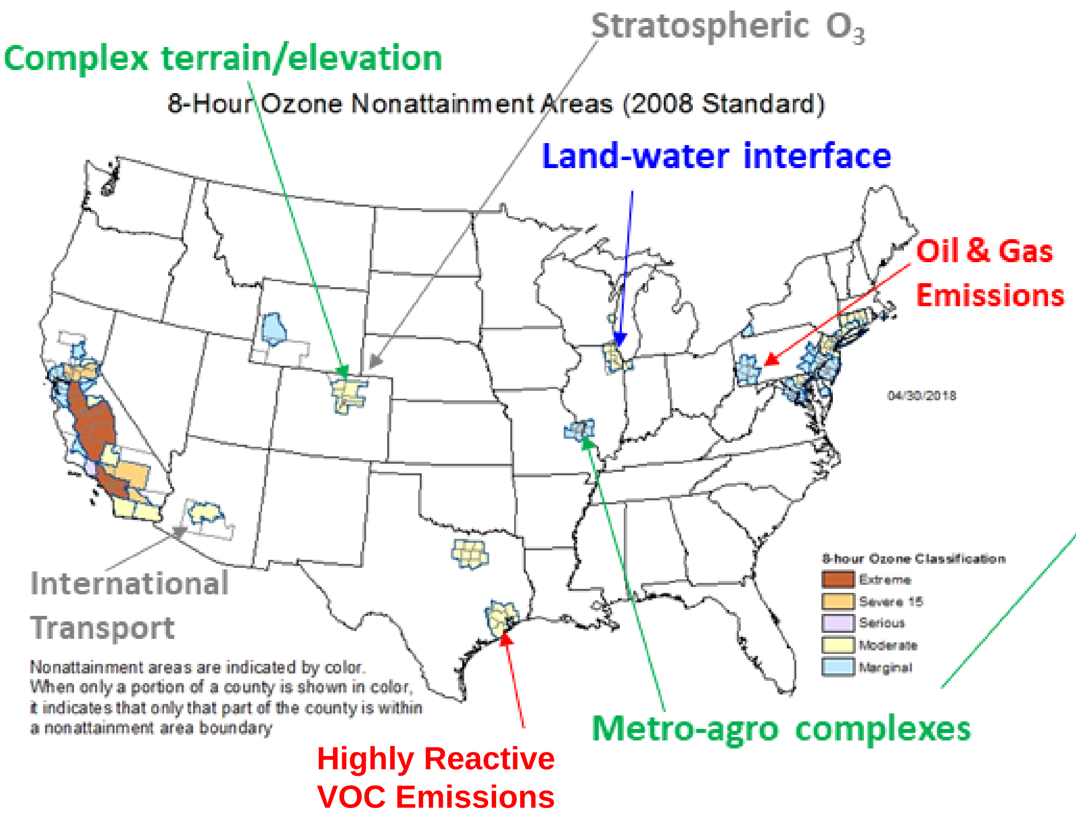
- There is a need for accurate representation of key atmospheric processes across global to local scales
- Increasing importance of long range transport (LRT) contributions as National Ambient Air Quality Standards (NAAQS) are updated

Local nonattainment problems require *individualized* approaches

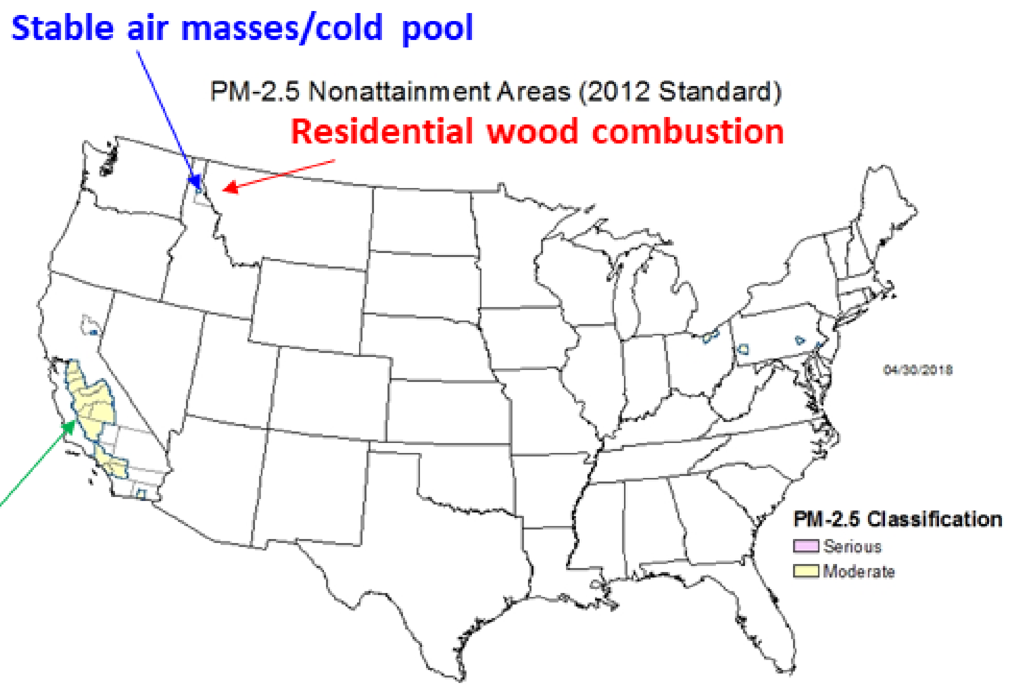
Problem

Local nonattainment presents ***unique process and modeling challenges*** due to a combination of unique emission sources, meteorological conditions, geographical features, and/or non-controllable sources.

Nonattainment Classification: O_3



Nonattainment Classification: $PM_{2.5}$

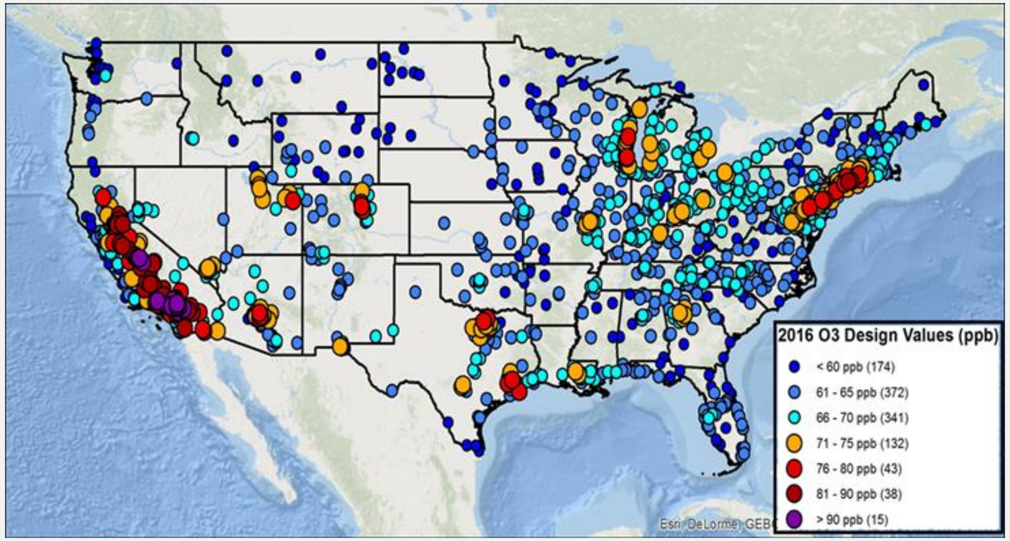


➡ **Fine-scale air quality modeling capabilities developed for a particular nonattainment area may not necessarily be transferable to another area**

Increasing Need to Quantify Natural Contributions and Anthropogenic Enhancements

Problem

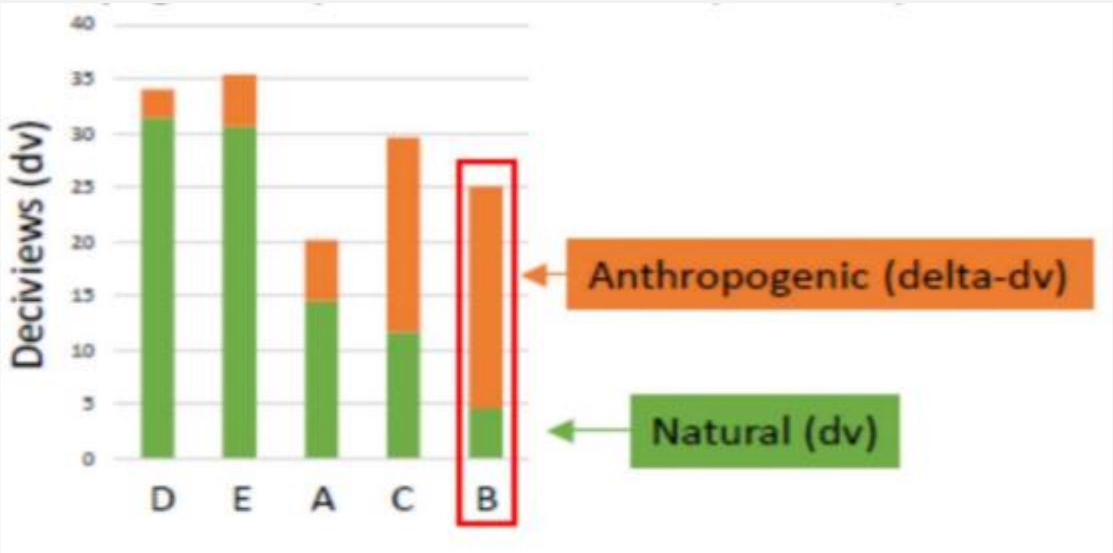
O_3 NAAQS



2016 Daily-max 8-Hour Ozone (DM8O_3) Design Values across the US

< 60 ppb 61-65 ppb 66-70 ppb 71-75 ppb 76-80 ppb 81-90 ppb >90 ppb

Regional Haze



- Updated standards place ***greater/renewed emphasis*** on the ability of models to
  - Simulate the *entire spectrum of concentrations*
  - Accurately represent *(smaller) contributions from numerous sources*
  - Represent atmospheric physics and chemistry over *larger space and time scales*
  - Incorporate *uncertain emissions* from (i) regions outside the US; (ii) sectors (international shipping, soil NO_x)
  - "Anthropogenic impairment" vs. natural contributions
  - Aerosol optical properties (composition & *size*)

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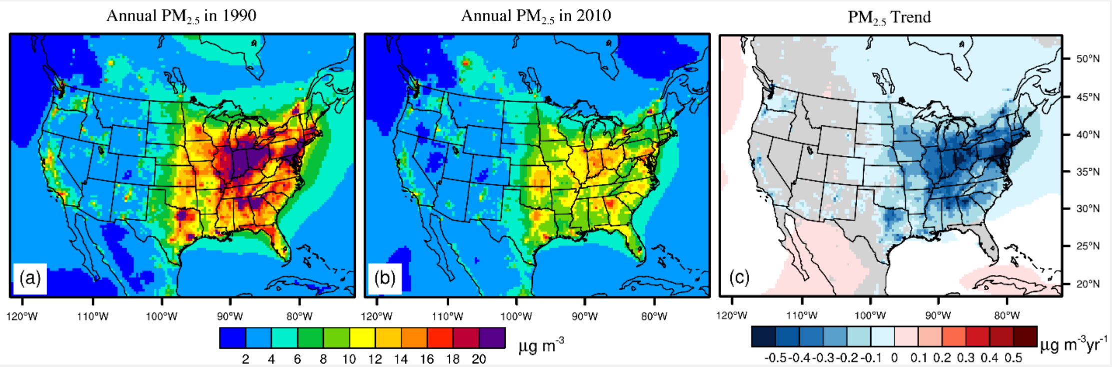
CMAQ Modeling System

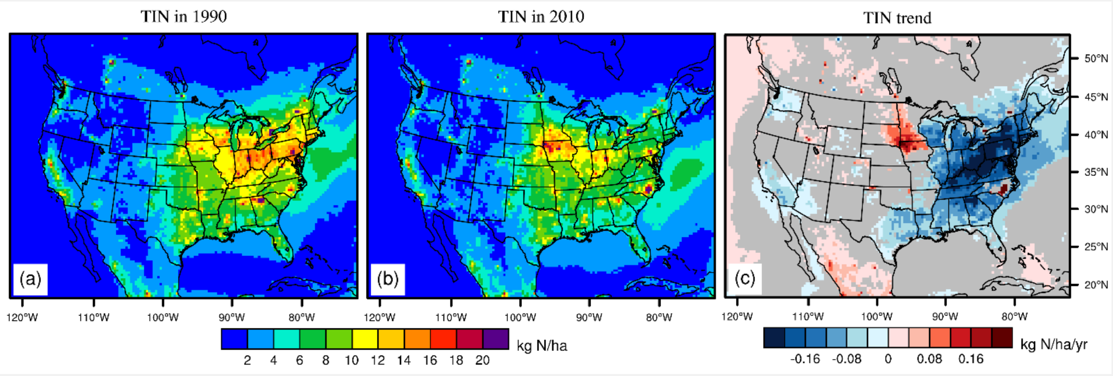
- **Comprehensive Chemical Transport Model**
  - Emission, advection, diffusion, chemistry, deposition
- **Multiscale: Hemispheric → Continental → Regional → Local**
- **Multi-pollutant & multi-phase**:
  - **Ozone (O_3)** photochemistry
    - NO_x + VOC (biogenic & anthropogenic) → O_3
  - **Particulate Matter (PM)**
    - Inorganic chemistry & thermodynamics → Sulfate, Nitrate, Ammonium
    - Organic aerosol → primary, secondary
    - Geogenic aerosol → wind-blown and fugitive dust, sea salt
  - **Acidifying and eutrophying atmospheric deposition**
    - Aqueous chemistry, Wet and Dry Deposition
  - **Air Toxics**
    - Benzene, formaldehyde, mercury etc.

Approach

Simulated Trends (1990-2010) in Ambient $PM_{2.5}$



Simulated Trends (1990-2010) in N Deposition



Zhang et al., ACP, 2018

Download CMAQ at https://www.epa.gov/cmaq/access-cmaq-source-code

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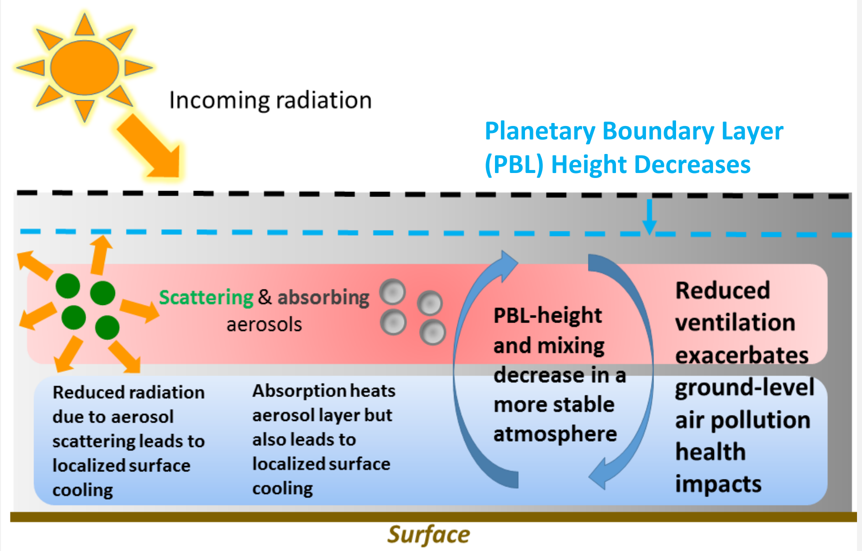
CMAQ Modeling System

Approach

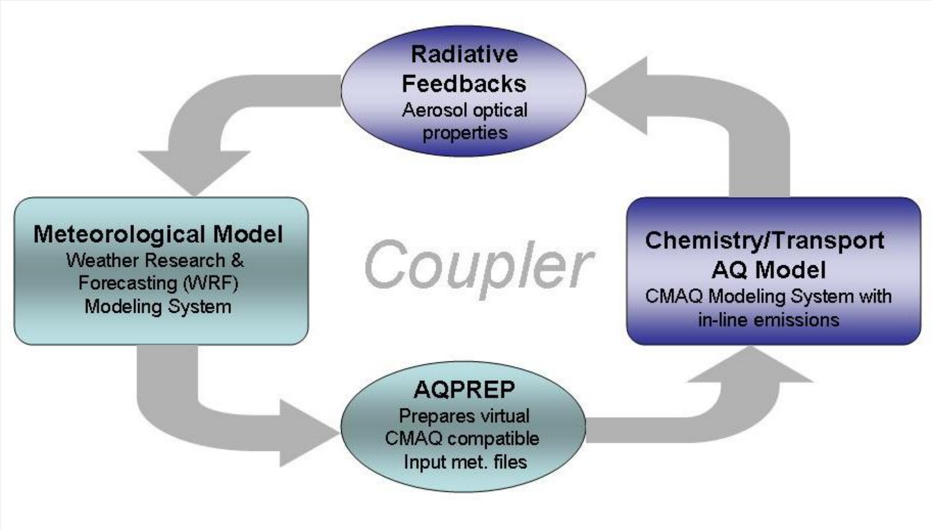


Assessing impacts of pollution on public health requires accurate accounting of the interactions between pollutants and meteorology, which may drive or exacerbate additional impacts

CMAQ is integrated directly with meteorological models to meet this challenge

2-Way Coupled to the Weather Research & Forecasting (WRF) – CMAQ System

- Enables higher temporal frequency coupling between dynamics and chemistry essential for fine scale applications
- *2-Way Coupled* enables consideration of aerosol radiative effects



CMAQ Users

CMAQ is widely used for Air Quality Assessments & Design/Implementation of NAAQS

States

- State Implementation Plans to attain NAAQS
- Regional Haze Rule

EPA

- National Rulemaking
  - Clean Air Interstate Rule
  - Clean Air Mercury Rule
  - Renewable Fuel Standard Act-2

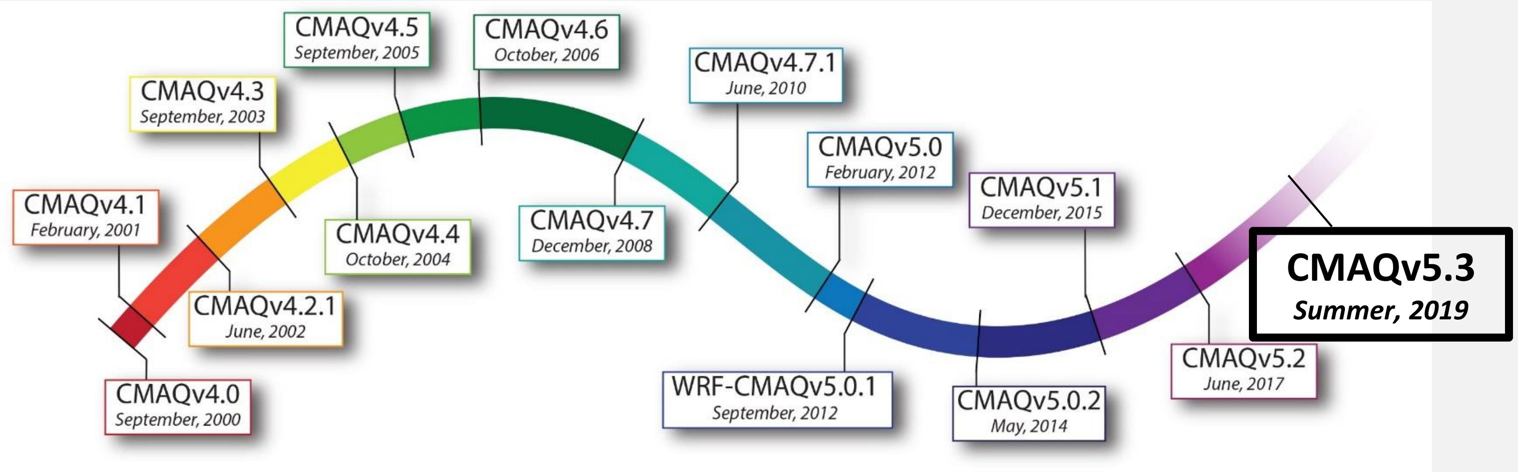
Other Federal Agencies

- Deployed in **NOAA/National Weather Service's** National Air Quality Forecast Capability
  - Guidance for next-day air quality public health forecast
- **Centers for Disease Control and Prevention** (CDC)
  - Tools for county-specific air quality information

International

- Worldwide: users in 125 countries

Periodic public releases of improved versions of the modeling system



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CMAQv5.3β: Now Available on GitHub

Science Application Goals

- **Improve capabilities for addressing local nonattainment issue**
  - Added new features to the Weather Research and Forecasting (WRF) model to support better meteorological prediction
  - Updated the underlying chemistry mechanisms based on the latest science
- **Enable examination of US air pollution in context of changing global emissions**
  - Updated marine chemistry to better represent long-range Ozone transport
- **Quantifying natural contributions vs anthropogenic enhancements, especially with lower NAAQS threshold**
  - Better representation of secondary pollutant formation in Clouds
  - Updated model of secondary organic aerosol formation from Biogenic VOCs
  - Harmonized the treatment of water uptake to aerosol organic phase – applications to chemistry, mixing state, optics, etc.
- **Improve cross-media application capability**
  - Incorporated latest science on deposition
  - Two deposition modules now available – M3dry (consolidated) and STAGE (tiled)

Results

- Greater transparency of emissions source options and online scaling
- Improved diagnostic tools for probing and understanding model results
- Increased numerical efficiency with expanded use of modern high performance computing techniques
- Improved user-oriented design features like better-organized output logs with consistent and expanded meta-data

User-Oriented Development Goals

https://github.com/USEPA/CMAQ/blob/5.3.b2/README.md

Multiphase Chemistry is Tailored to Application Needs

Chemistry Mechanism Title	Gas Species	Aerosol Species	Total Species	Gas-Phase Reactions	Comment
CB6r3-AERO7	137	80	217	338	Efficient regional chemistry
CB6r3-AERO7-KMT2	137	80	217	338	Cloud Processing
CB6r3-AERO7-Marine	172	82	254	452	Hemispheric Scale including transport over Oceans
CB6r3-AERO6	145	83	228	335	Backward Compatibility to support existing users and applications
CB6mp-AERO6	139	155	294	335	Air Toxics
RACM2-AERO6	164	82	246	407	Multiscale Chemistry
SAPRC07-AERO7	216	86	302	925	Detailed Organic Chemistry
SAPRC07-AERO7-KMT2	216	86	302	925	Cloud Processing with detailed Organic Chemistry
SAPRC07-AERO6	227	91	318	934	Backward Compatibility to support existing users and applications

Atmospheric chemistry mechanisms of varying complexity are available to support diverse applications across scales and explore extensions for emerging problems and contaminants

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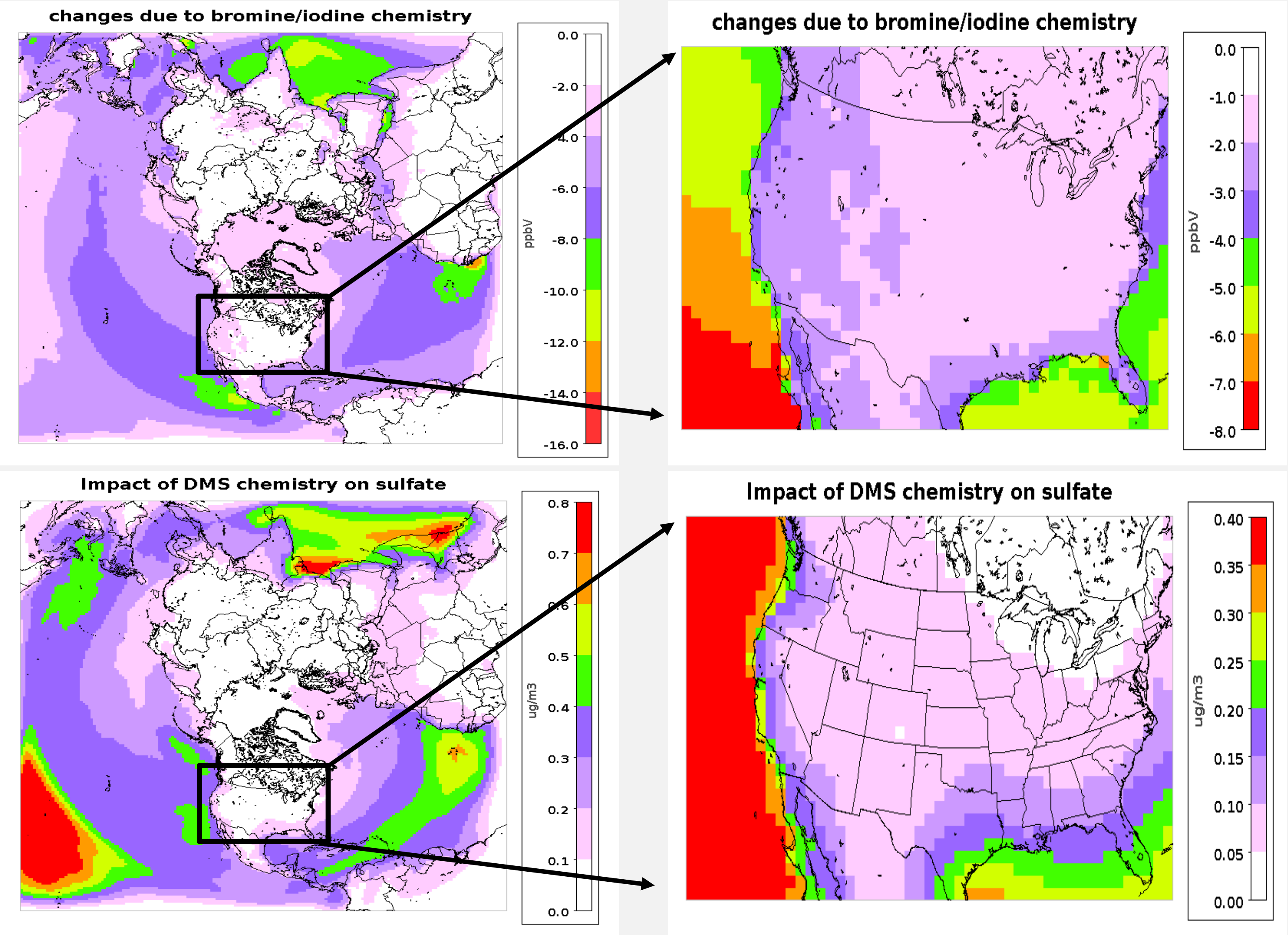
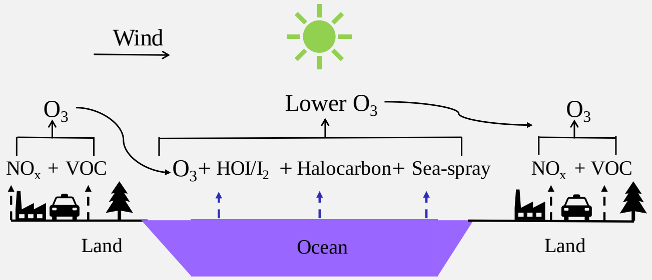
Improved Chemistry in Marine Environments

Results

ΔO_3

ΔSO_4^{2-}





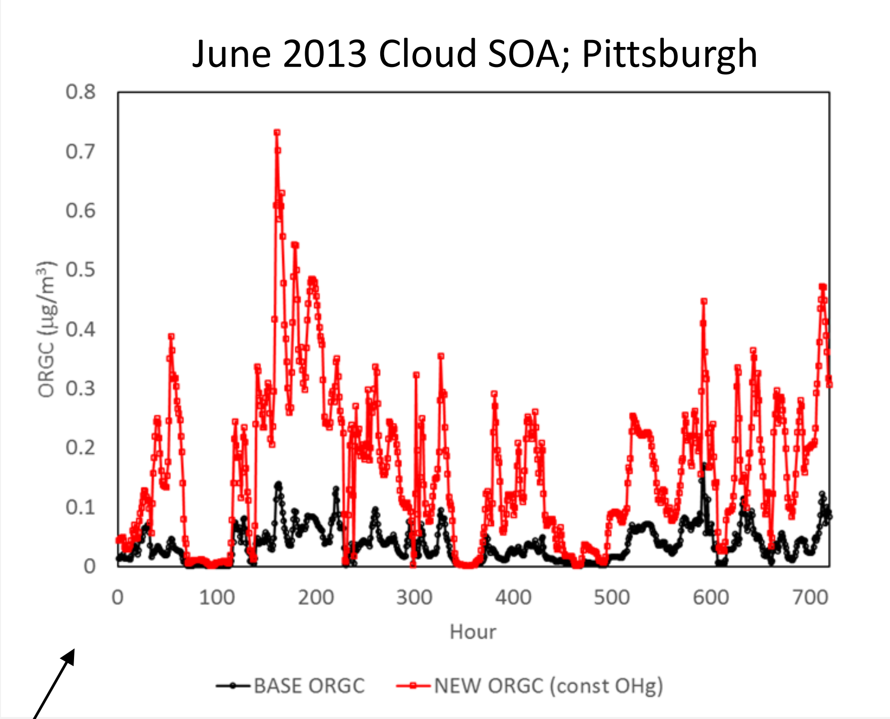
Oceanic halogen emissions can deplete O_3 in air masses that are transported inter-continentally

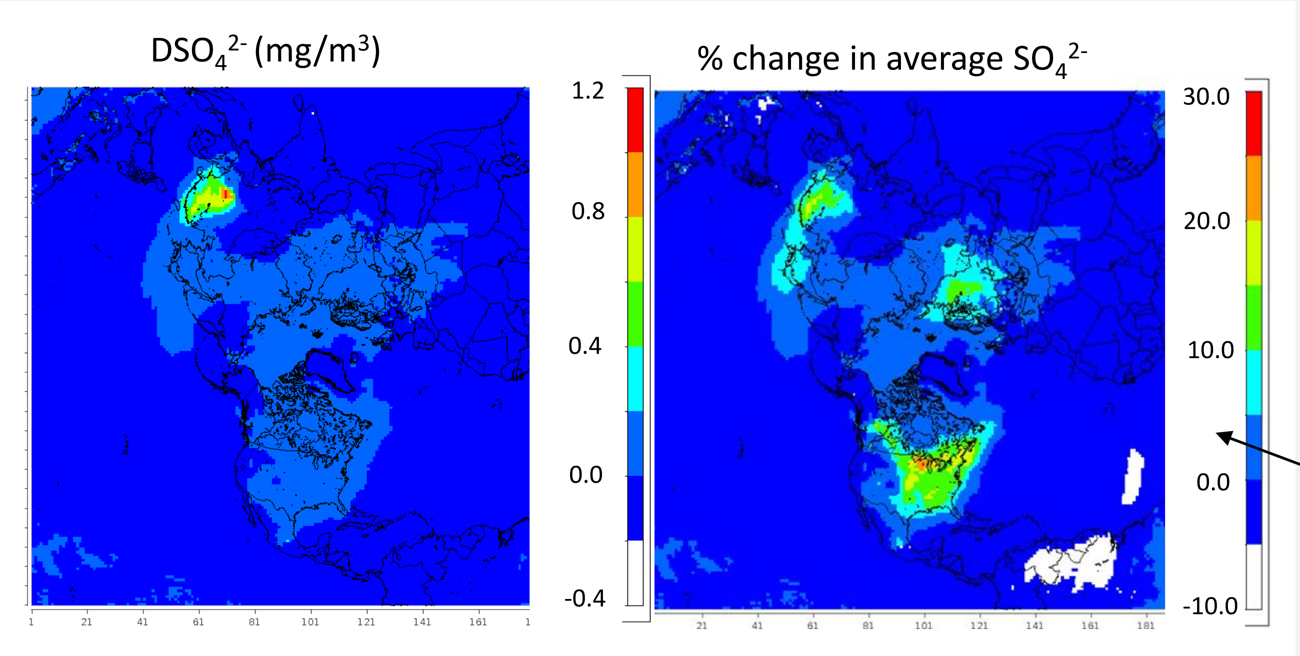
Oceanic Dimethyl Sulfide (DMS) emissions can modulate Sulfur Dioxide (SO_2) & aerosol Sulfate (SO_4^{2-}) in marine environments as well as background aerosol SO_4^{2-} over continents

Representation of chemistry in marine environments helps improve model predictions in coastal regions and long-range transported amounts

Exploring Cloud Chemistry Pathways to PM

- SO_4^{2-} + Organic Aerosol (OA) are major contributors to $PM_{2.5}$ levels around the globe (≥ 50% total mass)
- Secondary Organic Aerosol (SOA) is the dominant contributor to OA composition downwind of emission sources
- Accurately representing the major sources and production pathways of these species in Chemical Transport Models is necessary to assess the impacts of emissions changes on air quality/climate





Summer (June 2013, *Top right*):

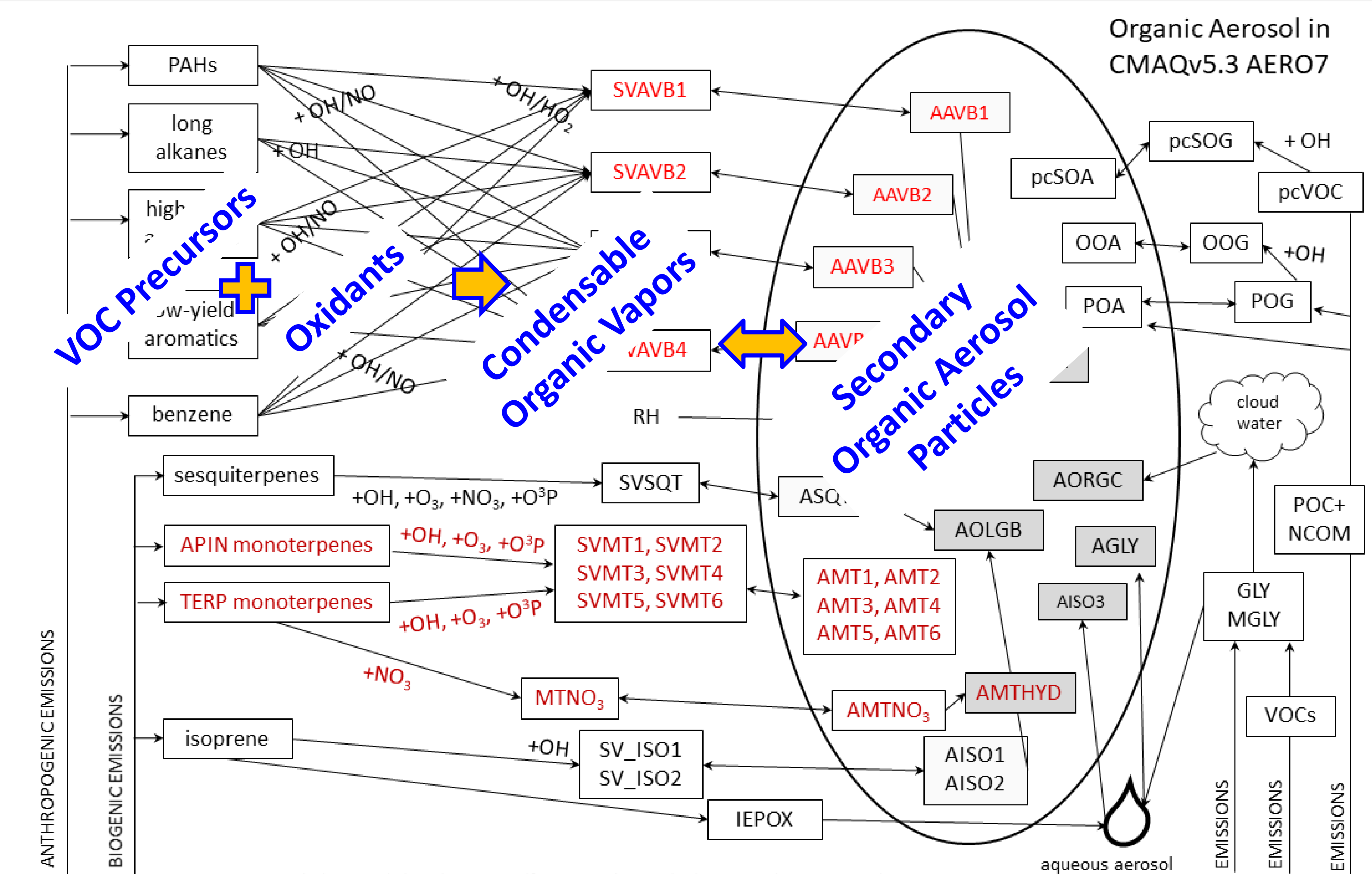
- 150-300+% increase in surface level "cloud SOA" in US

Winter (January 2016, *Bottom left*):

- SO_4^{2-} increased up to 27%. NO_3^- tends to decrease with a similar pattern

Results

Complex Organic Aerosol Formation Pathways Considered

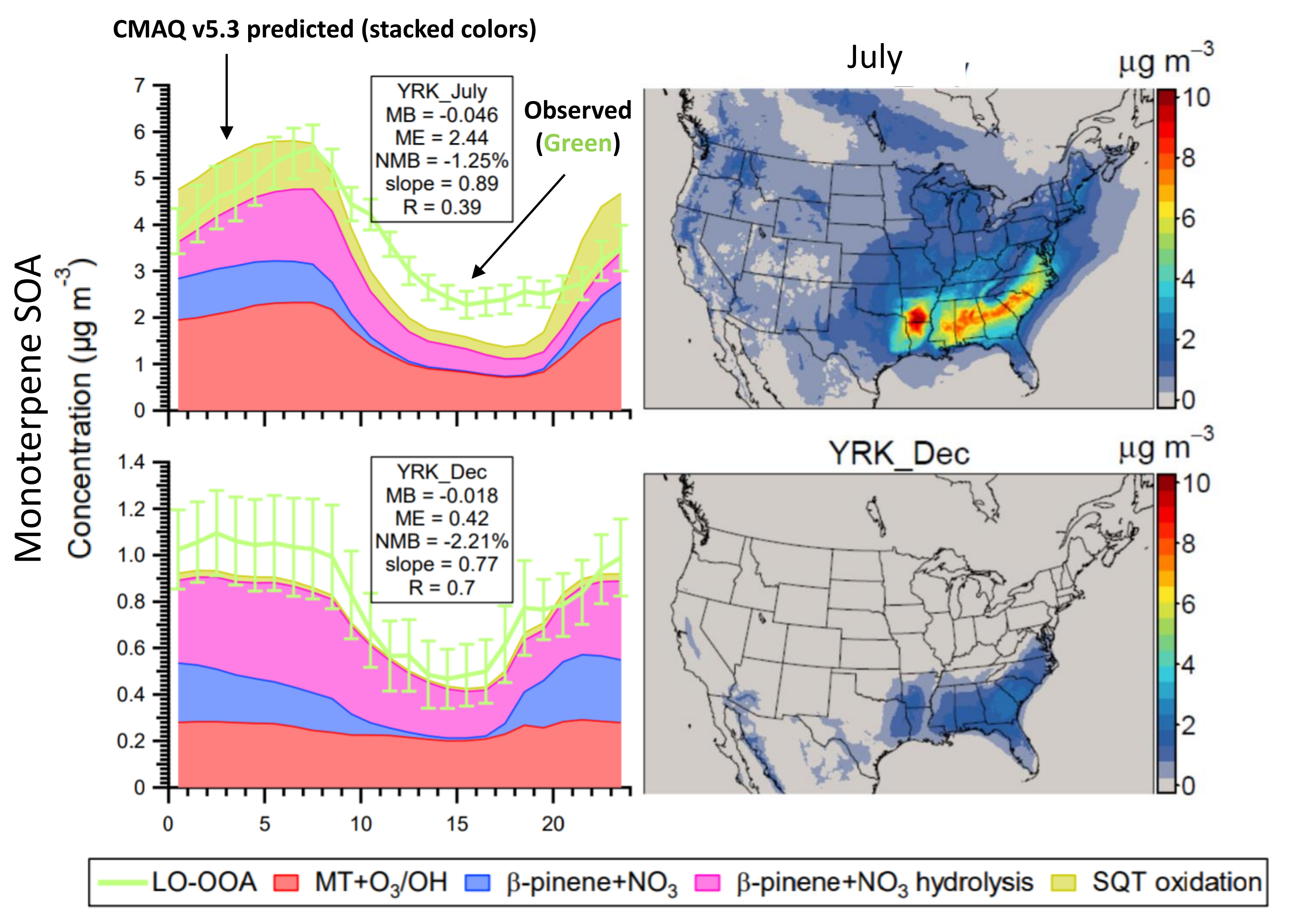


AERO7i: AISO3 tracked as 2-methyltetrols, organosulfates, etc and semivolatile isoprene dinitrates contribute to SOA

Results

CMAQ Accurately Predicts Formation of Monoterpene SOA

Results



Xu et al., 2018 ACP

- Monoterpenes ($C_{10}H_{16}$)
  - Emitted from trees
  - Examples: pinene, limonene, sabinene, myrcene, etc.
  - Oxidation predicted to account for 21% of the World Health Organization $PM_{2.5}$ health standard in the southeast
- Observations from around the southeast in 2012-2013 used to identify monoterpene SOA (MTSOA)
- CMAQ SOA chemistry updated with new laboratory evidence now matches observed monoterpene SOA in summer and winter

Improvements in representation of MTSOA formation pathways enables improved attribution of natural and anthropogenic contributions to airborne $PM_{2.5}$

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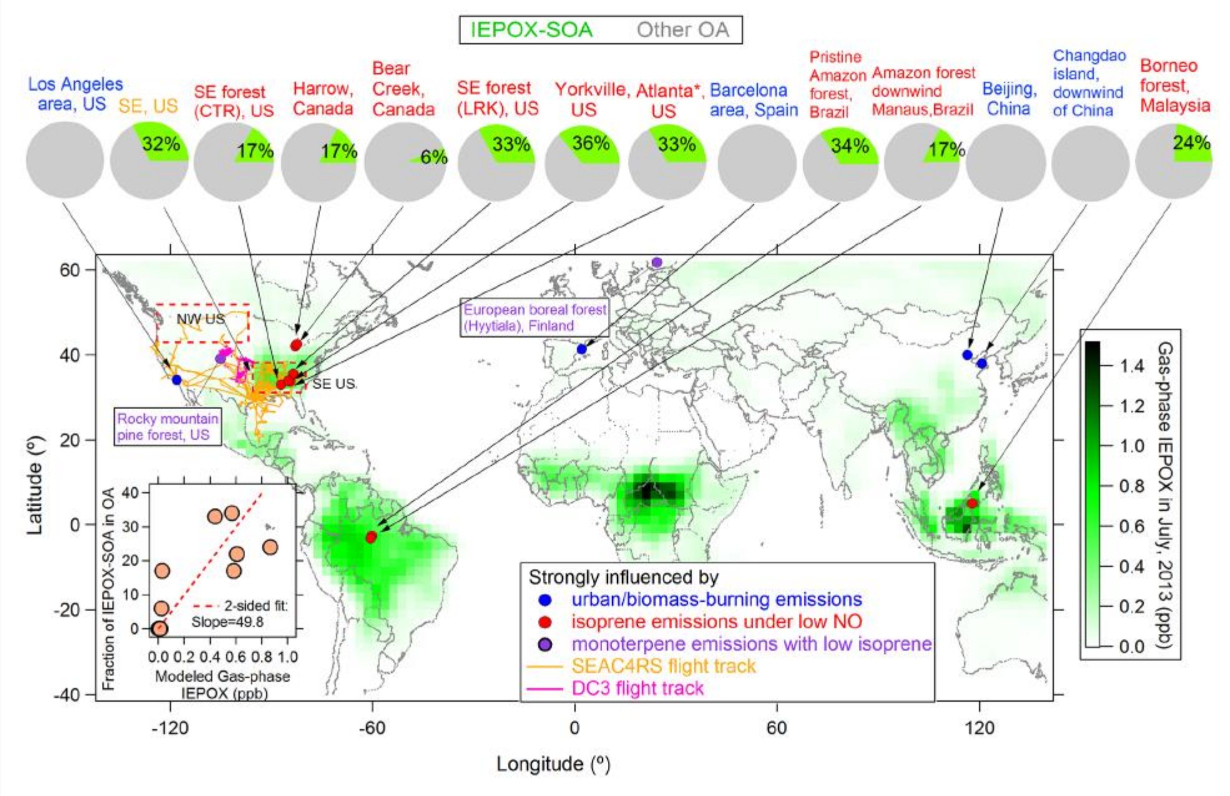
Anthropogenic Sulfur Emissions Enhance Biogenic SOA

Results

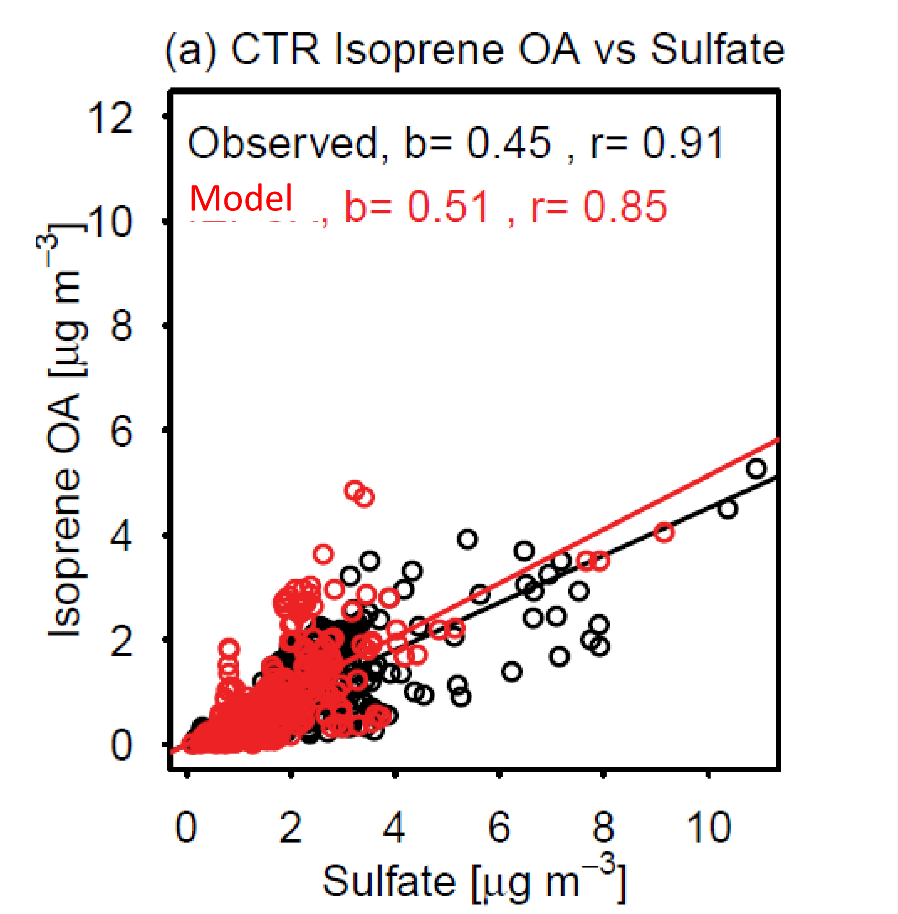
Isoprene Epoxide (IEPOX) SOA



Hu et al., 2015 ACP

(Percentage of total OA mass in **green**)

Better capture of Isoprene SOA dependence on aerosol sulfate

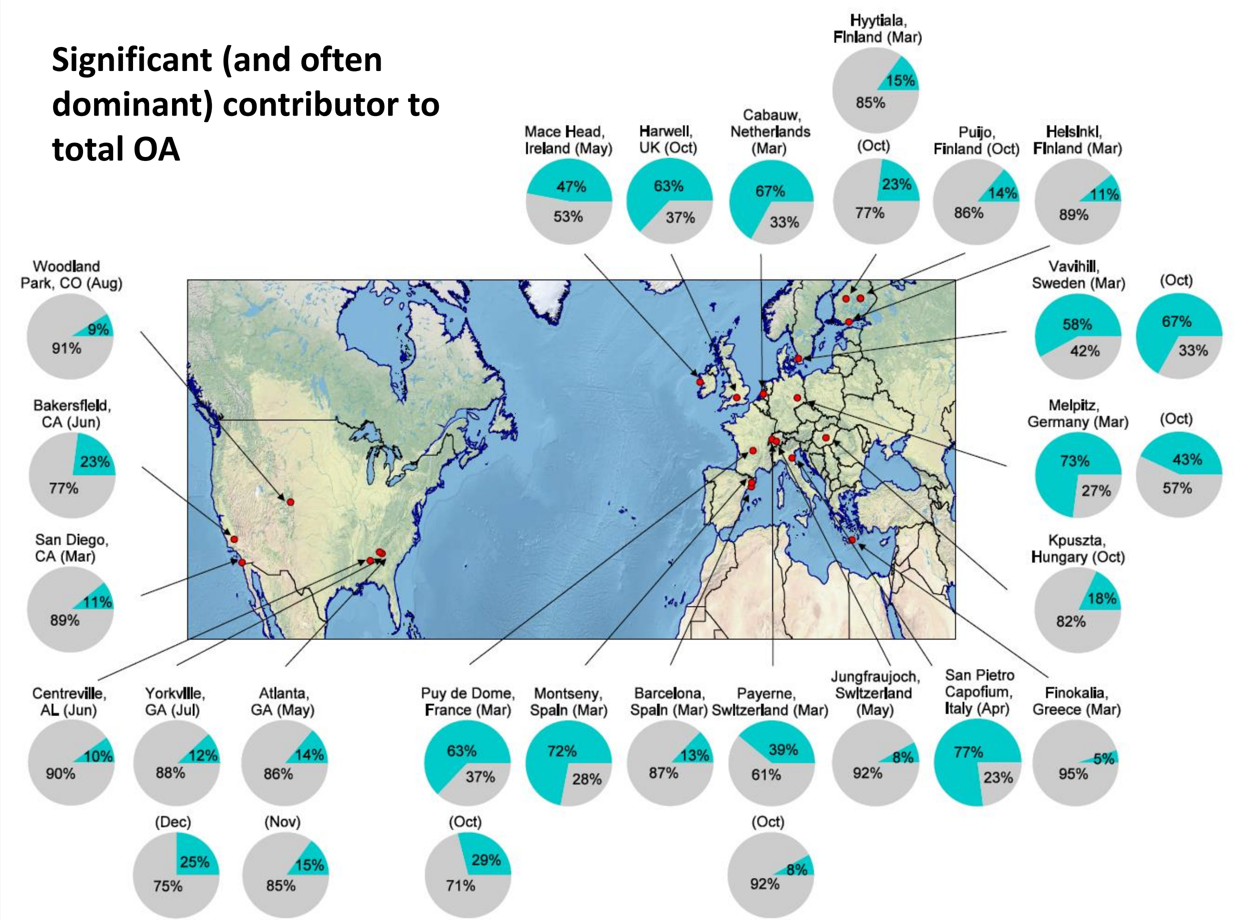


Pye et al., 2017 ACP

Improved representation of acid-enhanced SOA formation from biogenic hydrocarbons now indicates significant role of sulfur emissions to organic PM

Anthropogenic NO_x Emissions Enhance Organic Nitrate Formation

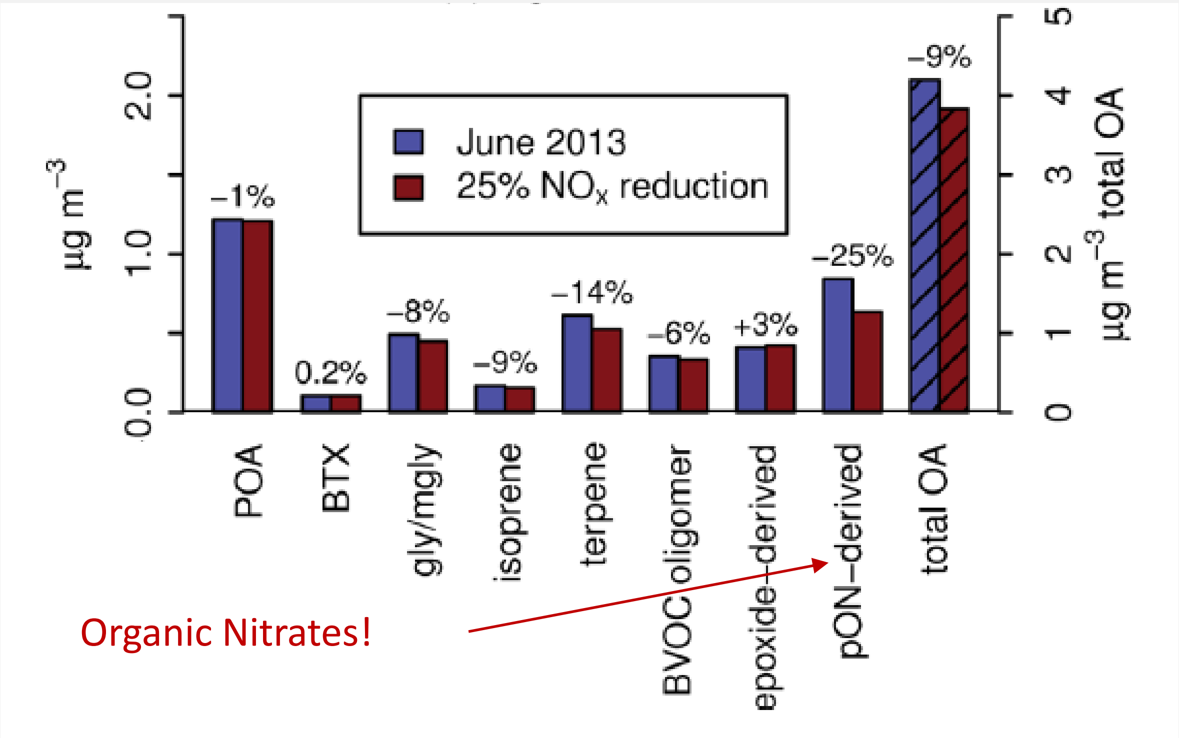
Particulate Organic Nitrate Aerosols



Ng et al., ACP, 2017

(Percentage of total OA mass in cyan)

NO_x reductions → substantial OA reductions via NO_x participation in organic nitrate formation



Pye et al., ES&T 2015

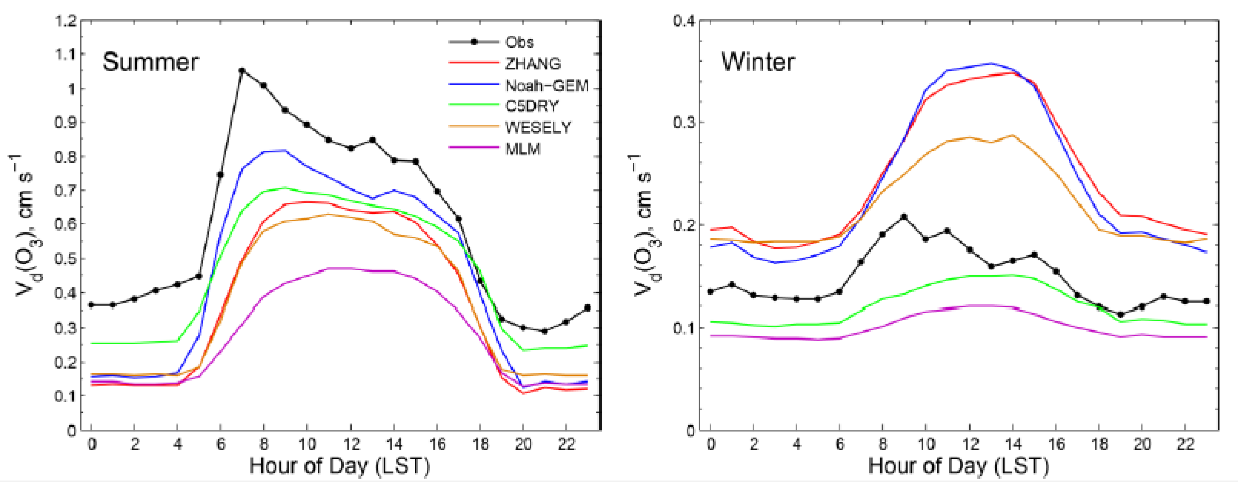
Organic nitrate formation is sensitive to NO_x emissions and reductions in NO_x can lead to substantial reductions in total OM via this pathway

Dry Deposition: Supporting Multiple Approaches

Results

Renewed emphasis on dry deposition of O_3

- *A persistent sink*
- *Current parameterizations vary widely:*



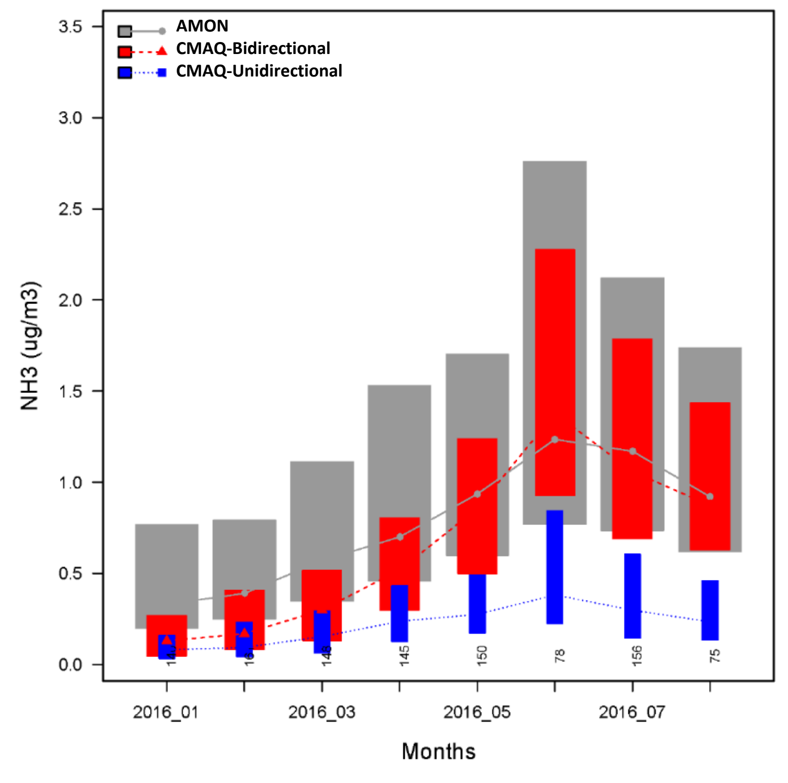
Wu et al., 2017

- Important for accurate representation of low-moderate O_3 mixing ratios
- Deposition to snow
  - Winter-time O_3
- Deposition to water
  - Urban areas along coasts and lakes
  - Background O_3: removal in air masses traversing the oceans

Consistency between unidirectional and bi-directional approaches

- Accurate representation of bi-directional ammonia (NH_3) flux at the surface is important for describing:
  - Ambient $PM_{2.5}$ concentrations & composition
  - Atmospheric N-deposition

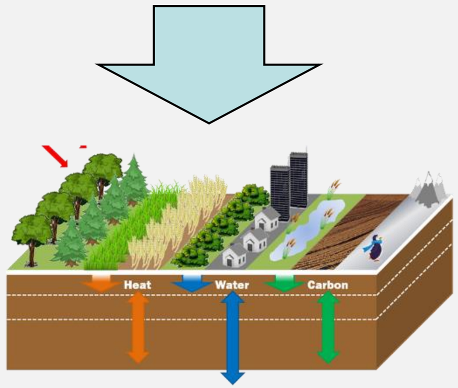
Monthly average model NH_3 with vs Ammonia Monitoring Network observations for Contiguous US 2016



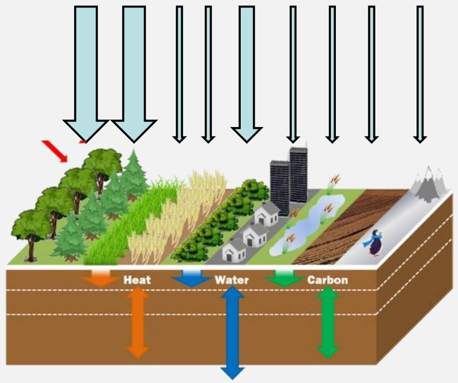
New Surface Deposition Module Supports Ecological Applications

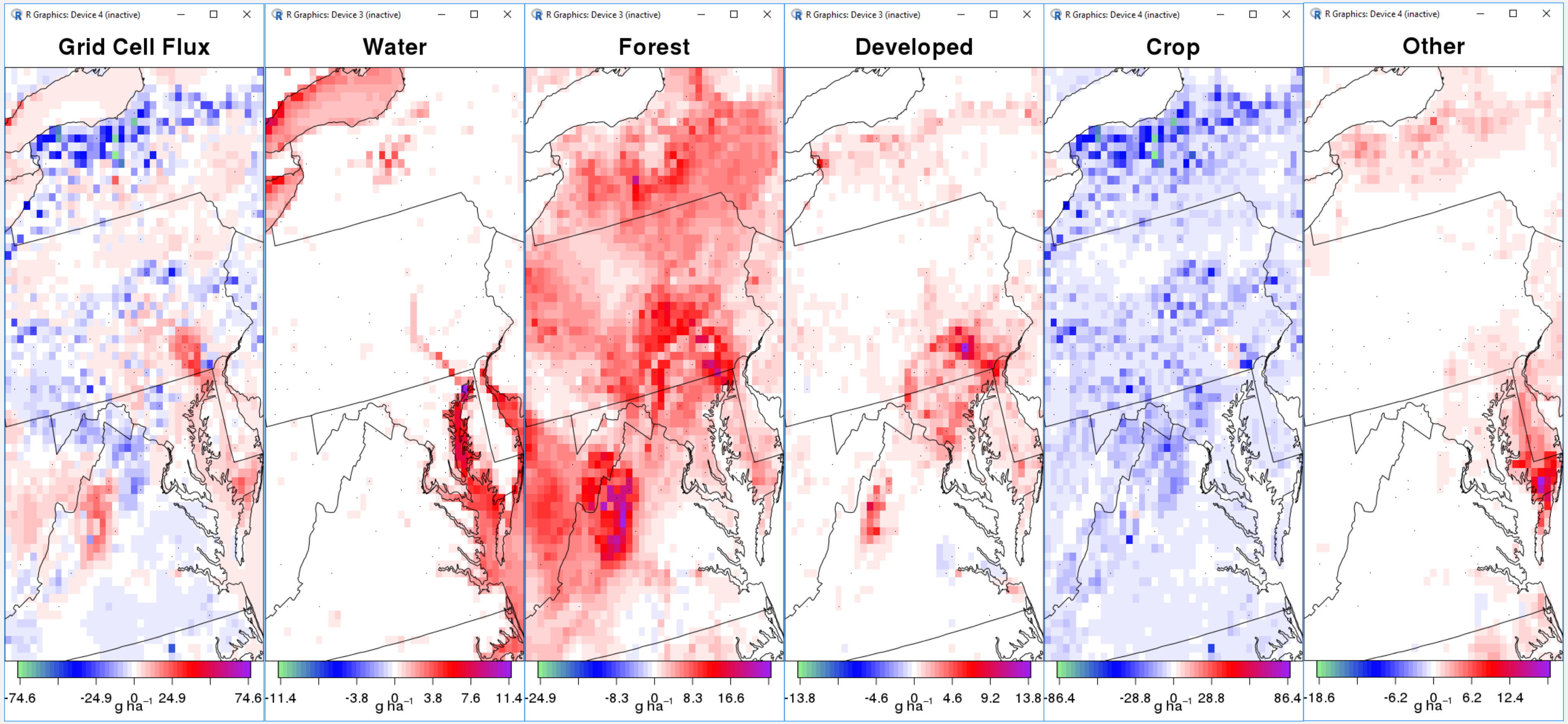
- Surface Tiled Aerosol and Gaseous Exchange (STAGE)
- Estimates land use specific deposition for each land use class in each grid cell
- Alternative scheme to support Total Maximum Daily Load (TMDL) and critical loads applications
- *LU-Specific Schemes* make it easier to test our understanding of the effects of individual types of land cover

Grid Cell Average Dry Deposition



LU Specific Dry Deposition





Results

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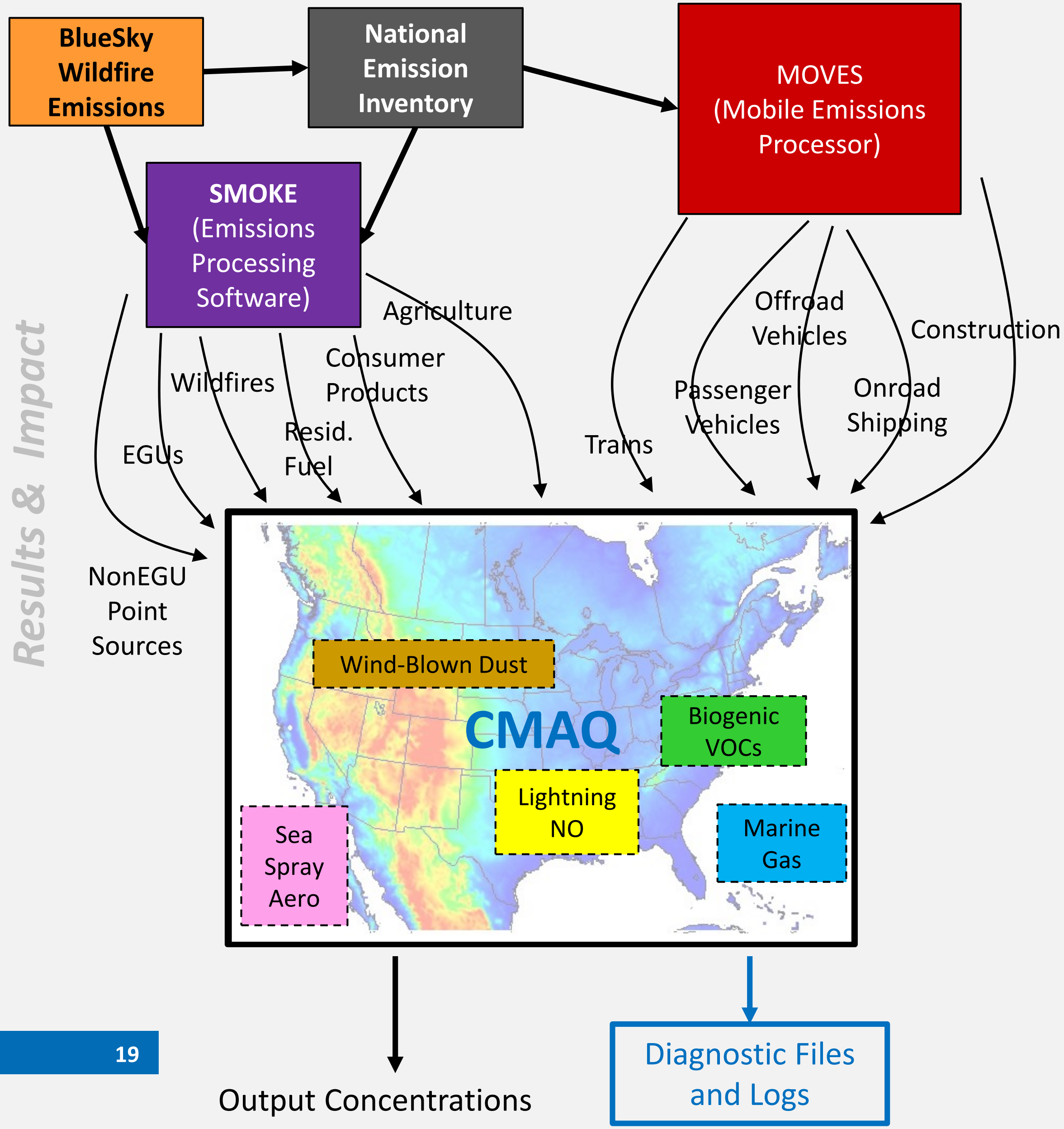
Flexibility in Emission Mapping and Perturbations

Results & Impact



Many tasks can now be completed with one line of instruction:

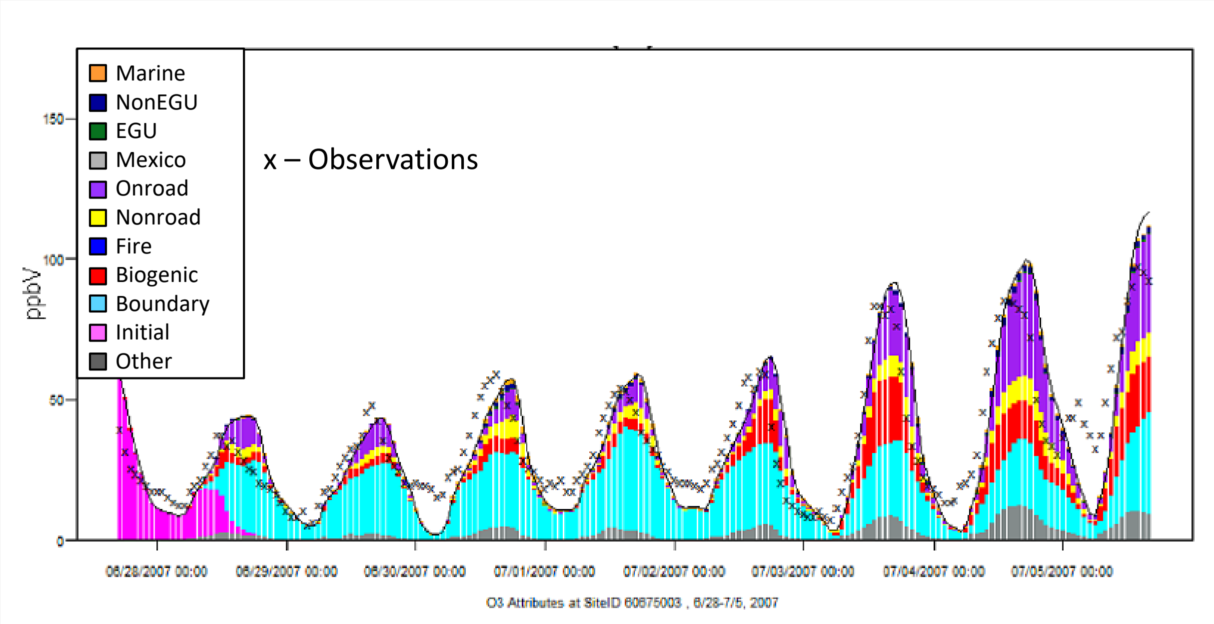
- How do I scale only emissions for one chemical species from one emissions source by a constant factor like 25% or 50%?
- How do I scale all surrogates from a given emission source?
- How can I introduce emissions of some new pollutant using emissions of something I have related it to, like CO or total VOCs?
- How do I scale an emissions source computed inside CMAQ like wind-blown dust, biogenic VOCs, etc
- How do I scale emissions from a particular source only over a specific region of the domain, like over one county, state or a group of states?
- We are learning more about the size of particles when they are emitted – how can I experiment with this parameter for different sources?
- And more…

New framework improves transparency & flexibility

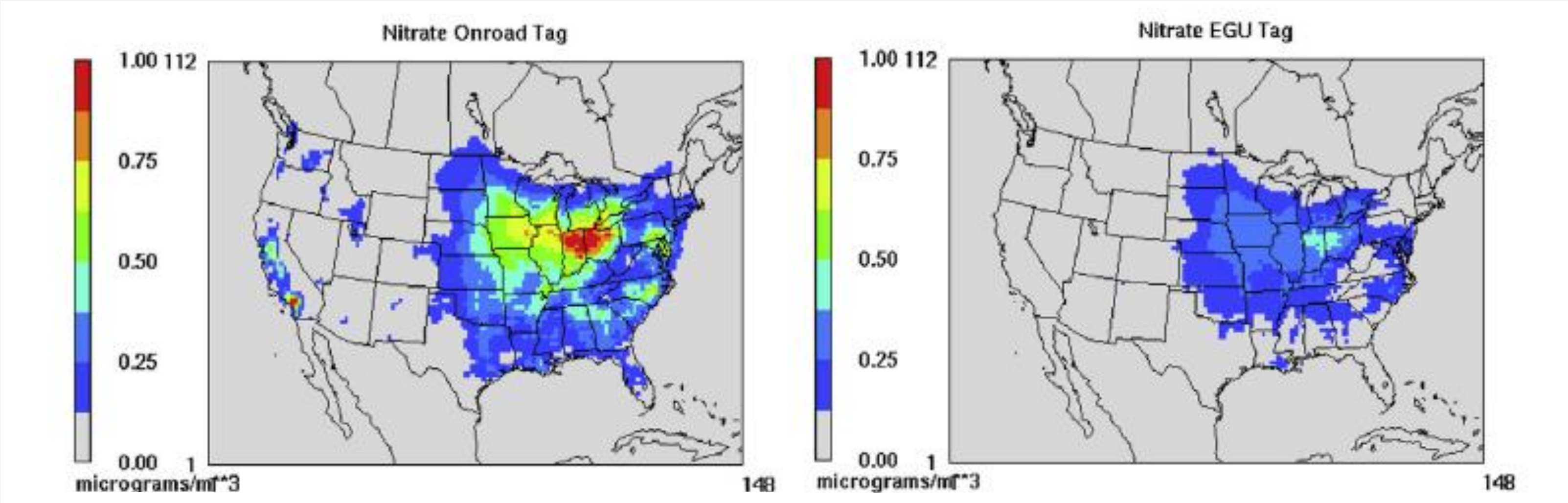
Incorporation of Source-Apportionment Technology

- Integrated Source Apportionment Technology (ISAM)
- One CMAQ model run provides output for a number of user-requested sources
- Contributions to O_3 in Sacramento are dominated by vehicles/trains, biogenic vapors, and long-range transport from outside the US
- Improved computational efficiency & numerical accuracy
- Incorporation with base model release

O_3 Source Attribution at Sacramento (Summer 2007)



Average PM NO_3 Source Attribution for Contiguous US, 2010



Kwok et al., Atmospheric Environment, 2013
Kwok et al., Geoscientific Model Develpoment, 2015

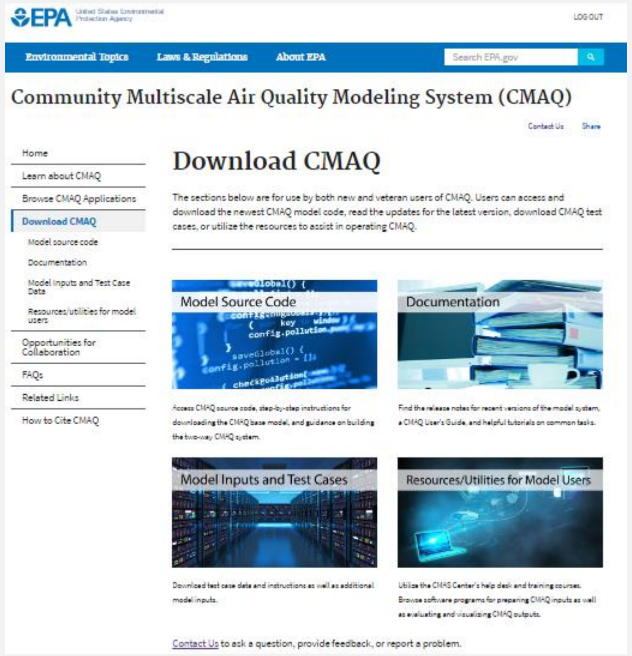
Results

Sound Science to Support Regulatory Actions & Implementation

Impacts

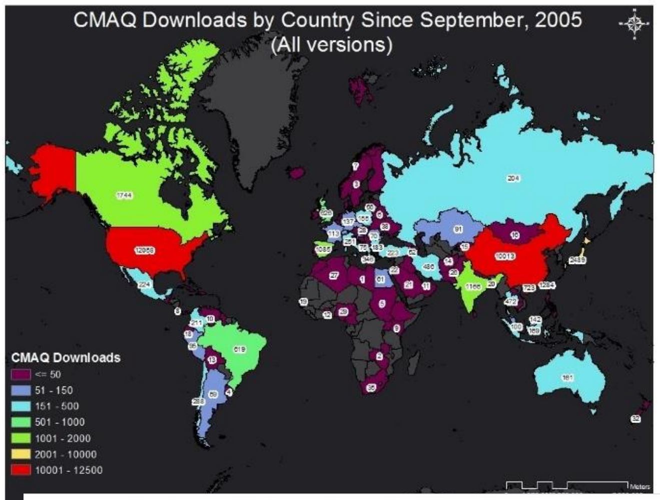
Transparency & Reproducibility

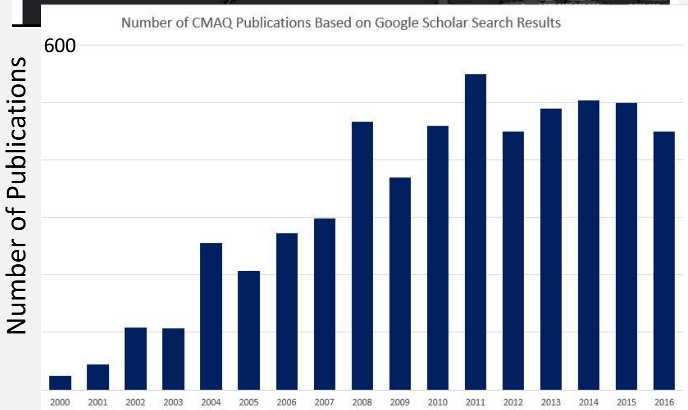
www.epa.gov/cmaq



- Documentation
- Source-code
- Data sets

Dissemination





Peer Review

- External panels comprising of Internation experts in atmospheric modeling & applications
- Five peer reviews since 2000; next in May 2019
- *Panel's findings and our responses accompany the public release of the model*

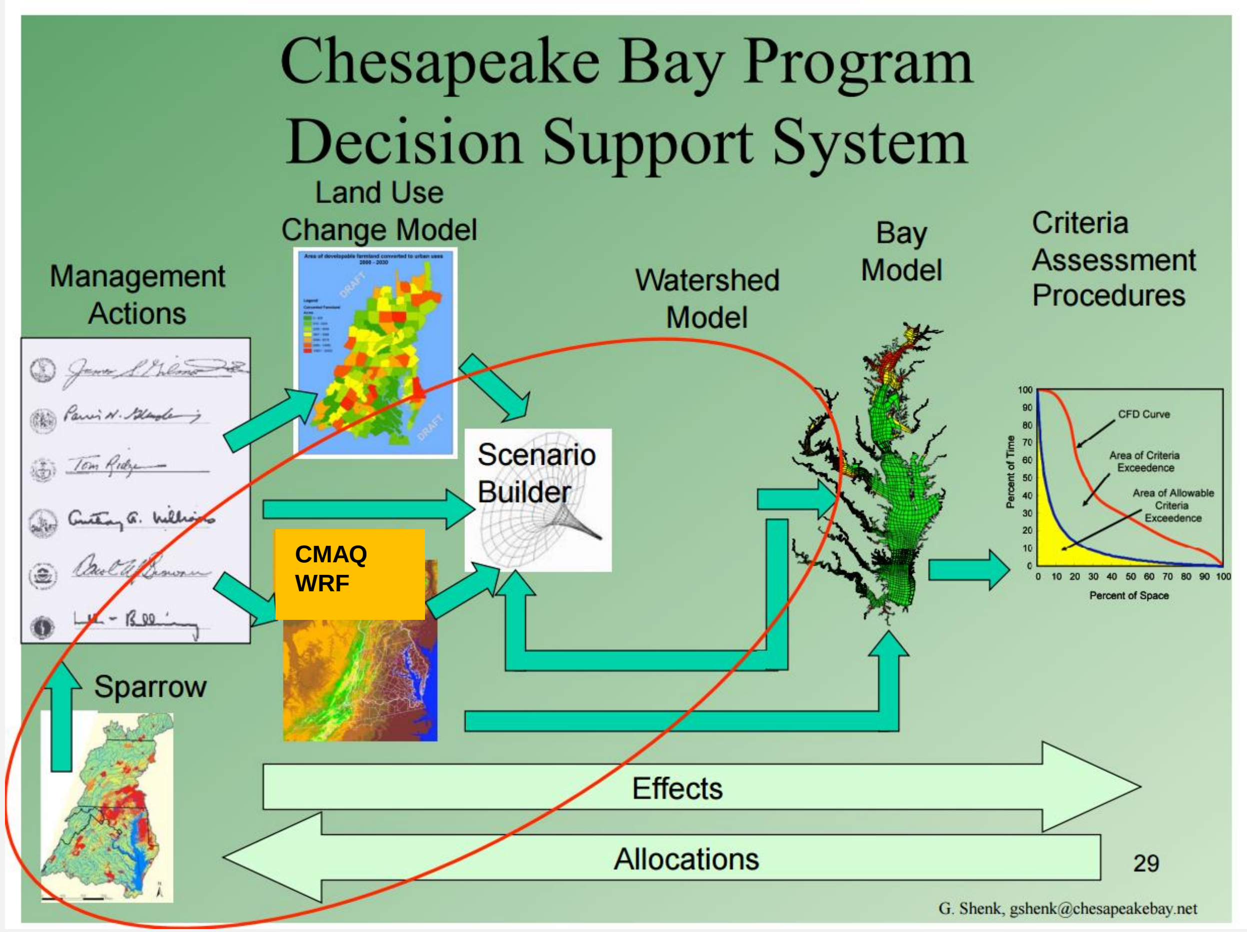
Periodic scientific updates to the CMAQ model have led to the creation of:

- *dynamic* and *diverse* user community
- more *robust* modeling system

Case Study: Chesapeake Bay Program

Impacts

- Approximately 164,000 square kilometers and home to more than 18 million people
  - Largest estuary in the US
  - Population increasing by about 150,000 people per year
- Encompasses parts of six states and Washington, D.C.
- Land-to-water ratio of 14:1
  - Largest of any coastal water body in the world
  - Sensitive to atmospheric deposition



- ➢ CMAQ plays a critical role in Chesapeake Bay environmental management efforts by providing quantitative estimates of changing atmospheric Nitrogen inputs
- ➢ Improves understanding of linked atmosphere-biosphere systems
- ➢ Using CMAQ, the assessment was able to demonstrate the improvements in water quality that have resulted from reductions in atmospheric Nitrogen deposition due to the Clean Air Act

Take Home Messages

- EPA and states have used EPA's CMAQ Modeling System, a computational tool that simultaneously models multiple air pollutants, including ozone, particulate matter and a variety of air toxics, for ***over 15 years***

- *CMAQ brings* together 3 kinds of models including: ***meteorological models*** to represent atmospheric and weather activities; ***emission models*** to represent man-made and naturally-occurring contributions to the atmosphere; and an ***air chemistry-transport model*** to predict the atmospheric fate of air pollutants under varying conditions

- Updates to CMAQ include:
  - Improve capabilities for addressing local nonattainment issue
  - Enable examination of US air pollution in context of changing global emissions
  - Quantify natural contributions vs anthropogenic enhancements
  - Improve cross-media application capability
  - Addresses user-oriented needs and goals

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