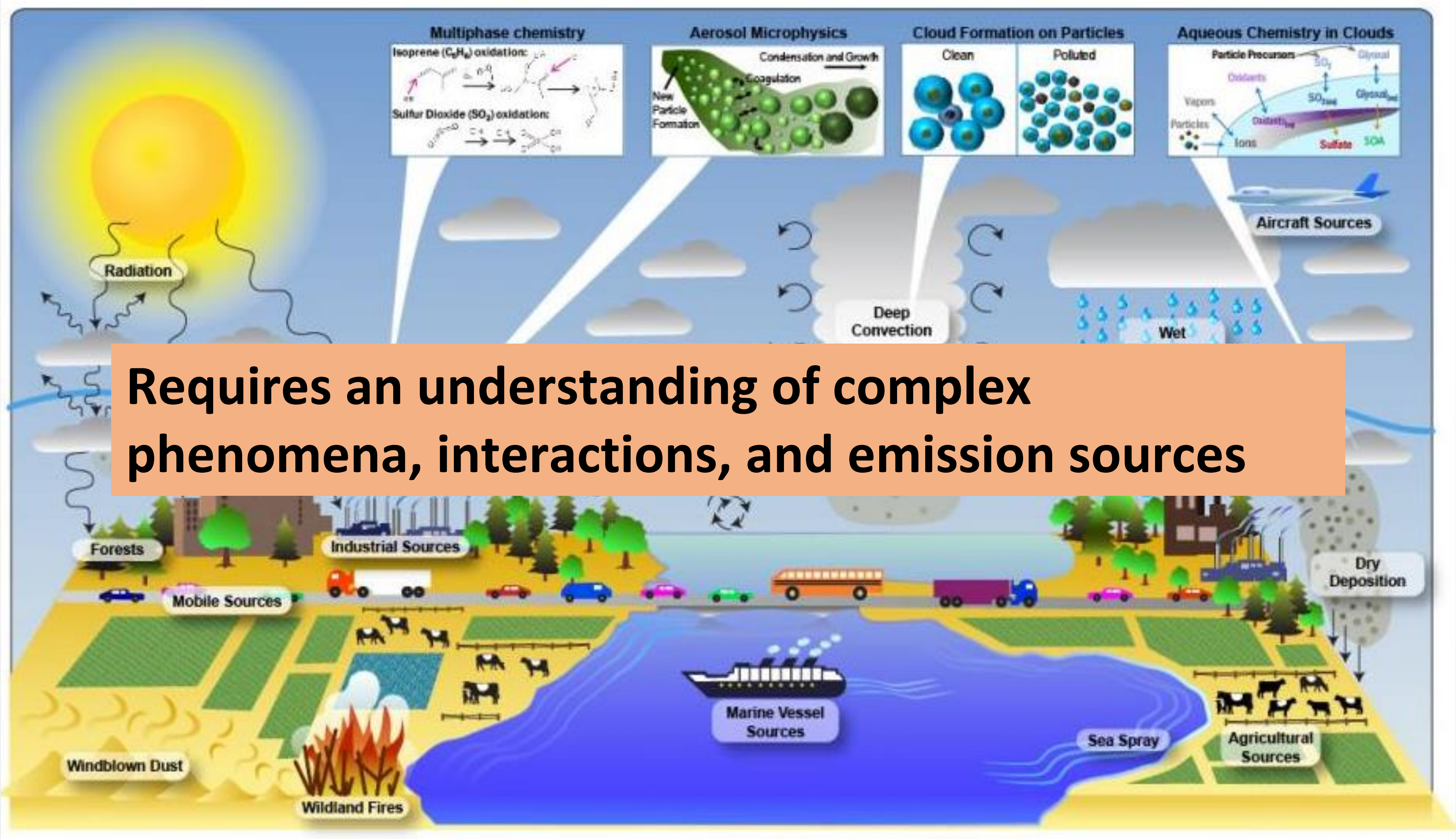
EPA Tools & Resources Webinar

The Community Multiscale Air Quality (CMAQ) Modeling System Version 5.4: An Overview

Presented by K. Wyat Appel
US EPA Office of Research and Development
Center for Environmental Measurement & Modeling

January 18, 2023

Managing Air Quality is Complex

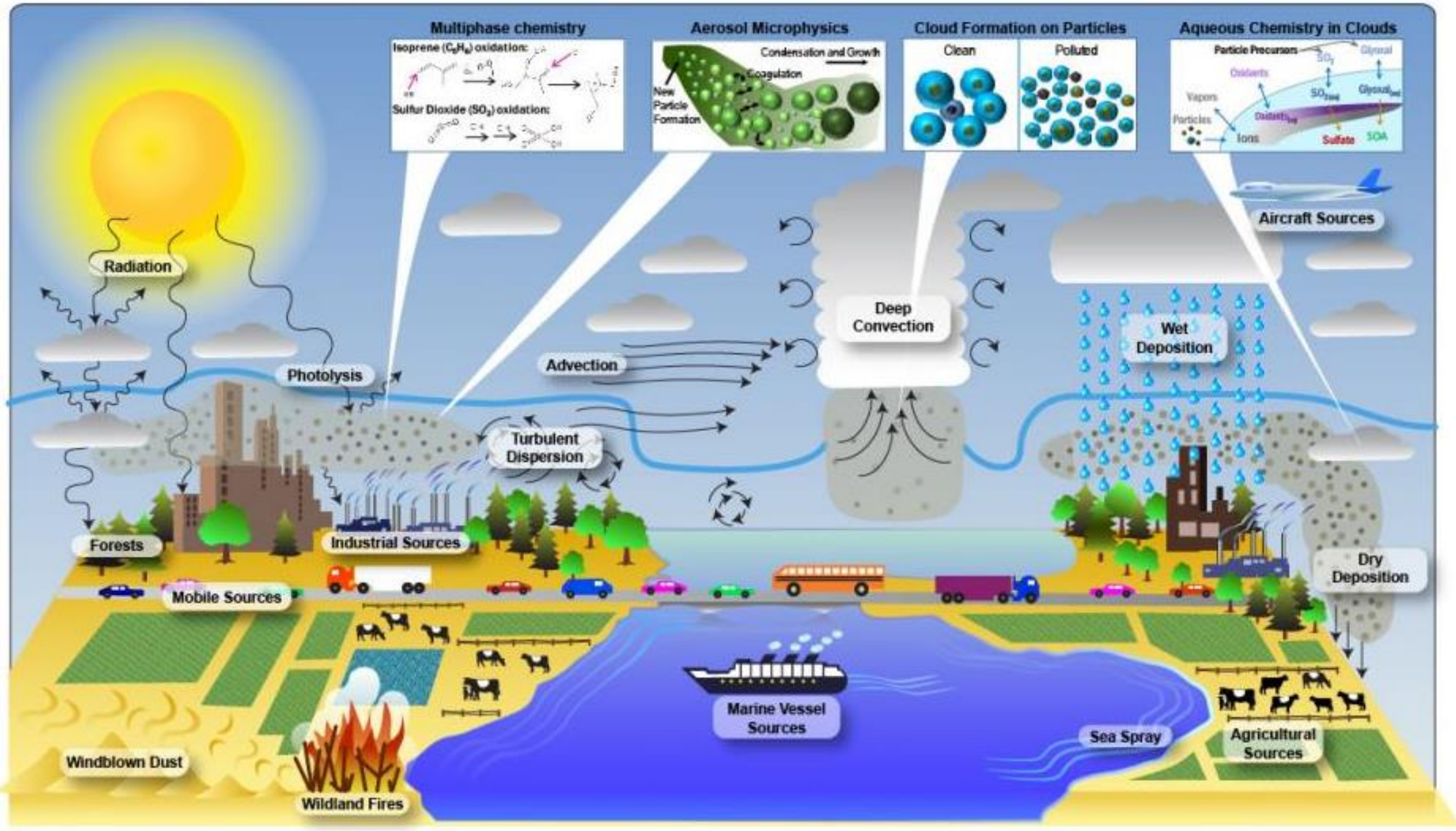


Requires an understanding of complex phenomena, interactions, and emission sources

Atmospheric Models are Essential Tools

- **Numerical modeling is required** because:
  - Pollutants of concern are not always directly emitted, but often created in the atmosphere
  - Atmospheric chemistry is complex and non-linear

- **Atmospheric models allow us** to:
  - Simulate the complexity of atmospheric chemistry
  - Understand future air quality
  - Fill in gaps spatially where monitors do not exist
  - Formulate and test potential control strategies



"*State Implementation Plan must provide air quality modeling performance to predict future pollution levels, as EPA Administrator prescribes*." 110(a)(2)(k)(i)

AQ Models: Implementing the *Clean Air Act*

Evolution of EPA's models guided by increasingly complex application & assessment needs

Single Pollutant
Non-reactive
Dispersion
Local/urban Scales

→

Single Pollutant
Reactive
Grid-based
Regional/urban Scales

→

Multi-pollutant,
Multi-scale
Reactive
Grid-based
Regional/urban Scales

→

Multi-pollutant
Multi-scale (***local to hemispheric***)
Interactions with climate forcing and air quality changes
Grid-based

→

Multi-pollutant
Near-source to global
Reactive
Atmospheric-hydrologic

Regulatory & Assessment Needs

- Standards Assessments
- PSD New Source Permitting
- O_3, PM attainment demonstrations; Regional Haze
- Mercury; Toxics
- Meteorology and Air Quality Interactions; Exposure
- Background air pollution; Met-AQ Interactions; Exposure & Health; Multimedia

Timeline:

- ***1970*** — AQDM, UNAMAP
- Regional Acid Deposition Model
- Regional Oxidant Model
  - Acid Deposition
  - Ozone
- ***1998*** — **CMAQ**
- **CMAQ For PM**
- Neighborhood Scale CMAQ
- Multi-pollutant CMAQ
- Coupled WRF-CMAQ
- ***2019*** — **CMAQv5.3**
- **CMAQ NextGen**
- ***2022*** — **CMAQv5.4**

Model Development & Applications

What is CMAQ?

CMAQ ***(see-mak)*** *is* an active open-source development project of the US EPA that consists of a suite of programs for conducting air quality model simulations.

For over two decades, EPA and states have used EPA's Community Multiscale Air Quality (CMAQ) Modeling System, a powerful computational tool for air quality management.

CMAQ brings together three kinds of models:

- **Meteorological models** to represent atmospheric and weather activities
- **Emission models** to represent man-made and naturally-occurring contributions to the atmosphere
- An **air chemistry-transport model** to predict the atmospheric fate of air pollutants under varying conditions

CMAQ Fact Sheet October 2022 (pdf)

CMAQ is used for Air Quality Assessments

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
- Updates to NAAQS

Other Federal Agencies

- Deployed in NOAA/National Weather Service's National Air Quality Forecast Capability
- Centers for Disease Control and Prevention (CDC)
  - Tools for county-specific air quality information
- *4th National Climate Assessment* (USGCRP)

Academia

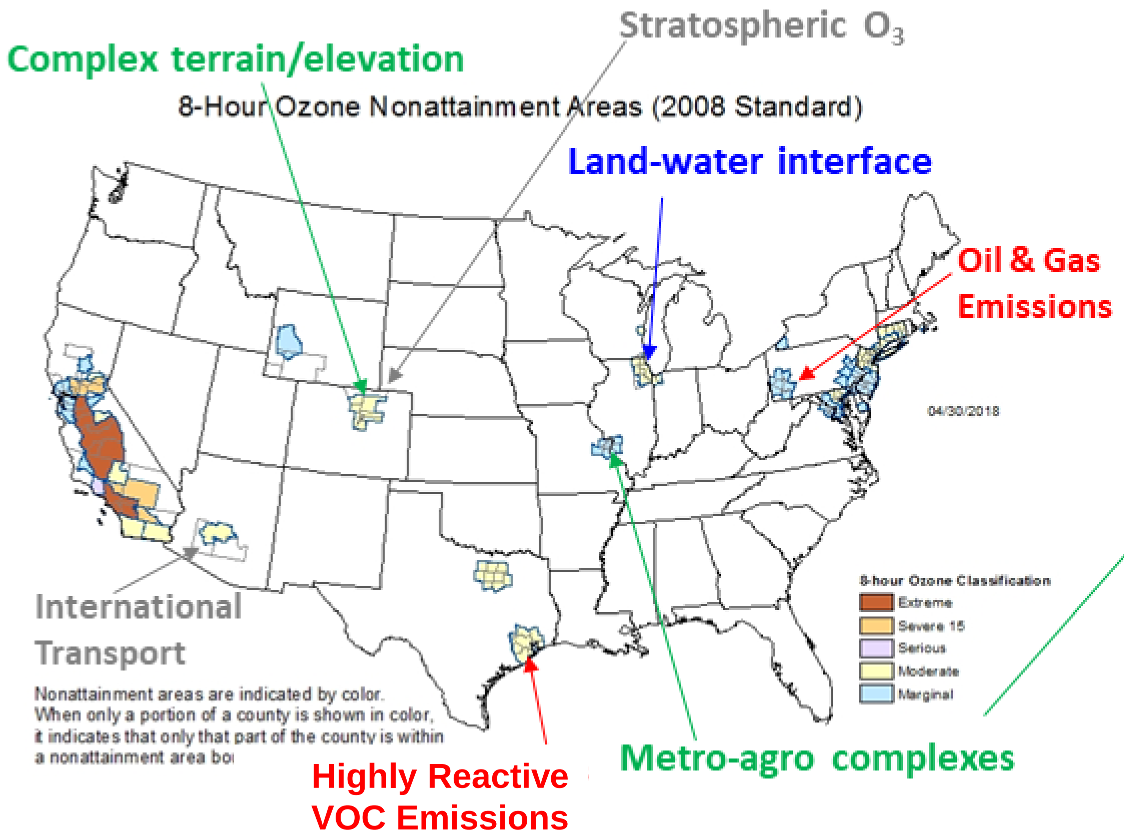
- Research tool

International

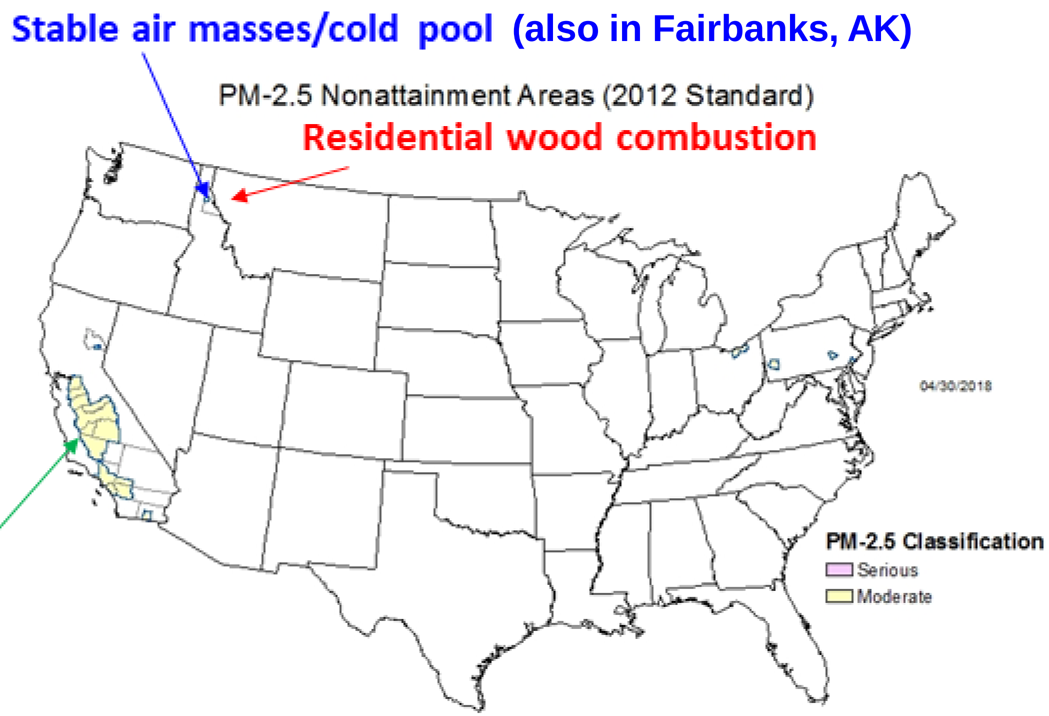
- Worldwide: users in 125 countries

Nonattainment Presents *Unique* Challenges

Nonattainment Classification: O_3



Nonattainment Classification: $PM_{2.5}$

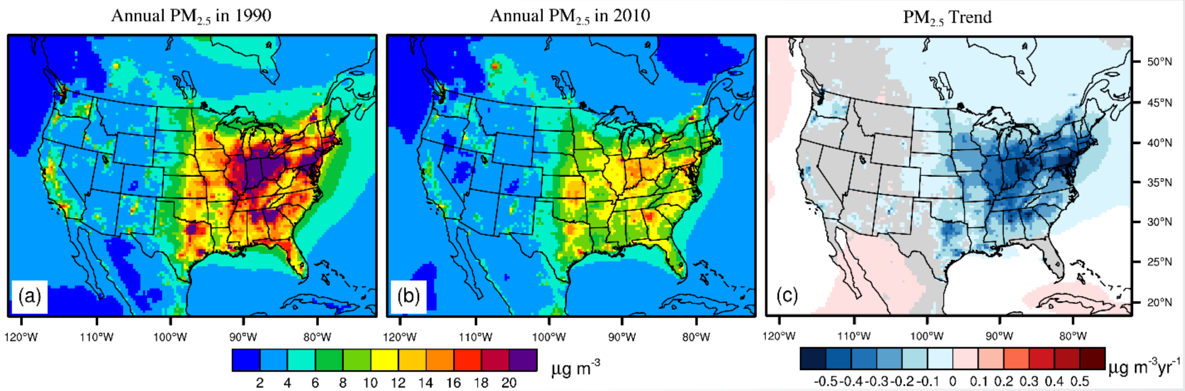


Modeling is often tailored to address local issues. Each location has unique process and modeling challenges from emission sources, meteorological conditions, geographical features, and/or non-controllable sources.

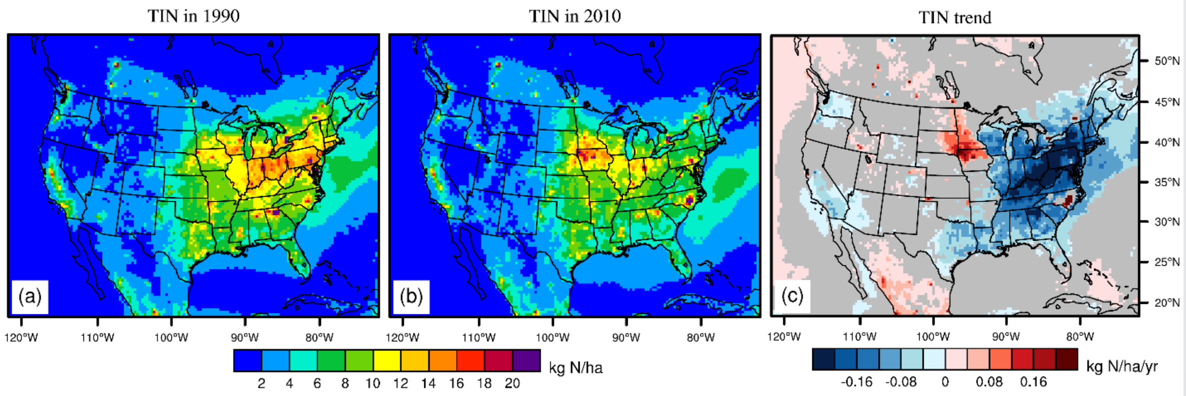
Features of the CMAQ Modeling System

- **Comprehensive Chemical Transport Model**
  - Emissions, advection, diffusion, chemistry, deposition
- **Multiscale: Hemispheric → Continental → Regional → Local**
- **Multi-pollutant & multi-phase**:
  - **Ozone (O_3)** photochemistry
  - **Particulate Matter (PM)**
    - Sulfate, nitrate, ammonium
    - Organic aerosol
    - Natural aerosol (wind blown dust, sea salt)
  - **Acidifying and eutrophying atmospheric deposition**
    - Wet and dry deposition
  - **Air Toxics**
    - Benzene, formaldehyde, mercury, etc.
- **Research/exploratory**
  - Pollen, nano-materials, PFAS

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



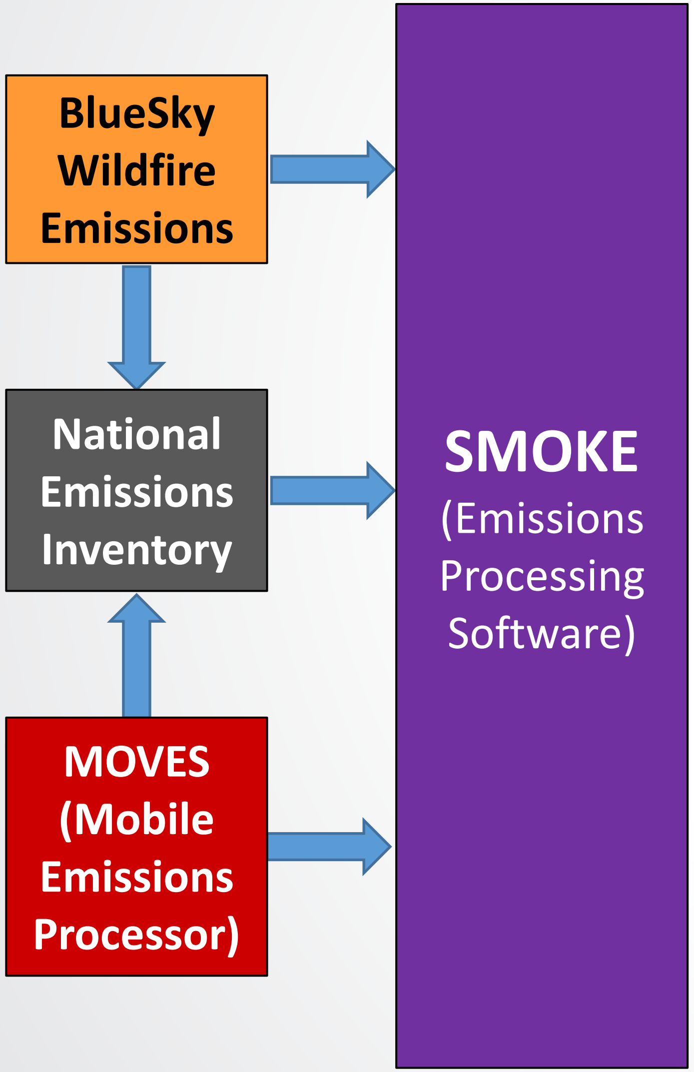
Simulated Trends (1990-2010) in Nitrogen Deposition



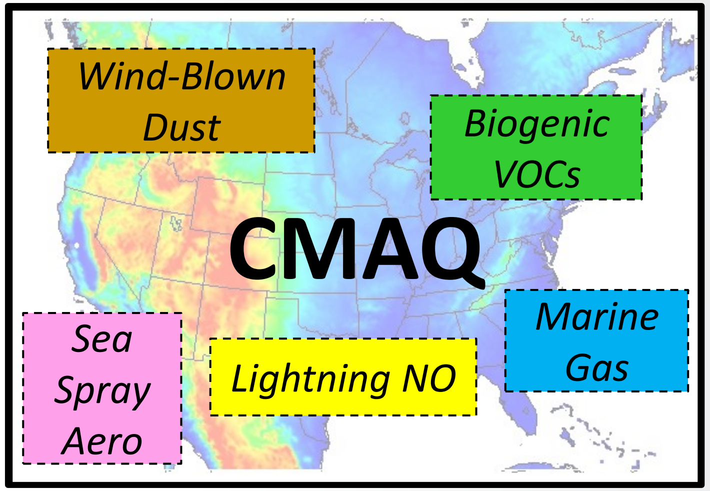
Zhang et al., ACP, 2018

Download CMAQ at https://www.epa.gov/cmaq/

Many Emissions Sources Considered in CMAQ



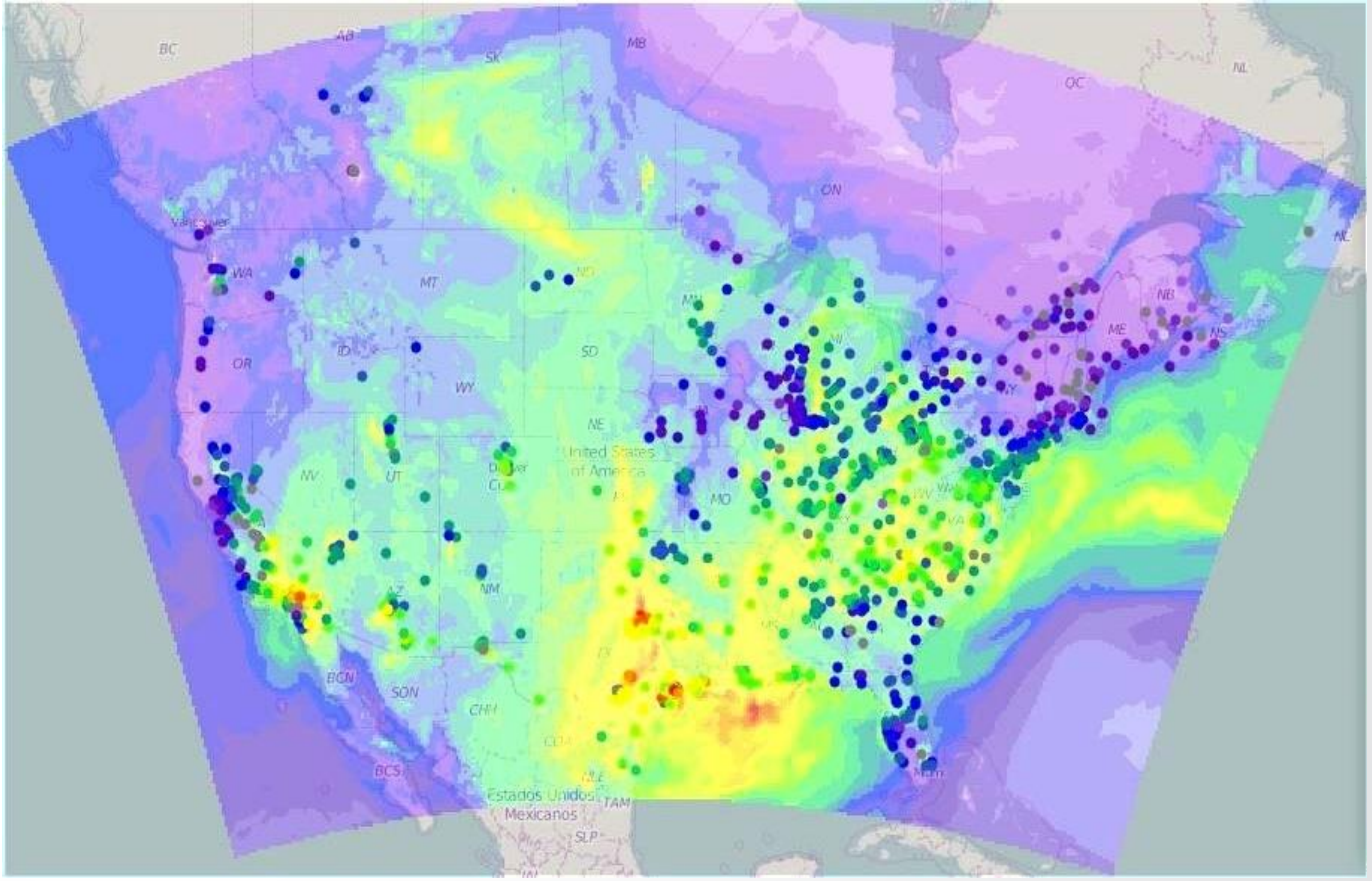
- *EGUs*
- *Non-EGU point sources*
- *Agriculture*
- *Trains*
- *Passenger vehicles*
- *Offroad vehicles*
- *Onroad shipping*
- *Construction*
- *Wildfires*
- *Residential fuel*
- *Consumer products*



- CMAQ allows direct scaling of emissions by species, sector, and location
- Easy to introduce emissions for new pollutants
- Direct scaling of emission sources computed inside CMAQ (e.g., wind-blown dust, biogenic compounds)

Primary Updates in CMAQv5.4

- Updated **chemistry** for ozone and PM from global-to-local scales
- Expanded **biogenic emissions** options
- Improved modeling of **aerosol dry deposition**
- Simplified **model evaluation** workflows
- Improved **visualization** of meteorology and air quality data
- Streamlined **coupling** of CMAQ with meteorological models
- Improved CMAQ **instrumented extensions**
- New **diagnostic and output tools**



Improving Estimates of Particulate Matter

Introducing the Community Regional Atmospheric Chemistry Multiphase Mechanism

- CMAQ historically has relied on empirically derived anthropogenic secondary organic aerosol (SOA), an important component of $PM_{2.5}$
- **CRACMM** (Pye et al., 2022 ACPD) provides a bottom-up approach to SOA formation and supports source apportionment of SOA
  - Emphasis on process-based design
  - Multi-phase chemistry approach
  - Incorporates autoxidation, aromatic chemistry, oxygenated hydrocarbons, organic nitrate chemistry
  - Developed with a specific consideration of health applications
- CRACMM available in CMAQv5.4 as a **research option**
- Currently, CRACMM expected to become the **“flagship” chemical mechanism** in CMAQ in 2025

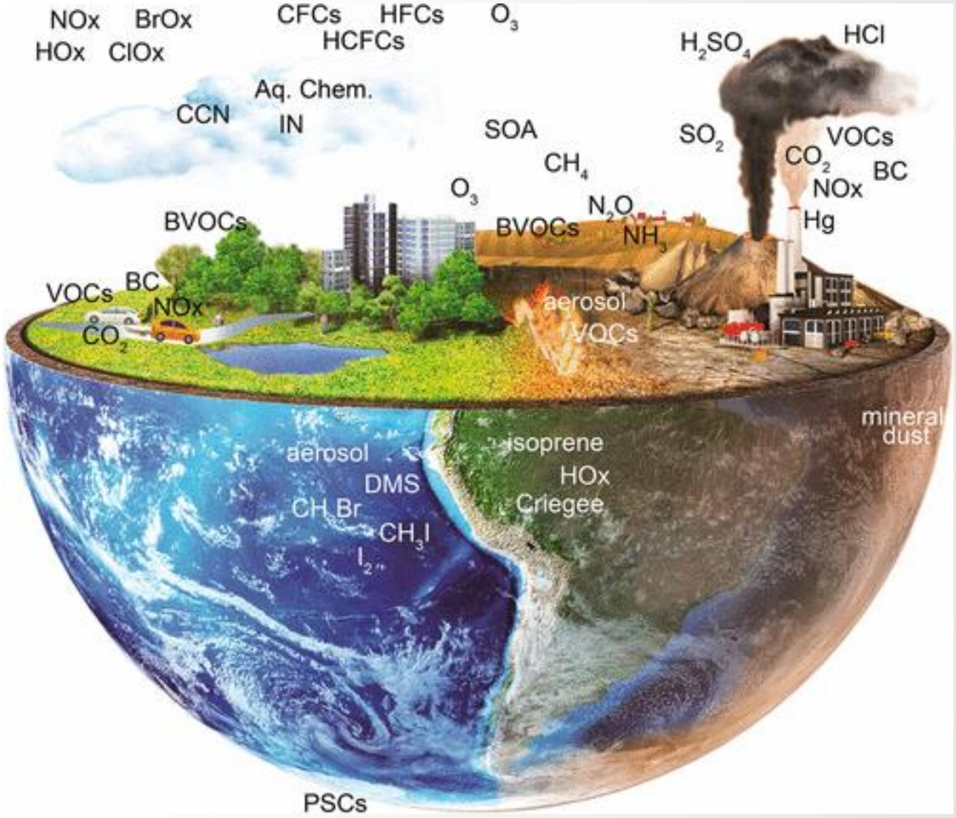
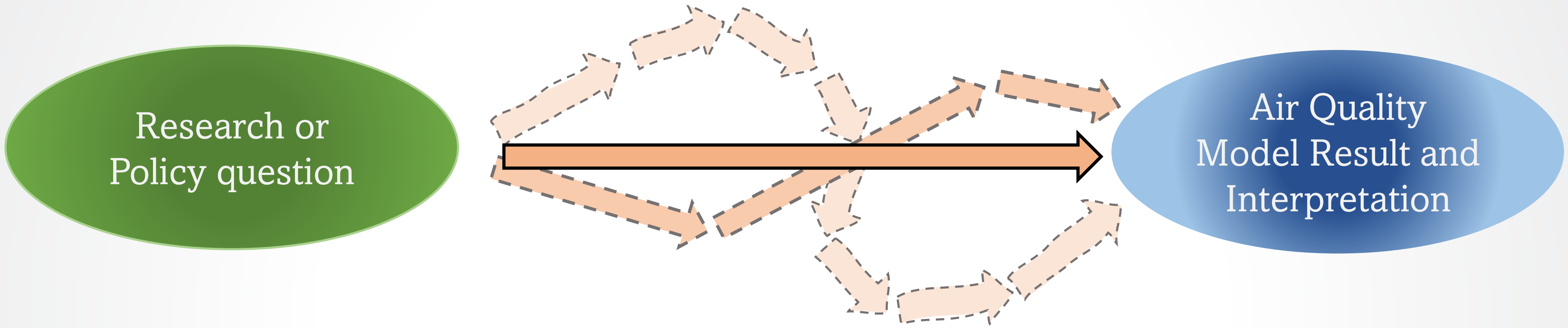


Image: Burkholder et al., ES&T, 2017

https://www.epa.gov/cmaq/cmaq-fact-sheets

Lead PI: Havala Pye

Tools for Air Quality Managers



DESID: Detailed Emission Scaling, Isolation and Diagnostics Module

- Allows easy scaling of input emissions
- Easy specification of regions and aggregated emission types
- Define any number of diagnostic files
- Sum multiple streams to one diagnostic file
- Choose individual variables, all variables, or sum variables

ELMO: Explicit and Lumped CMAQ Model Output Module

- Simplifies the CMAQ output files
- Reduces required post-processing of CMAQ output
- Online processing of aggregate variables (e.g., $PM_{2.5}$)
- Instantaneous and/or average files
- Reduces required disk space

Lead PI:
Ben Murphy

Accounting for Emissions from Ocean Water

- **Halogens (e.g., iodine, bromine) from oceans can affect ozone concentrations in air**
- Including these reactions in CMAQ improves accuracy of ozone concentrations:
  - in simulations with large expanses of open ocean (e.g., hemispheric and global simulations)
  - near coastal regions (e.g., southern CA, Houston, NY-NJ-CT) in regional CMAQ simulations
- **Updates in CMAQv5.4 further refined and improved the marine chemistry treatment in CMAQ**

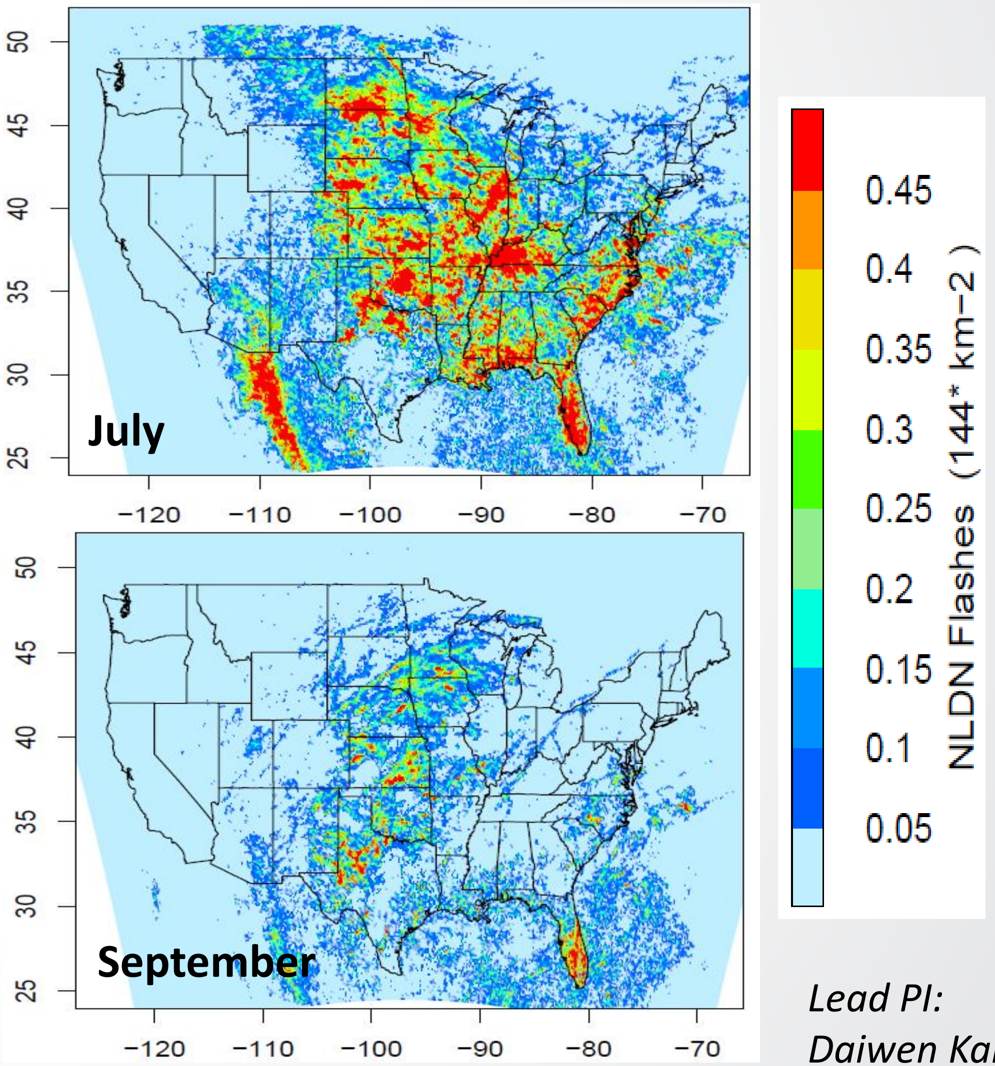
https://www.epa.gov/sciencematters/modeling-research-shows-how-salty-ocean-air-impacts-ozone-pollution

Lead PI:
Golam Sarwar

Estimating NO_x Emissions from Lightning

- **Lightning strikes are an important natural source for NO_X emissions**
- Lightning has important implications for simulating:
  - **Ozone**
  - **Nitrate deposition**
- Lightning NO (LNO) production in CMAQ uses either:
  - observed lightning flash data (NLDN) or
  - climatological lightning data and meteorology
- **CMAQv5.4 has been updated to use alternative and readily available sources of lightning flash data**, such as the World Wide Lightning Location Network (WWLLN) and satellite retrievals

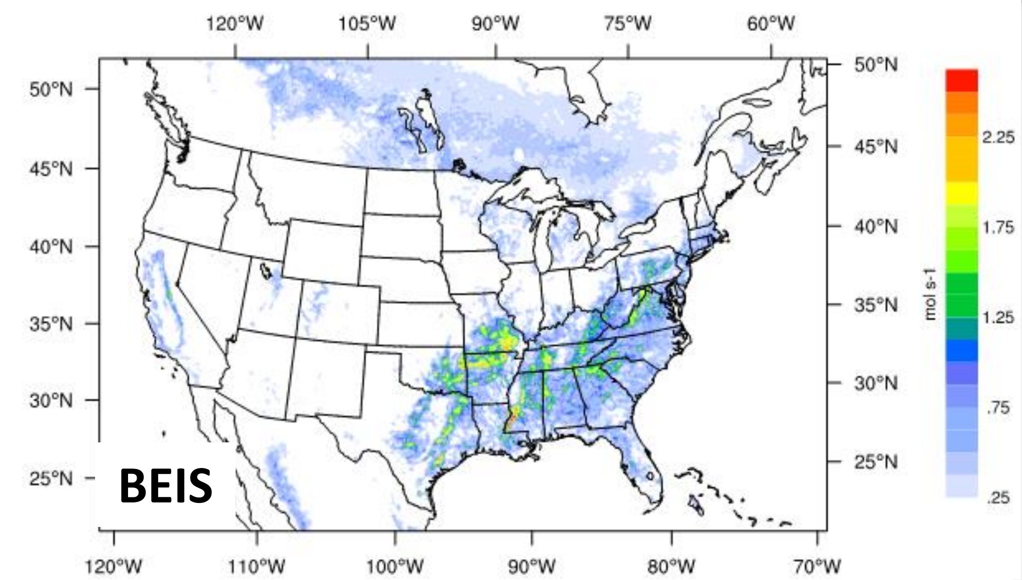
National Lightning Detection Network

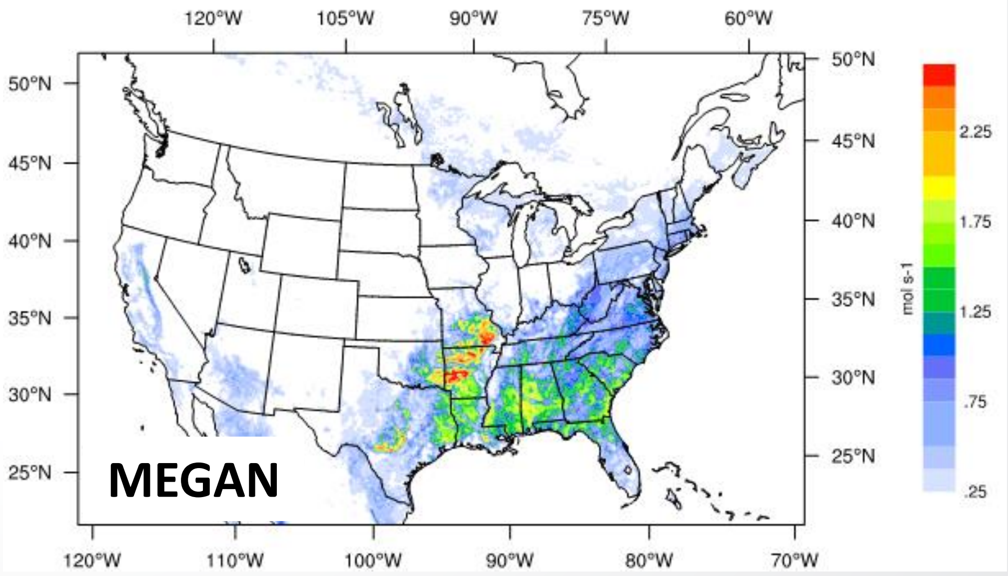


Lead PI: Daiwen Kang

Generating Biogenic Emissions within CMAQ

- **Biogenic (e.g., plant, tree, soil) emissions are an important natural source of emissions (e.g., isoprene, terpenes, NO)**
- Biogenic emissions have important implications for simulating:
  - **Ozone**
  - **Secondary organic aerosol (SOA)**
- Prior to CMAQv5.4, the only option for inline biogenic emission production in CMAQ was the **Biogenic Emissions Inventory System (BEIS)**
- As of CMAQv5.4, the **Model of Emissions and Gases from Nature (MEGAN)** is also available. MEGAN can be used for simulations beyond the US



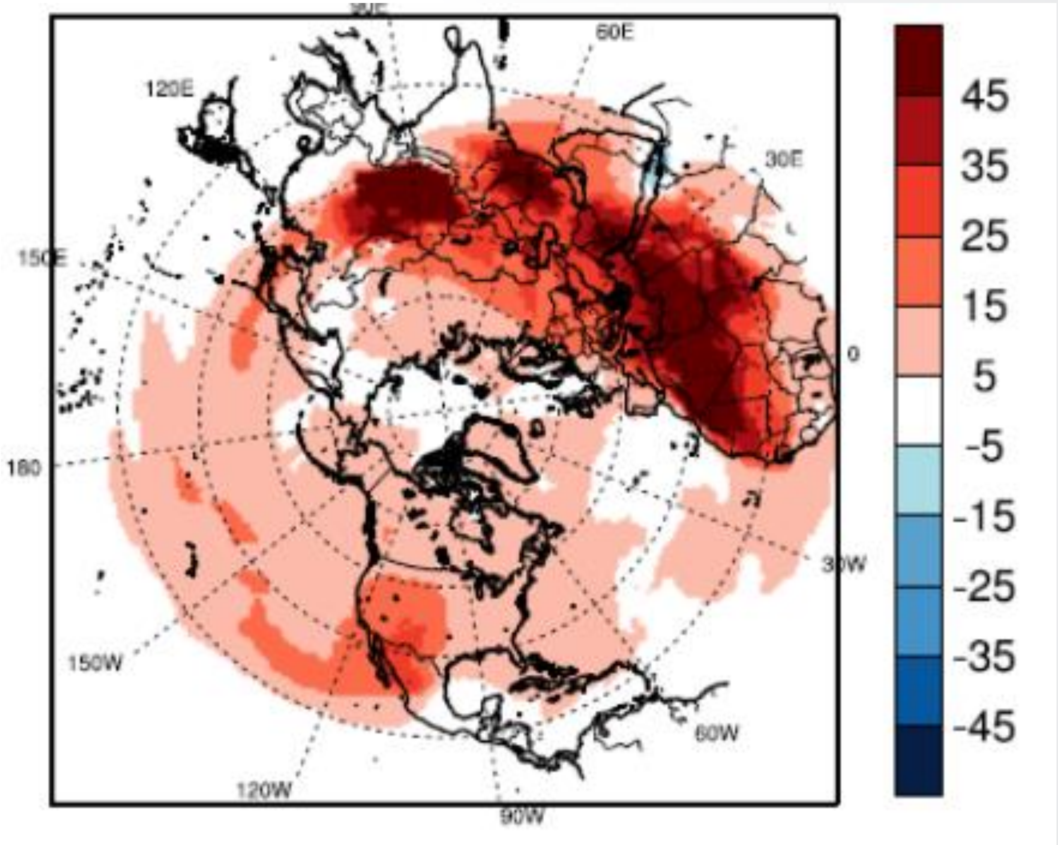


Lead PI: Jeff Willison

Generating Wind-Blown Dust in CMAQ

- **Wind-blown dust (WBD) is an important natural source of particulate matter**
- WBD has important implications for simulating:
  - **$PM_{2.5}$ and PM_{10}**
  - **Solar radiation and ozone (indirectly)**
- WBD production in CMAQ relies on:
  - Meteorology (e.g., wind speed, precipitation)
  - Land-use characteristics
  - WBD model in CMAQ
- Updates to the WBD model and other updates in CMAQv5.4 result in **increased dust emissions** across the Northern Hemisphere

Percent difference in WBD emissions between CMAQv5.3.3. and CMAQv5.4



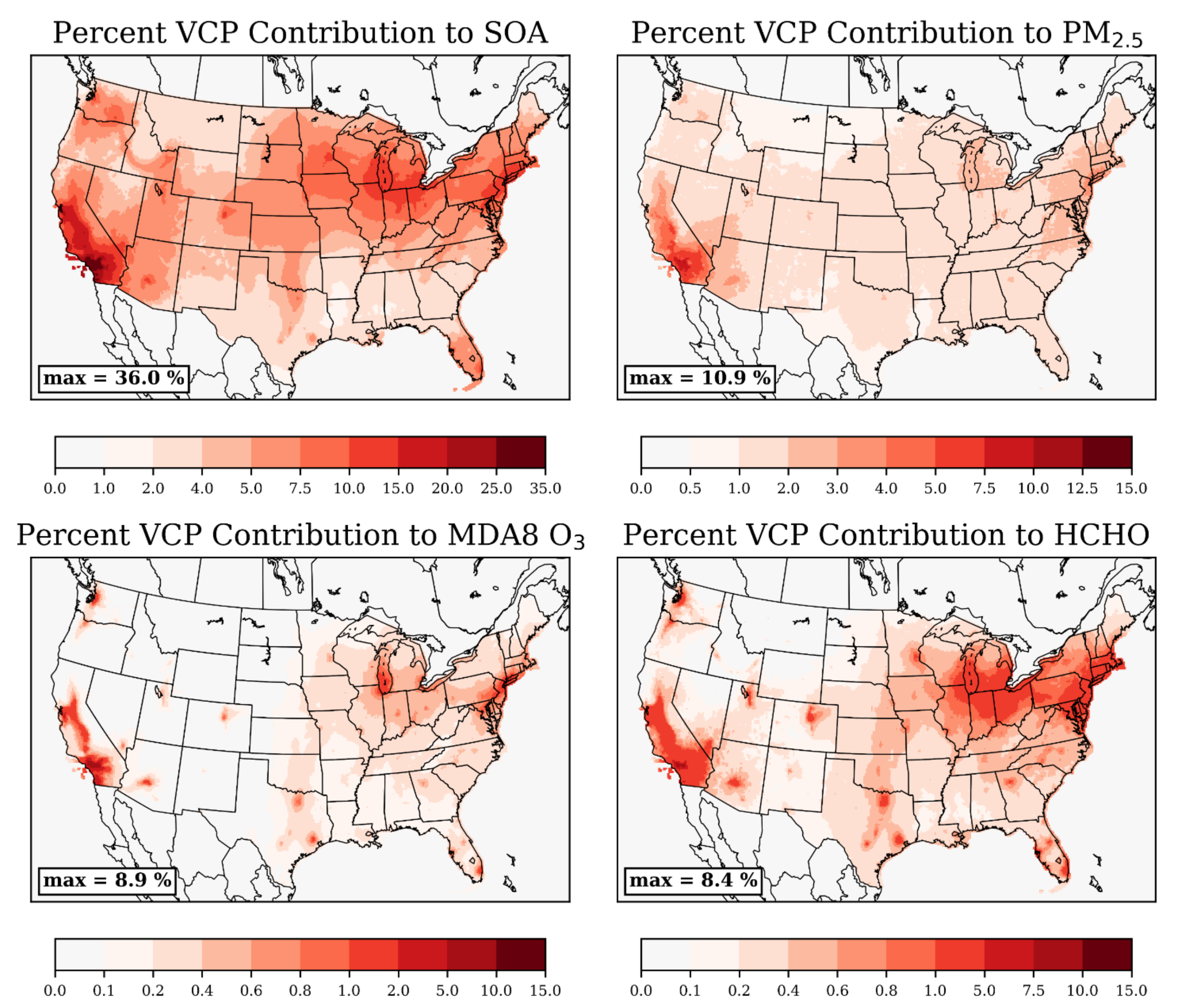
Lead PIs:
Fahim Sidi (EPA) and Hosein Foroutan (VA Tech)

Impact of Volatile Chemical Products on PM

As **VCPs take on a greater role in $PM_{2.5}$**, research suggests that the National Emissions Inventory (NEI) may underrepresent some VCPs by a factor of 2-3.

Emissions from VCPs are added to CMAQ to examine impacts on PM, O_3, and toxics.

Photo: https://esrl.noaa.gov/csd/news/2018/231_0416.html



Annually:

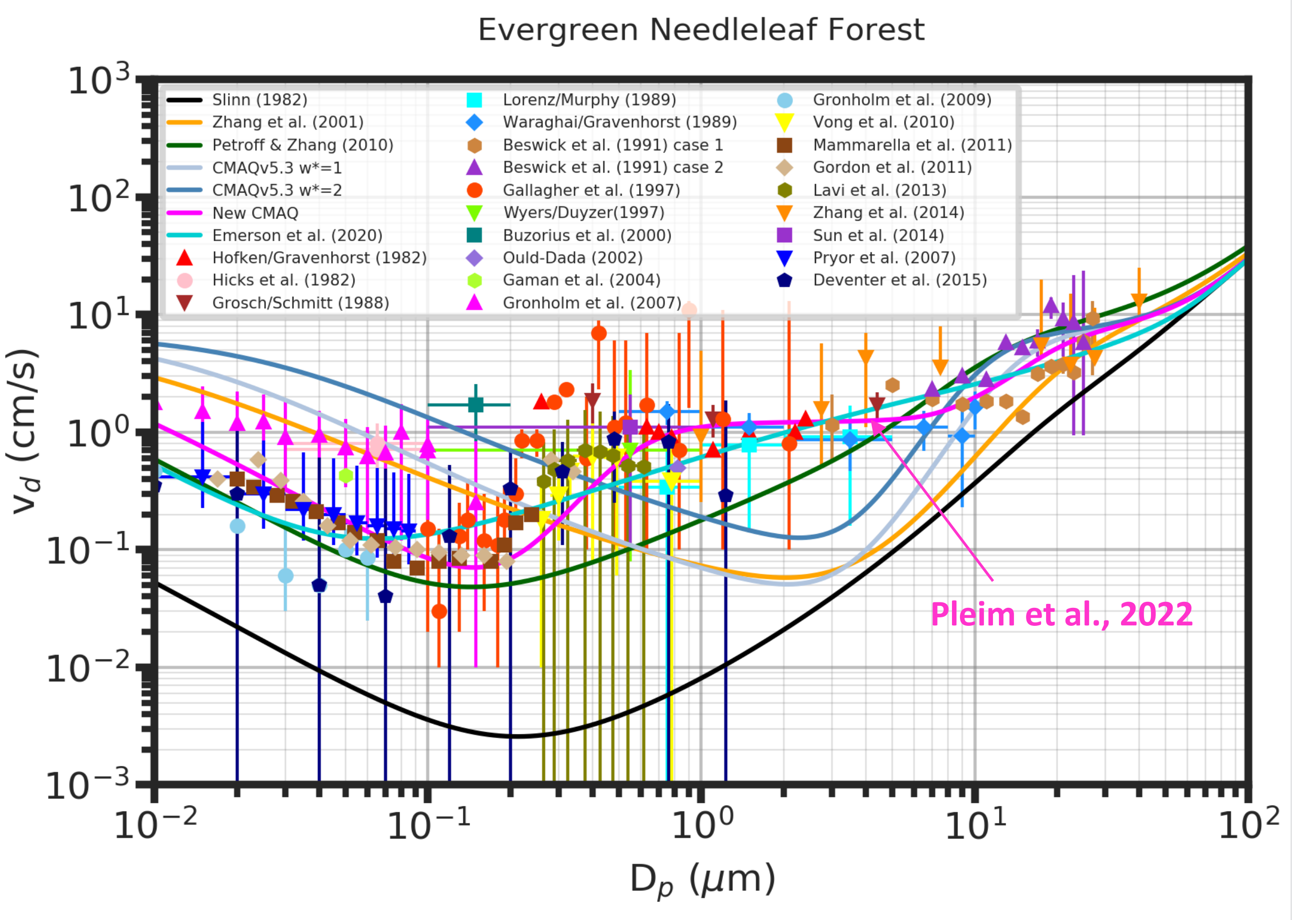
VCPs contribute:

- up to 0.55 $\mu g\ m^{-3}$ to annual $PM_{2.5}$
- up to 3 ppb to annual MDA8 O_3
- to formaldehyde as well

Lead PIs:
Havala Pye
Karl Seltzer

Aerosol Dry Deposition Updates

- CMAQ contains two dry deposition models, **M3Dry and STAGE**
- Both models were updated in CMAQv5.4
- **M3Dry** updates include:
  - New representation of "leaf-level" microscale features to correct underestimation of PM dry deposition
  - Increases deposition to forested areas, resulting in 10-40% reductions in regional $PM_{2.5}$
- **STAGE** updates include:
  - Option to toggle between multiple deposition models (i.e., Emmerson et al. (2020), Pleim et al., (2022))
  - Reduced redundant land-use categories
  - Easier control of species and land-use specific data



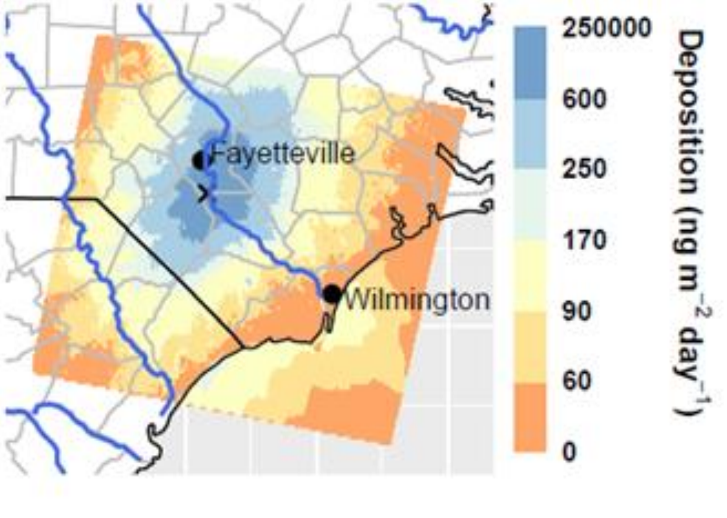
Lead PI (M3Dry): Jon Pleim

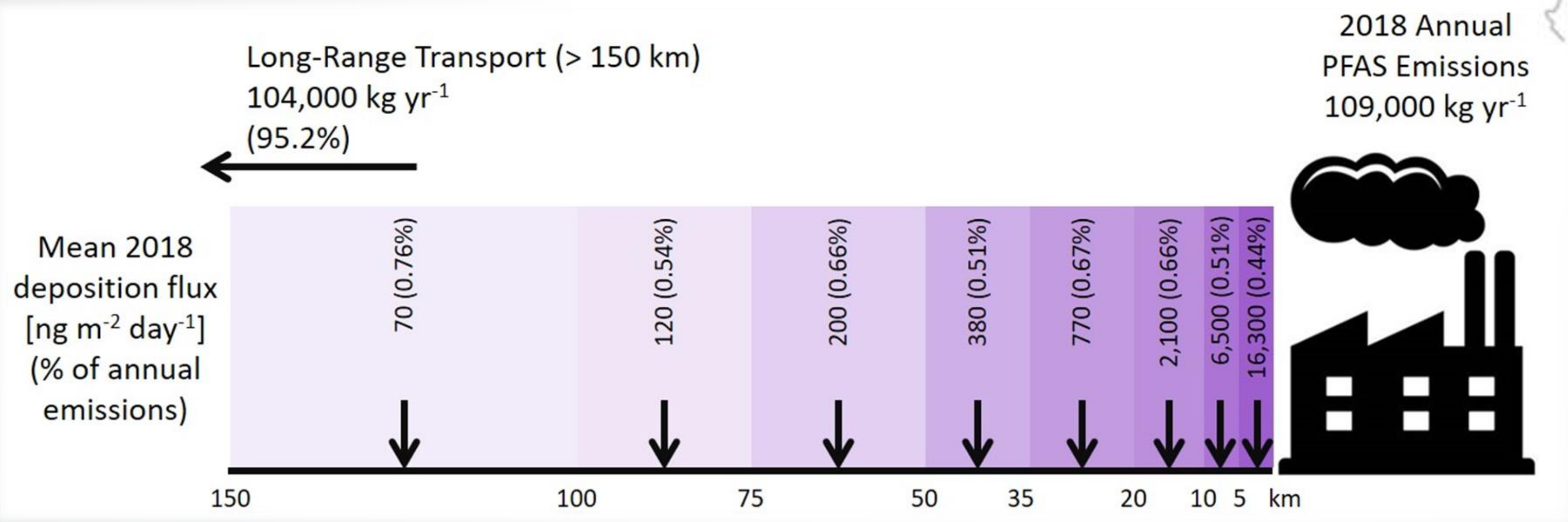
Lead PI (STAGE): Jesse Bash

Simulating Emerging Pollutants of Concern

CMAQ is used to simulate local atmospheric fate and transport of per- and polyfluorinated substances (PFAS).

- Model a production facility with documented air emissions
- 26 individual PFAS and 1 additional lumped species were added to CMAQ





Deposition and air concentrations are highest near the facility, decreasing rapidly with distance.

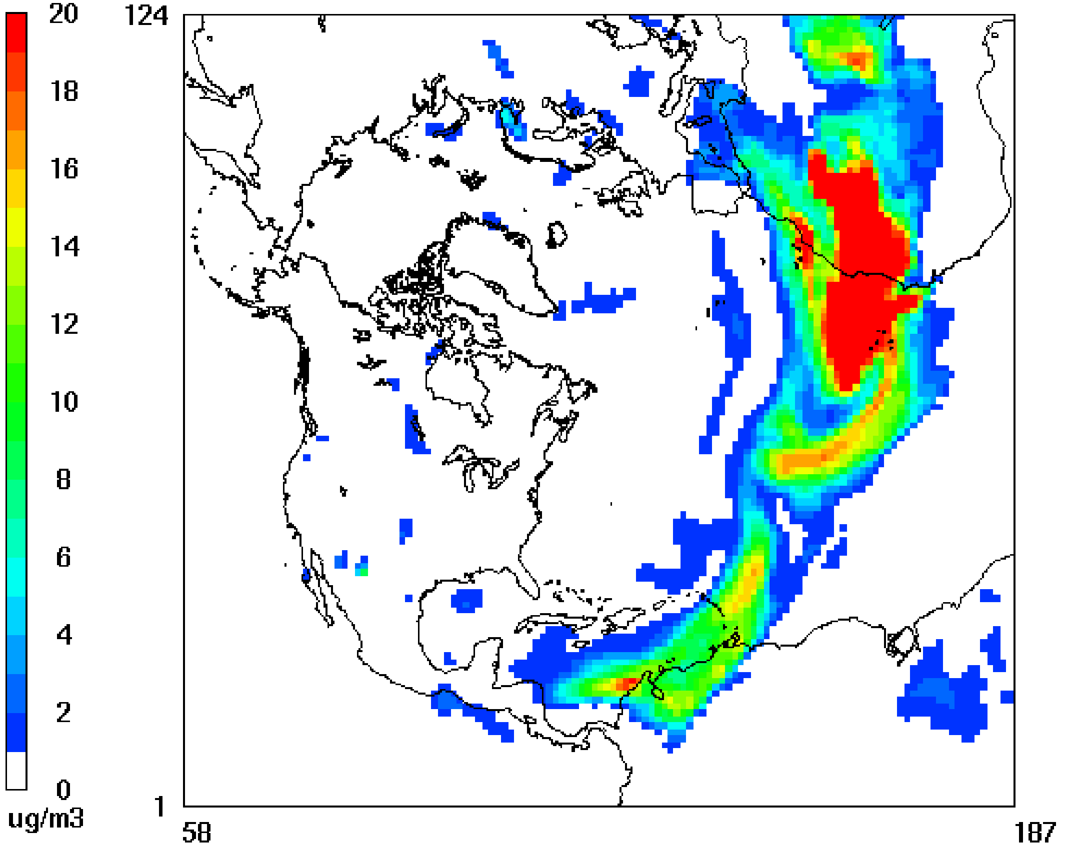
5% of total emissions by mass are deposited within ~150 km of the facility; the remaining mass is transported farther.

D'Ambro et al., ES&T, 2021

Lead PIs:
Emma D'Ambro
Benjamin Murphy

Air Quality: A Global Transport Issue

CMAQ Simulation of
Trans-Atlantic Transport of Saharan Dust



Examining US air quality in context of the changing global atmosphere

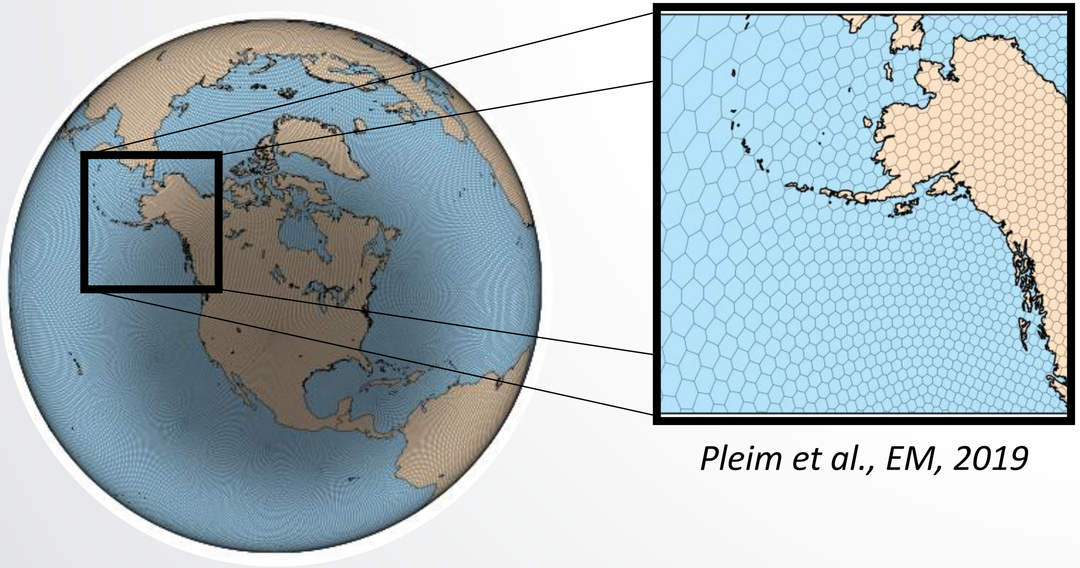
- Pollutants near the Earth's surface can be lofted to higher altitudes where **strong winds can efficiently transport** then from one continent to another
- Need to **accurately represent the global emission and transport** of pollutants to **estimate US background pollution** concentrations

Lead PI:
Rohit Mathur

Simulating Global Influences on Local AQ

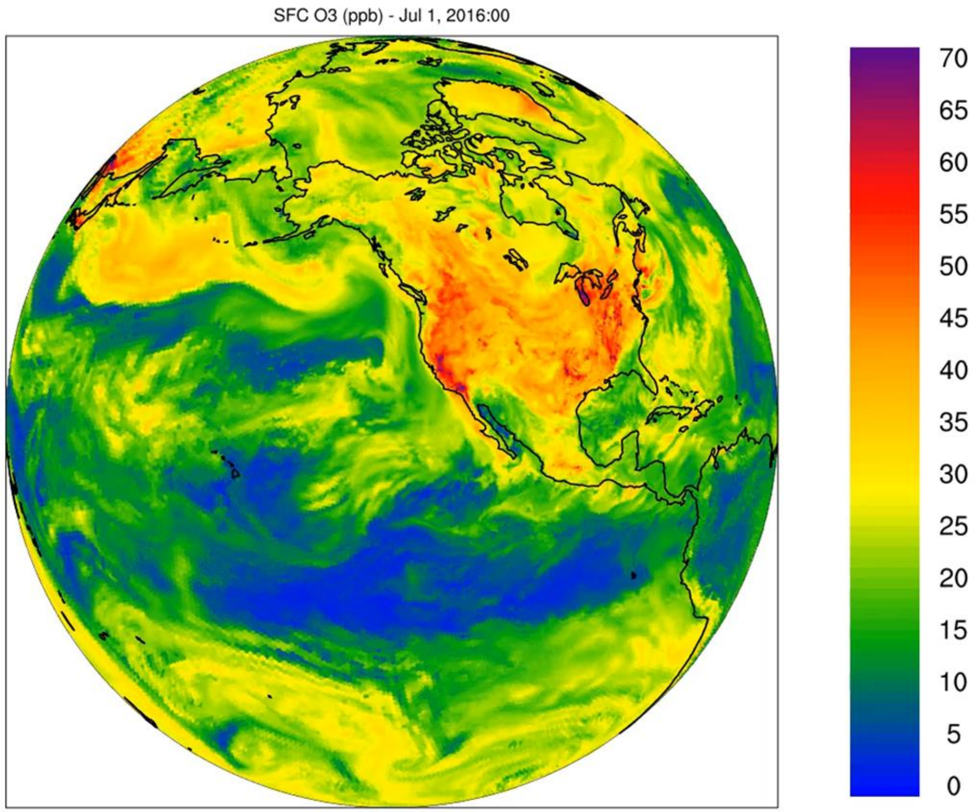
Consistent Representation of Air Pollution Process-Interactions Across Scales (MPAS-CMAQ)

- Linking CMAQ with the Model for Prediction Across Scales (MPAS)
- Seamless mesh refinement to local scales
  - **Finer resolution in regions of interest**
  - **Lack of discontinuities at boundaries improves results**



Pleim et al., EM, 2019

Long-range O_3 Transport

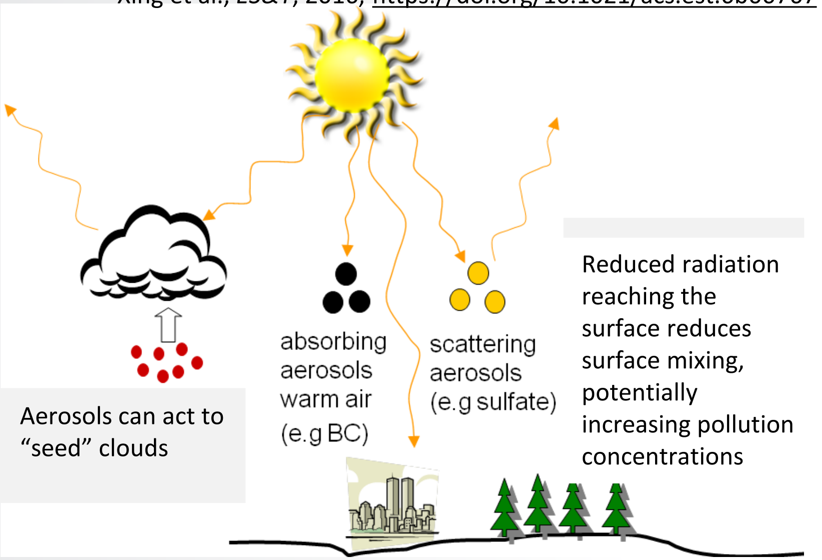


Lead PI:
Jonathan Pleim

Air Quality-Meteorology-Climate Interactions

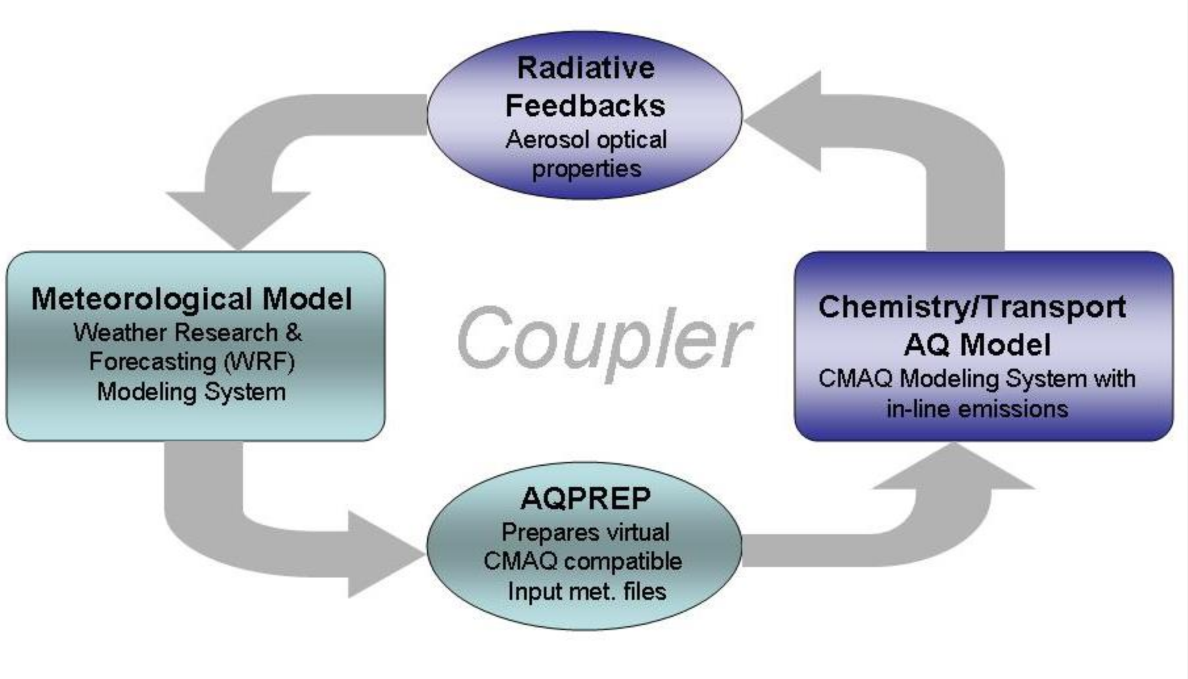
Optical and Radiative Properties of Particulate Matter

Xing et al., *ES&T*, 2016, https://doi.org/10.1021/acs.est.6b00767



Two-Way Coupled WRF-CMAQ

Wong et al, 2012, https://doi.org/10.5194/gmd-5-299-2012



Particle concentrations and composition need to be considered to accurately simulate air quality and the effects of a changing climate. **CMAQ specific requirements for two-way coupled WRF-CMAQ are included in the latest WRF model release.**

Tailored Model Evaluation Strategies

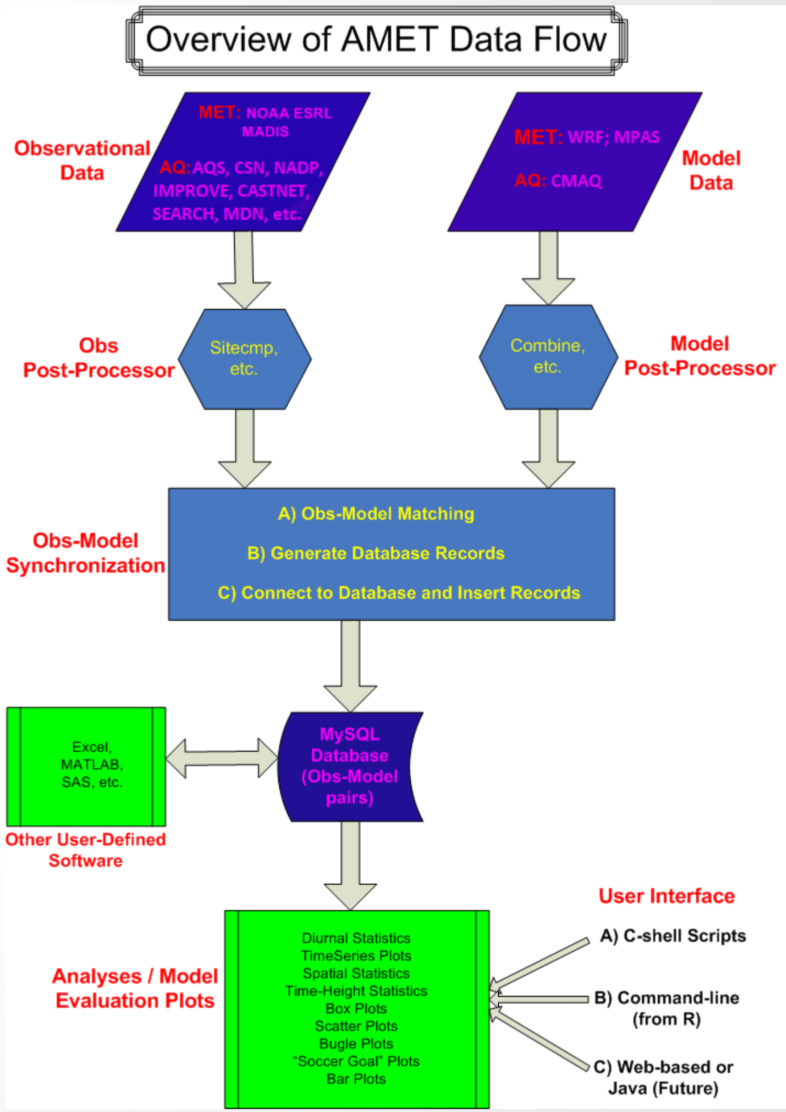
Atmospheric Model Evaluation Tool (AMET)

- Packaged software for evaluating AQ and Met models
  - MySQL database for data storage and access
  - Fortran and R post-processing tools
  - R software for database interface and analysis

- Advantages of AMET
  - Capable of managing large datasets efficiently
  - Partially automated system, therefore easy to use
  - Relational database allows for unique querying of data
  - Pre-defined analysis scripts for common analysis across groups
  - Users can easily develop their own custom analyses in R

EPA Link: AMET Description and Download Information

Lead PIs:
Wyat Appel
Rob Gilliam

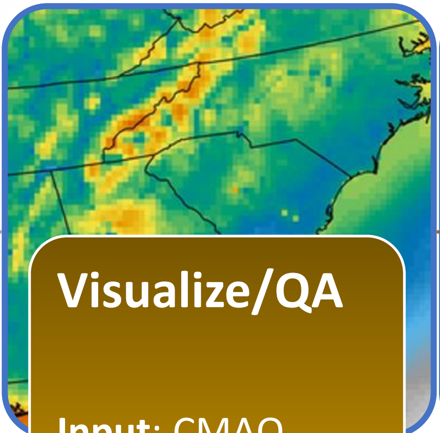


Extensive Evaluation Against Observations

Pre-process

Input: CMAQ data

Output: Aggregated files



Visualize/QA

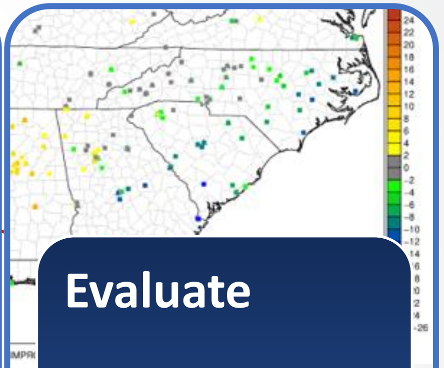
Input: CMAQ post-processed output

Output: graphics files, html

Match to Obs

Input: CMAQ post-processed output + observations

Output: .csv



Evaluate

Input: .csv files

Output: database, graphics files

4 TB Model Data

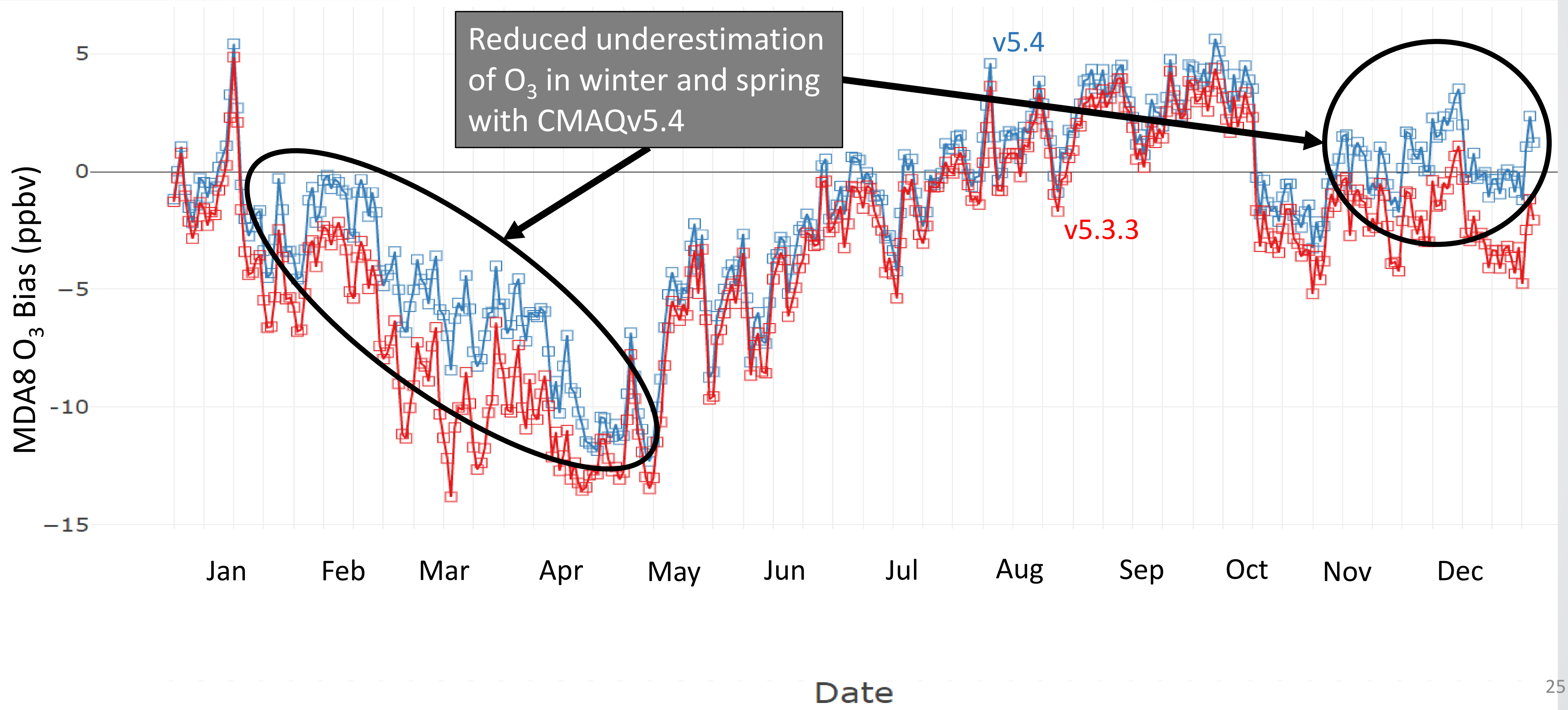
90 GB Model Data

0.5 GB Obs Data

1 GB Paired Model/Obs Data

Post-processing 1 month of model output for the continental US

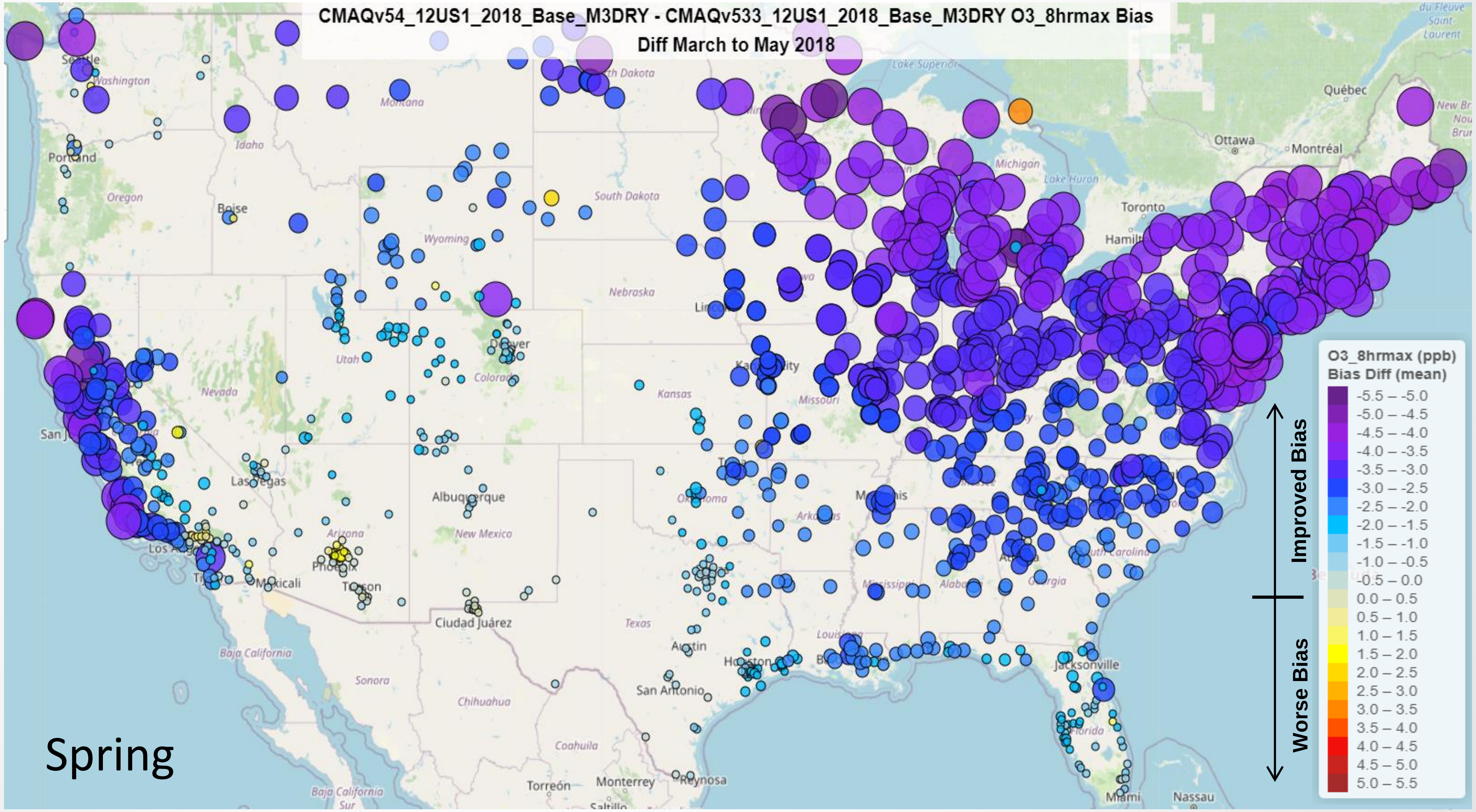
Ozone estimates improve with CMAQv5.4



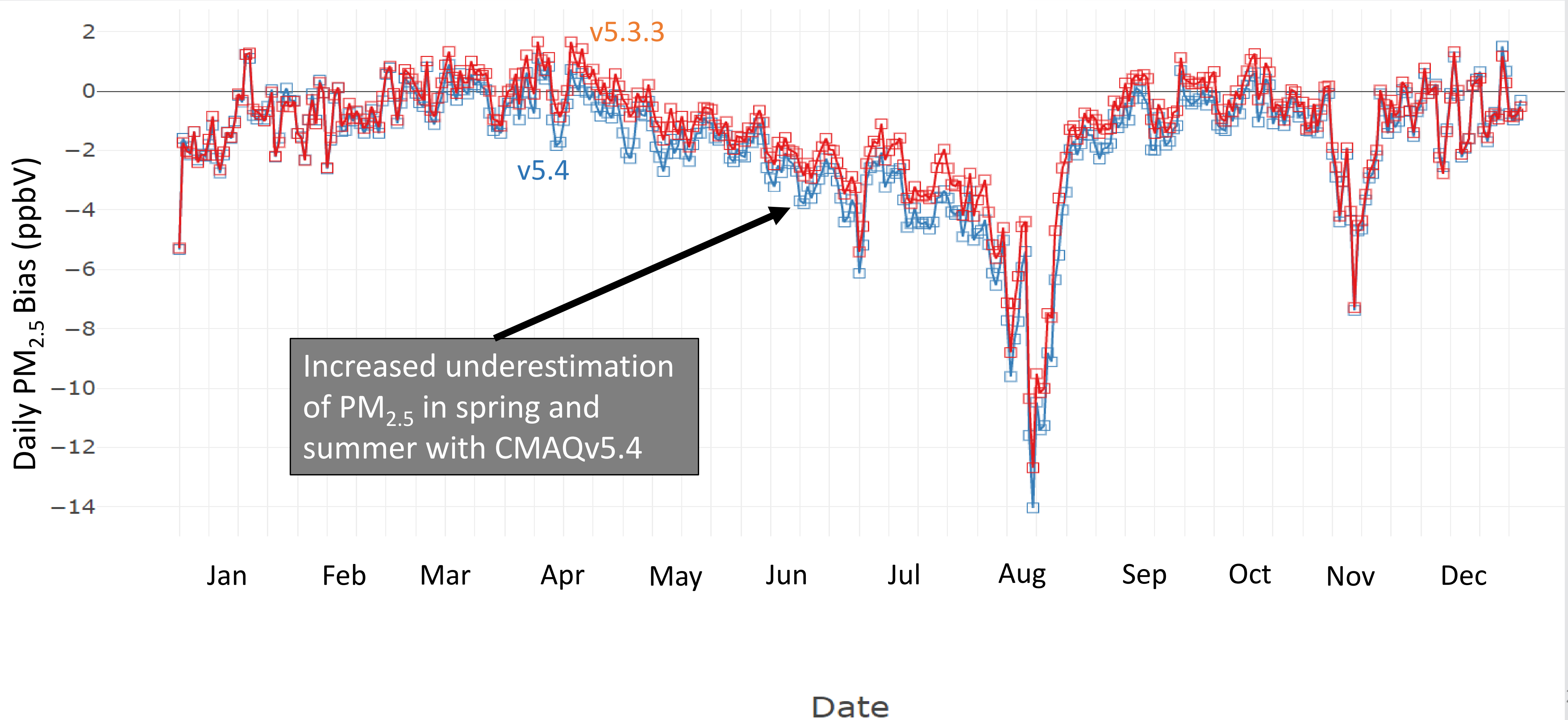
Large improvement in O_3 in Spring

Difference in seasonal MDA8 O_3 bias between CMAQv5.4 and v5.3.3

Along with temporal comparisons, evaluations include **spatial comparisons** to observations

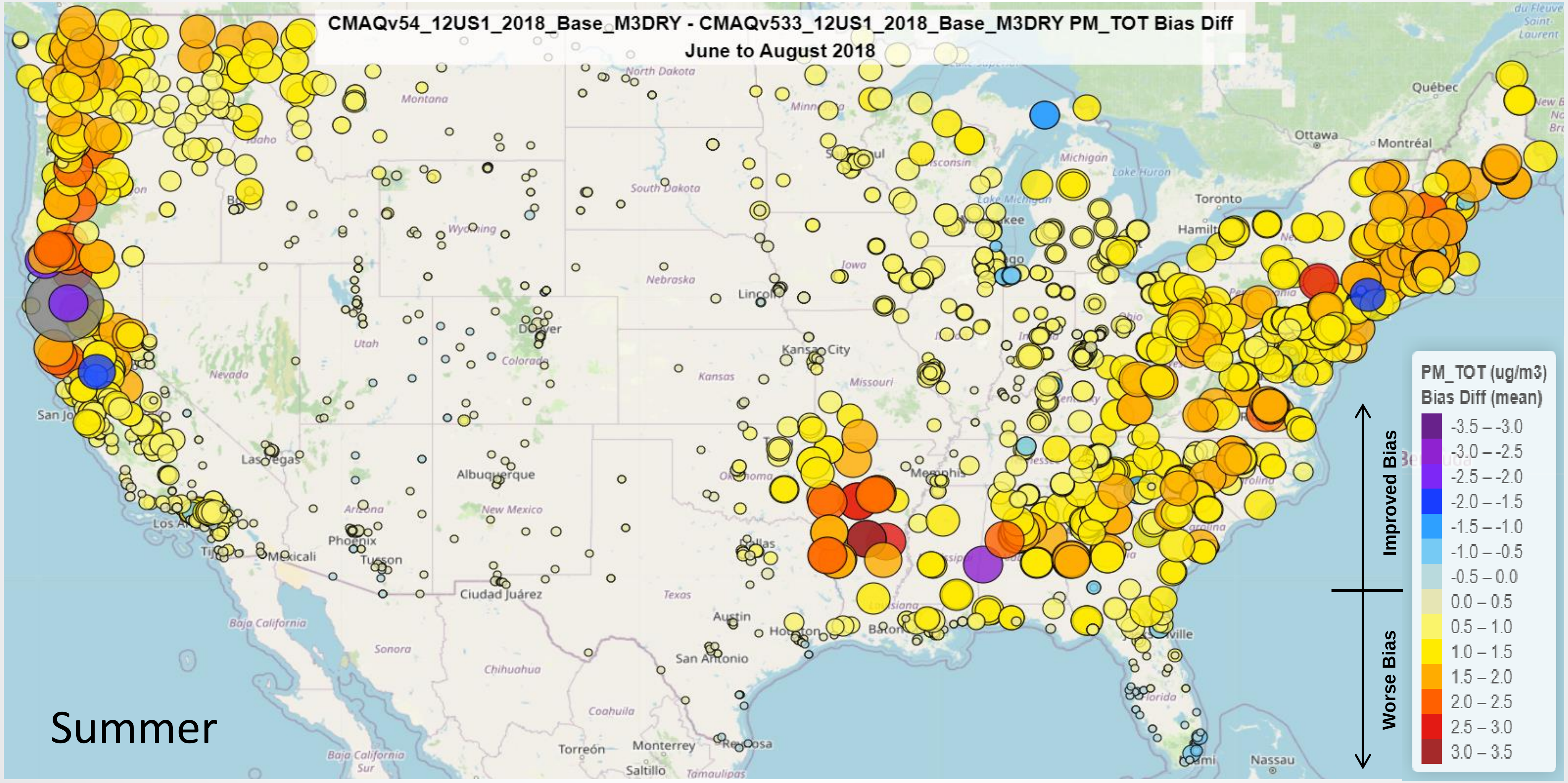


$PM_{2.5}$ Estimates Similar with CMAQv5.4

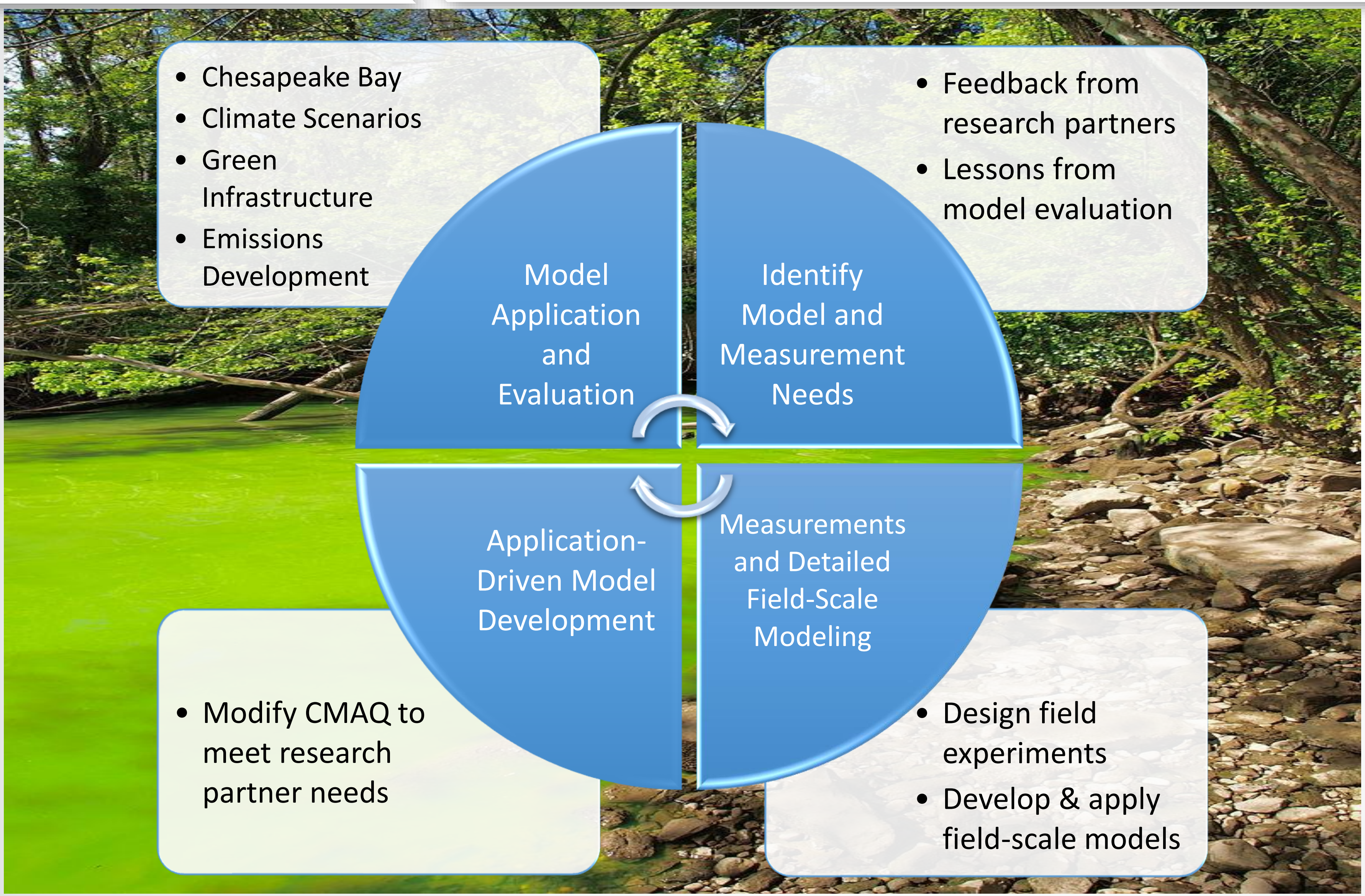


Higher Bias in $PM_{2.5}$ in Summer w/ CMAQv5.4

Difference in summer $PM_{2.5}$ bias between CMAQv5.4 and v5.3.3



Application-Driven Model Development



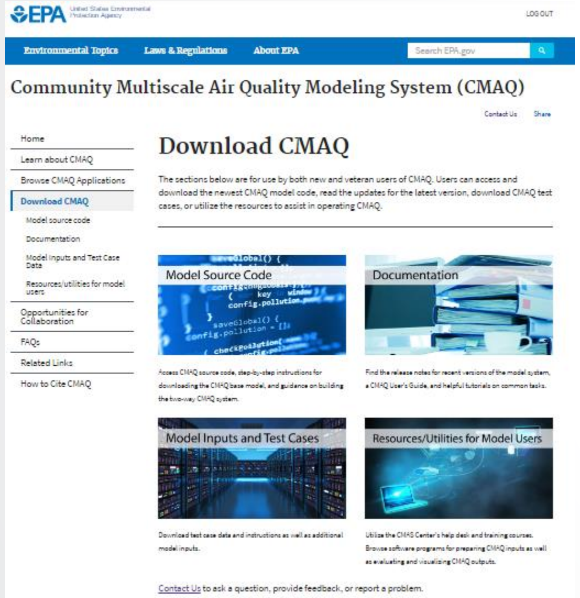
CMAQ development draws from partner needs. It includes a feedback cycle that links development, evaluation, and applications. It incorporates suites of observations to inform scientific advancement for Agency needs.

Image adapted from J. Bash

Sound Science is a Foundation for Regulatory Actions and Implementation

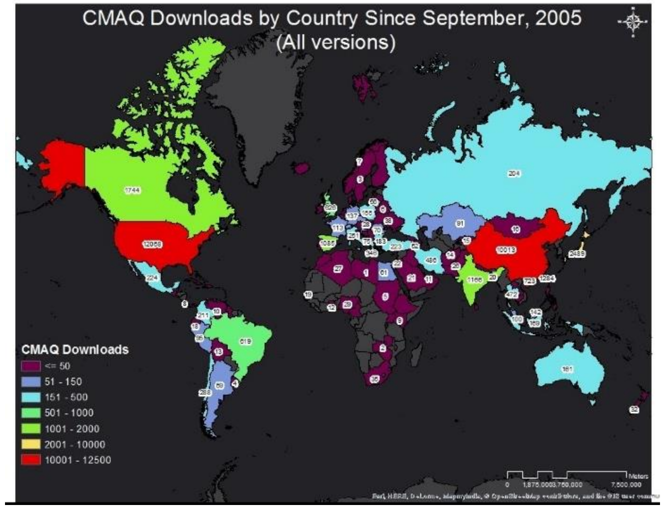
Transparency & Reproducibility

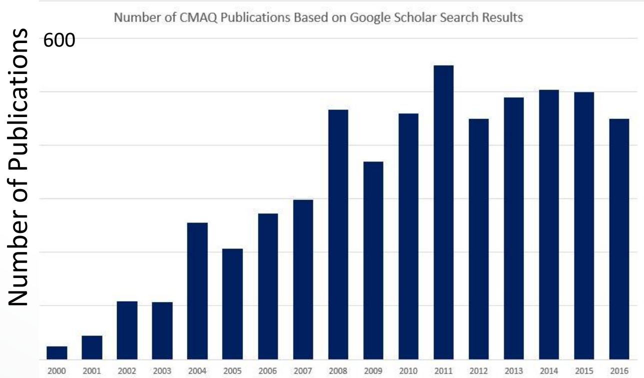
https://www.epa.gov/cmaq



- Documentation
- Source code
- Datasets

Dissemination

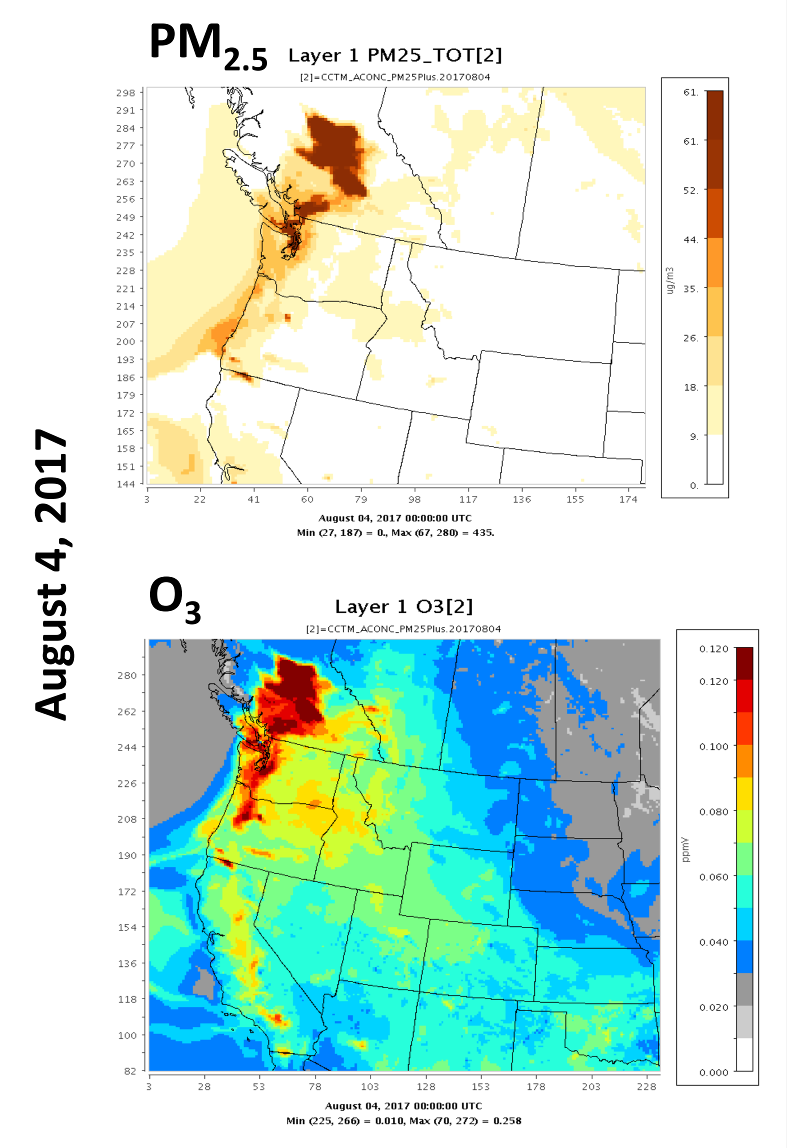




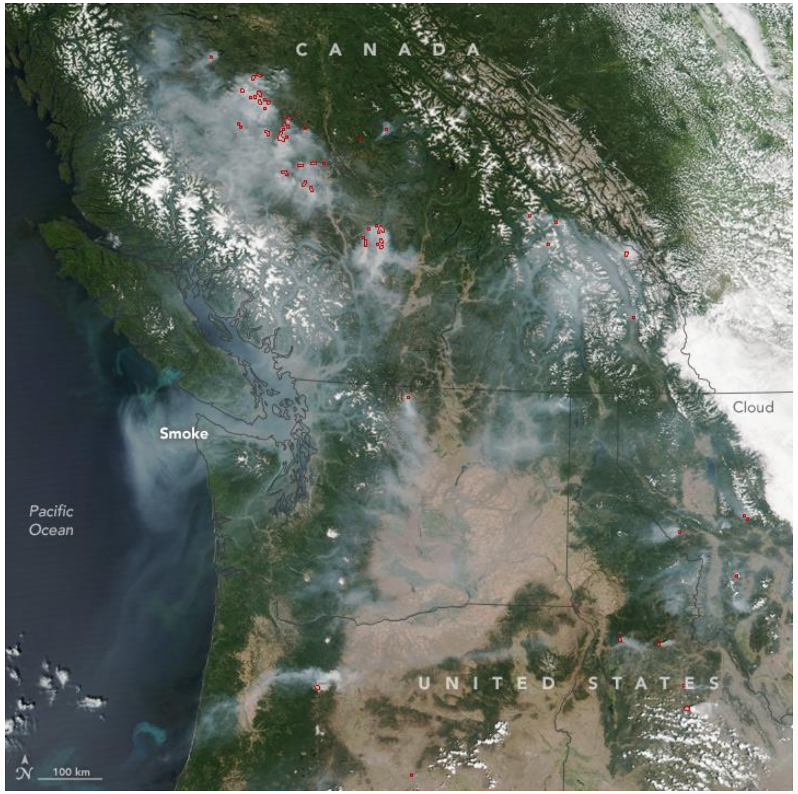
External Peer Review

- External panels comprised of International experts in atmospheric modeling & applications
- Six peer reviews since 2000; most recent in May 2019
- Panel's findings and our responses accompany the public release of the model
- CMAQ is open source and free, with a large userbase that acts as a de facto peer-review

Partner Need: Quantifying Wildfire Impacts



Fighting to breathe in the face of Canada's wildfire emergency
By **Mika McKinnon** in Kamloops, British Columbia
www.newscientist.com



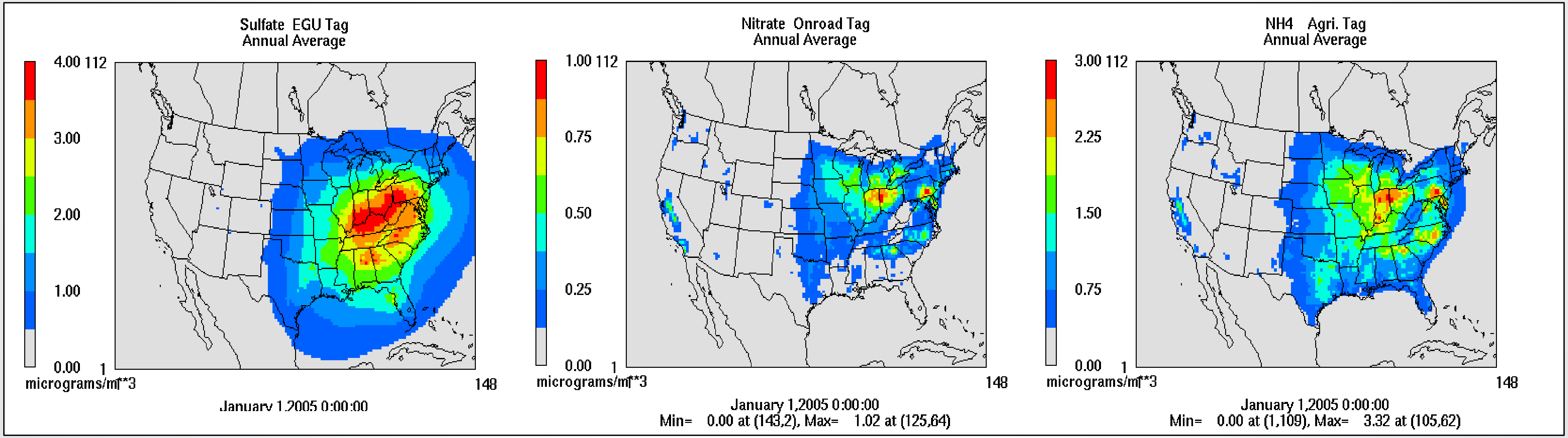
https://earthobservatory.nasa.gov/NaturalHazards/view.php?id=90695

Haze hangs over Seattle as smoke from B.C. wildfires drifts into Washington
by: KIRO 7 News Staff Updated: Aug 2, 2017 - 6:25 PM

CMAQ not only predicts movement of smoke from wildfires, but also simulates the atmospheric chemistry related to wildfire emissions.

Partner Need: Quantifying Impact of Emissions

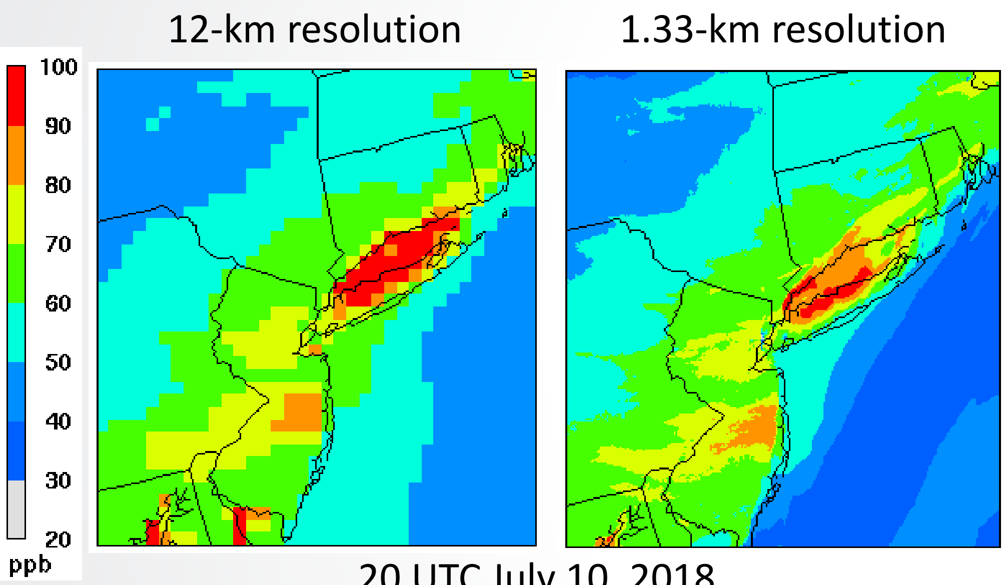
- For policy applications it is often the **response of model predictions to emission changes** that inform decision making
- The **Integrated Source Apportionment Method (CMAQ-ISAM)** quantifies the contributions of various emissions to pollutant levels



Lead PI:
Sergey Napelenok

Partner Need: Local Air Quality Characterization

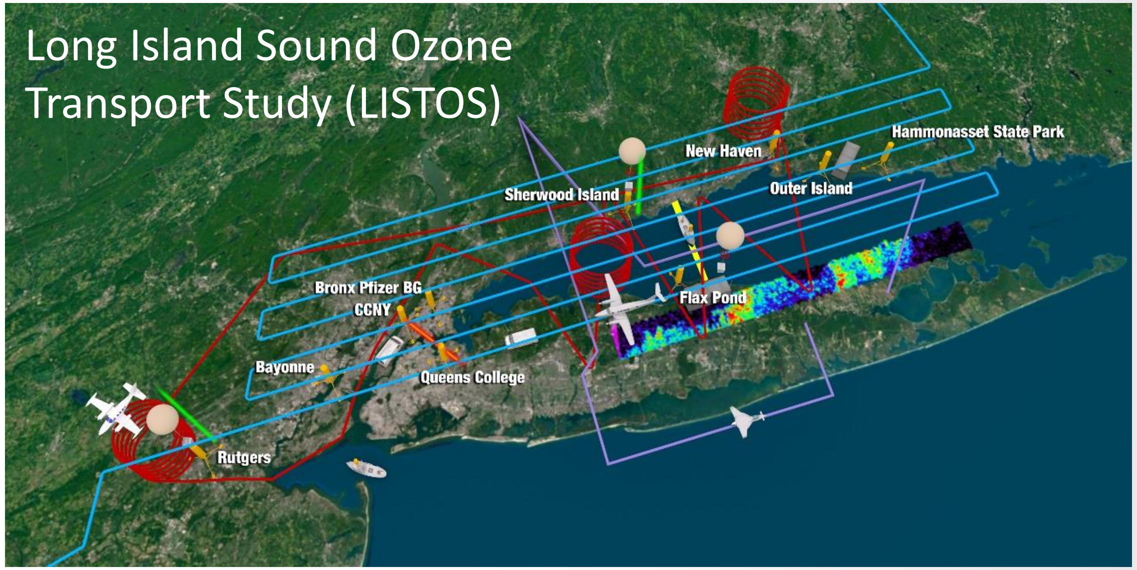
O_3 Transport across the Long Island Sound



20 UTC July 10, 2018

Responding to needs from EPA Regions 1 and 2, higher resolution modeling enables better representation of:

- Pollution transport across the sound
- Impacts on locations along the Connecticut shore-line
- Regional strategies to address nonattainment



This work will ultimately improve the science in CMAQ with better representation of:

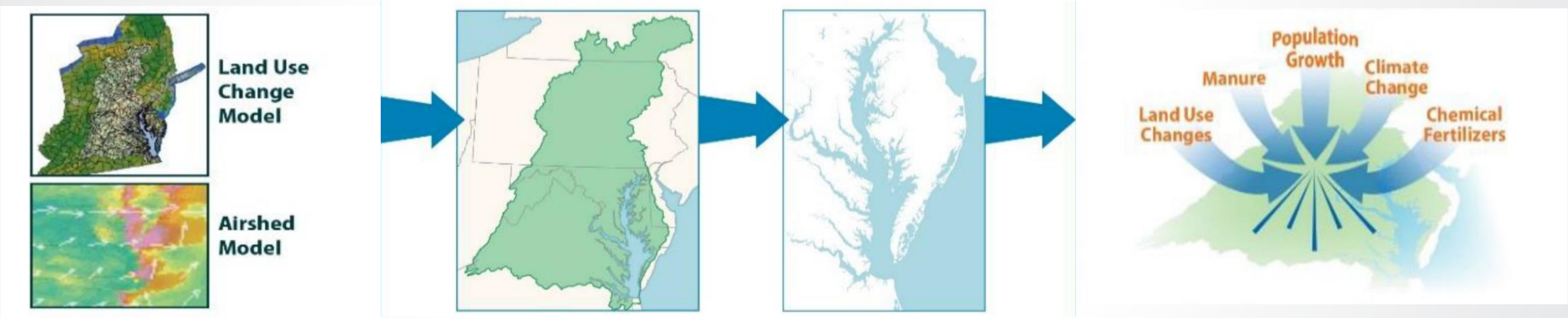
- **Land/sea breeze circulations**
- **Low-level "jets" (airflow)**
- **Urban-scale physical processes**

Lead PI: Jon Pleim

Partner Need: Deposition to Chesapeake Bay

ORD has a very long history working with Maryland and other groups on deposition to Chesapeake Bay.

Model Data Input | *Watershed Model* | *Estuary Model* | *Prediction of Impacts*



CMAQ application and development has been an important part of the Chesapeake Bay work.

Lead PI:
Jesse Bash

Partner Need: Alaskan Wintertime $PM_{2.5}$

- Fairbanks, Alaska and regions near the North Pole **exceed daily fine particulate matter ($PM_{2.5}$) standards**
- **High wintertime $PM_{2.5}$ episodes** are characterized by low winds, strong temperature inversions, and high home heating emissions
- The Alaska Pollution and Chemical Analysis (ALPACA) field campaign aims to **better understand PM formation in these areas**
- ORD researchers are working with Region 10, the State of Alaska, and other partners to **use CMAQ to simulate the areas at a fine scale**
- The **sulfur tracking capability in CMAQ** is used to understand the role of SO_2 emissions and sulfate formation in wintertime exceedances

Lead PIs:
Kathleen Fahey, Sarah Farrell, George Pouliot, and Rob Gilliam

CMAQ in the Cloud: Computing, Analysis, Data

Exploring cloud computing and data storage for CMAQ

Goal: enable states and Multi-Jurisdictional Organizations (MJOs) to more easily receive/send large data sets and to conduct modeling and analysis in the Cloud, which could:

- Provide a cost-effective data sharing and modeling solution
- Improve ability of states/MJOs to conduct simulations to meet their needs
- Improve sharing of information between states/MJOs and EPA
- Improve efficiency of OAQPS sharing data sets and assisting states/MJOs in configuring simulations
- Support research groups

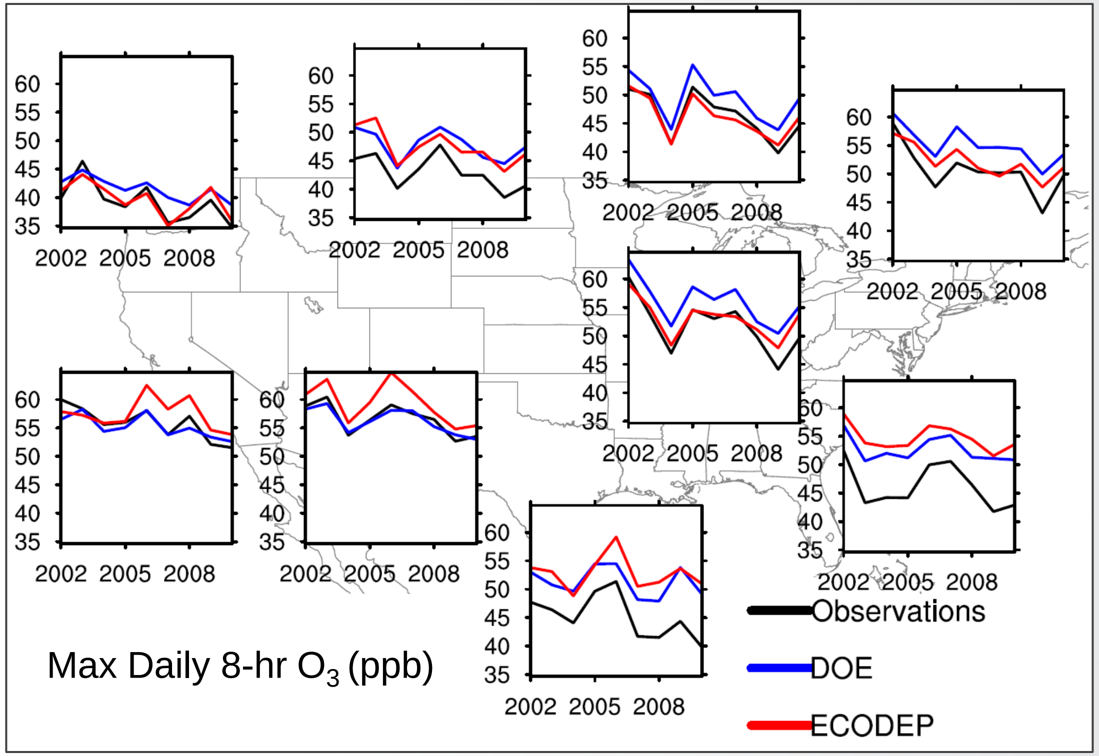
Image: Knowarth Technologies via Medium

Lead PIs:
Fahim Sidi
Kristen Foley

EQUATES: *EPA's Air QUAlity TimE Series*

- Long-term CMAQ simulations:
  - Decadal CMAQ simulations have been used for a wide variety of applications, e.g., **epidemiological studies, critical loads analyses, local and global air quality trends**
  - CMAQ modeling of **2002–2019** has been created for the **Northern Hemisphere** and **contiguous US** using updated models and emissions datasets
  - Model output will be available to collaborators
- EQUATES team members include ORD (CEMM) and OAR (OAQPS, OTAQ)
- Additional information on EQUATES is available at https://www.epa.gov/cmaq/equates.

CMAQv5.0.2 2002-2010 Trends

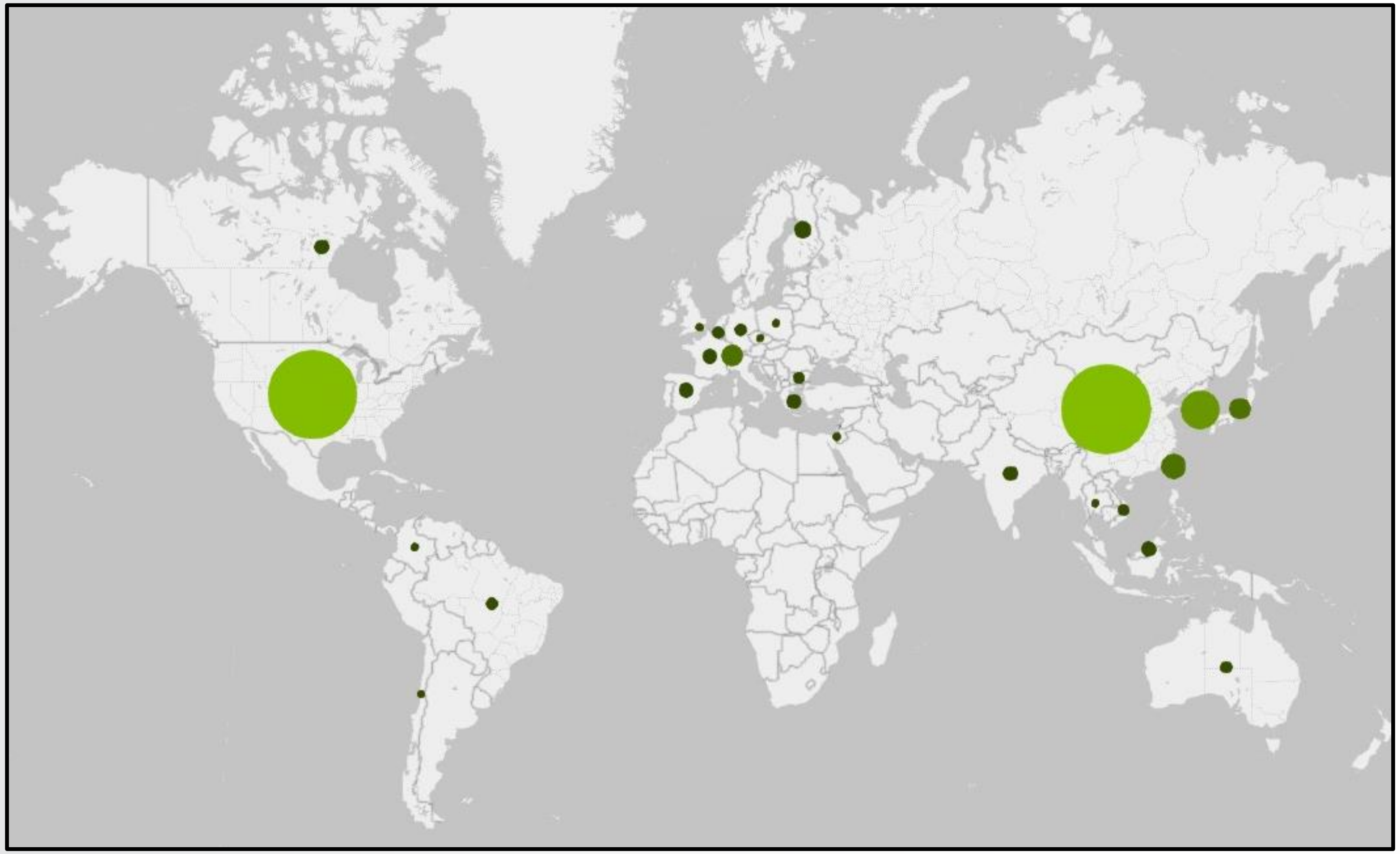


EQUATES modernizes the version of CMAQ (v5.3.2) and supersedes the previous time series based on CMAQv5.0.2 to unify modeled data for applications.

Lead PIs:
Kristen Foley and George Pouliot

CMAQ Research Impact

2021 CMAQ Publications per Coauthoring Country



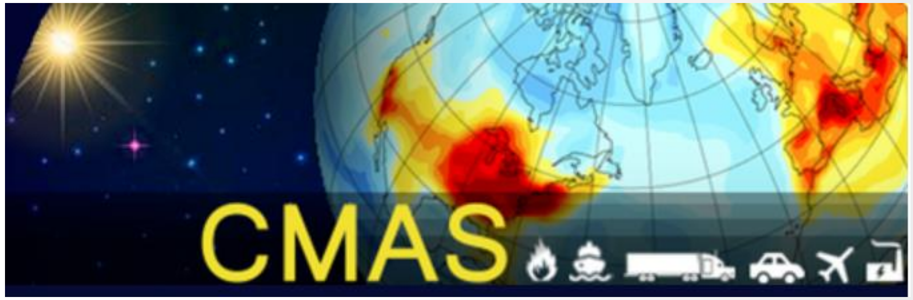
2021 Publications Metric Analysis (Courtesy: EPA-RTP Library)

- ❑ **53 journal & conference proceeding** titles
- ❑ Authors from **355 organizations** across **26 countries**
- ❑ Over **57%** of 2021 publications **already cited** resulting in **>340 citations**
- ❑ The 5 journals with most CMAQ mentions in 2020 are in **top quartile** based on impact factors

Supporting the CMAQ Community

We are partnered with the **CMAS Center** at University of North Carolina to support CMAQ and affiliated software products.

- Training (on-site, online, and across the globe)
- Advanced CMAQ testing
- Outreach
- Model support (via https://forum.cmascenter.org)
- Annual technical conference
- Data Warehouse
- Mutual research initiatives

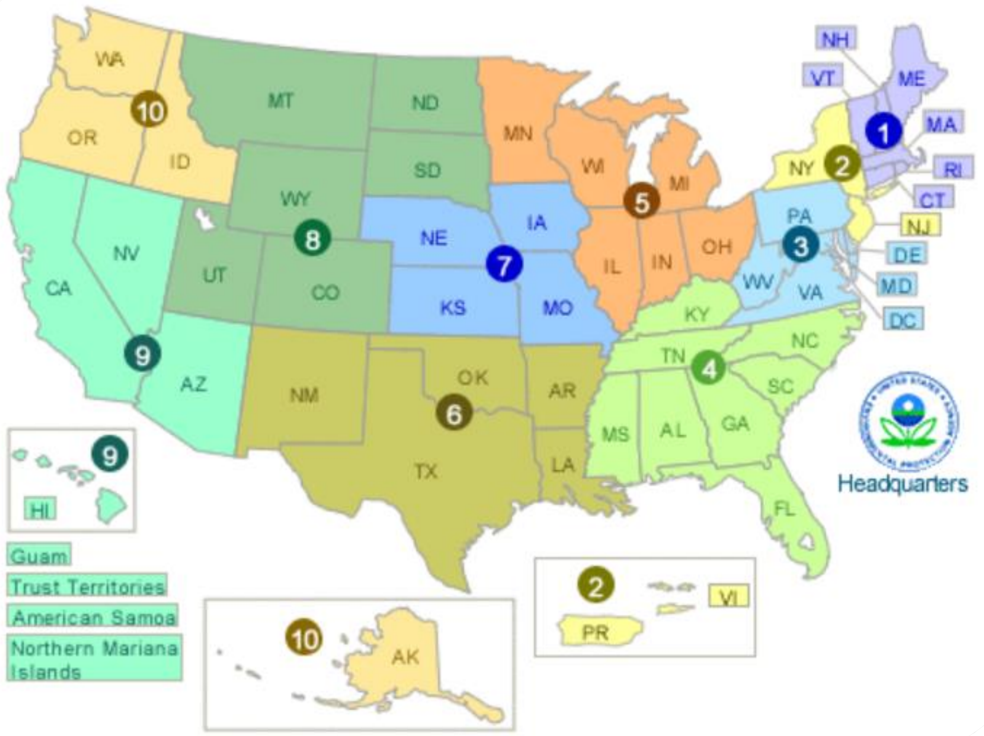


https://www.cmascenter.org/

UNC | INSTITUTE FOR THE ENVIRONMENT

EPA Regional Air Modeling Contacts

- Each of the 10 EPA Regions maintains experts and points of contact for air modeling functions within the Region
- Experts are available for various needs:
  - ➢ SIP Modeling
  - ➢ Permit Modeling
  - ➢ Mobile Source Modeling
  - ➢ Air Toxics Modeling



https://www.epa.gov/scram/air-modeling-regional-contacts

Contact

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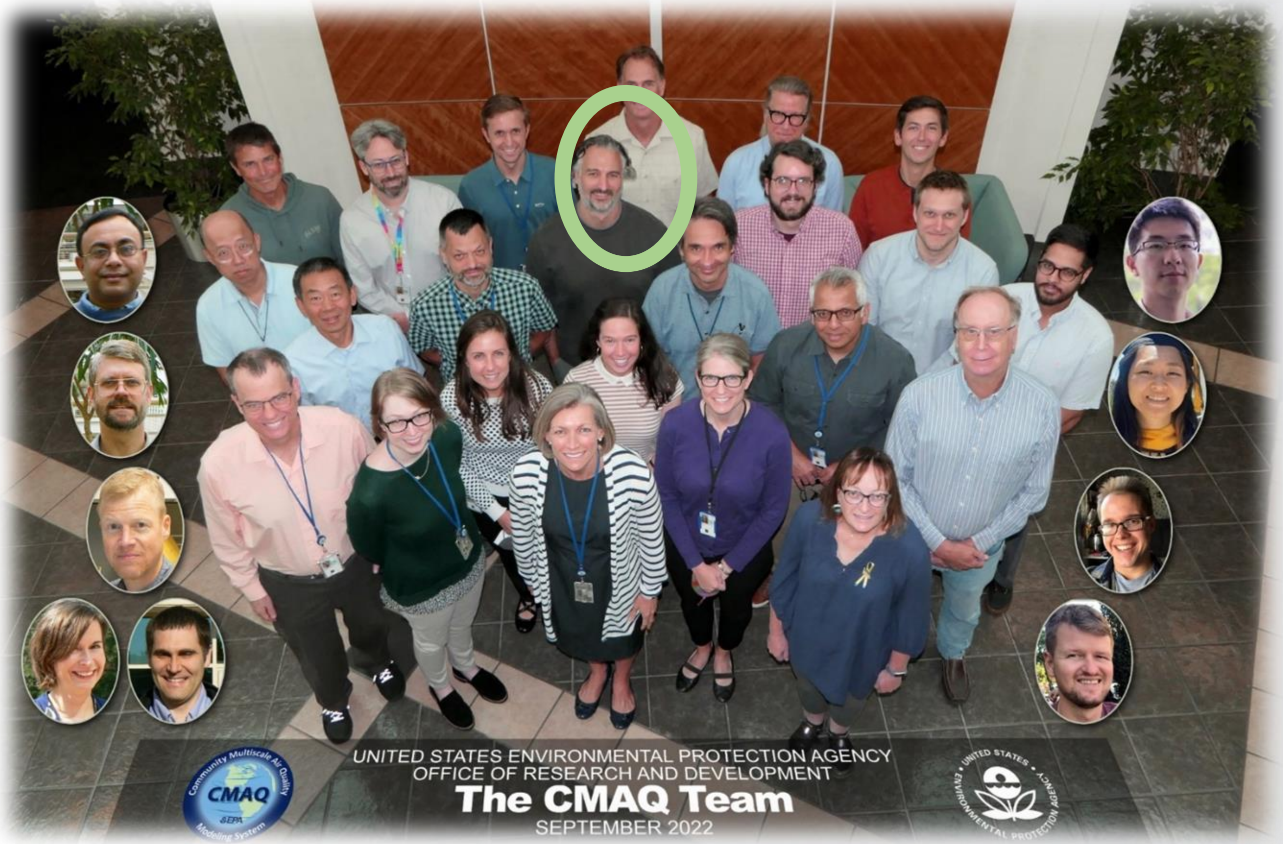
appel.wyat@epa.gov



Disclaimer: The views expressed in this presentation are those of the authors and do not necessarily reflect the views or policies of the US EPA.

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