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

The CMAQ Team

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Presentation Overview

- **Purpose:** *Provide Regions, States, and Tribes with summary of scientific updates included in new release of EPA's Community Multiscale Air Quality (CMAQ) modeling system (v5.2)*

- **Outline:**
  - **Background on CMAQ** (Rohit Mathur)
  - **Relevance of scale interactions**
  - **Process updates**
    - Meteorology–chemistry linkages (Jon Pleim)
      - PBL/LSM, clouds & precipitation, stratosphere-troposphere exchange
    - Chemistry (Ben Murphy)
    - Aerosols
  - **Evaluation** (Wyat Appel)
  - **Summary**

Evolution of Air Quality Models

To address increasingly complex applications and assessments

Application 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

NATA
&
Air Quality
Forecasting

- Hg
-Toxics

Meteorology
- Air Quality
Interactions

Exposure

Background
air pollution

Met-AQ
Interactions

Exposure &
Health

Multimedia

AQDM UNAMAP

RADM-ROM
Eulerian Grid Models
- Acid Deposition
- Ozone

MODELS3

CMAQ
For PM

Neighbor
Scale CMAQ
- CFD

NAM-CMAQ

Multi-
pollutant
CMAQ

Coupled
WRF-CMAQ

CMAQv5.2

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

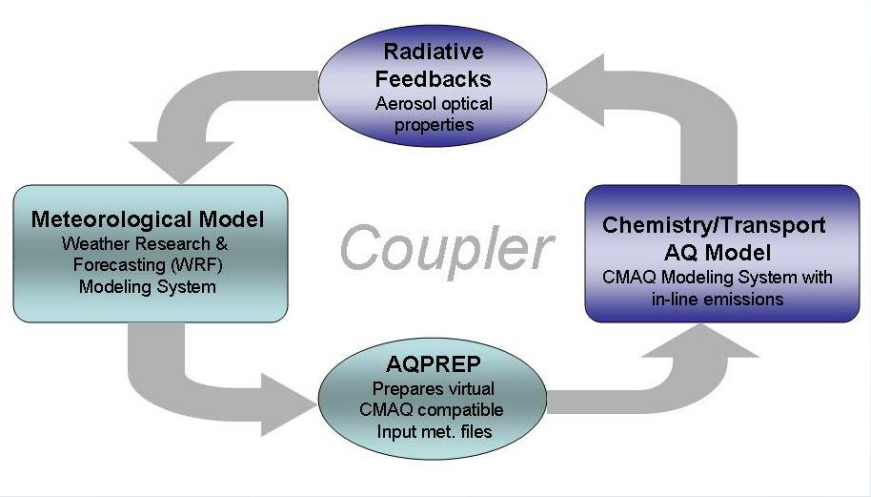
Multi-pollutant
Multi-scale (***local to hemispheric***)
Interactions with Climate forcing
and Air Quality changes
Eulerian Grid

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

Model Development

The Community Multiscale Air Quality (CMAQ) Modeling System

- **Comprehensive Eulerian Chemical Transport Model**
  - Emission, advection, diffusion, chemistry, deposition
- **Multi-scale: Hemispheric → Continental → Regional → Local**
- **Multi-pollutant & multi-phase:**
  - **Ozone** Photochemistry
    - NO_x + VOC (biogenic & anthropogenic) → O_3
  - **Particulate Material (PM)**
    - Inorganic chemistry & thermodynamics → Sulfate, Nitrate, Ammonium
    - Organic aerosol → primary, secondary
    - Geogenic aerosol → wind-blown and fugitive dust, sea salt
  - **Acid deposition**
    - Aqueous chemistry, Wet deposition
  - **Air Toxics**
    - Benzene, Formaldehyde, Hg, etc
- **Coupled to the Weather Research & Forecast (WRF) Model**
  1. "Off-line" – sequential operation
  2. "On-line" – 2-way coupled



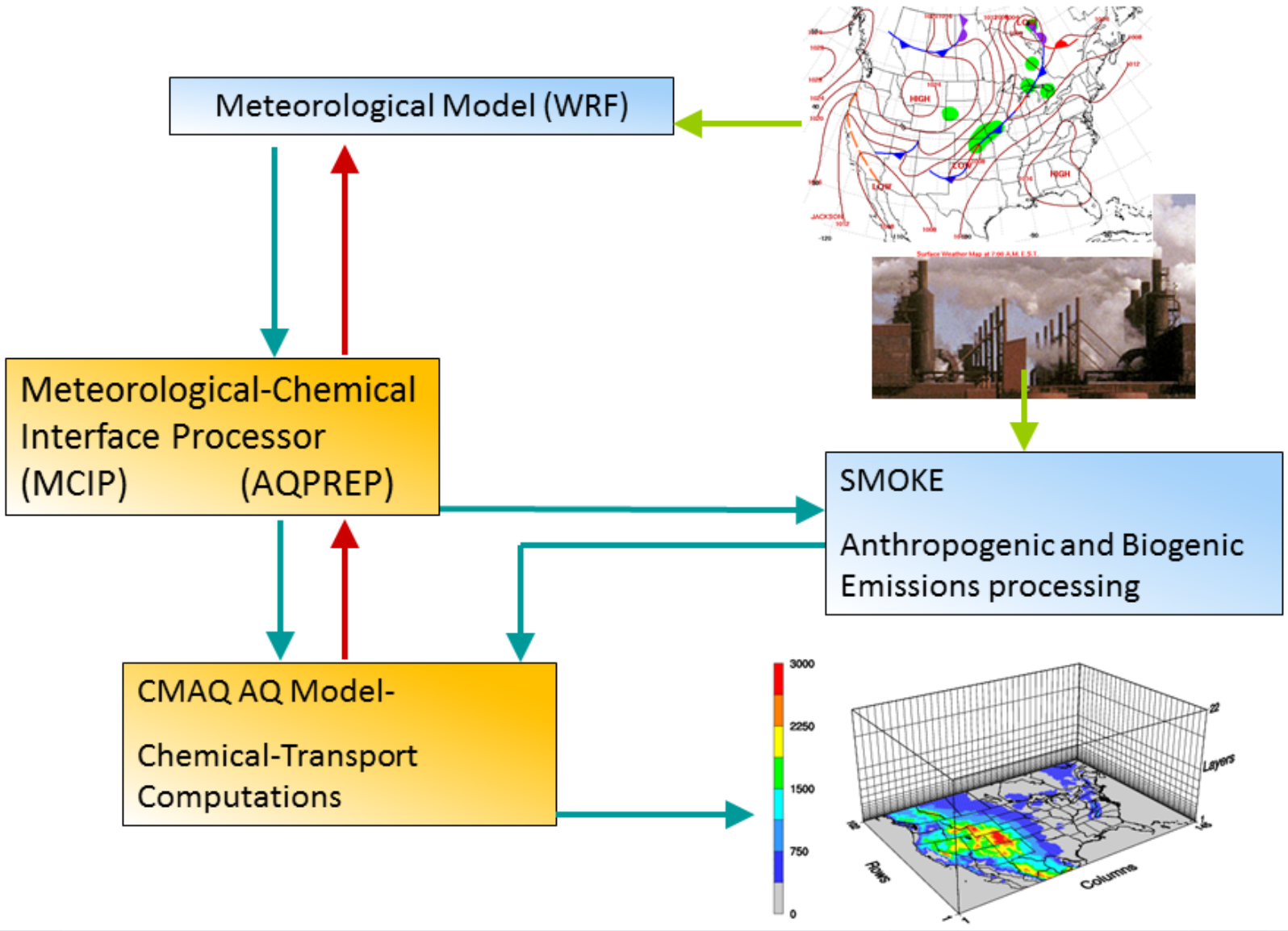
Recent CMAQ Versions

Periodic public release of improved versions of the modeling system

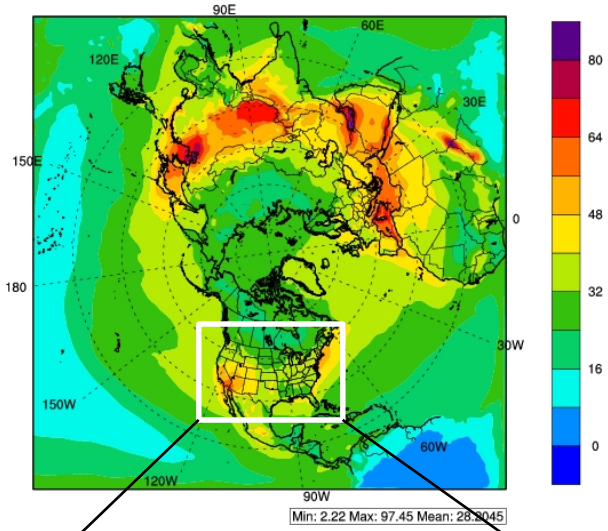
- **CMAQv4.7 (Fall 2008) and CMAQv4.7.1 (June 2010)**
  - *Supporting evaluation*: Foley et al, Geoscientific Model Development, 2010
- **CMAQv5.0 (Feb. 2012)**
  - Updates to gas-aqueous-aerosol chemistry and photolysis
  - Improved advective and turbulent transport
  - Major structural upgrades that improve flexibility and maintainability
  - 2-way coupling between WRF-CMAQ
  - Bi-directional exchange: NH_3 and Hg
- **CMAQv5.0.2 (May 2014)**
  - Instrumented Models (*Direct Decoupled Method (DDM), Source Apportionment, Sulfur Tracking*)
  - Community Contributions (*Volatility Basis Set* (*VBS*))
- **CMAQv5.1 (October 2015)**
  - Revised gas chem and Photolysis
  - Aerosol updates: New pathways for SOA production
  - Improve computational performance
  - *Supporting Evaluation: Appel et al., GMDD, 2016*
- **CMAQv5.2 (β-version in November 2016; final version in June 2017)**
  - New Organic aerosol treatment
  - New wind-blown dust model
  - CB6 chemical mechanism
  - Lightning – NOx and assimilation
  - Instrumented models compatible with process updates
  - Process options for hemispheric configuration

CMAQ Modeling System

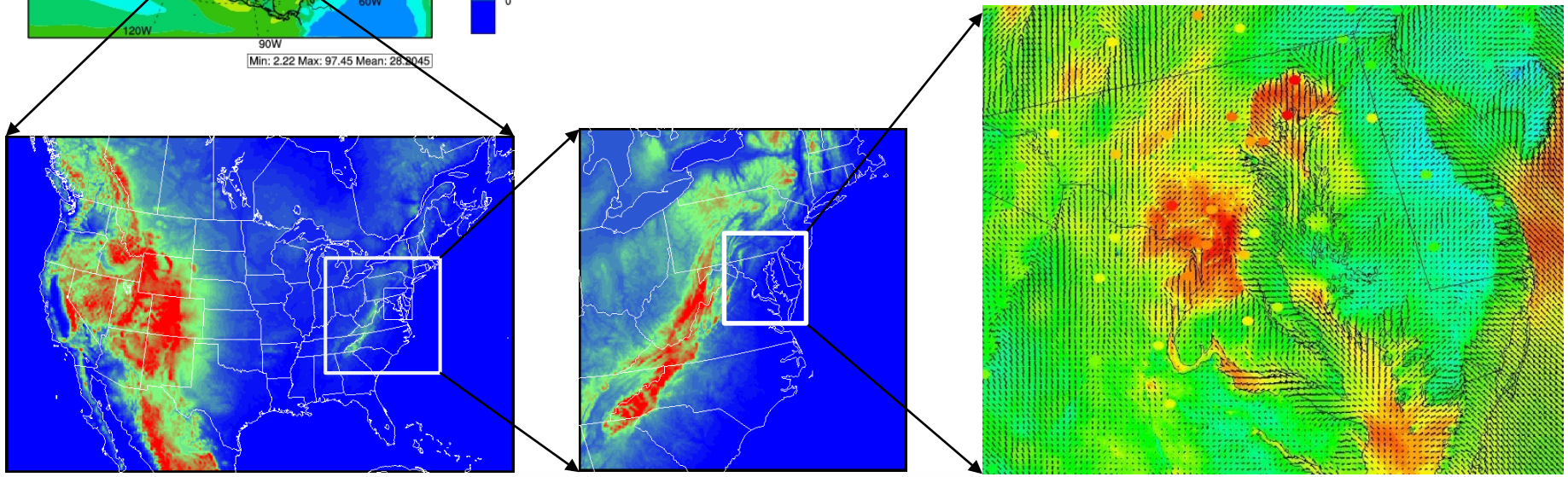
"Numerical Laboratory" to synthesize our evolving understanding of processes (& interactions) regulating air pollution



Current Multi-scale Modeling



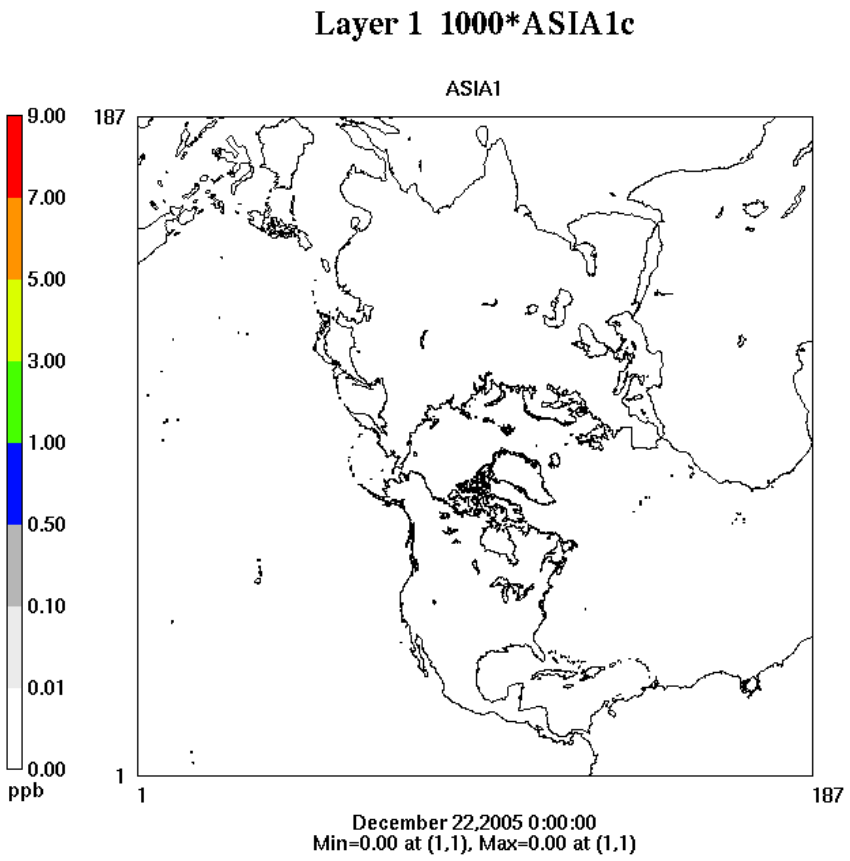
- Hemispheric model needed to provide lateral boundary conditions (LBCs) for US Domain
  - Increasing importance of long range transport (LRT) contributions as NAAQS are reduced
- Fine scales:
  - Urban Environments
  - Linkage with human exposure & health studies
  - Residual non-attainment

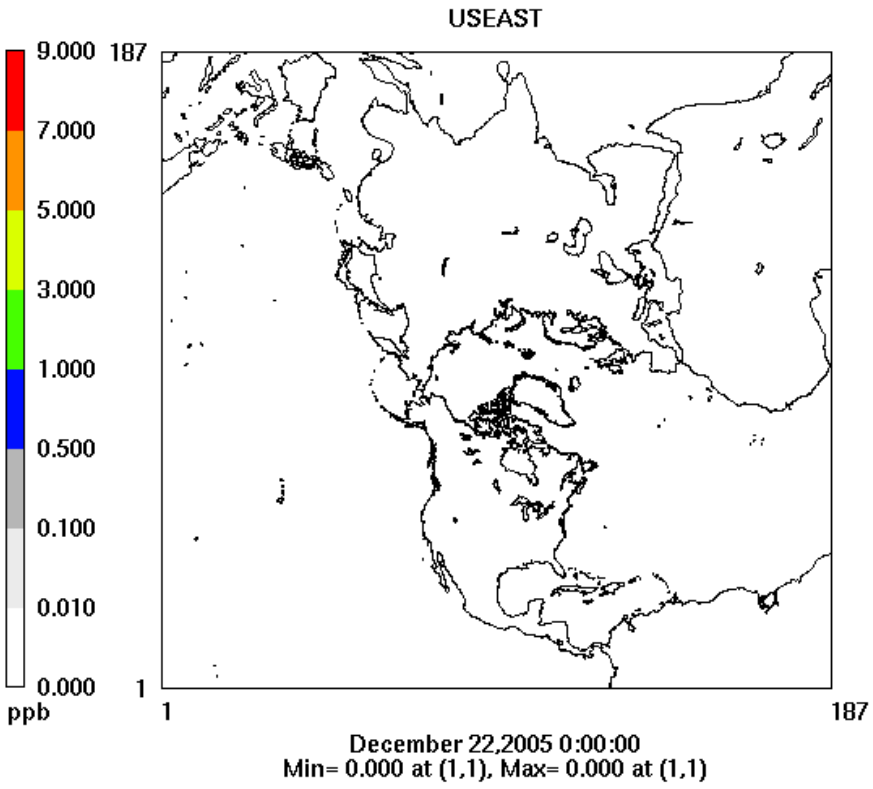


Hemispheric model at 108 km provides LBCs for 12 km CONUS with nests to 4 km and 1 km

Long-Range Pollutant Transport

Example: Tracer transport at 850 mb

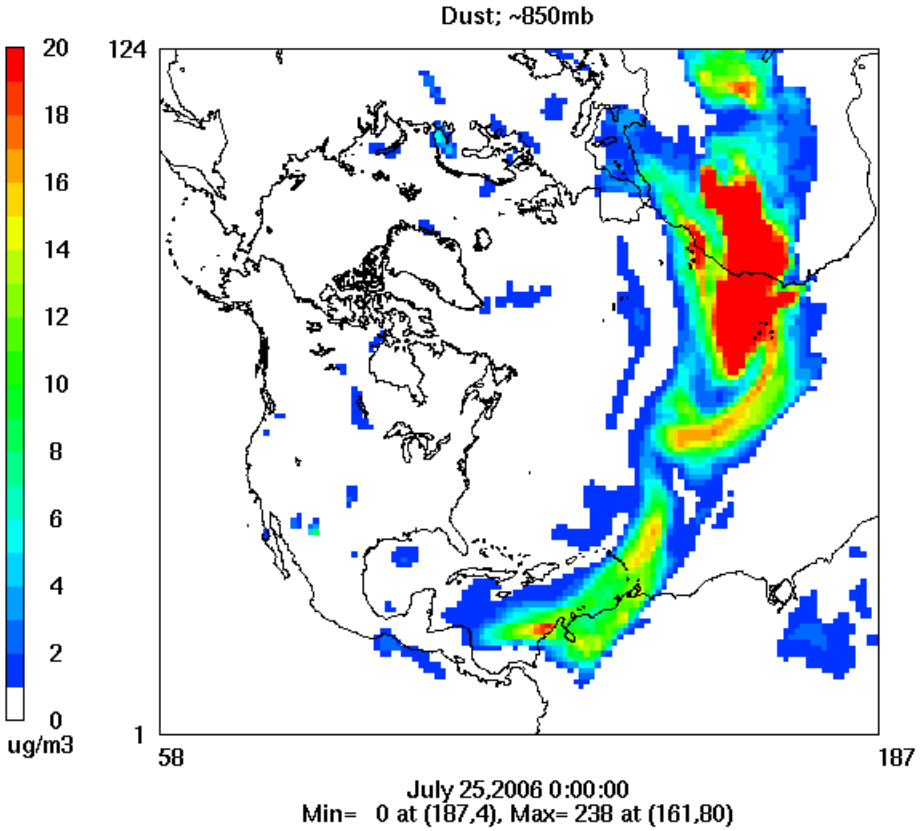




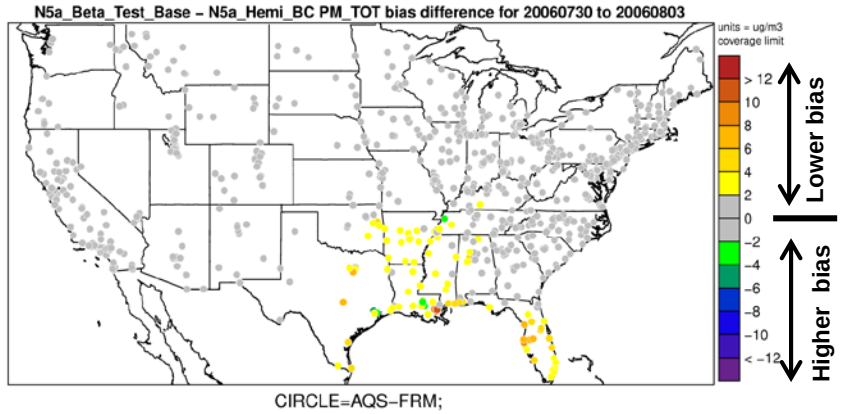
Tightening NAAQS and greater emphasis on characterizing "background" air pollution requires ***improved representation of scale interactions***

Trans-Atlantic Transport of Saharan Dust

Impact on surface-level $PM_{2.5}$ in the Gulf States



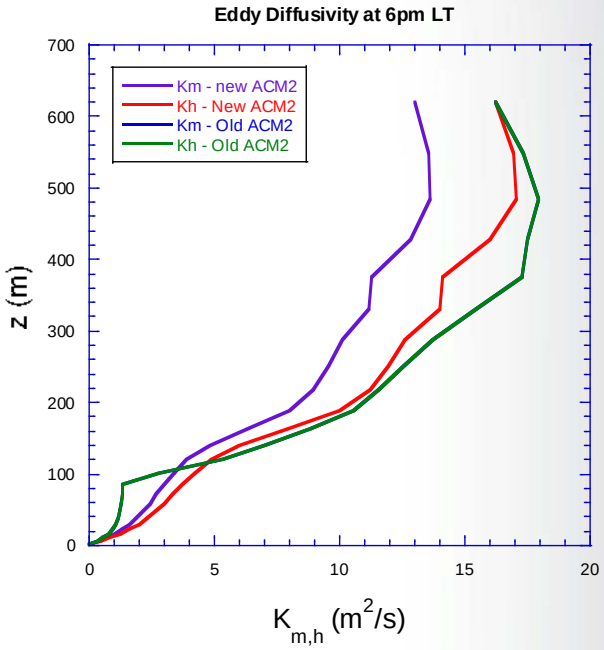
Reduction in bias in simulated surface $PM_{2.5}$



Space and time varying LBCs from hemispheric CMAQ helped capture impacts of long-range transport on episodic Saharan dust intrusion events

Recent updates to Planetary Boundary Layer (PBL) and Land Surface Model (LSM)

- The Asymmetric Convective Model version 2 (ACM2) in WRF-CMAQ
  - Designed especially for AQ applications
  - Consistent PBL transport of meteorology and chemistry
  - Combined local and non-local closure scheme for convective conditions
  - Combines local scaling and boundary layer scaling for eddy diffusivities
  - Updates to ACM2 in WRFv3.7 and WRF v3.8
    - Different K_m and K_h ($Pr = K_m/K_h \neq 1$)
    - New eddy diffusivities for stable conditions

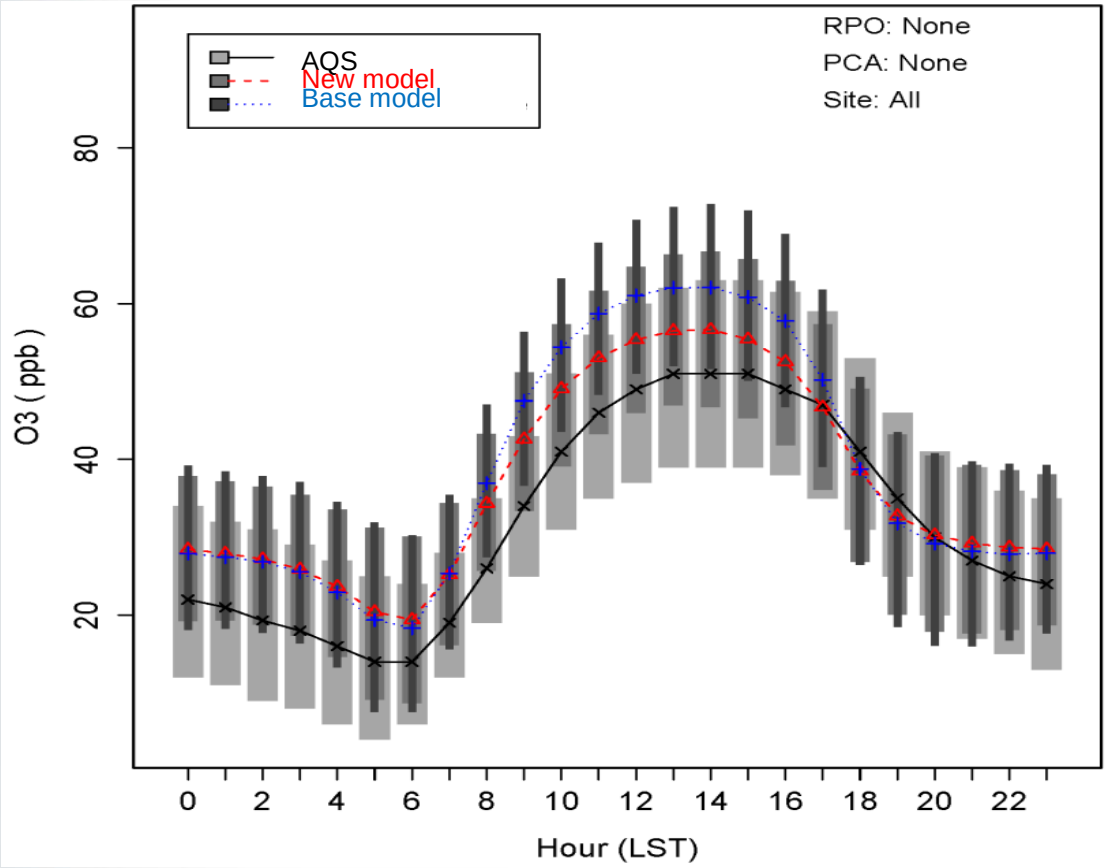


- PX Land Surface Model in WRF-CMAQ
  - Designed for consistent treatment of heat, moisture, and momentum fluxes in WRF and chemical fluxes (dry dep, bi-directional) in CMAQ
  - Updates to PX LSM:
    - Modified stomatal conductance function for PAR (F1) (WRFv3.8)
    - Reduced heat capacity of vegetation (WRFv3.7)

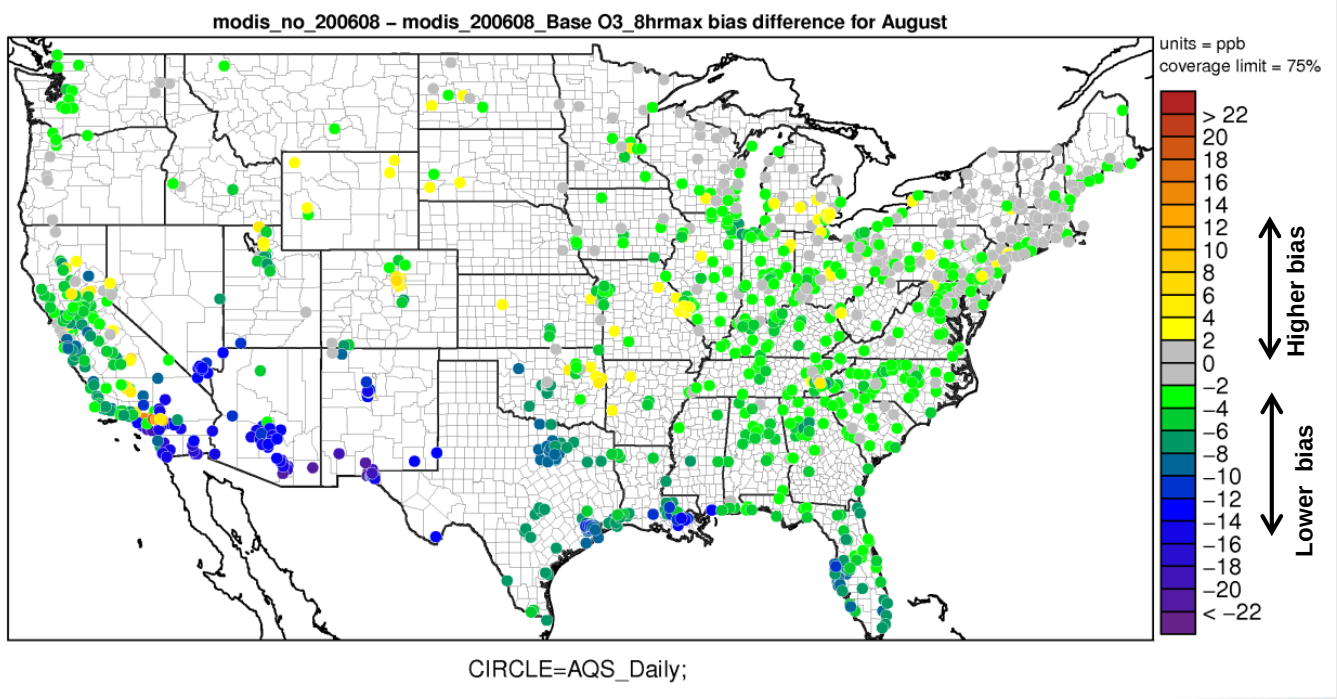
Together updates to PBL and LSM reduce biases in meteorology (particularly T and Q) mostly at night

Updates also reduce over-prediction of ground level emitted species (e.g. NOx, CO, EC)

Effects of PBL and LSM Updates on O_3



Max 8-h bias difference → New - Base

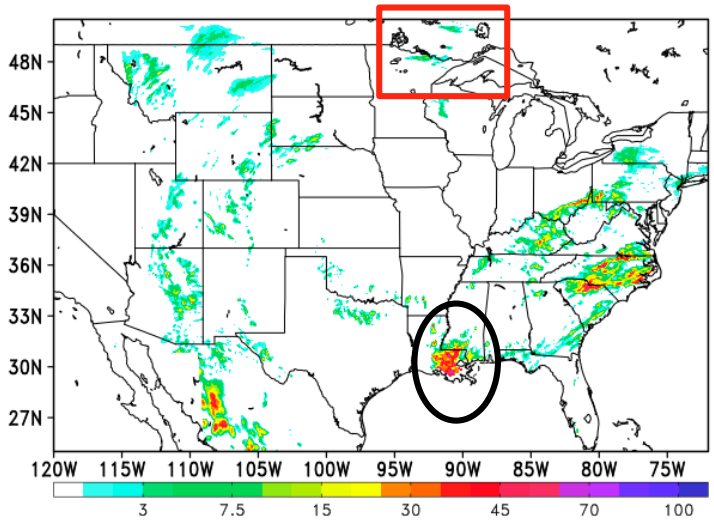


Δx = 12 km : Aug. 10 to Aug. 30, 2006

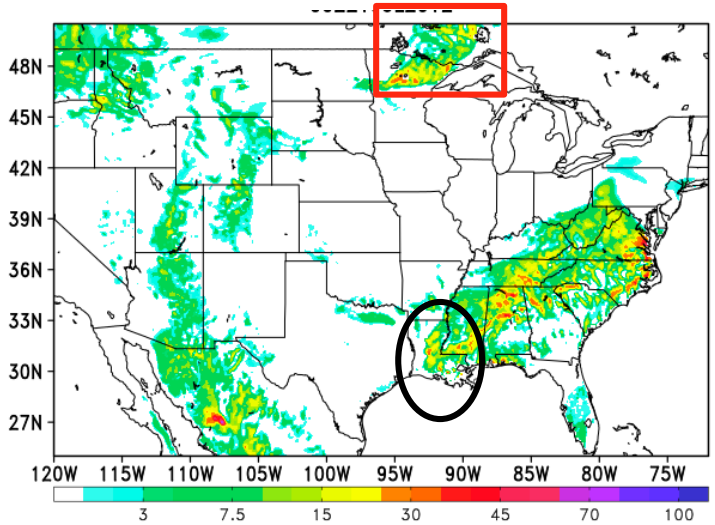
Changes to PBL and LSM tend to reduce ozone during mid-day hours, resulting in reductions in the MD8hr O_3 bias

Improvements in Clouds, Radiation, and Precipitation

Observations



Base Case

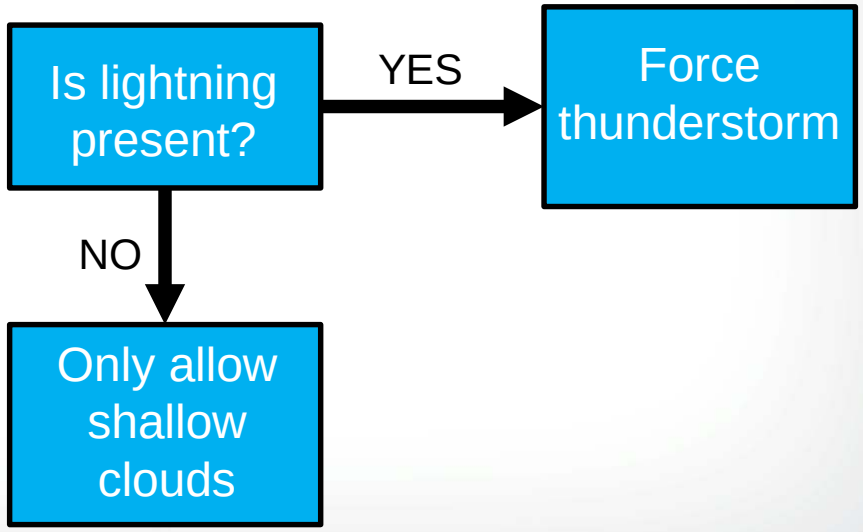


Predicting clouds and precipitation is challenging.

Example on the left shows both over- and underestimation of precipitation.

WRF Lightning Assimilation in Kain-Fritsch

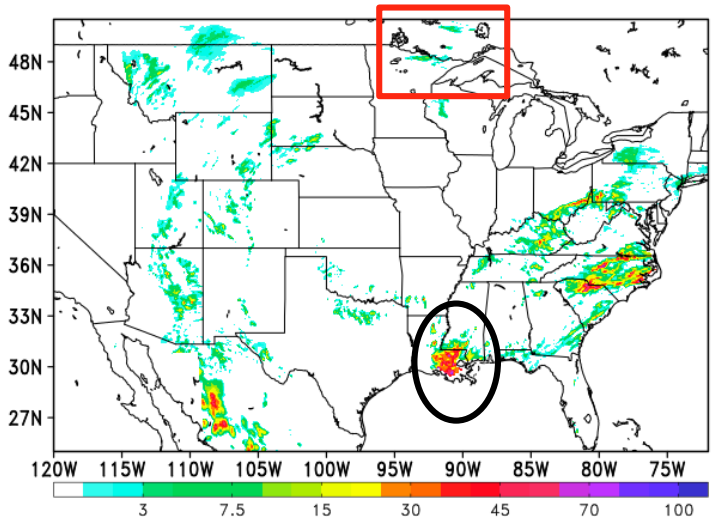
- Use lightning data from the National Lightning Detection Network (NLDN)
- Simple, computationally efficient approach: (builds off of Mansell et al. 2007)
  - ❖ Force deep convection where lightning is observed
  - ❖ Only allow shallow clouds where it is not



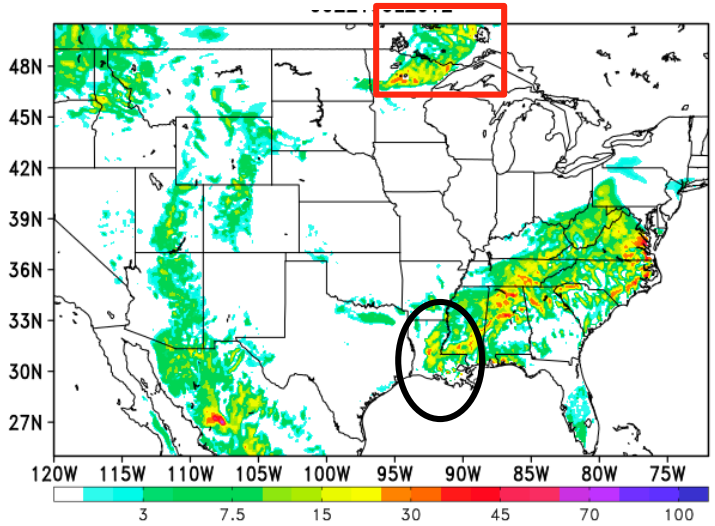
Heath et al., JAMES, DOI: 10.1002/2016MS000735, 2016

Improving Precipitation in WRF-CMAQ through Lightning Assimilation

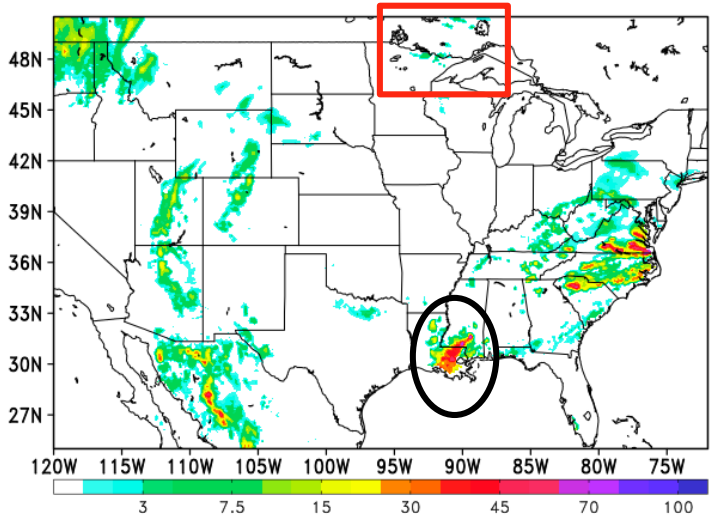
Observations



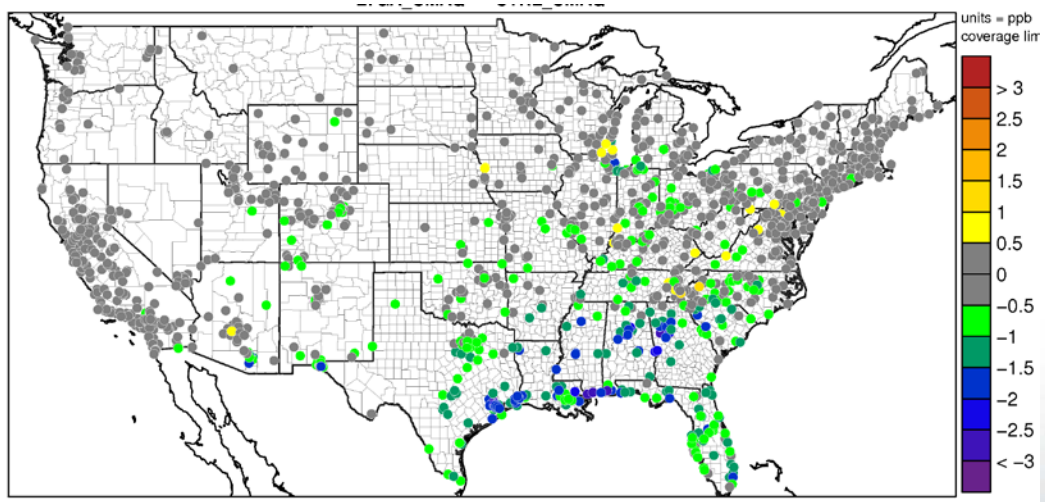
Base Case



Lightning Assimilation



Reduced O_3 Bias at 71% of AQS sites (July 2011)

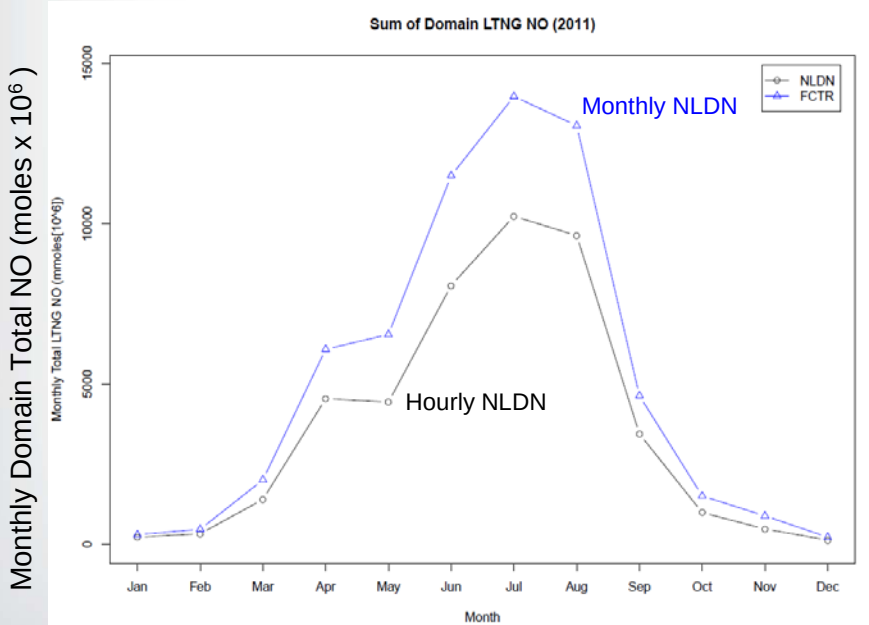


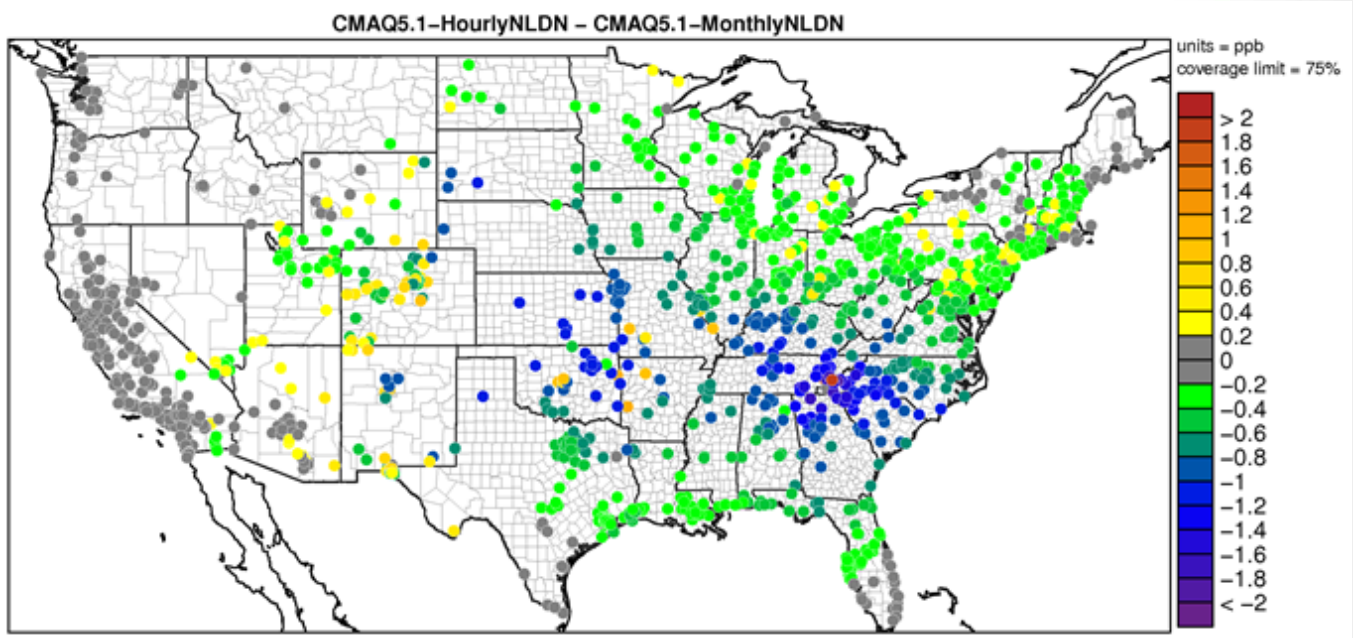
Lightning assimilation methodology improves clouds, precipitation, and O_3.

Improving Estimates of Lightning NO Generation

CMAQv5.1: monthly climatological data from the National Lightning Detection Network (NLDN) were associated with WRF's gridded convective rainfall rate to distribute lightning strikes per grid cell.

CMAQv5.2: hourly raw NLDN data are now used to generate gridded hourly LNO, resulting overall in ~30% decrease in LNO.





Impact of using hourly NLDN Data:
Bias in hourly O_3 predictions decreased at 79% of the sites

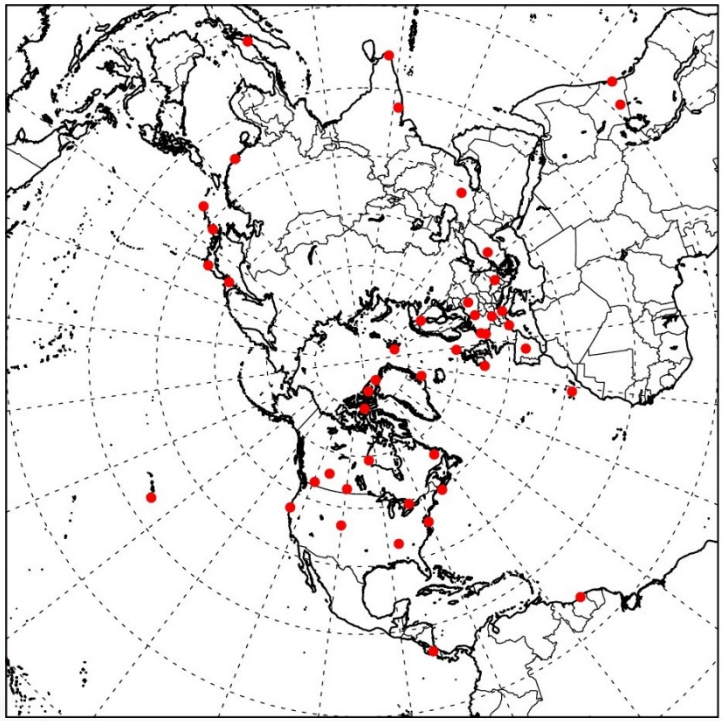
Courtesy: Daiwen Kang

CMAQv5.2 Updates:

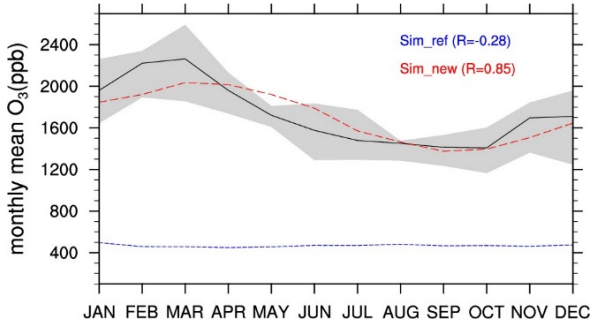
Impact of stratosphere-troposphere exchange on tropospheric O_3

- Modeled O_3 specified by enforcing the condition of proportionality to Potential Vorticity: ***$[O_3] = c \cdot PV$***
- Used recent CMAQ multi-decadal simulations to develop a robust relationship that varies spatially and temporally: $O_3/PV = F(spatial) \times G(temporal)$

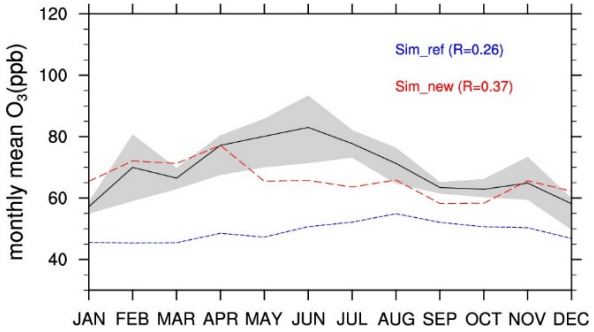
Used observed O_3 data from 1990-2010 from 44 WOUDC sites



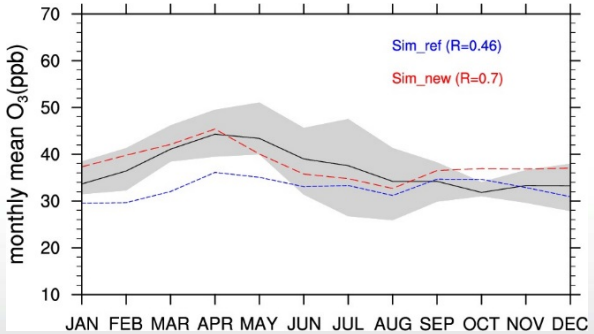
UTLS
P<100mb



Mid-Troposphere
300mb<P<500mb



PBL
P>800mb



Comparison of Observed O_3 with Reference simulation and New PV scaling

Xing et al, ACP, 2016

CMAQv5.2 Updates:

Gas-phase chemistry

CMAQ includes different mechanisms so that mechanism can be matched to application

Mechanism family	Specific mechanisms in CMAQ
Carbon Bond	CB05tucl, CB05e51 (expanded nitrates), CB05e51h (with halogens), CB6r3
SAPRC	SAPRC07T (explicit toxics), SAPRC07tic (expanded isoprene)
RACM	RACM2

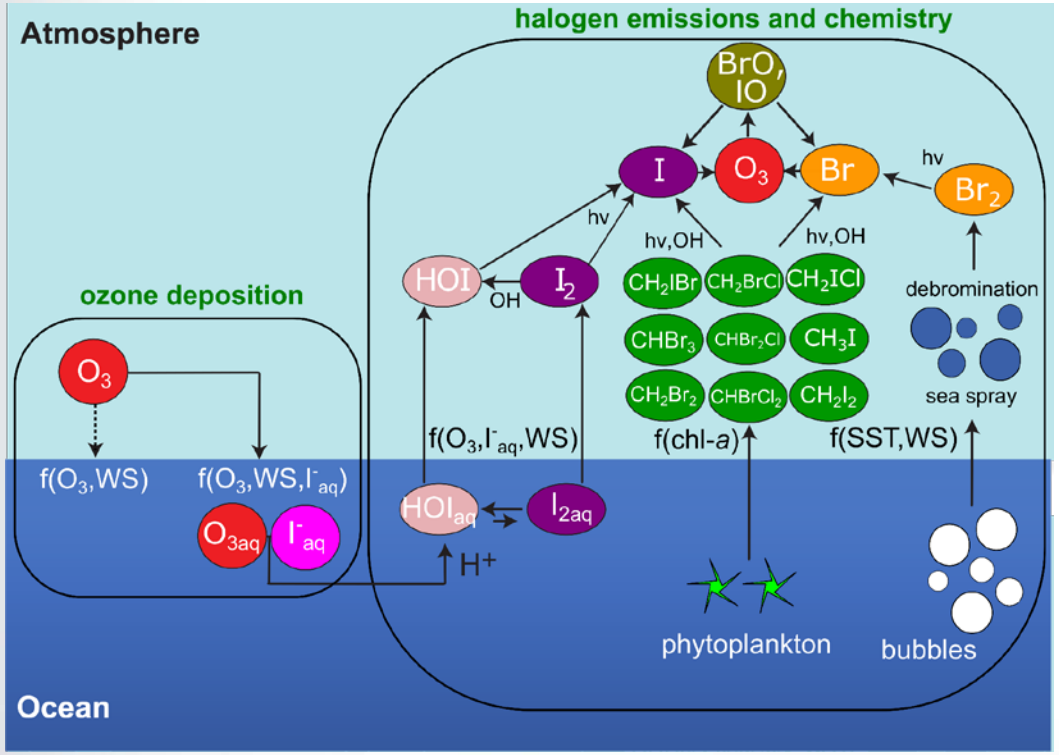
New in CMAQ v5.2 is CB6 (r3) mechanism:

- **Updated reaction rates and yields *(matches current science recommendations)***
- **Updated nitrate yields in low temperatures *(winter simulations)*; 3 nitrates instead of 1 in CB05tucl**
- **More high-emitted, longer-lived species, including acetone, benzene, propane, carbonyls *(slower reacting, more transport)***
- **CMAQ extensions to CB6r3:**
  - **Customized to interface with SOA improvements**
  - **Can modify for emerging issues/pollutants *(respond faster to science updates and new research findings)***

CMAQv5.2 Updates:

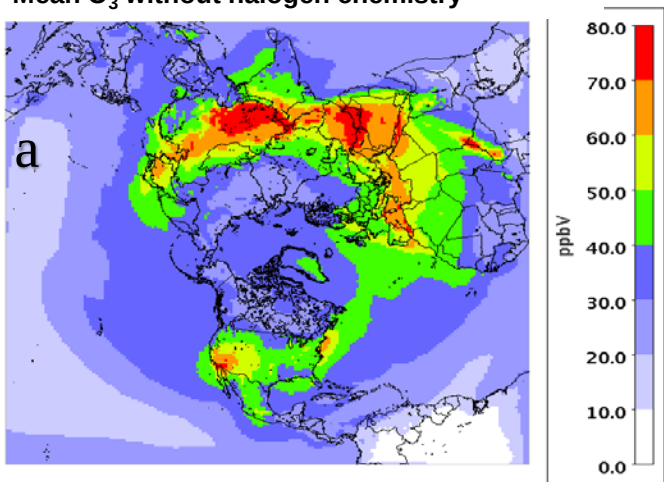
Improving representation of marine environments

Issue: Halogen chemistry and deposition to water are key sinks for O_3 in marine environments; their accurate representation impacts predictions of both long-range transport and ambient levels in coastal areas.

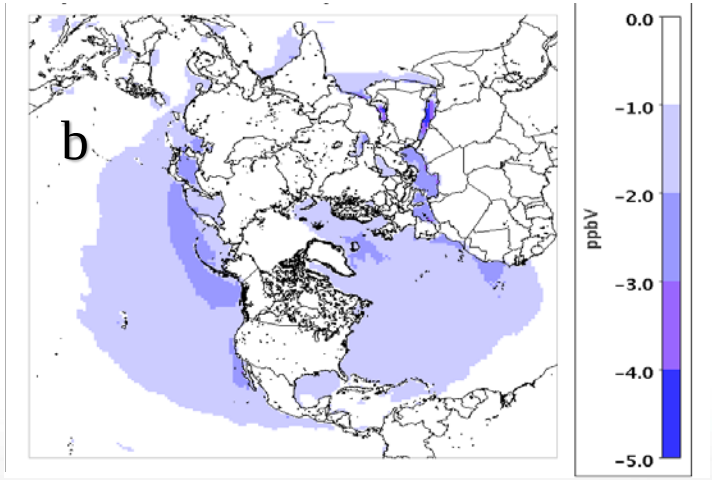


Sarwar et al., ES&T, 2015

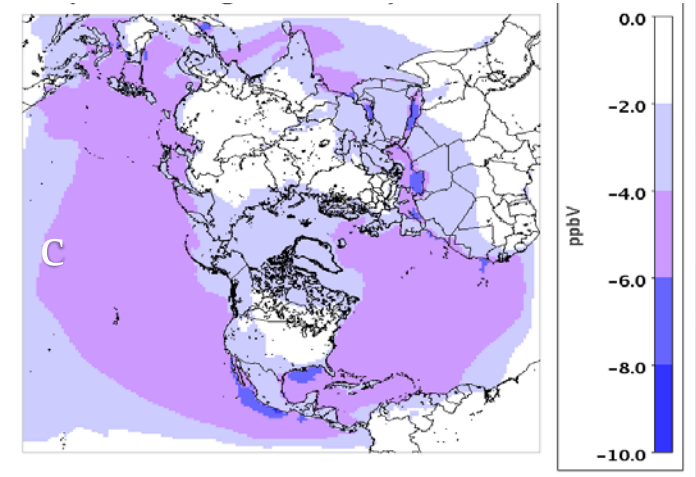
Mean O_3 without halogen chemistry



Impact of enhanced deposition on ozone



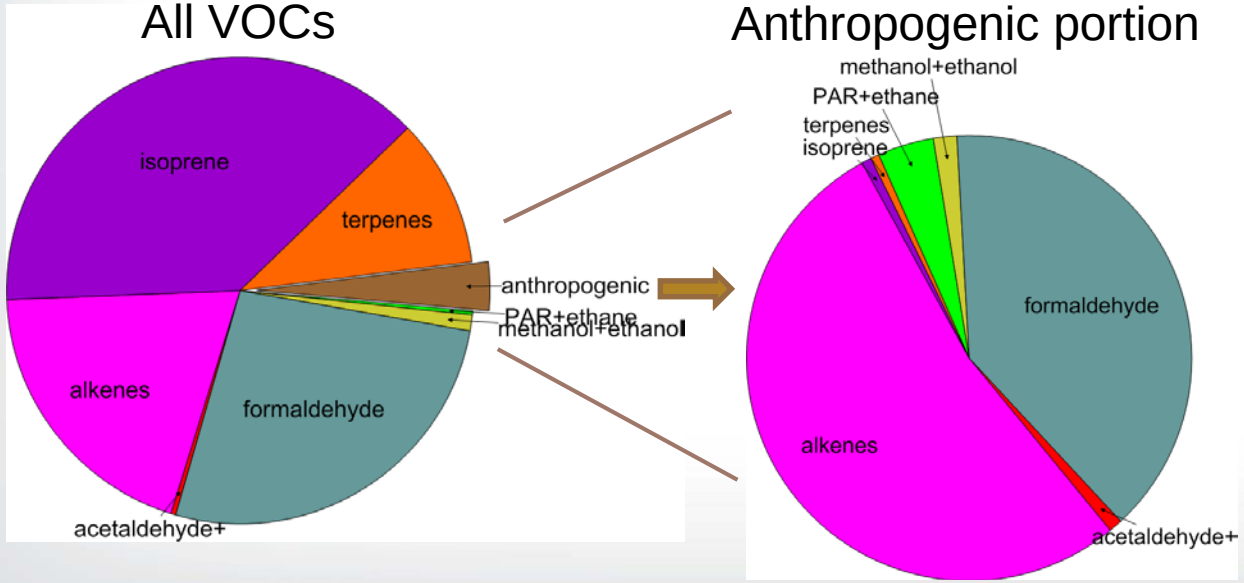
Impact of halogen chemistry on ozone



CMAQv5.2 Updates:
Gas-phase chemistry for HAPs

- **CB6r3 extended to predict concentrations of 41* Hazardous Air Pollutants (HAPs), used in 2014 National Air Toxics Assessment, to identify those air toxics which are of greatest potential concern in terms of contribution to population risk**

Example: Use of CMAQ to quantify the VOCs that contribute the most to ambient formaldehyde in the Southeast from all VOCs (left) and breakdown from anthropogenic sources (right)

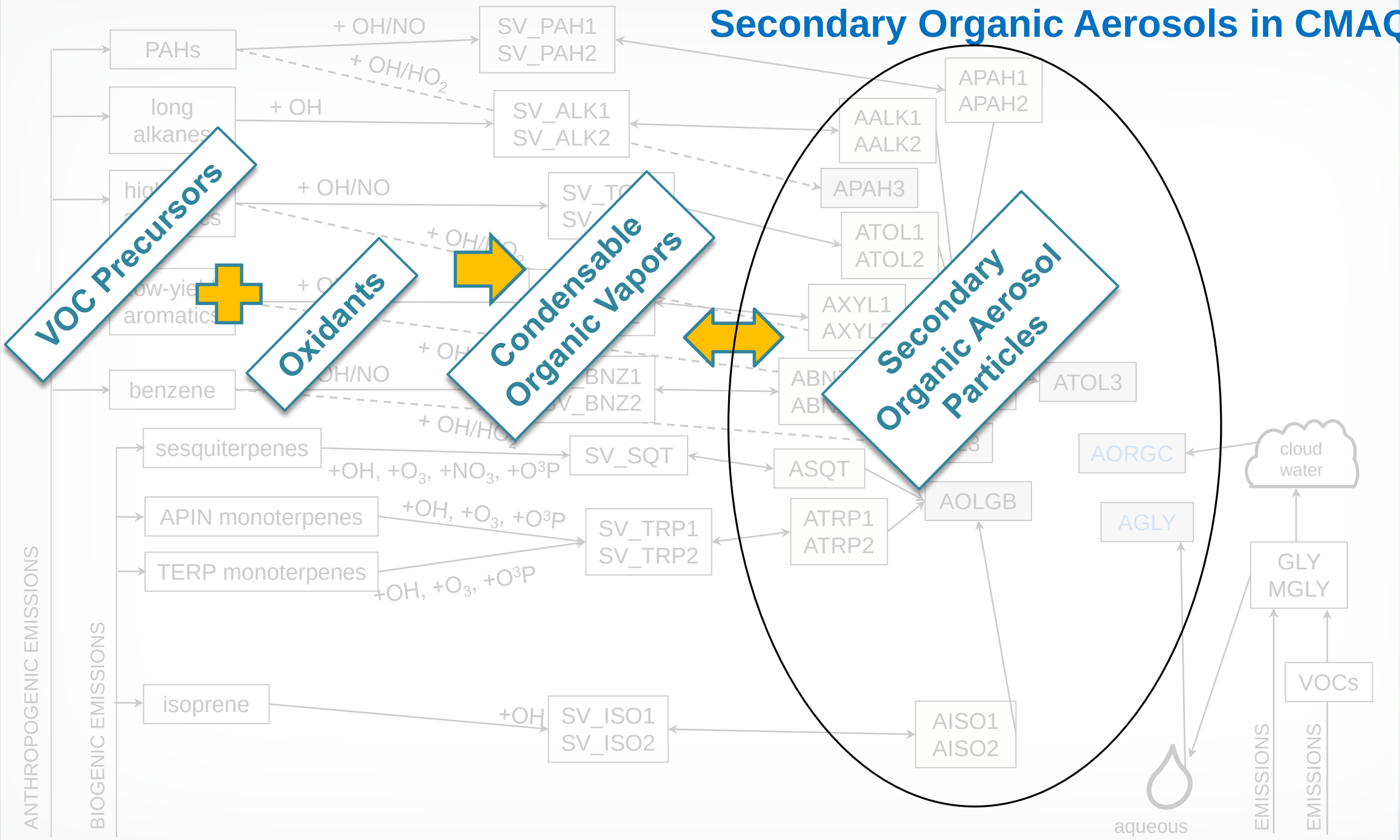


Example: Some of the important HAPs predicted by CMAQv5.2, including those which have been identified as national and regional cancer and noncancer hazard drivers.

HAP name	
formaldehyde - total and emitted	acetaldehyde - total and emitted
acrolein - total and emitted	1,3-butadiene
Benzene	Napthalene
Carbon tetrachloride	p-dichlorobenzene
Chloroprene	1,3-dichloropropene
Ethylbenzene	Chlorine
Ethylene oxide	Hexamethylene 1-6-diisocyanate,
Chromium 6 - fine and coarse modes	Arsenic - fine and coarse modes
Nickel - fine and coarse modes	Diesel PM elemental carbon - fine modes
Mercury - elemental and gas	Lead - fine and coarse modes

* users can now easily change model output to subset the 41 HAPs for their own applications

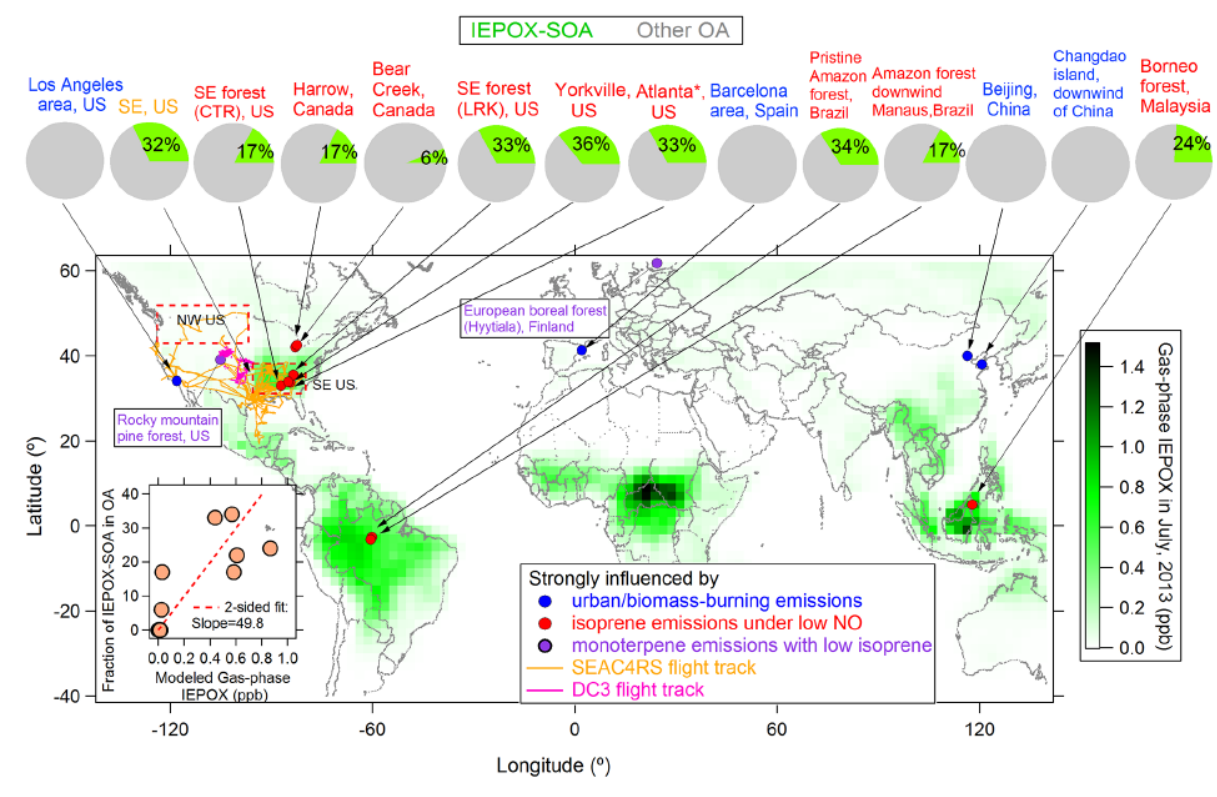
Secondary Organic Aerosols in CMAQv5.2



CMAQv5.2 Updates:

Biogenic Secondary Organic Aerosol

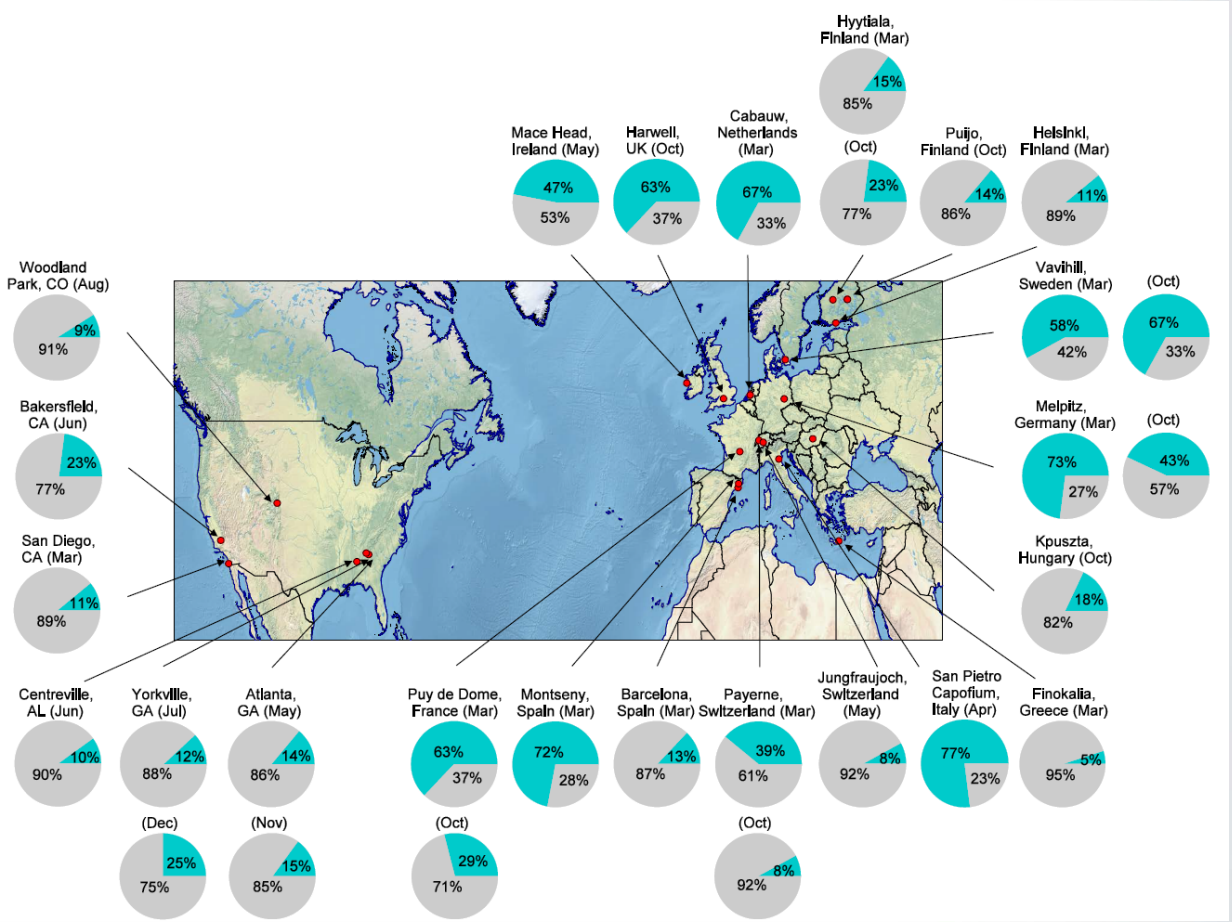
Isoprene Epoxide (IEPOX) SOA



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

Hu et al., 2015 ACP

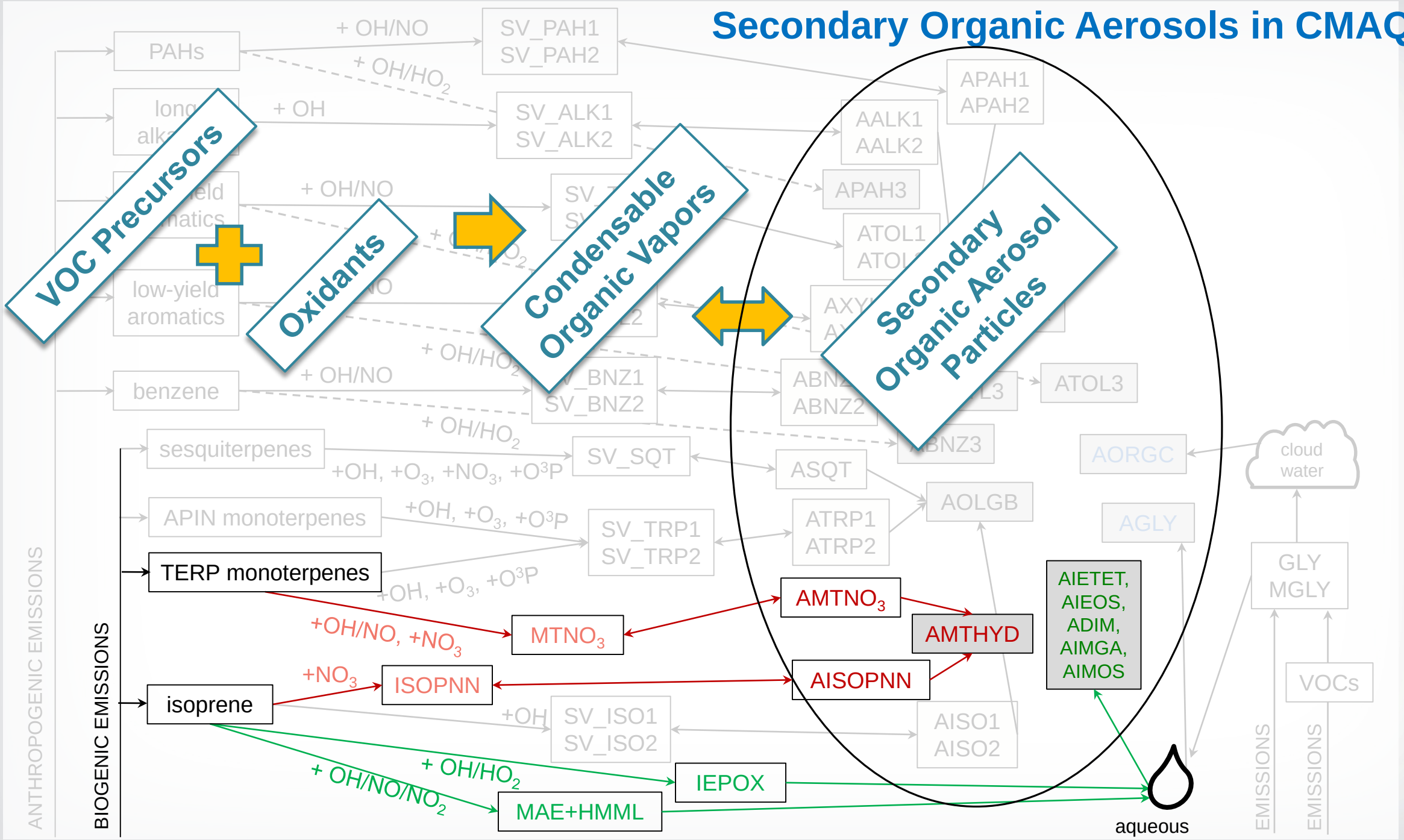
Particulate Organic Nitrate Aerosols



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

Ng et al., accepted ACP

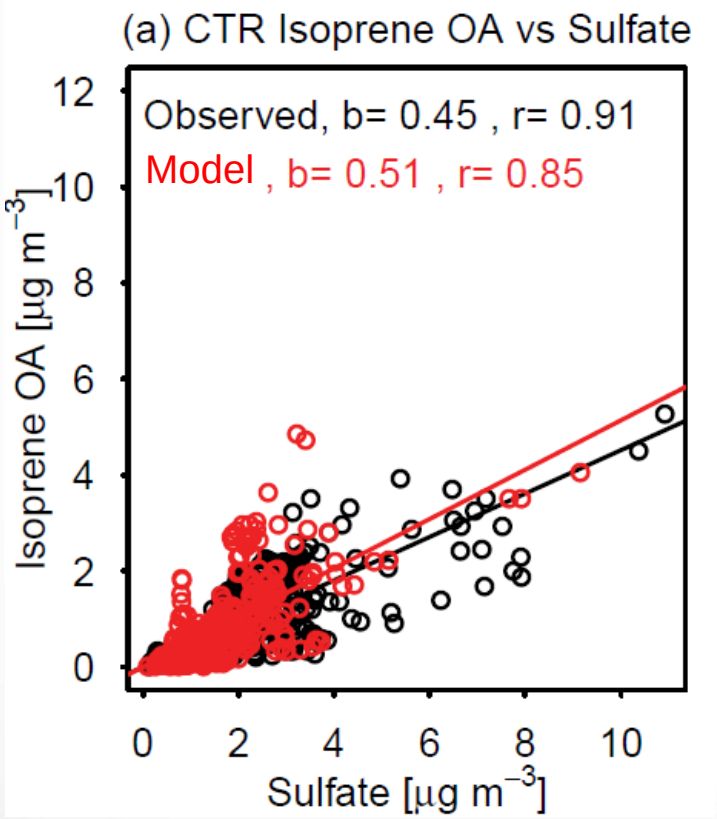
Secondary Organic Aerosols in CMAQv5.2



CMAQv5.2 Updates:

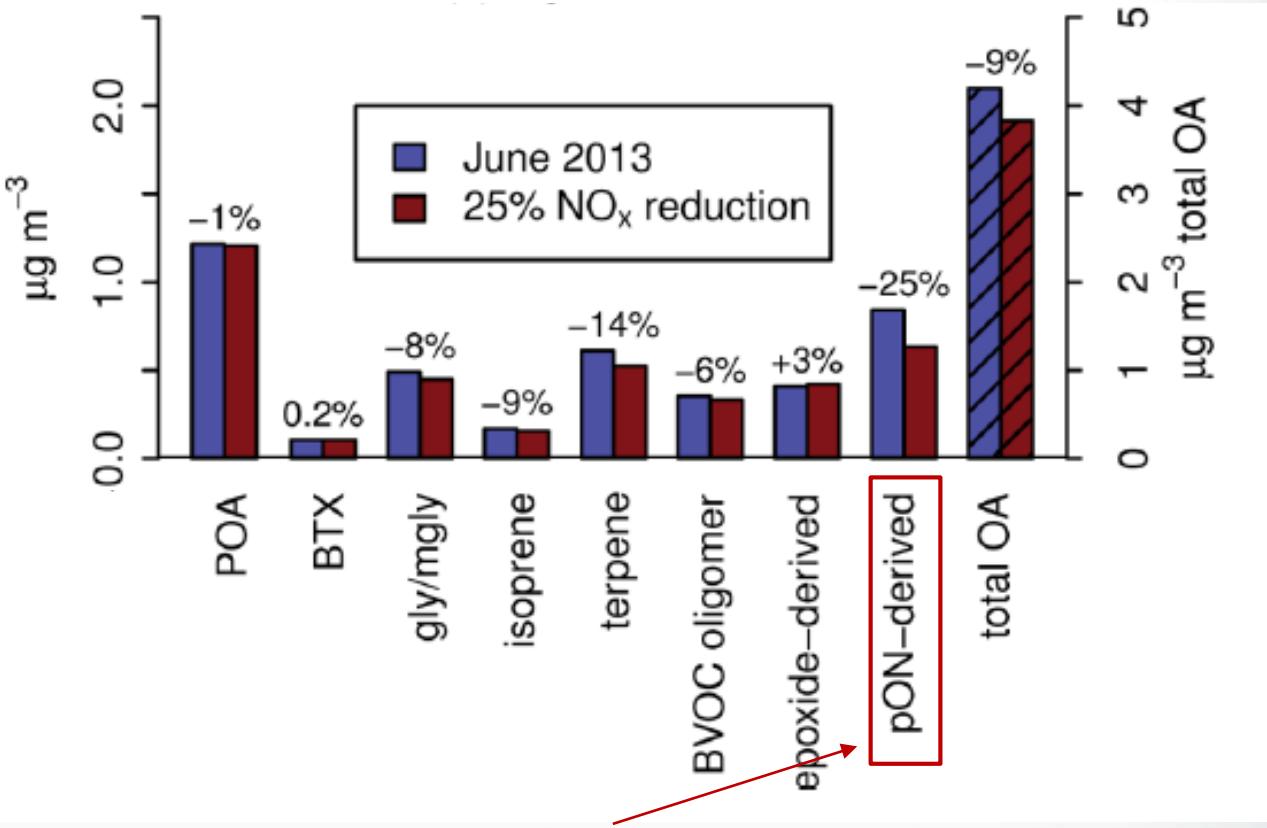
Organic aerosol co-benefits from SO_x and NO_x reductions

Better capture of Isoprene SOA dependence on aerosol sulfate



(*Pye et al., 2017 ACP, Mao et al., in review ACPD*)

NO_x reductions lead to substantial OA reductions via NO_x participation in organic nitrate formation



Organic Nitrates!

(*Pye et al., 2015 ES&T*)

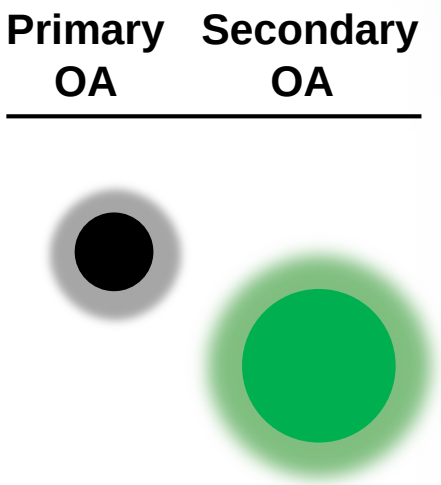
CMAQv5.2 Updates:
Anthropogenic Organic Aerosol

Organic aerosol in the atmosphere:

- is a significant contribution to mass throughout the world
- is becoming relatively more important for $PM_{2.5}$ predictions as PM sulfate and nitrate concentrations fall
- has been shown to evaporate with dilution from near-source to ambient conditions

  (Lipsky et al., *Environ Sci Technol*, 2006, Huffman et al., 2009, Grieshop et al., *ACP*, 2009, May et al., *Atmos. Environ*, 2013)
- is primarily comprised of oxygenated compounds

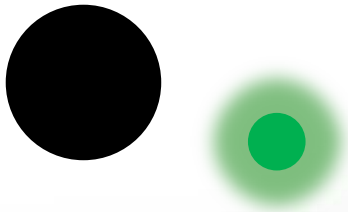
  (Ng et al., *ACP*, 2010; Zhang et al., *Anal Bioanal Chem*, 2011)



Organic aerosol in CMAQ<u>v5.1</u>:

- is dominated by primary, nonvolatile organic mass
- underestimates the response of OA to photooxidation in urban areas

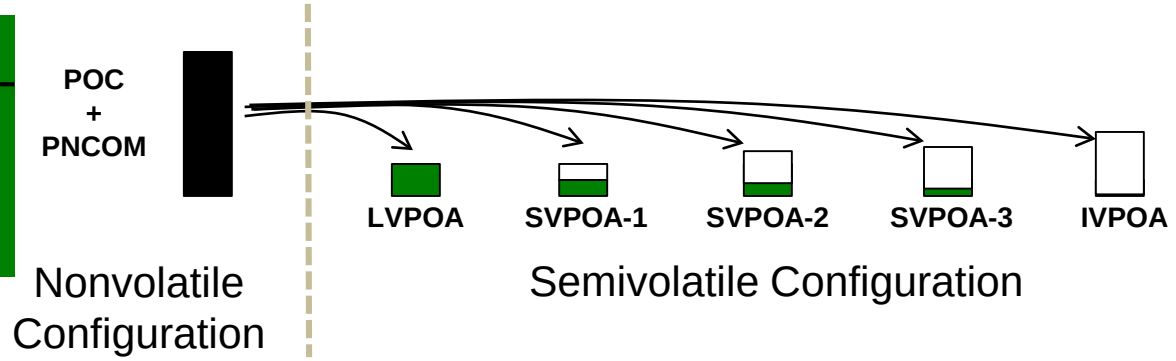
  (Woody et al., *ACP*, 2016)
- overestimates OA observations in winter (due to high POA concentrations)
- underestimates OA observations in summer (due to low SOA concentrations)



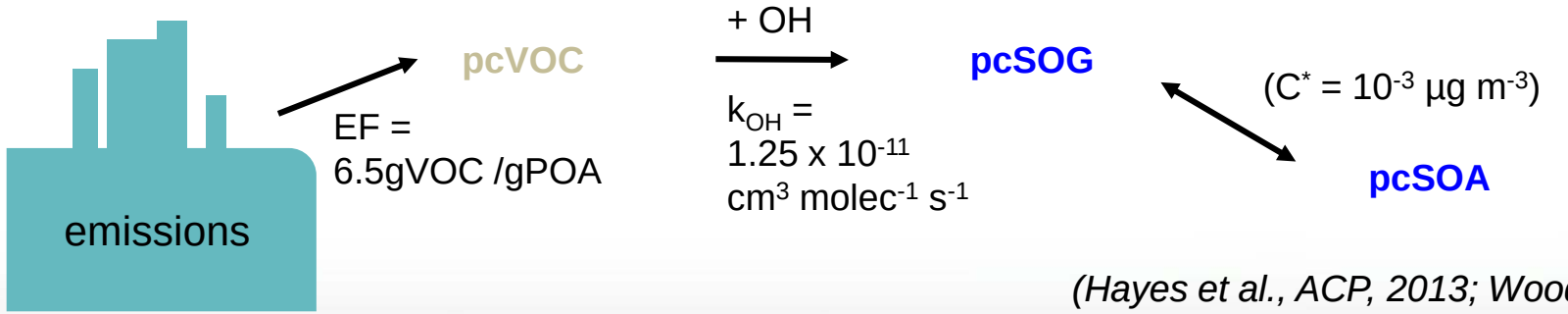
CMAQv5.2 Updates:
Anthropogenic Organic Aerosol

- Semi-volatile POA
  - The research community and our own models tell us a significant fraction of POA should be volatilized.
  - Distributed POA from inventory into separate species based on Volatility:

Class	C^* (µg m^{-3})
ELVOC	$C^* < 10^{-3}$
LVOC	$10^{-3} \leq C^* < 10^{0}$
SVOC	$10^{0} \leq C^* < 10^{3}$
IVOC	$10^{3} \leq C^* < 10^{6}$



- New Anthropogenic SOA model species
  - Lump The uncertain processes into one NEW model surrogate: Potential SOA from Combustion Emissions (pcSOA)

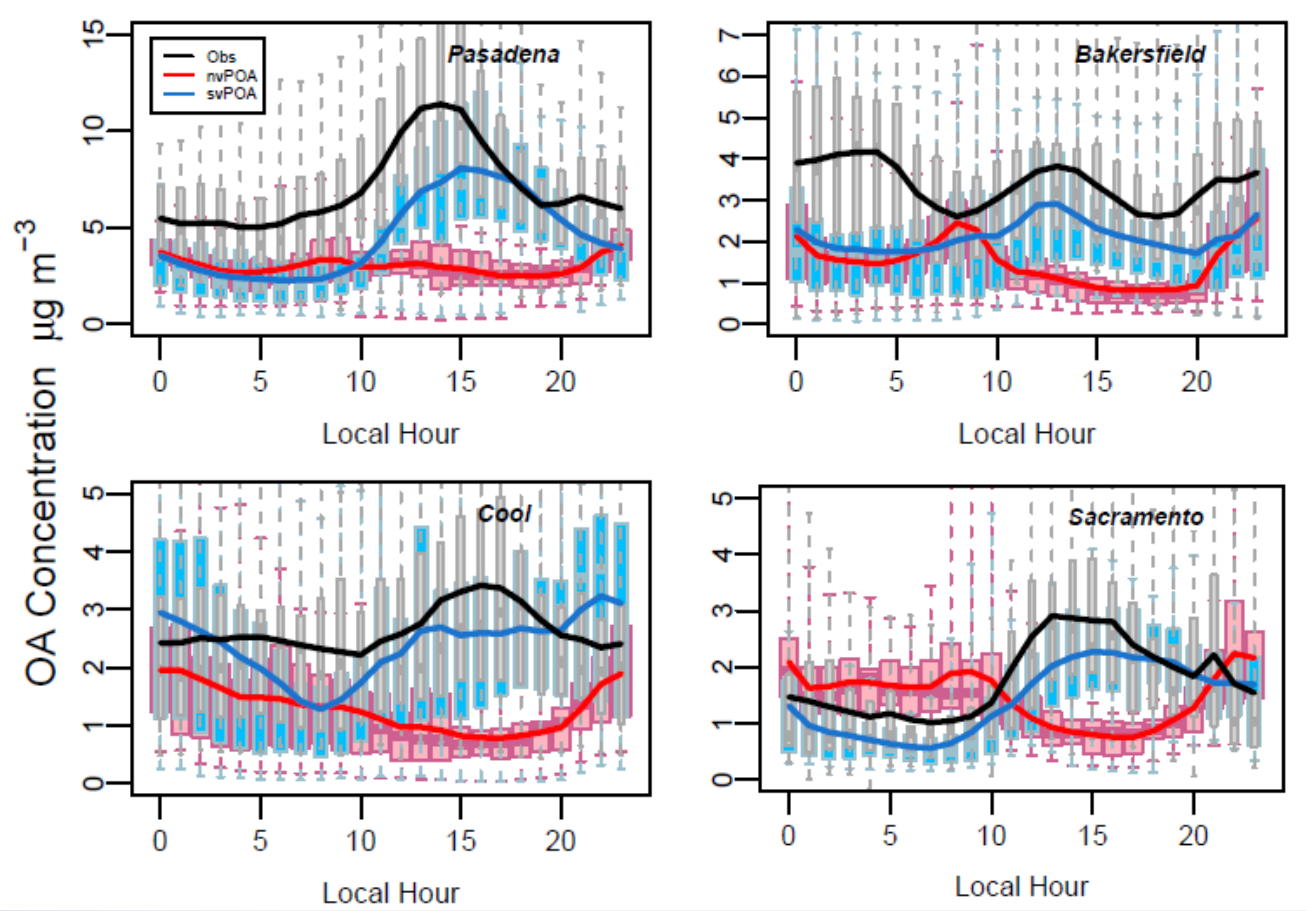


(Hayes et al., ACP, 2013; Woody et al, ACP, 2016)

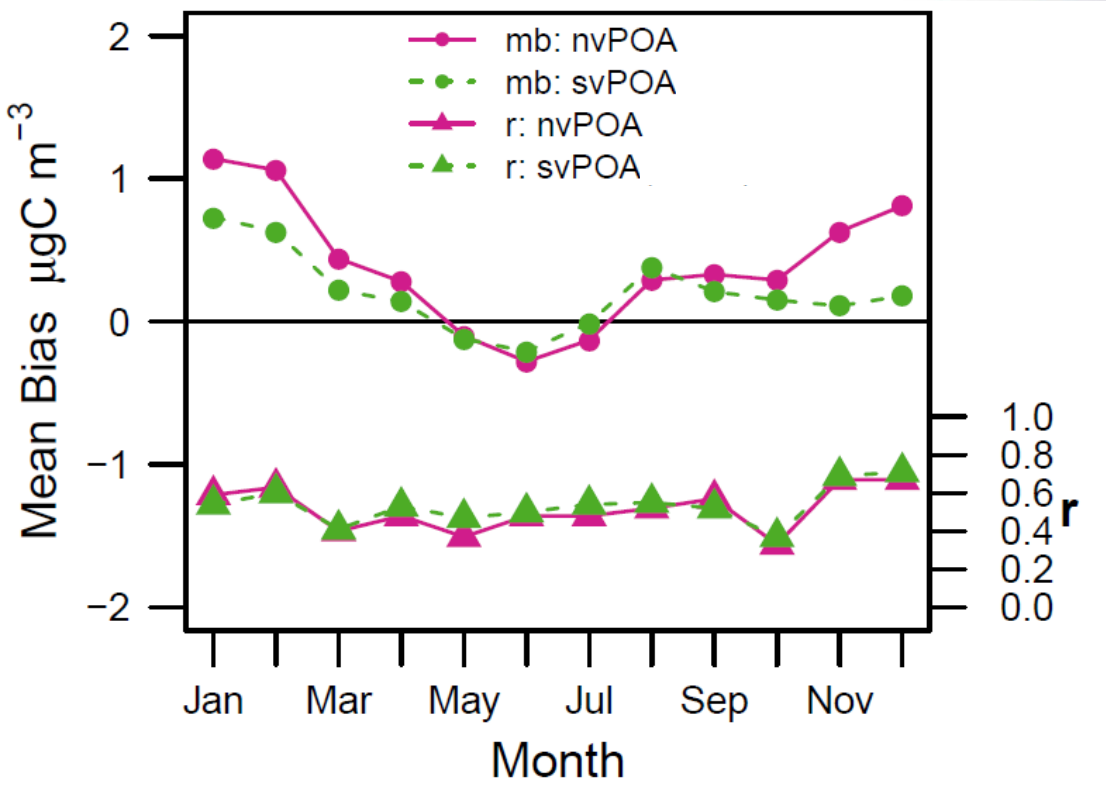
- Nonvolatile POA is still available in CMAQv5.2 for backwards compatibility

CMAQv5.2 Updates:
Anthropogenic Organic Aerosol

OA Diurnal profiles for California 4-km simulation. May-June 2010.

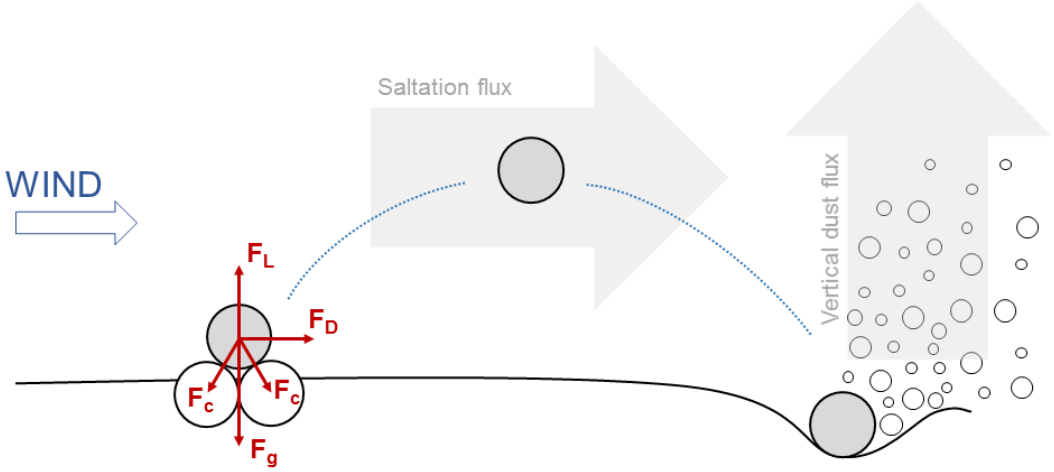


Seasonal performance indicators for CONUS 2011 simulation



CMAQv5.2 Updates:

New physics-based windblown dust model



- Particles are mobilized when the aerodynamic drag and lift *exceed* gravitational and inter-particle cohesive forces
- Particles striking back to the surface result in vertical emission flux

Update	Implications
Threshold friction velocity	More realistic values of the threshold velocity smoothly distributed
Roughness factor	Include the effect of roughness elements (both solid and vegetation)
Surface roughness	Develop a new relation for surface roughness based on data from several different studies
Vegetation cover fraction	Spatially and temporally variable vegetation fraction based on satellite observations

Foroutan et al., JAMES, in review, 2017

CMAQv5.2 Updates:
Evaluation of windblown dust improvements

CMAQv5.1 windblown dust model Issue

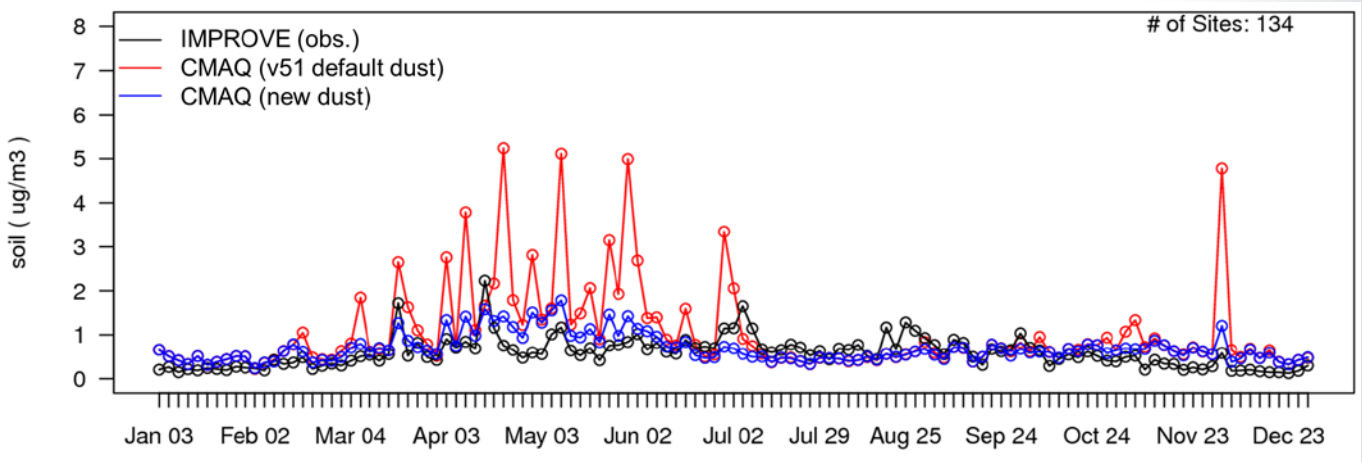
Tendency to occasionally produce unrealistically high emissions

Extensive updates to the windblown dust module for CMAQv5.2 release

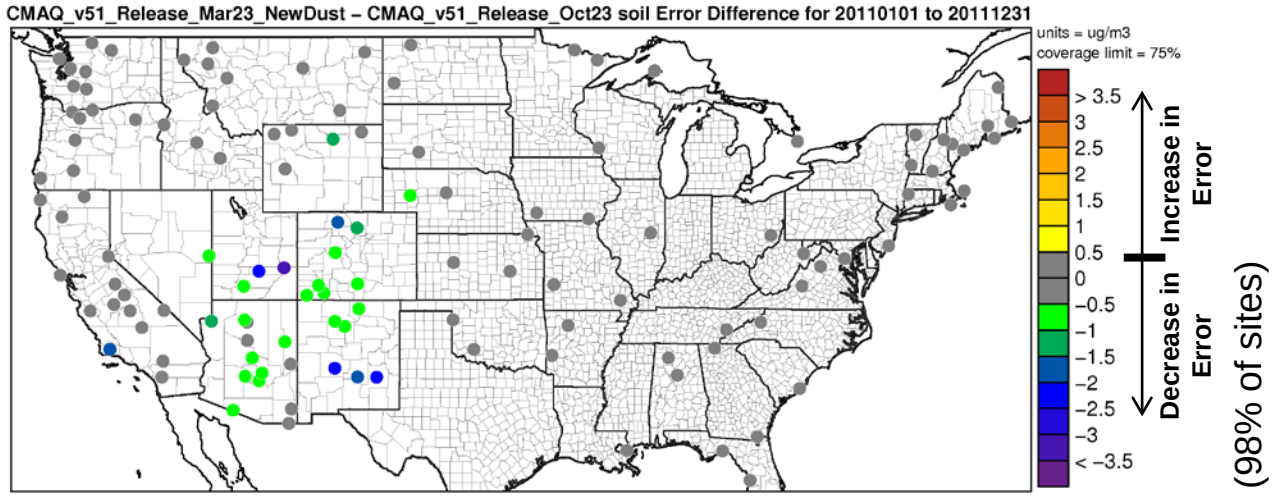
Foroutan et al., *JAMES* (in review)

Massive dust storm in Phoenix, AZ

Time series of fine particulate soil for all IMPROVE sites (CONUS, 2011)



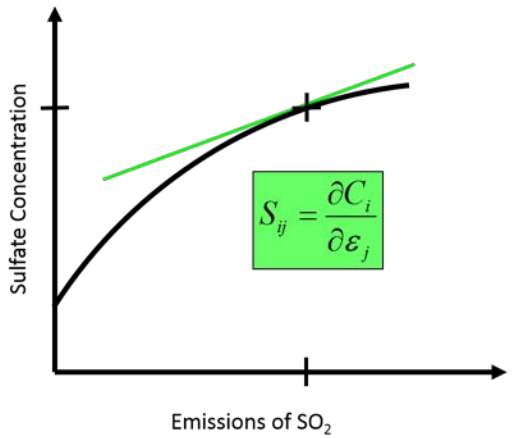
Difference in the soil error for entire year 2011 (CMAQv5.2 – CMAQv5.1)



CMAQv5.2 Instrumented Models

Decoupled Direct Method in Three Dimensions (DDM-3D)

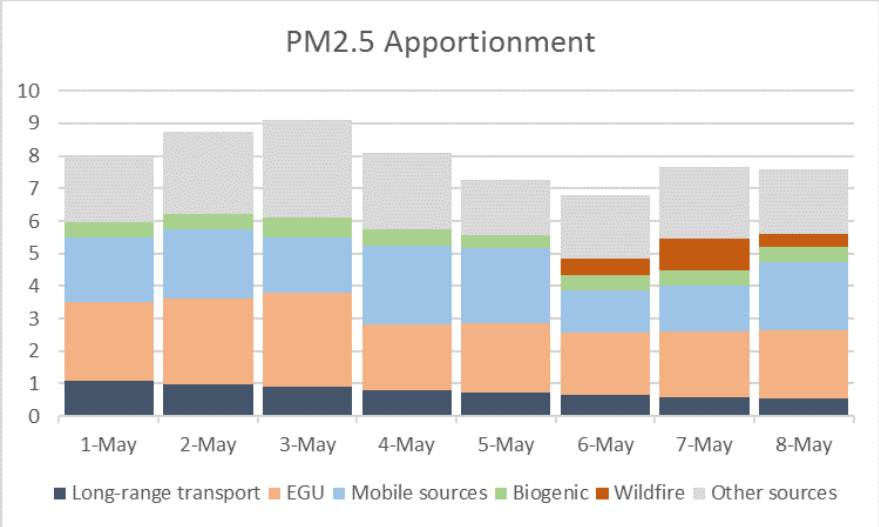
- CMAQ-DDM-3D enables sensitivity calculations simultaneously with the standard concentrations and deposition calculations using the existing core model algorithms. Sensitivities are with respect to:
  - Emissions (gridded, point, biogenic, lightning, etc)
  - Boundary and/or Initial conditions
  - Reaction rates
  - Potential Vorticity
  - Region or Time of emission
- Second order sensitivity calculation (sensitivity of sensitivity) is also available.



A hypothetical relationship between emissions of SO2 and sulfate concentrations. The green tangent line illustrates the sensitivity of sulfate concentration to emissions of SO_2.

Integrated Source Apportionment Method (ISAM)

- CMAQ-ISAM allows for source attribution calculations for both gaseous (O_3, VOC, and NO_x) and particulate species (SO_4, NO_3, EC, OC, etc.) in a single model run.
- O_3 attribution is classified into VOC/NO_x limited regimes.
- All reactive VOCs are explicitly tracked.
- Source attribution for user-defined combinations of emissions sectors and regions.
- Each simulation tracks IC/BC contributions as well as an other category to reconstruct the full bulk concentration.



An example of source-resolved particulate concentrations. This scenario demonstrates the effect of a wildfire plume impacting the receptor on May 6.

Courtesy: Sergey Napelenok

Incremental Testing of the CMAQv5.2 Modeling System

V5.1 Base

WRF3.7
2011NEI v2
CB05e51
Geos-Chem BCs

Updates in CMAQv5.2 reduce high bias in summer O_3 and low bias in summer $PM_{2.5}$ across much of the US. Changes in high bias in winter $PM_{2.5}$ are more spatially heterogeneous.

WRF3.8 with lightning assimilation

Lightning assimilation:
- Decreases summer O_3
  → Improves bias
- Mostly increases sulfate in eastern US in summer
- Increases nitrate in eastern US in winter

Other changes in WRF3.8 have much smaller impact

V5.2 with CB05e51 chemical mechanism

- Increases $PM_{2.5}$ in summer due to SOA updates
- Decreases $PM_{2.5}$ in winter due to addition of semivolatile POA

→ Improves bias in both seasons

- Impact on summer O_3 is mixed

V5.2 with CB6r3 chemical mechanism

- Decreases summertime O_3 and NO_2
  → Improves bias
- Small decrease in summer SOA in the southeast

Update to Calculation of NO from Lightning

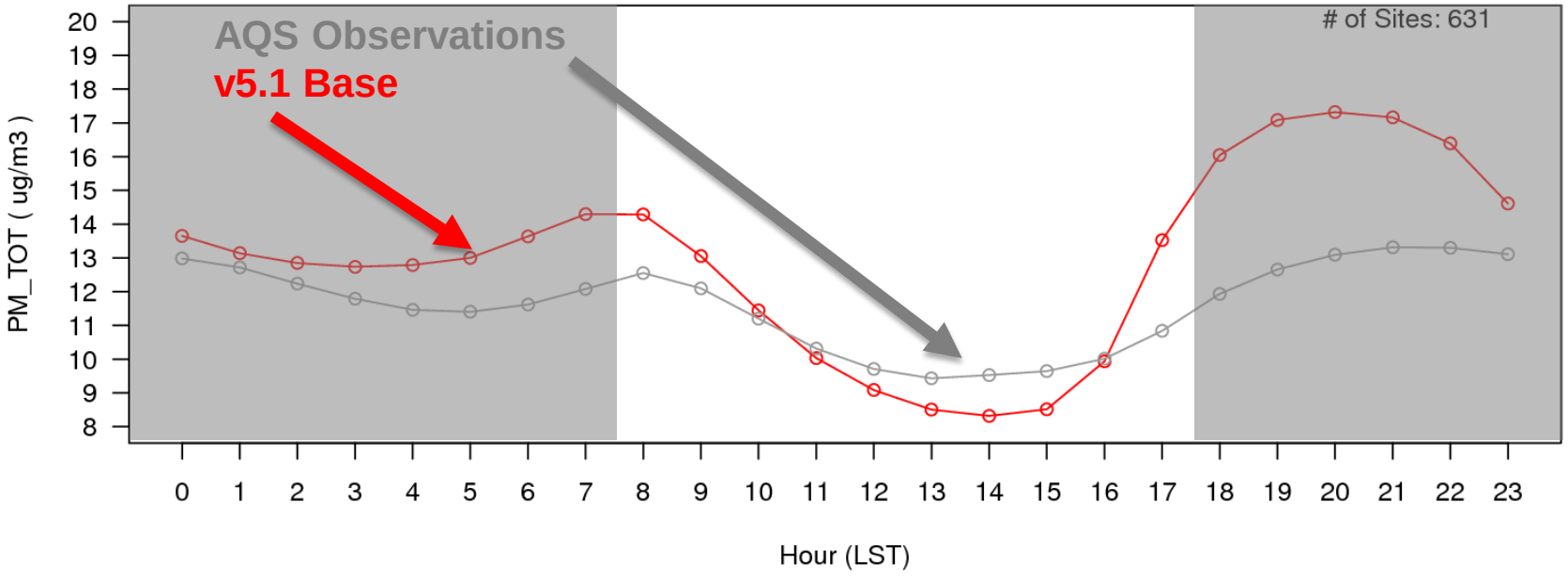
- Decrease in summertime O_3

Hemispheric CMAQ BCs

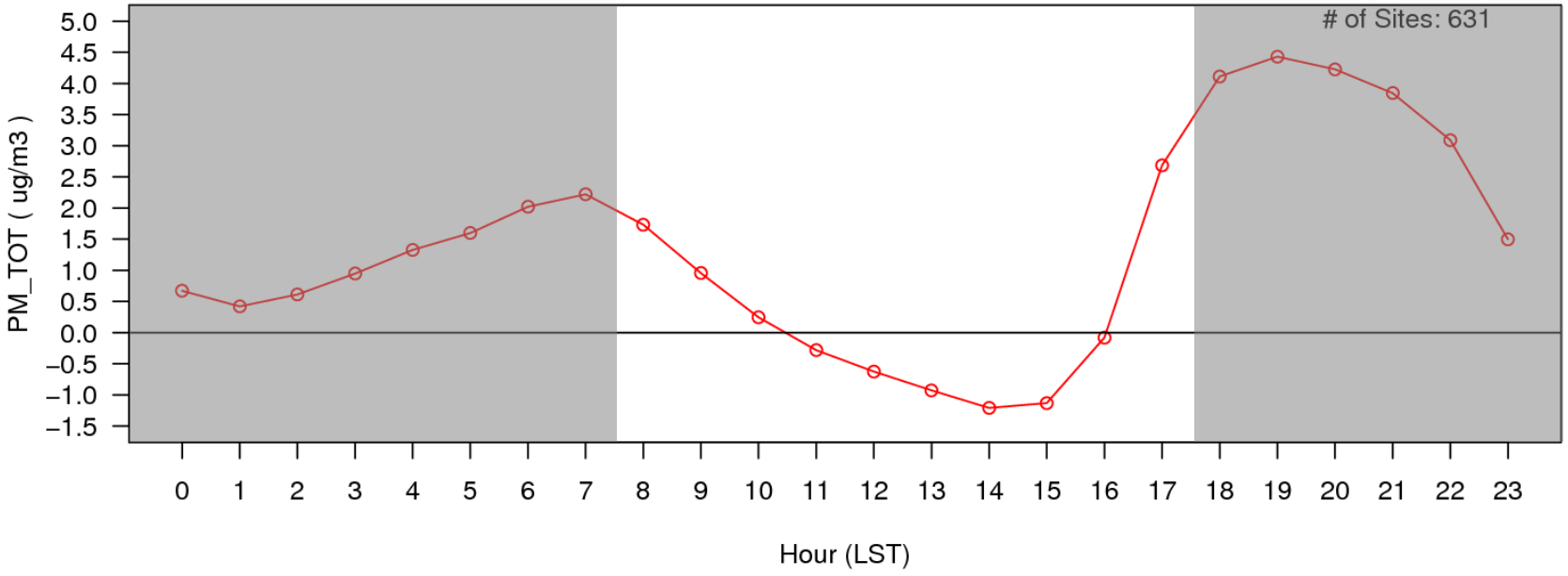
- Decreases summertime O_3 across much of the domain. Exception is over the Pacific.
  → Improves bias
- Increases $PM_{2.5}$ in summer
- Decreases nitrate in winter

January 2011 Incremental Testing for $PM_{2.5}$

$PM_{2.5}$ Concentration – January 2011

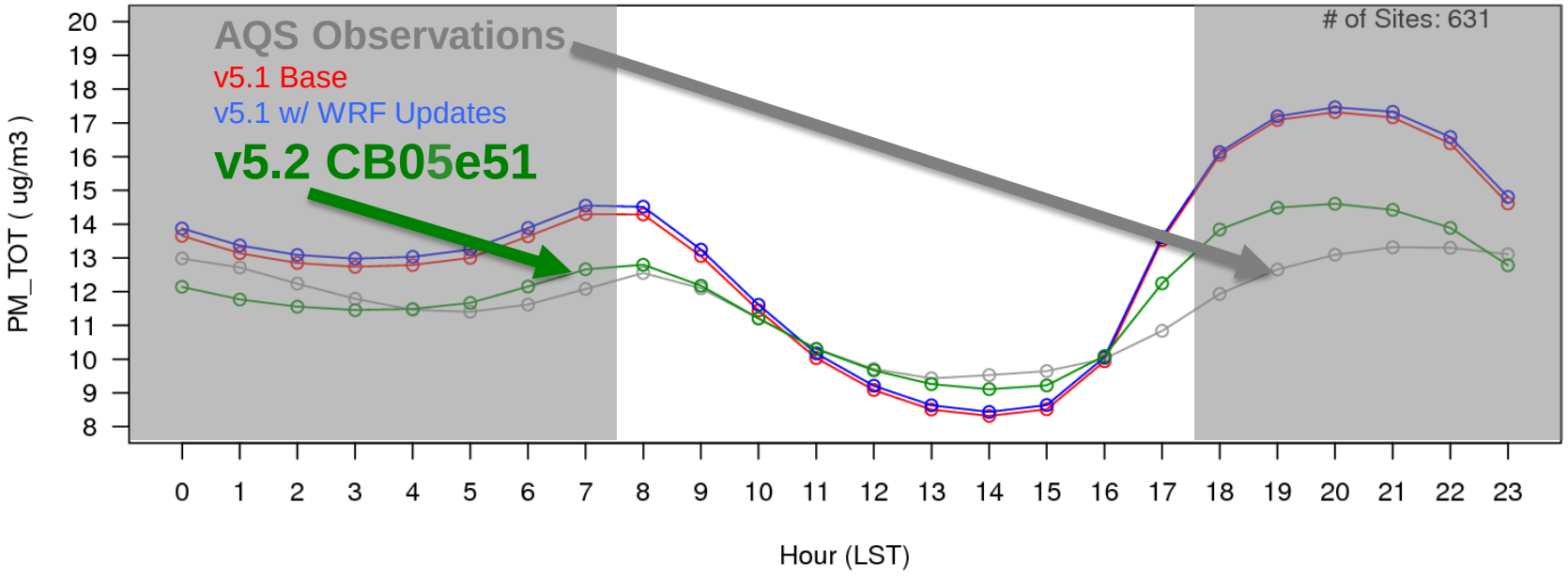


$PM_{2.5}$ Bias

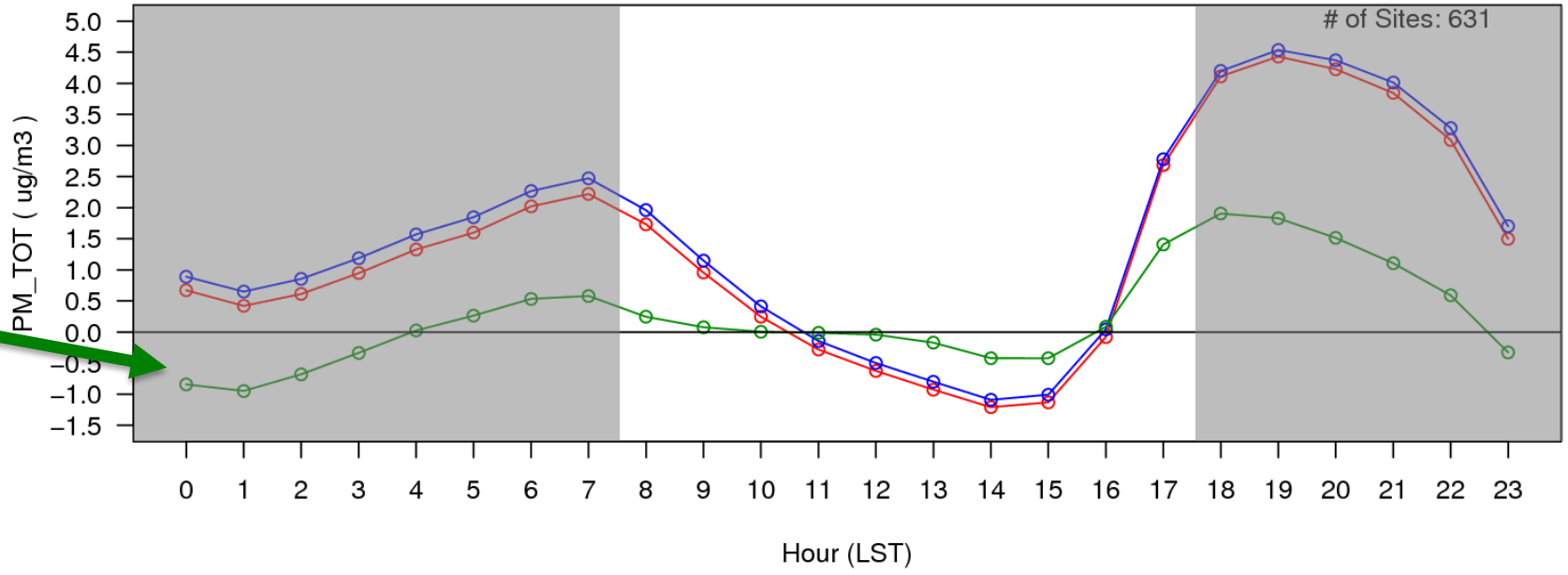


January 2011 Incremental Testing for $PM_{2.5}$

$PM_{2.5}$ Concentration – January 2011



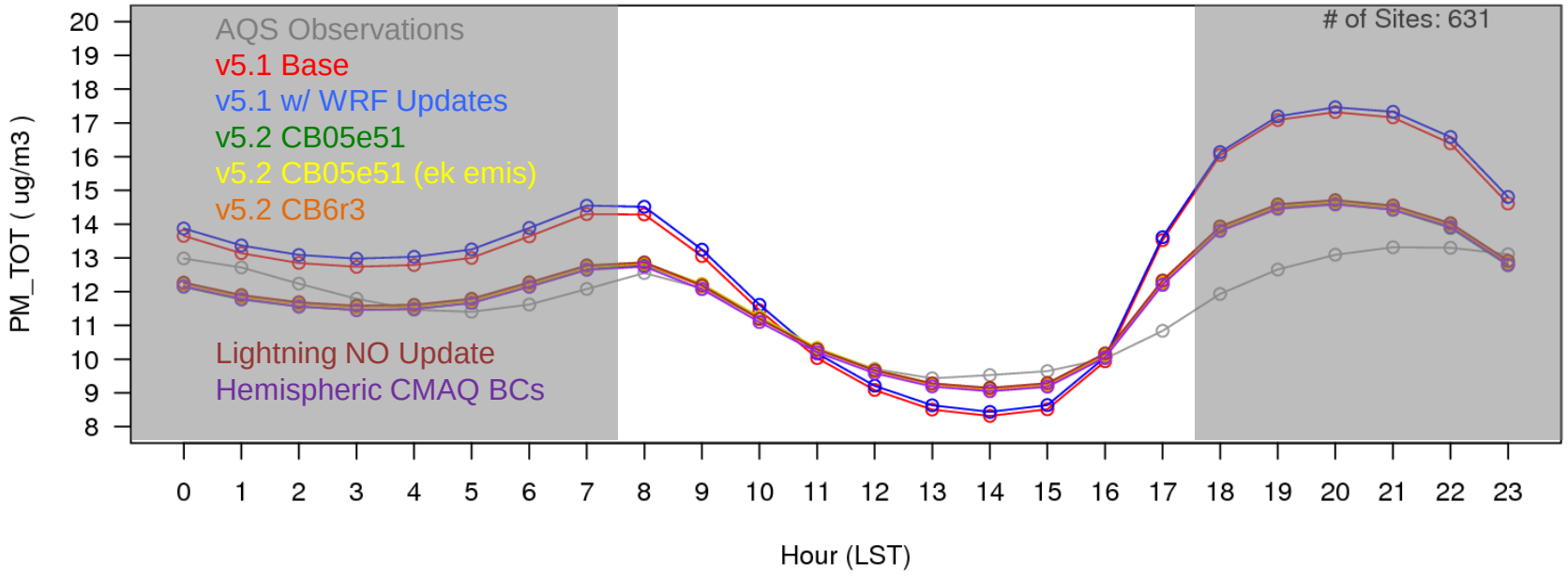
$PM_{2.5}$ Bias



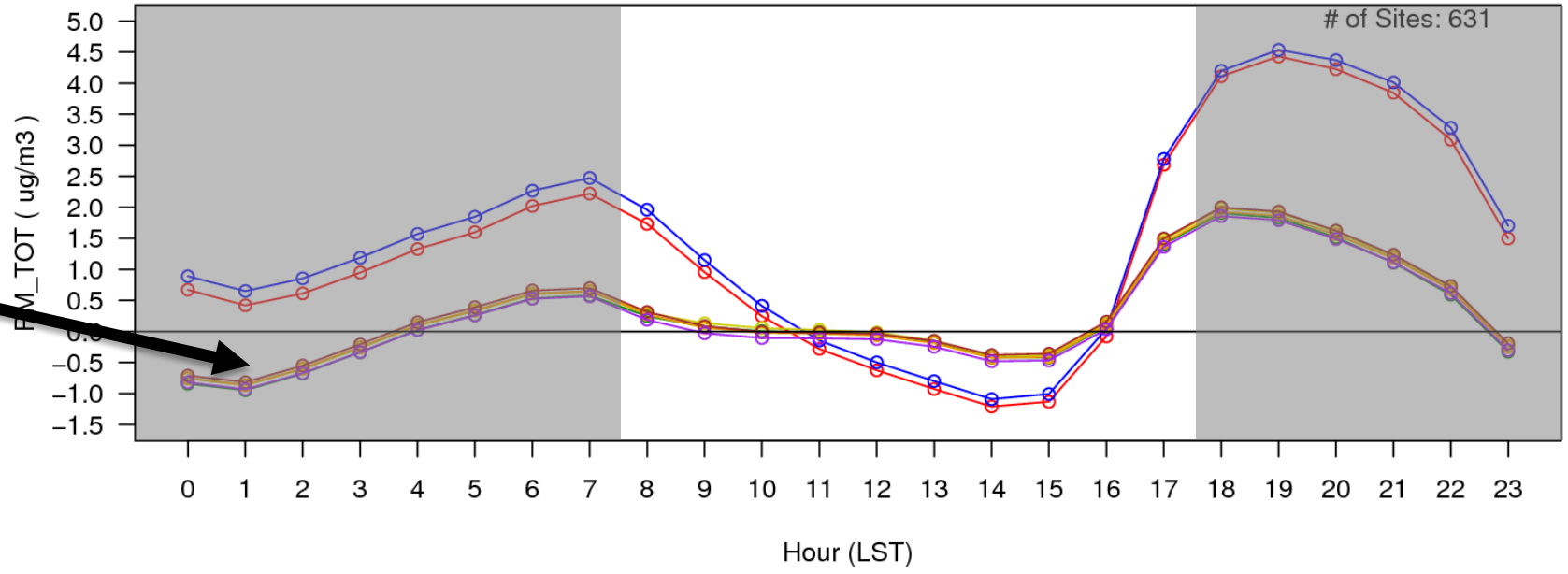
Improvements in bias due primarily to organic aerosol updates in v5.2 CB05e51.

January 2011 Incremental Testing for $PM_{2.5}$

$PM_{2.5}$ Concentration – January 2011



$PM_{2.5}$ Bias

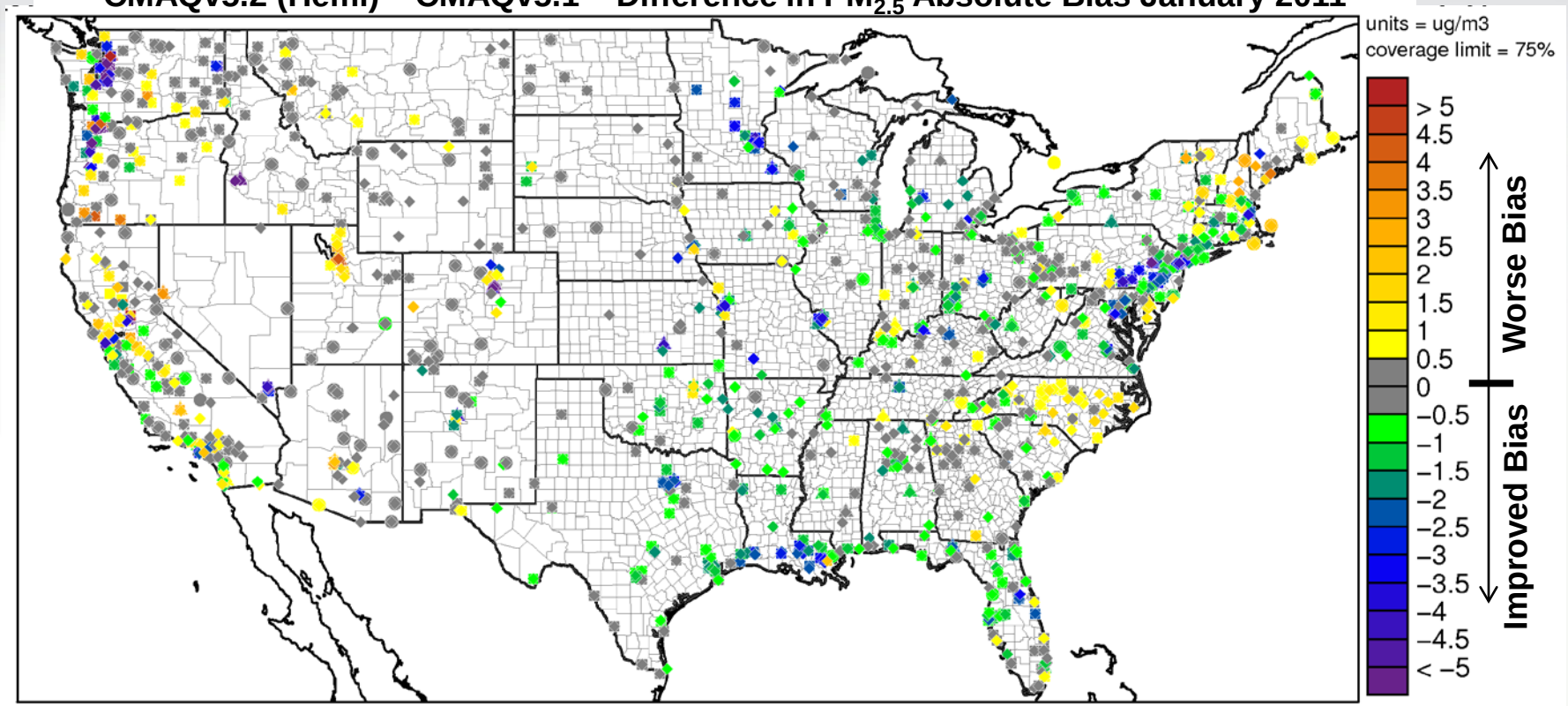


Other model updates have less impact on mean bias.

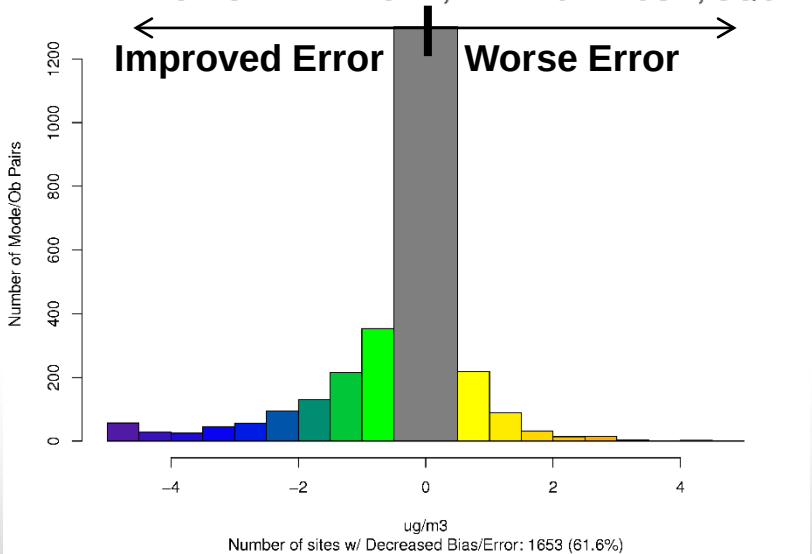
January 2011

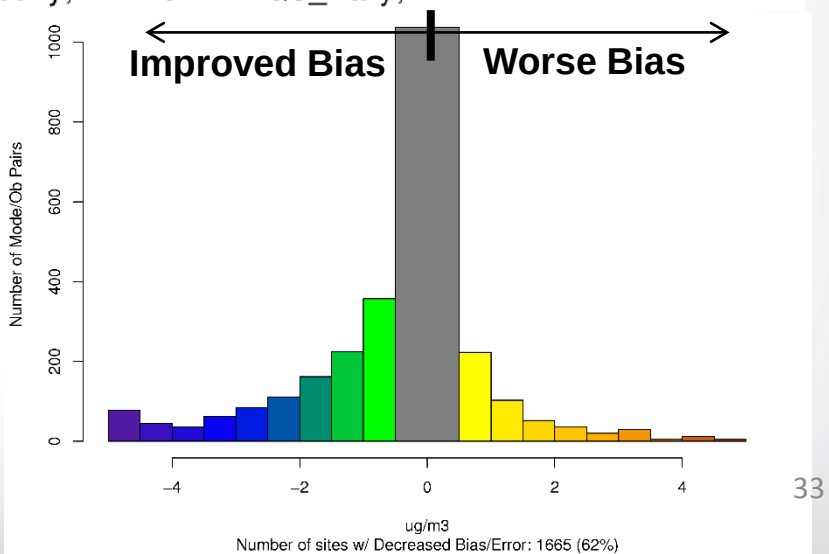
Improvement in $PM_{2.5}$ diurnal profile leads to decrease in bias at most locations

CMAQv5.2 (Hemi) – CMAQv5.1 – Difference in $PM_{2.5}$ Absolute Bias January 2011



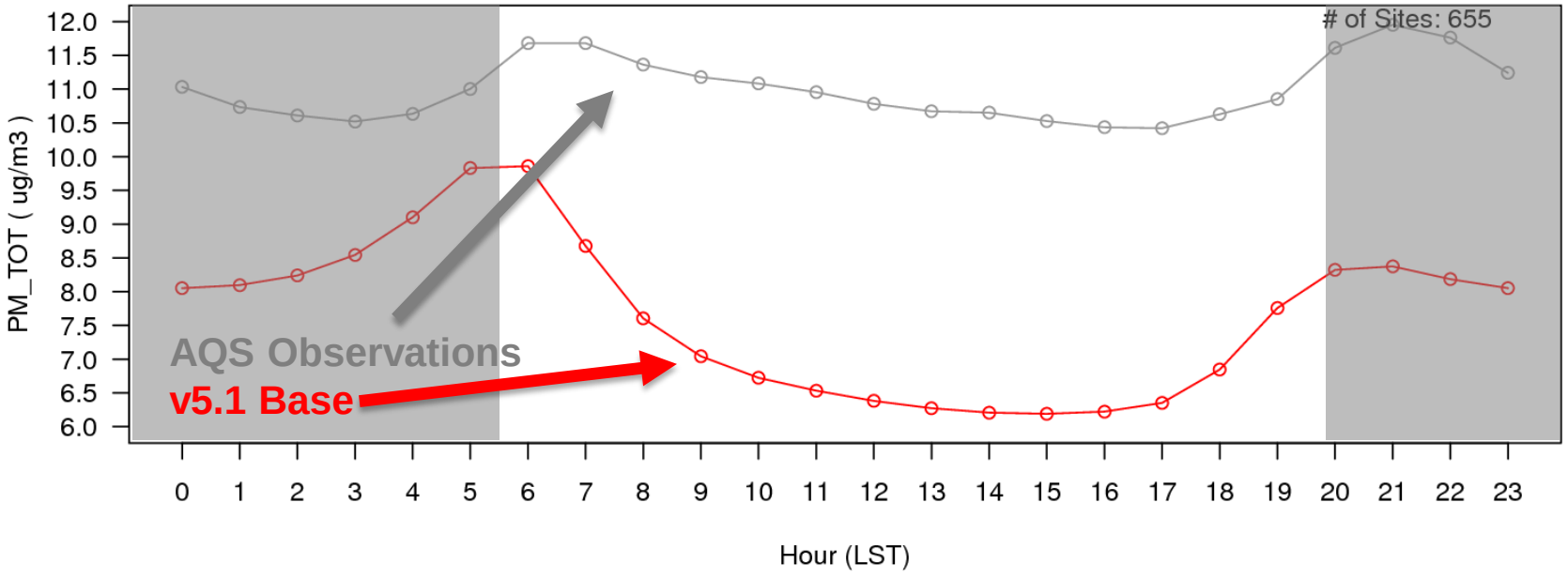
CIRCLE=IMPROVE; TRIANGLE=CSN; SQUARE=AQS_Hourly; DIAMOND=AQS_Daily;



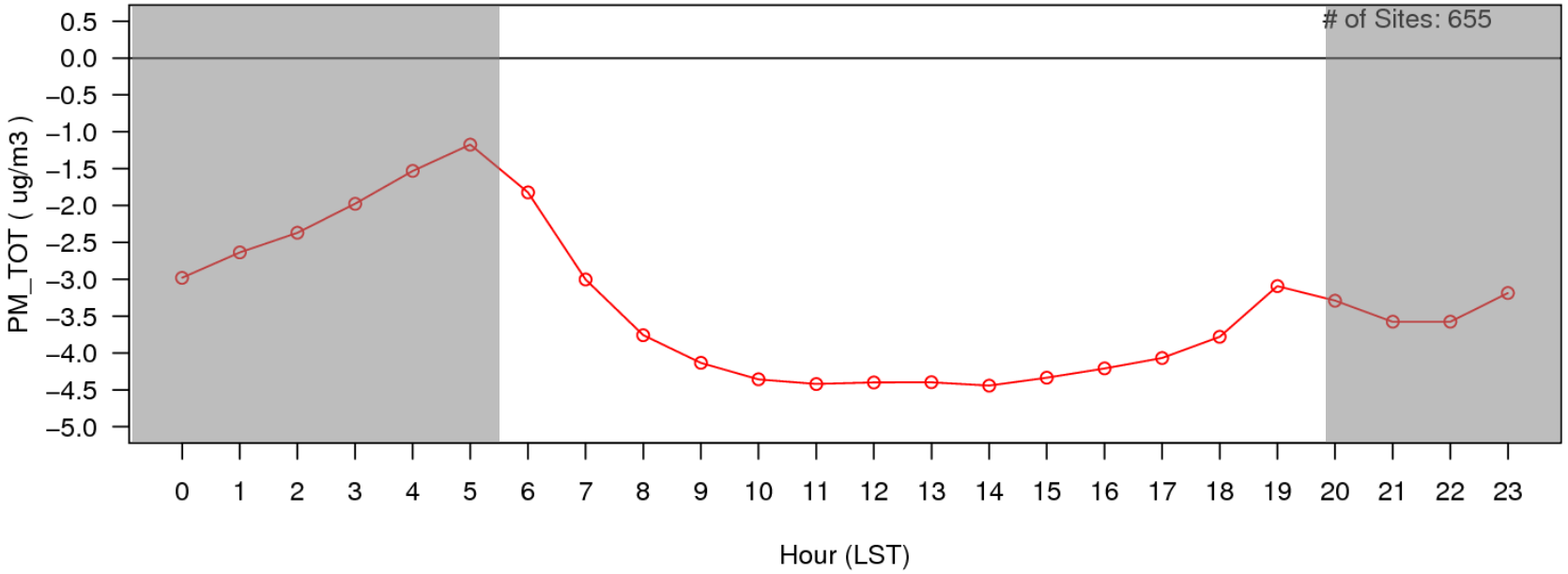


July 2011 Incremental Testing for $PM_{2.5}$

$PM_{2.5}$ Concentration – July 2011



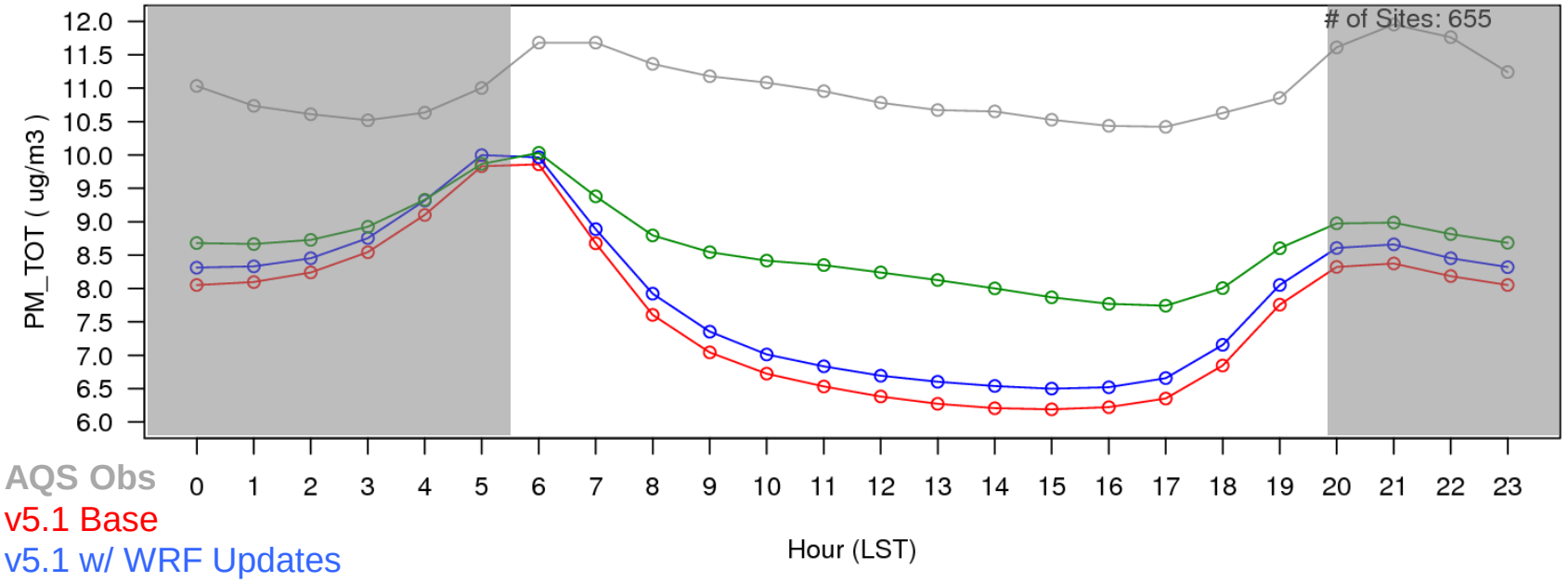
$PM_{2.5}$ Bias



July 2011 Incremental Testing for $PM_{2.5}$

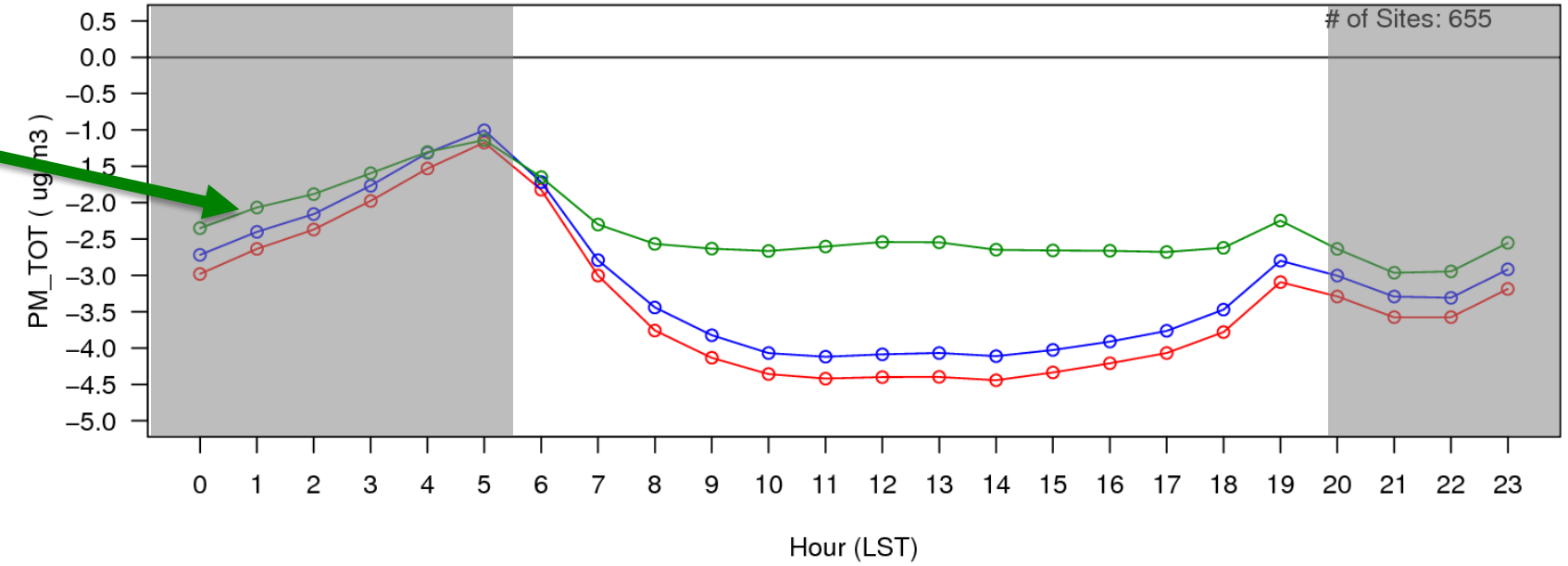
Improvements in bias due primarily to organic aerosol updates in v5.2 CB05e51.

$PM_{2.5}$ Concentration – July 2011



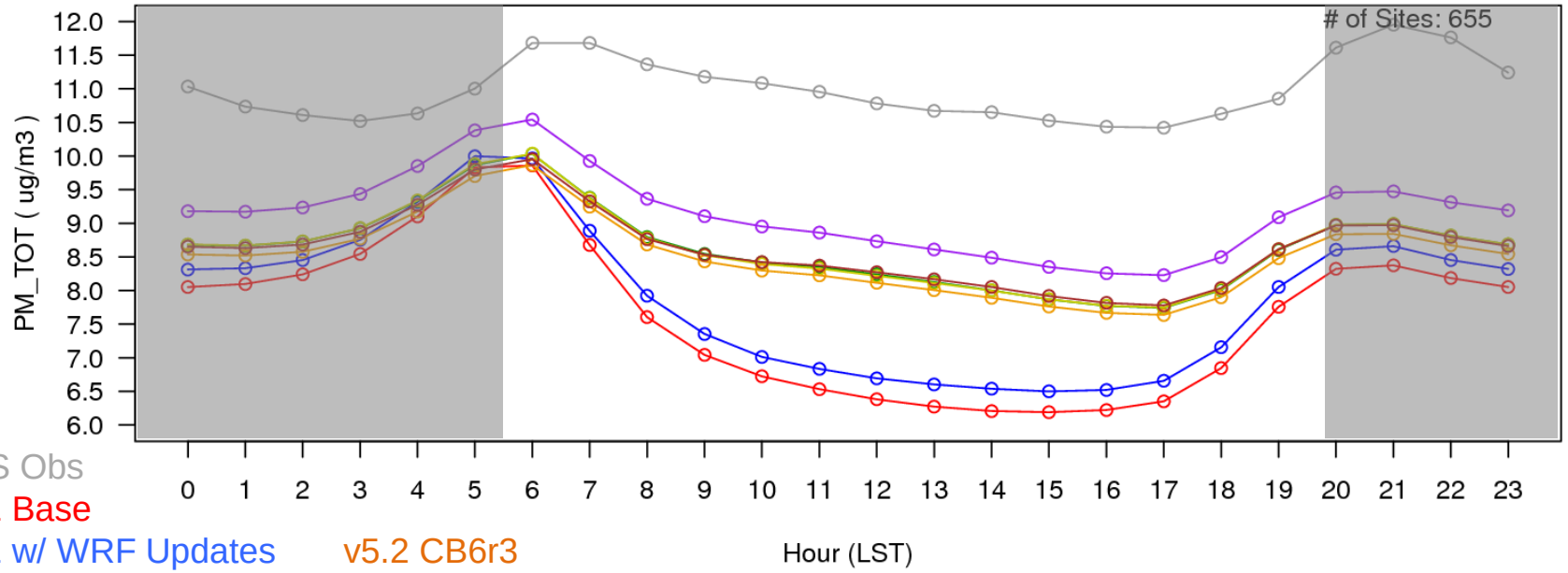
AQS Obs
v5.1 Base
v5.1 w/ WRF Updates
v5.2 CB05e51

$PM_{2.5}$ Bias



July 2011 Incremental Testing for $PM_{2.5}$

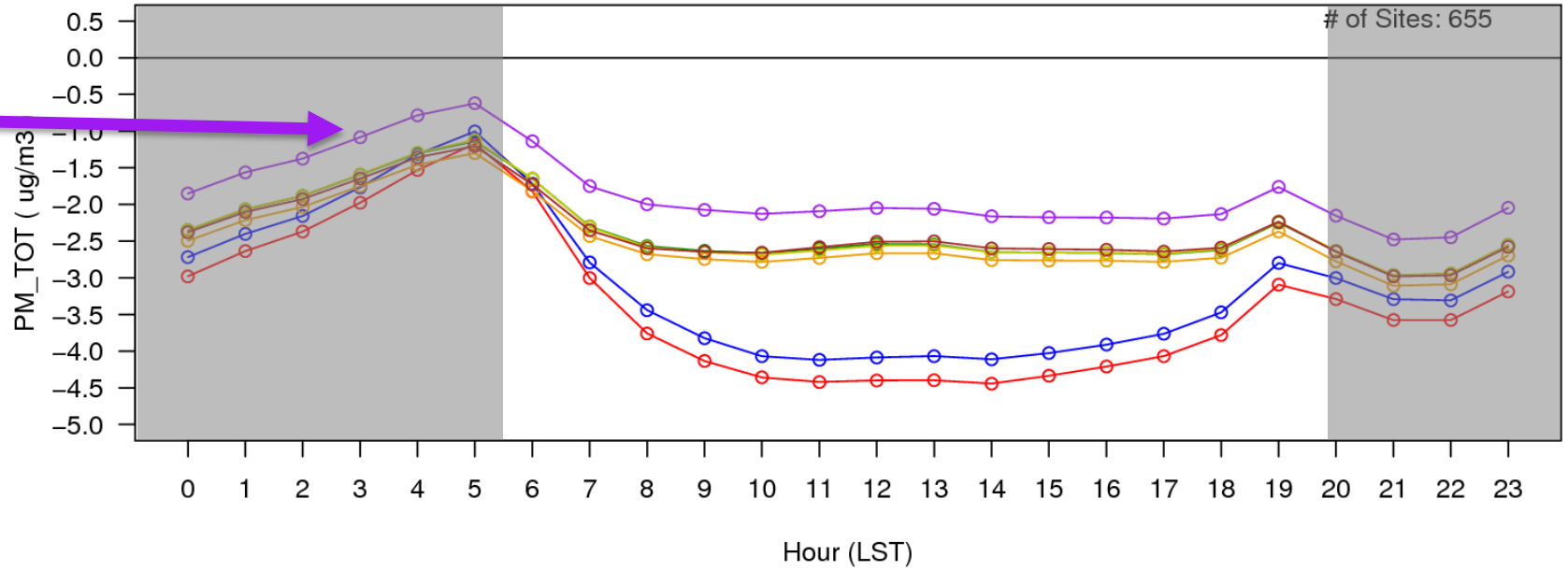
$PM_{2.5}$ Concentration – July 2011



AQS Obs
v5.1 Base
v5.1 w/ WRF Updates
v5.2 CB05e51
v5.2 CB05e51 (ek emis)
v5.2 CB6r3
Lightning NO Update
Hemispheric CMAQ BCs

Switch to boundary conditions from Hemispheric CMAQ also decreases bias.

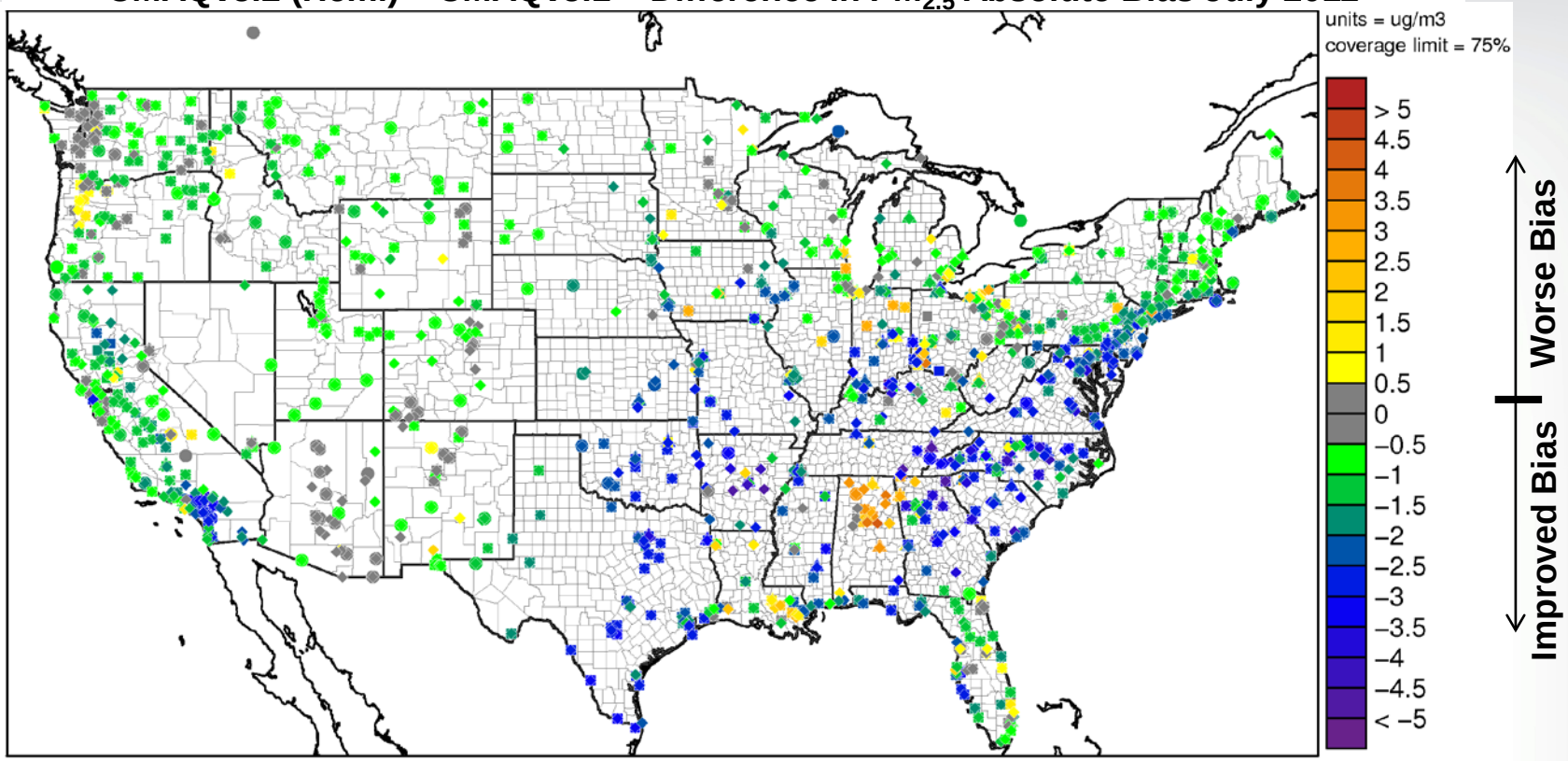
$PM_{2.5}$ Bias



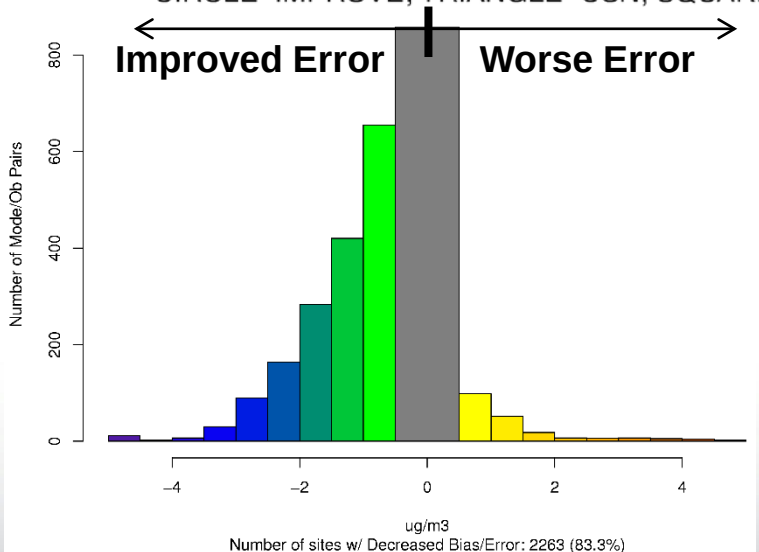
July 2011

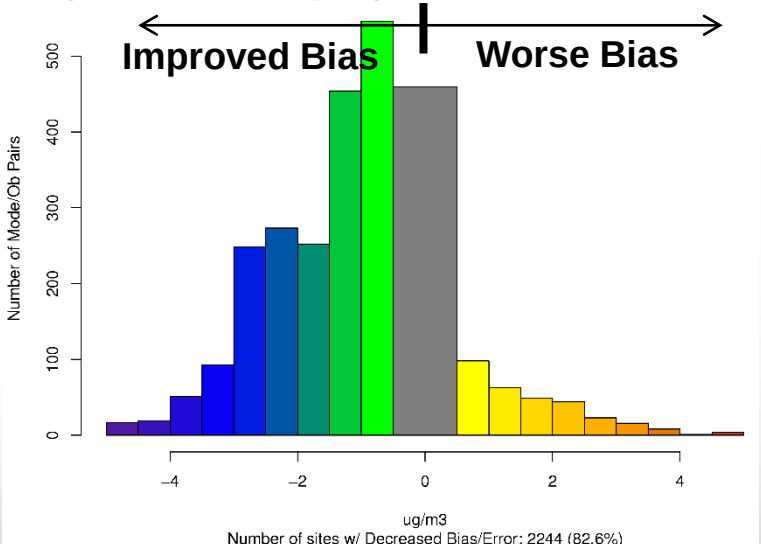
Bias in modeled $PM_{2.5}$ decreases at most locations from v5.1 to v5.2

CMAQv5.2 (Hemi) – CMAQv5.1 – Difference in $PM_{2.5}$ Absolute Bias July 2011

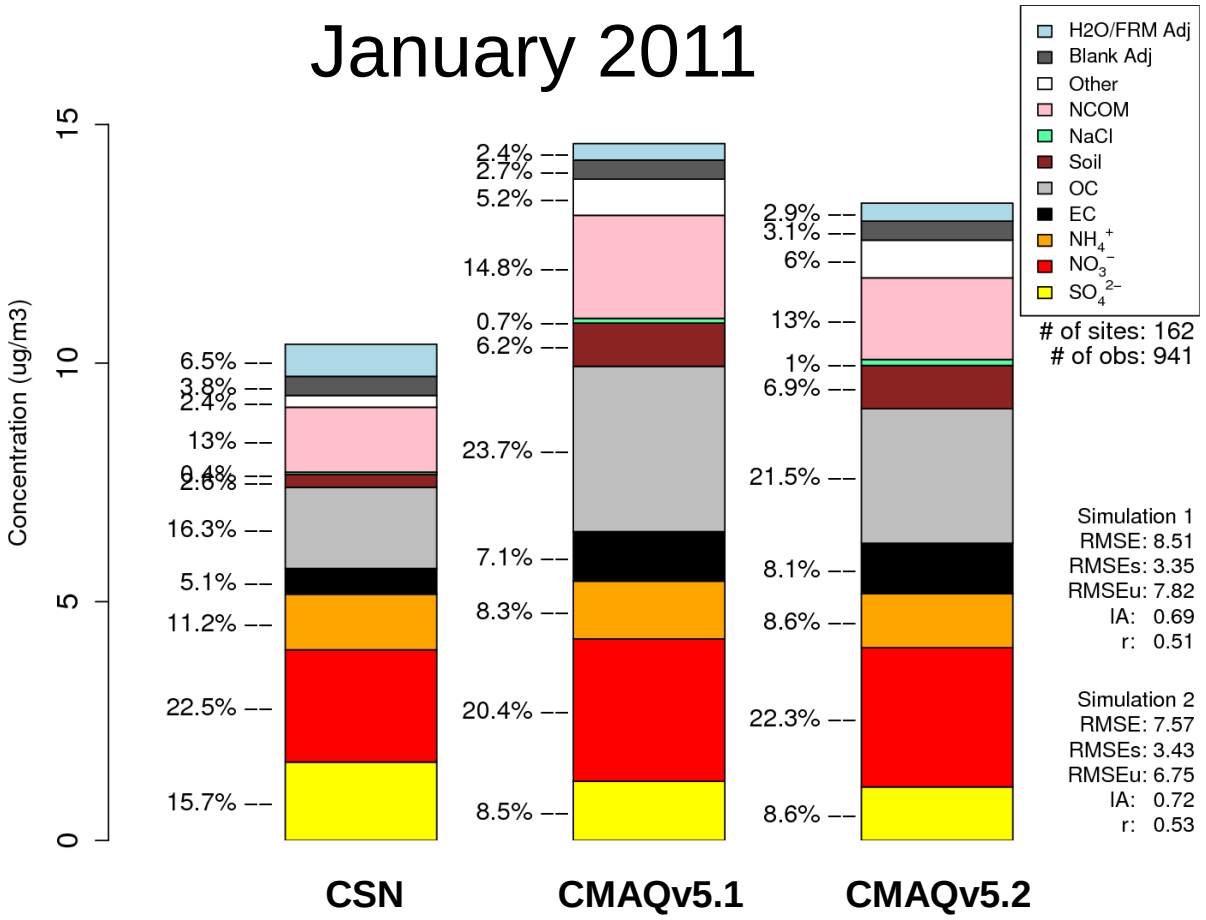


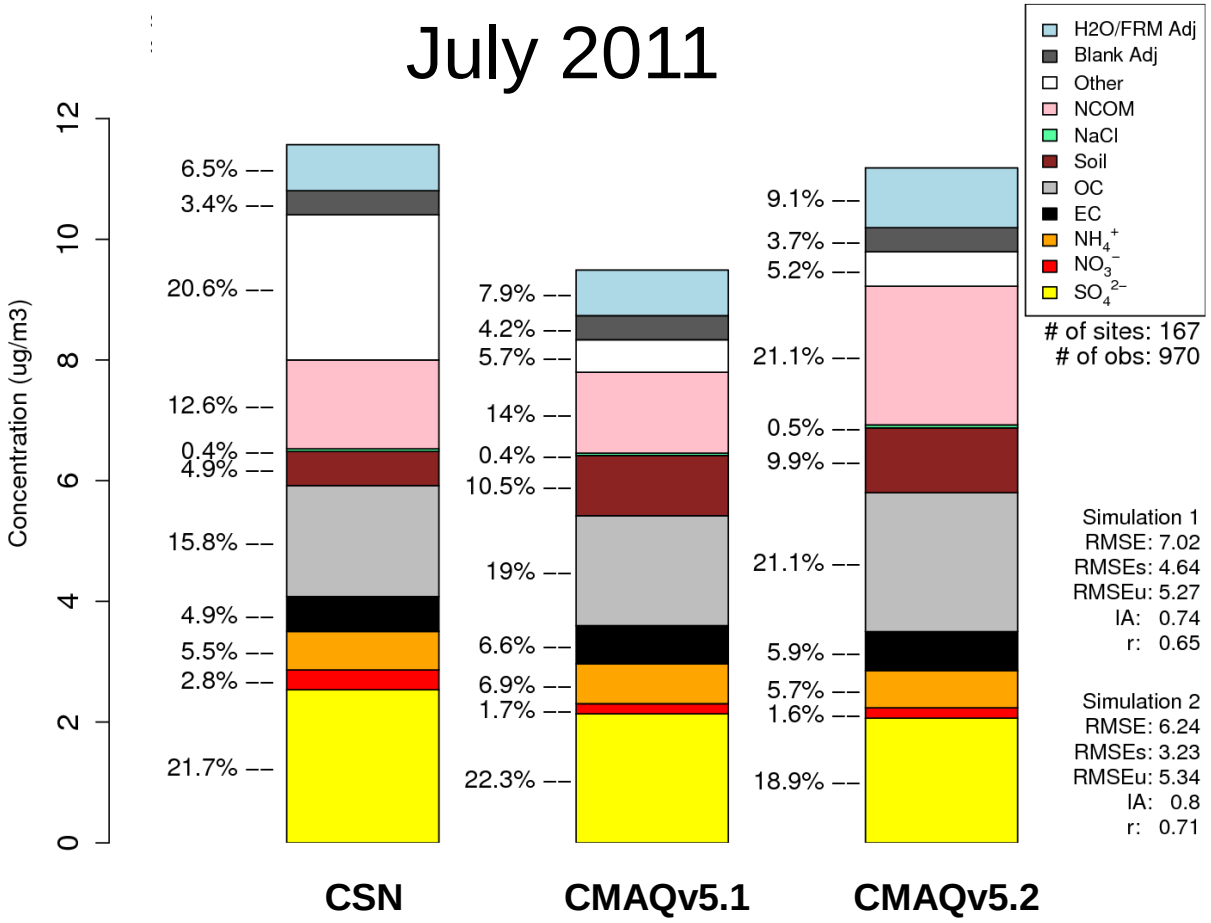
CIRCLE=IMPROVE; TRIANGLE=CSN; SQUARE=AQS_Hourly; DIAMOND=AQS_Daily;



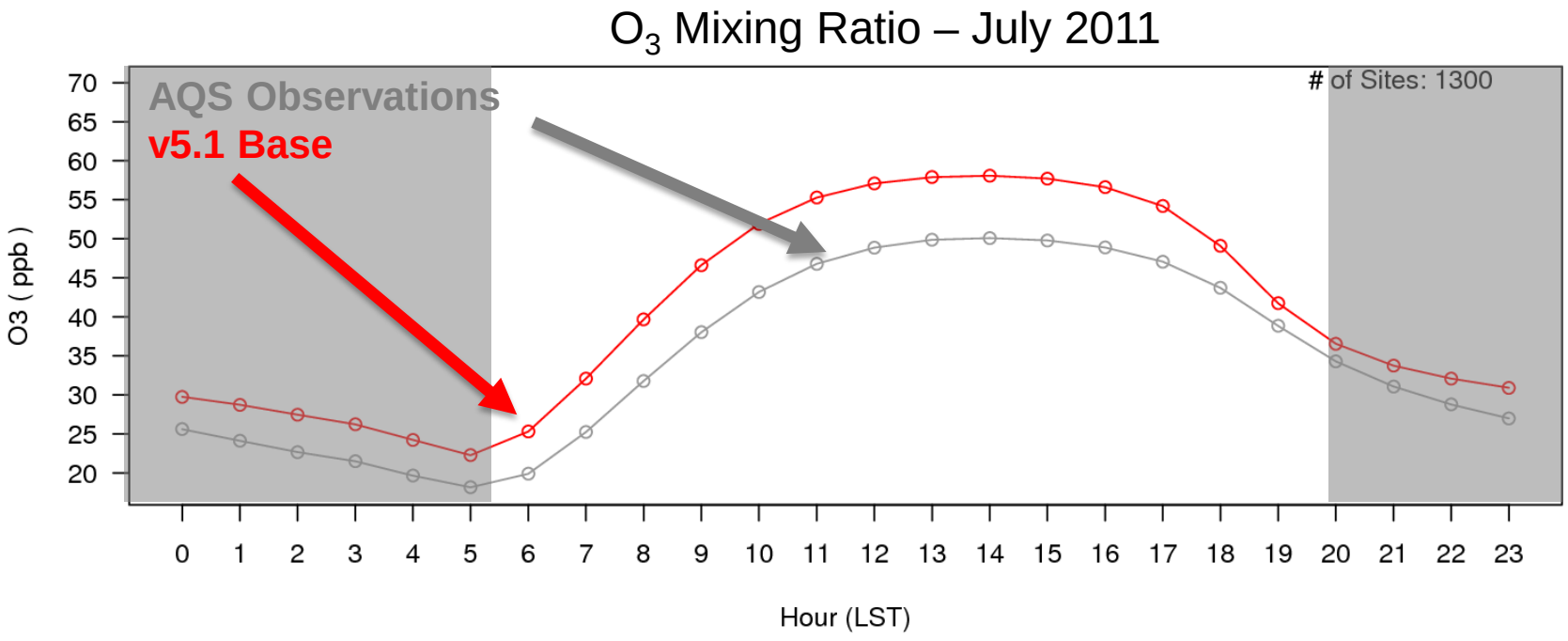


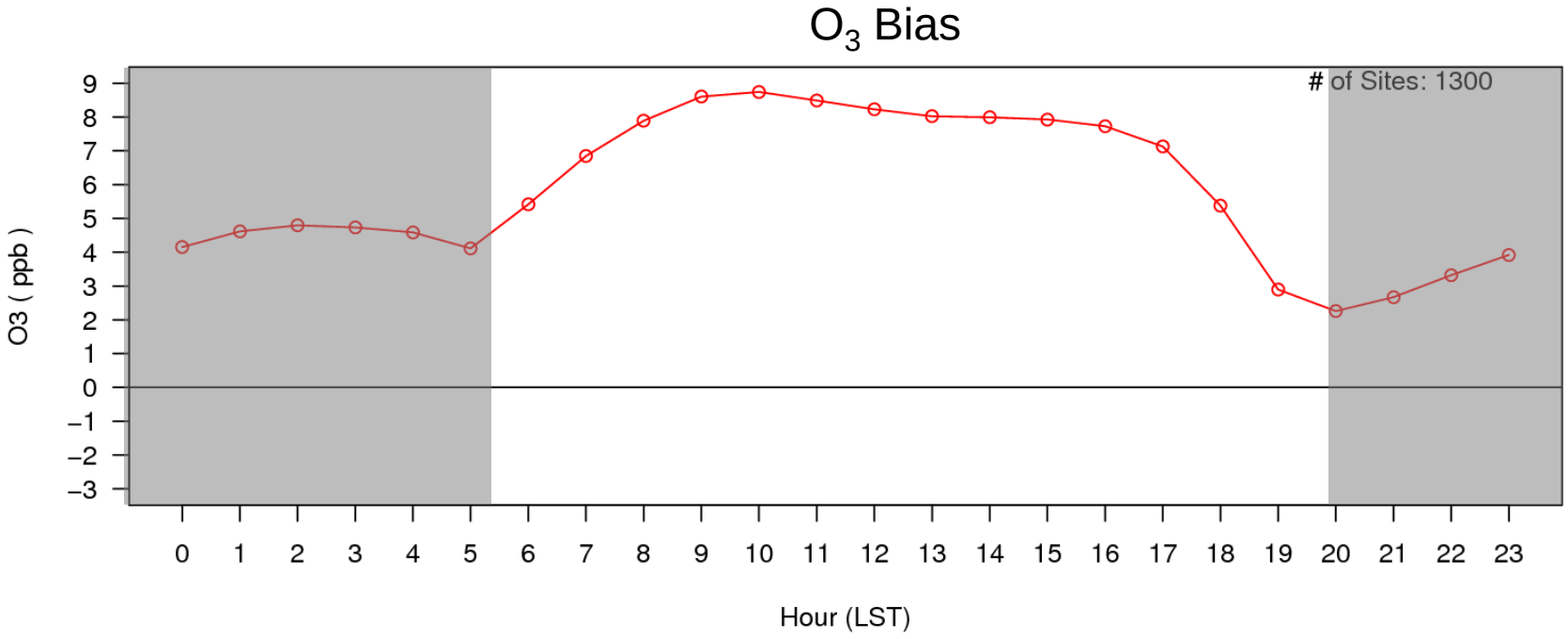
$PM_{2.5}$ Speciated Stacked Bar Plot





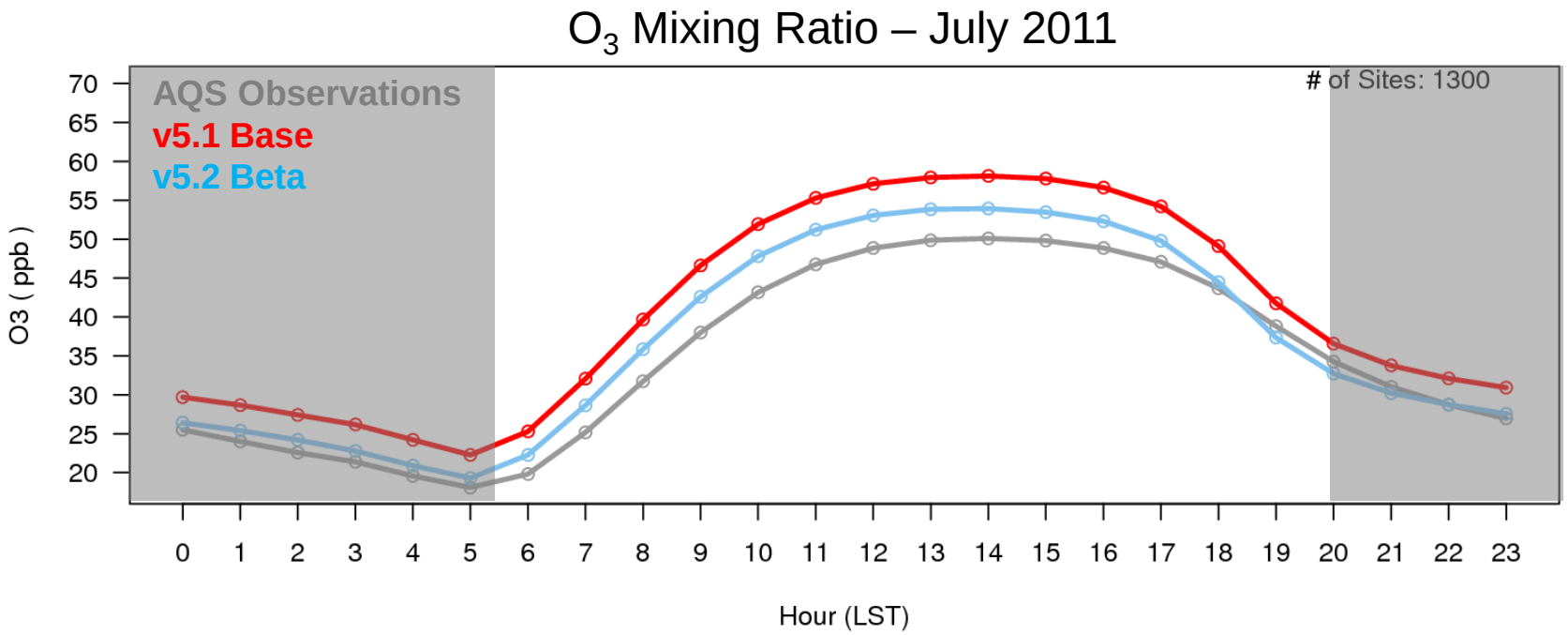
July 2011 Incremental Testing for O_3

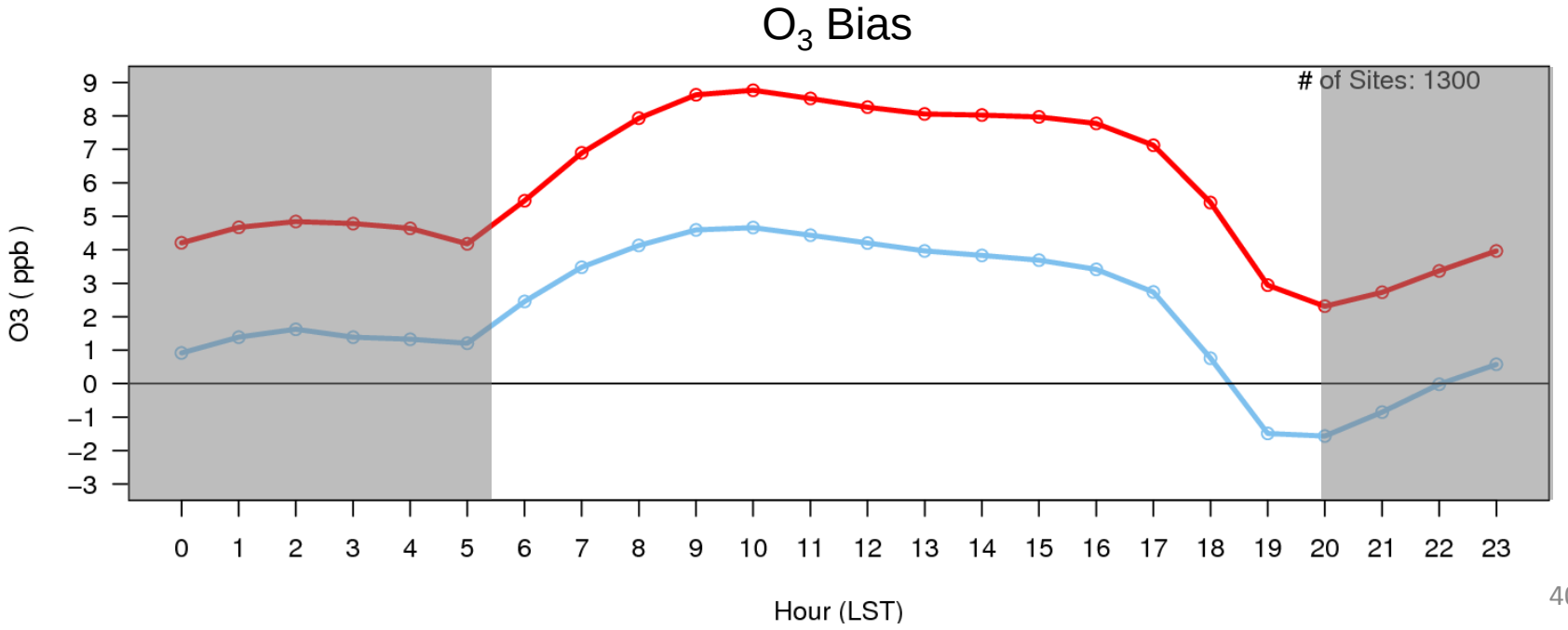




July 2011 Incremental Testing for O_3

Consistent decrease in O_3 bias across all hours in v5.2 compared to v5.1.

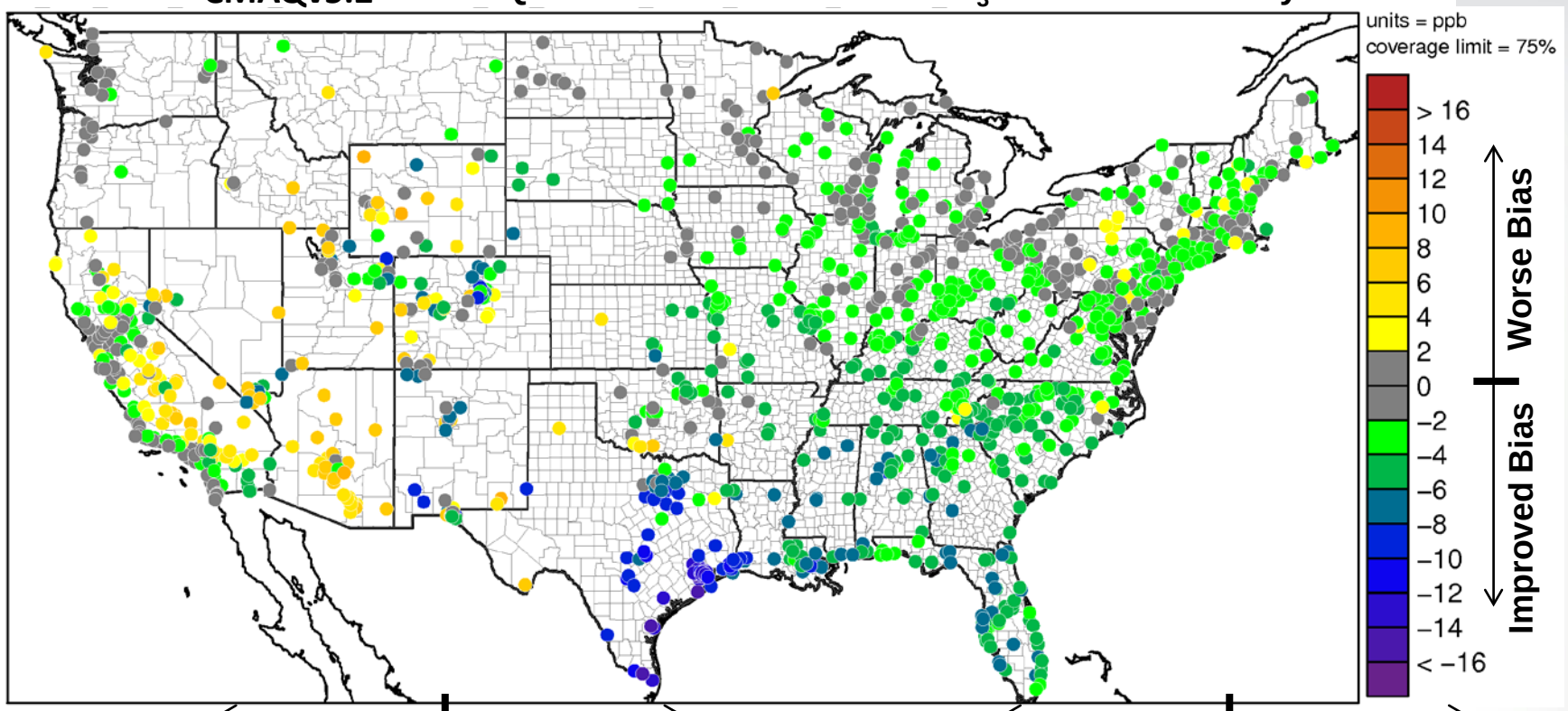


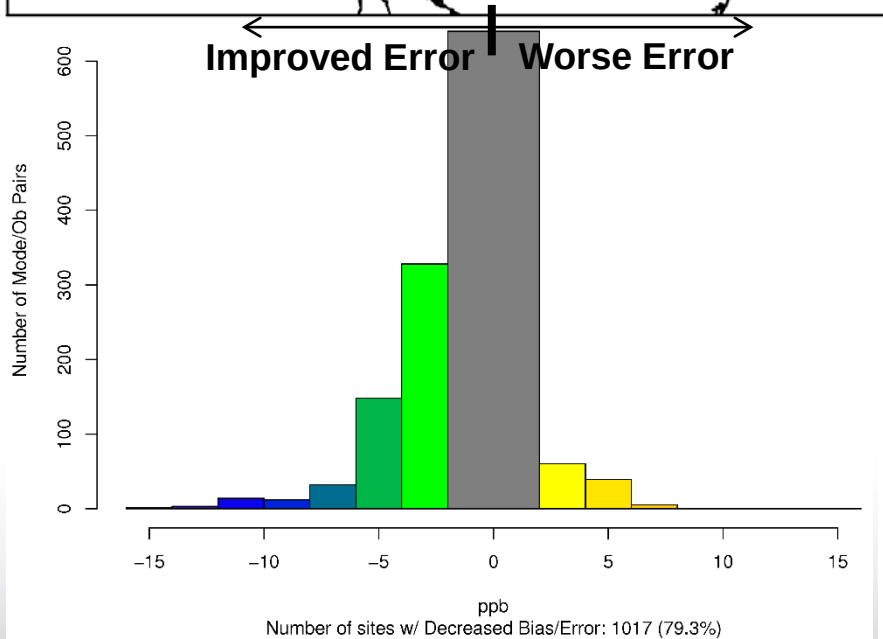


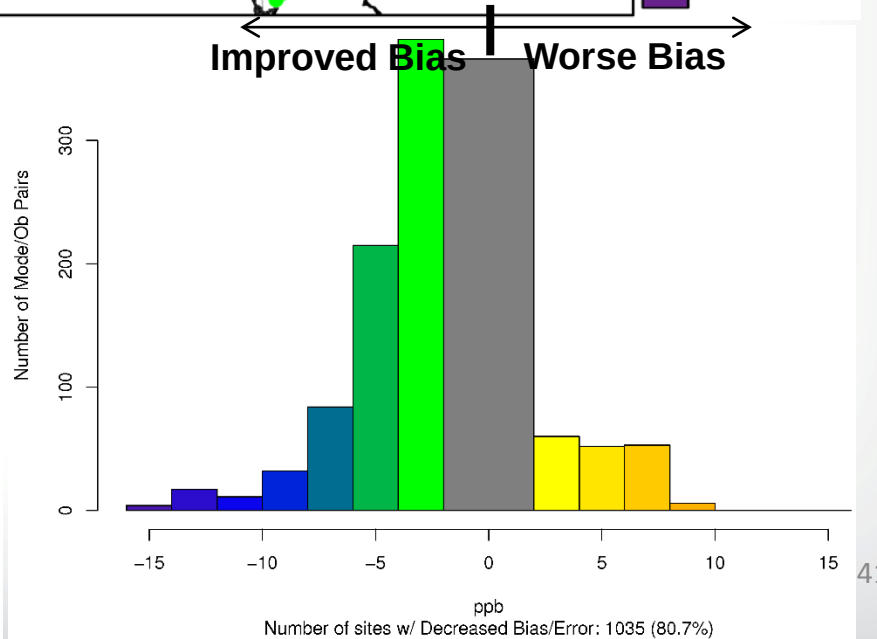
July 2011

Bias in modeled O_3 decreases at most location from v5.1 to v5.2

CMAQv5.2 – CMAQv5.1 – Difference in MDA8 O_3 Absolute Bias July 2011







CMAQ Evaluation Documentation and Tools

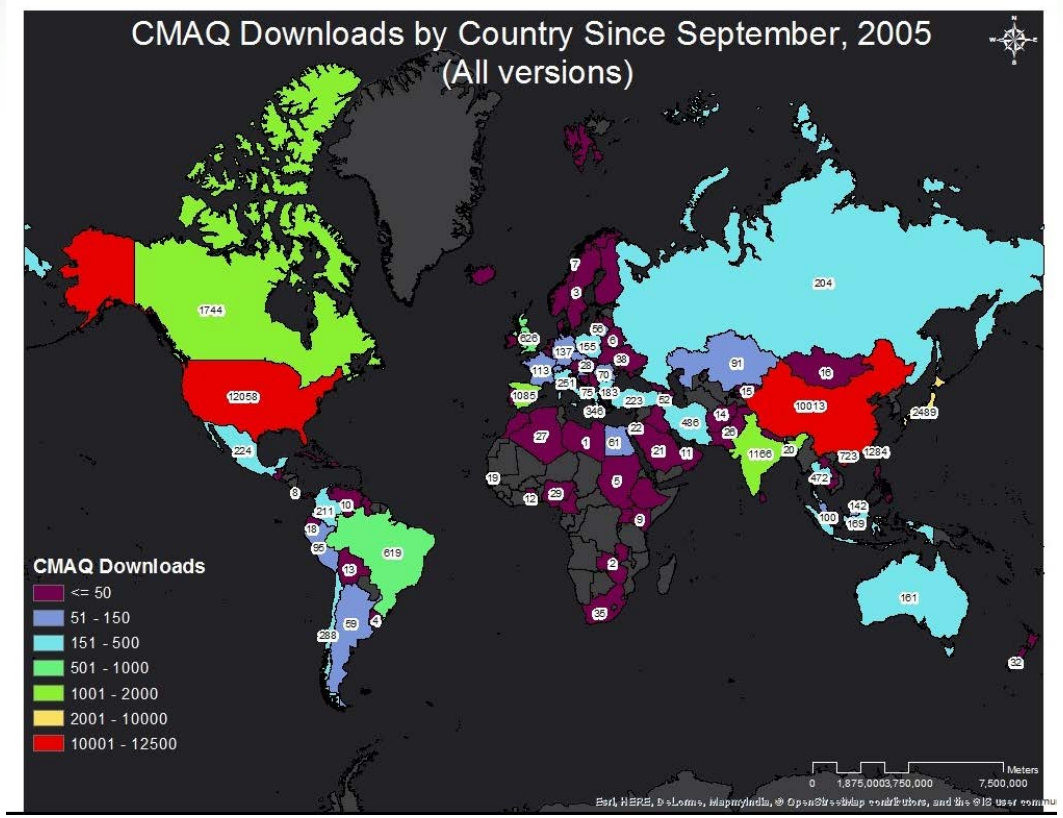
- **Model performance for v5.1 documented online:**

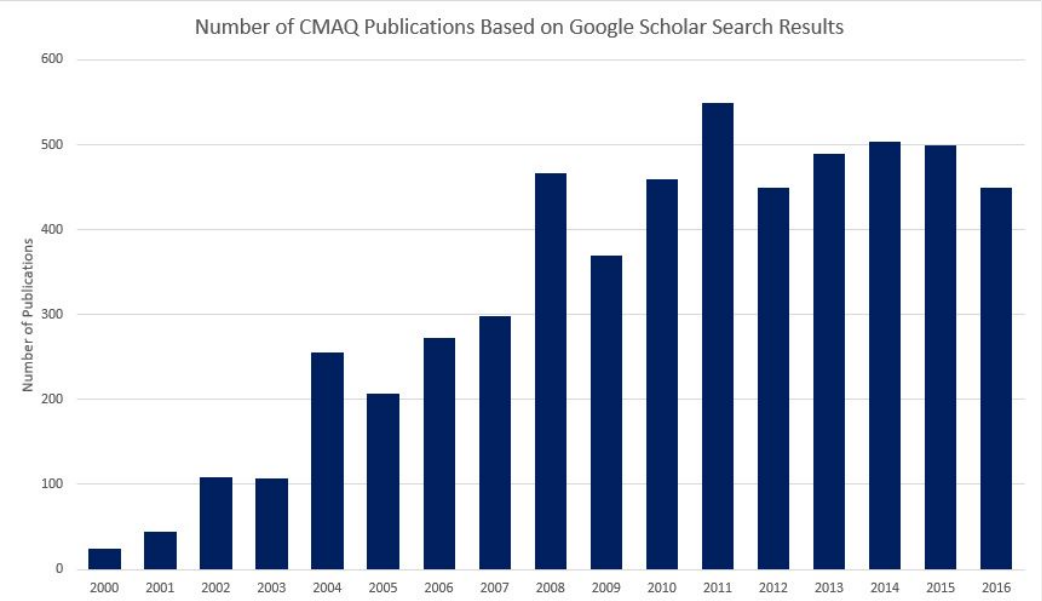
  Appel et al. (2017). Overview and evaluation of the Community Multiscale Air Quality (CMAQ) model version 5.1. Geosci. Model Dev. Disc., 1-41.

- **The release of v5.2 in June will correspond to updates in several evaluation tools:**
  - **New version of AMET (easier installation)**
  - **Updates to programs and scripts for post-processing CMAQ output to prepare for evaluation**
  - **New resources for users on CMAQ's new website: www.epa.gov/cmaq**

    (available June 2017)

Outreach & Dissemination

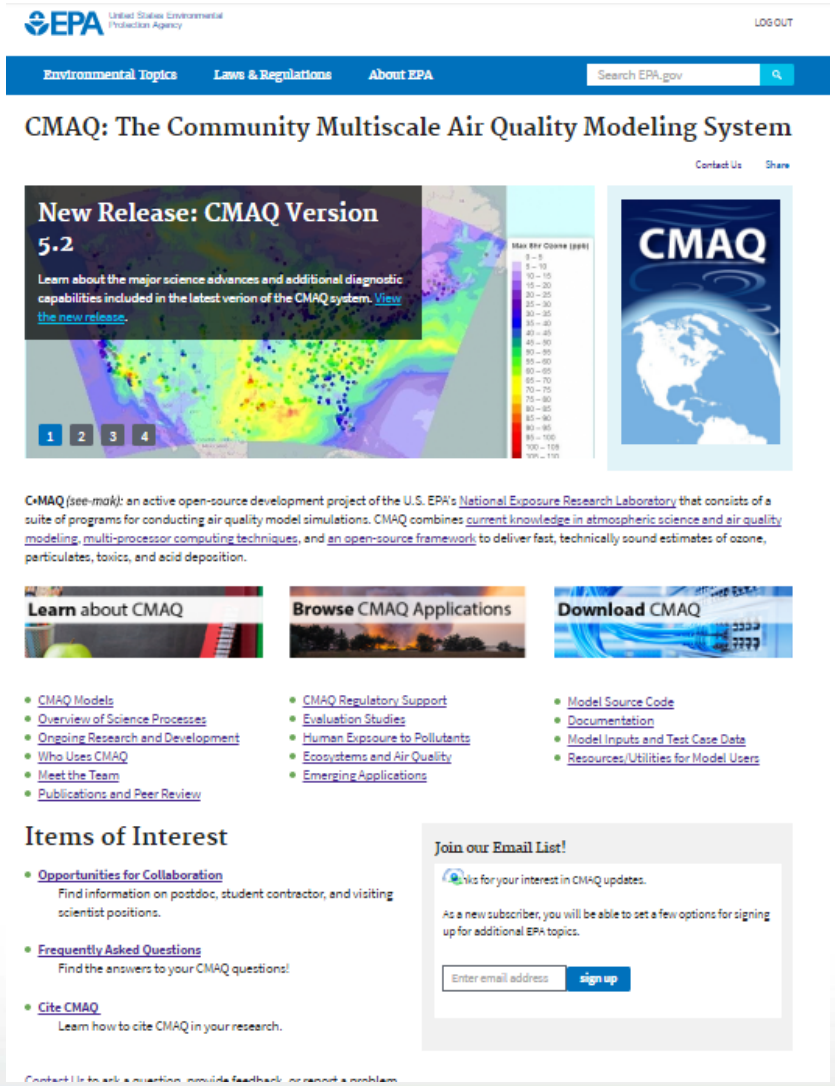


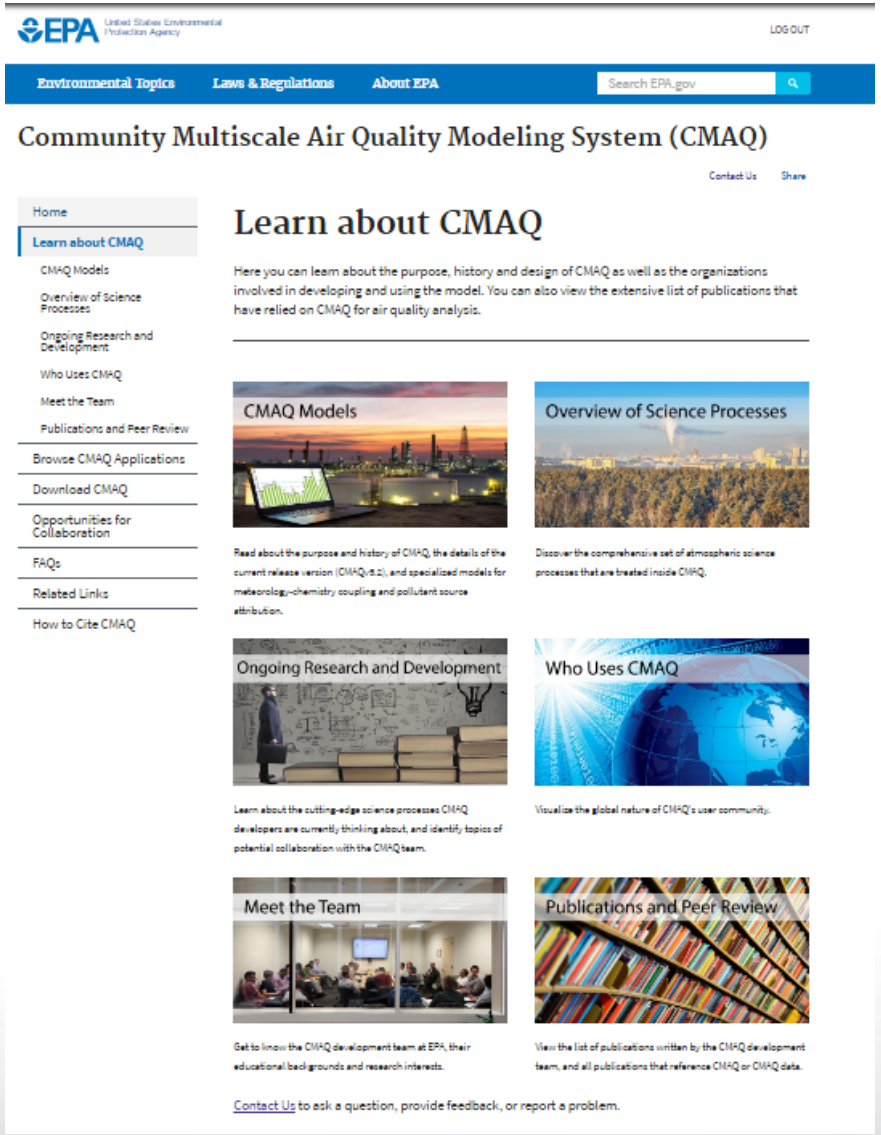


Periodic scientific updates to the CMAQ model have led to the creation of :

- Dynamic and diverse user community
- More robust modeling system
- Diverse applications supporting
  - Regulatory analysis by EPA & States (State implementation plans and rulemaking, Clean Air Interstate Rule, Clean Air Mercury Rule, Renewable Fuels Standard Act-2)
  - Air quality forecasting & public health advisories (NOAA, internationally)

www.epa.gov/cmaq [June 2017]





www.epa.gov/cmaq [June 2017]

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Download CMAQ

The sections below are for use by both new and veteran users of CMAQ. Users can access and download the newest CMAQ model code, read the updates for the latest version, download CMAQ test cases, or utilize the resources to assist in operating CMAQ.

Access CMAQ source code, step-by-step instructions for downloading the CMAQ base model, and guidance on building the two-way CMAQ system.

Find the release notes for recent versions of the model system, a CMAQ User's Guide, and helpful tutorials on common tasks.

Download test case data and instructions as well as additional model inputs.

Utilize the CMAS Center's help desk and training courses. Browse software programs for preparing CMAQ inputs as well as evaluating and visualizing CMAQ outputs.

Contact Us to ask a question, provide feedback, or report a problem.

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Community Multiscale Air Quality Modeling System (CMAQ)

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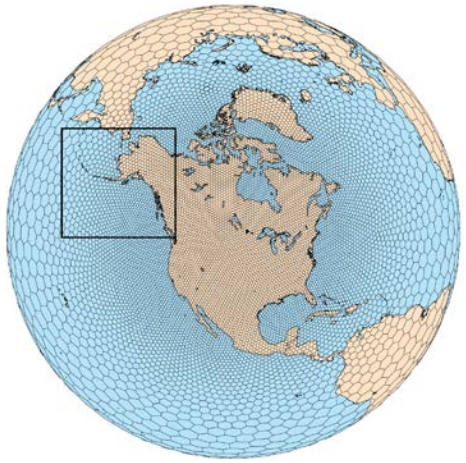
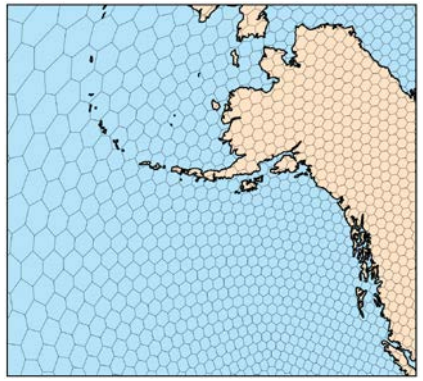
The CMAQ system has been used to address major environmental issues. Below are examples of how the CMAQ system provides information to help communities, states and countries determine the most effective strategies for reducing exposure to pollution.

Contact Us to ask a question, provide feedback, or report a problem.

Vision for Next Generation Model

- **The Next Generation model will be a 1-D AQ component coupled to meteorology models**
  - Chemical tracers to be transported in meteorology model
  - Can couple to multiple Meteorology models
- **Three configurations of flexible systems:**
  - On-line global variable grid (e.g. MPAS, OLAM)
  - Online regional (WRF-AQ)
  - Offline regional (WRF-AQ with offline chem transport)
- **One dimensional AQ component**
  - Gas, aerosol, aqueous in modular box
  - Modules for biogenic emissions, dry dep/bidi, wind-blown dust, photolysis, etc
- **Transport in met models for online systems (adv, diffusion)**
  - Ensure mass conservation
  - Consistency with met parameters
  - Minimize numerical diffusion and dispersion





MPAS

Additional Information

- **Download CMAQv5.2beta: https://github.com/USEPA/CMAQ**

- **For additional information, contact Shawn Roselle (roselle.shawn@epa.gov)**