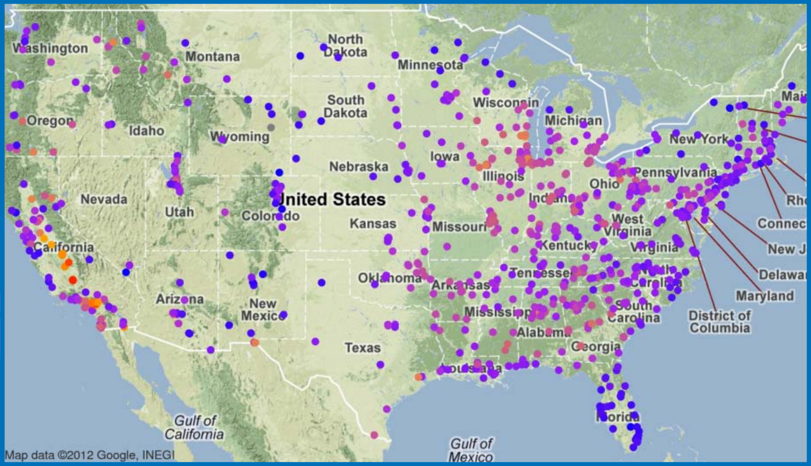
Single-Model Case Study: AQ Modeling for $PM_{2.5}$ NAAQS Regulatory Impact Analysis



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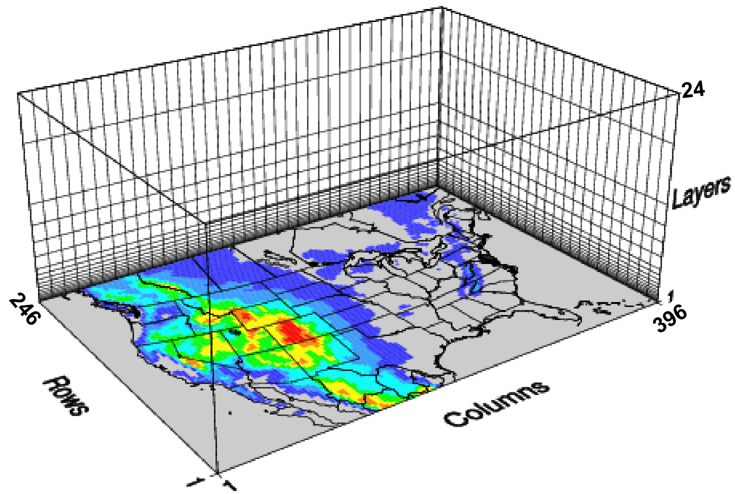
Outline

I. Background on air quality models
II. Single-model case study: $PM_{2.5}$ NAAQS RIA
III. Key considerations in single-model air quality projections
IV. Considerations in potential use of multiple models
V. Final thoughts

Air Quality Models

- AQ models simulate ozone, particulate matter ($PM_{2.5}$), toxics, acid deposition, visibility, etc. on 3-D fixed grid
- AQ models require inputs for emissions, meteorology, and initial & boundary conditions
- Two deterministic air quality models are used for regulatory modeling in US: CMAQ and CAMx*



Typical Configuration

- Horizontal resolution: 12 km x 12 km
- Vertical resolution: 24 layers
  - Lowest layer about 35 m deep
  - Model top at about 17.6 km
- Simulation period: 1 year

**CHIMERE is frequently used in Europe*

Source: Figure adapted from S. Arunachalam, http://airquality.gsfc.nasa.gov/uploads/data/CMAQ-Introduction-for-ARSET.ppt

Case Study Overview
$PM_{2.5}$ NAAQS Regulatory Impact Analysis

- In December 2012, US EPA strengthened the annual $PM_{2.5}$ National Ambient Air Quality Standards from 15 $\mu g/m^3$ to 12 $\mu g/m^3$
- US EPA was required to estimate the costs and benefits of the rule as part of a Regulatory Impact Analysis (RIA)
  - AQ modeling provided key inputs to the cost-benefit calculations performed in the RIA
- The purpose of the RIA is to provide information rather than to form the basis of AQ management decisions*
  - However, similar general approaches are used by states in air quality management decision-making for attaining AQ standards

**NAAQS levels are set based on health effects, not cost considerations*

AQ Modeling for the $PM_{2.5}$ NAAQS RIA

- **Goal:** To estimate future exceedances of the revised standard and the emissions reductions required for attainment
- **Steps:**

Project AQ to Future

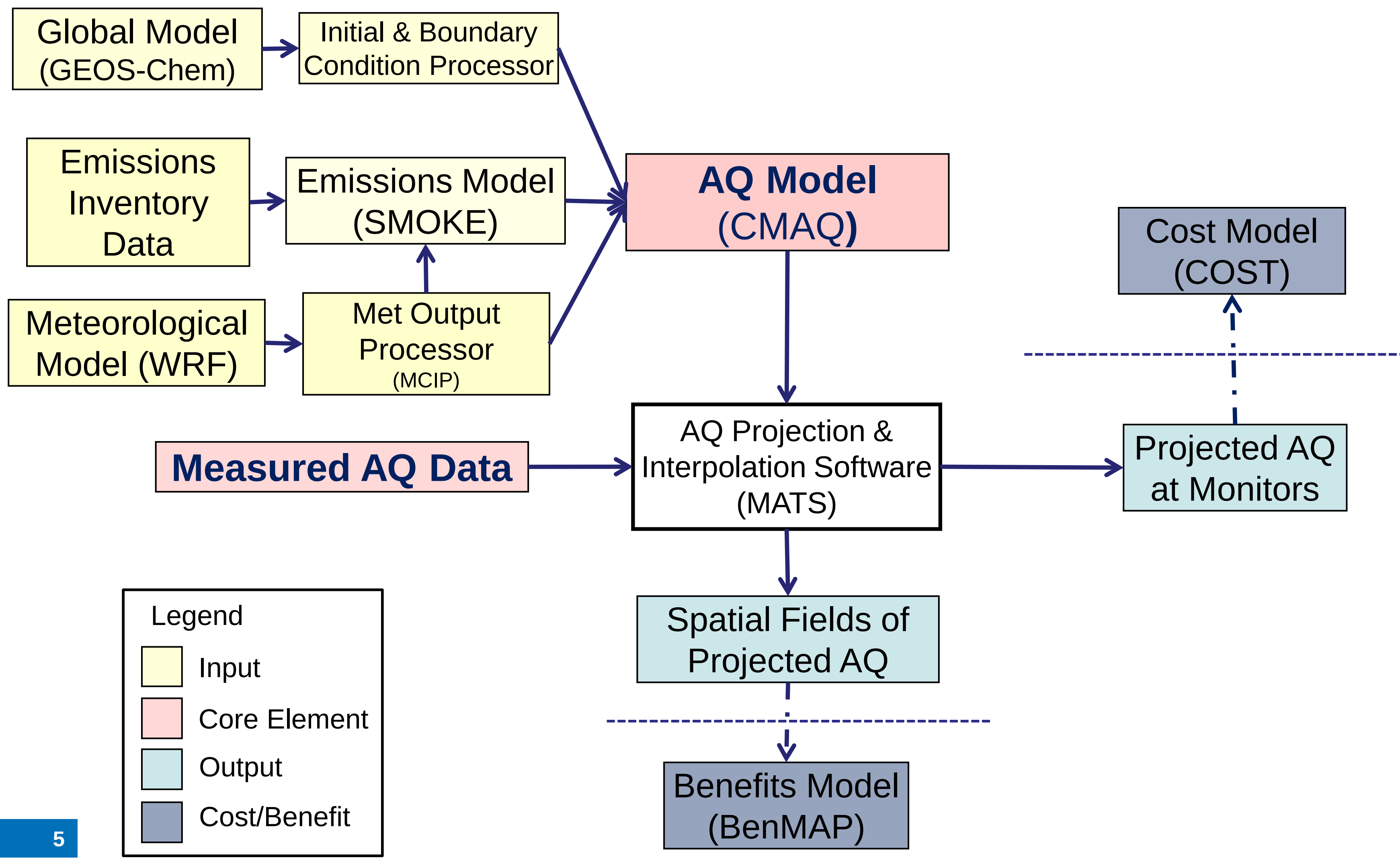
1) Calculate base-year ambient AQ value using observations
2) Simulate AQ for base year
3) Simulate AQ for future year
4) Project AQ value from the base year to the future year

Meet NAAQS Levels

5) Develop AQ response factors for emissions changes
6) Estimate the required emissions reductions and the costs and benefits of meeting the revised standard

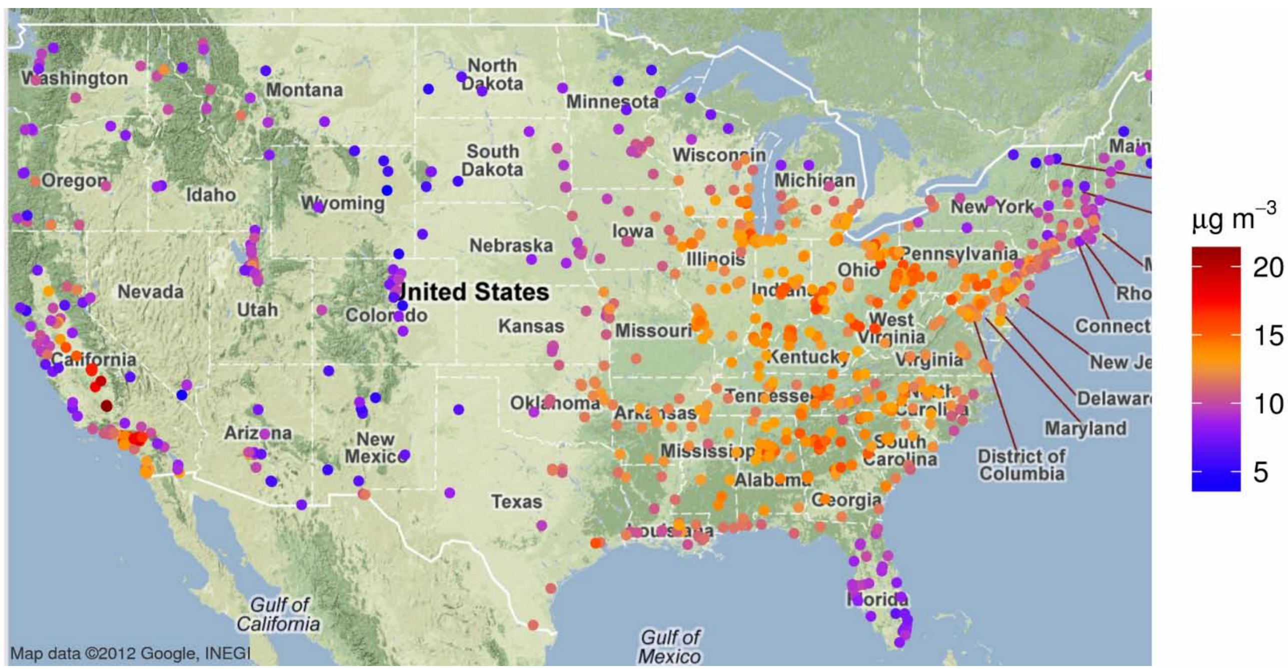
[*]The discussion of the PM2.5 NAAQS RIA is simplified in this presentation for clarity;
For details on the RIA, see the following: http://www.epa.gov/pm/2012/finalria.pdf

AQ Modeling Platform Components



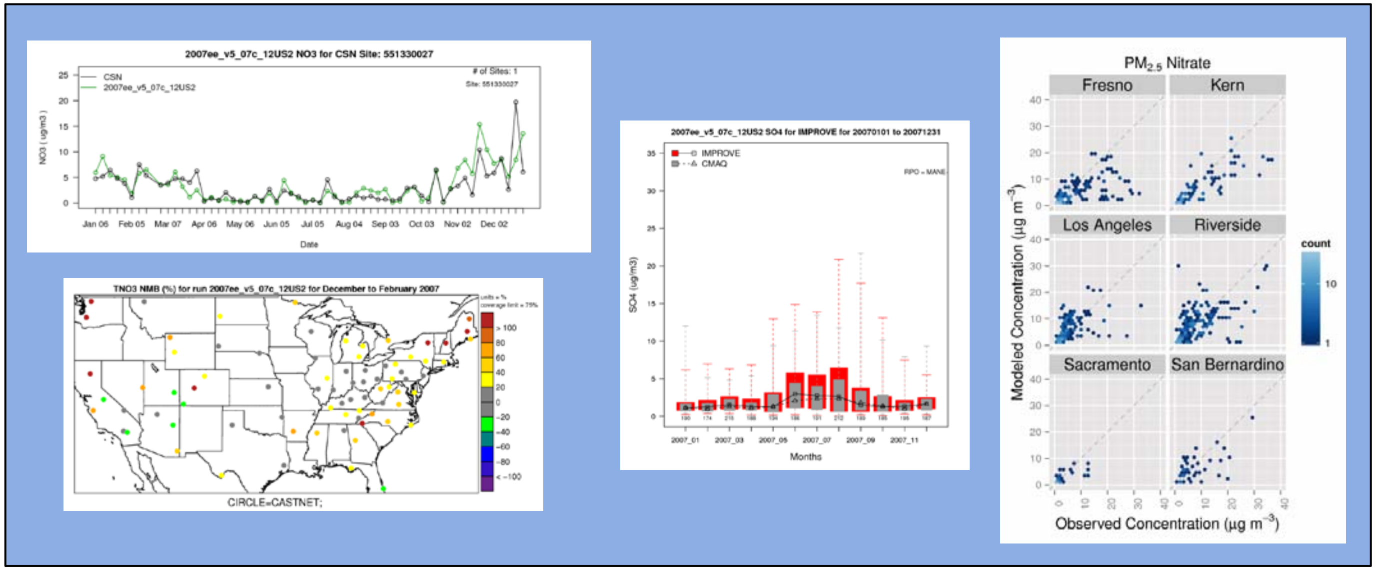
Step 1: Calculate Base-Year Ambient AQ Value

- Ambient base-year $PM_{2.5}$ is characterized using a 5-year weighted average of $PM_{2.5}$ observations at US sites
  - Average of three 3-year averages: 2005-2007, 2006-2008, & 2007-2009



Step 2: Simulate Base-Year Air Quality

- Create AQ model inputs for 2007 base year
  - Emissions: EGUs, mobile sources, residential wood combustion, etc.
  - Meteorology: Conduct simulation with WRF model & evaluate w/ observations
  - Boundary AQ: Conduct simulation with GEOS-Chem global AQ model
- Simulate AQ in US in 2007 using the CMAQ model*
- Evaluate predictions with observations: e.g.,

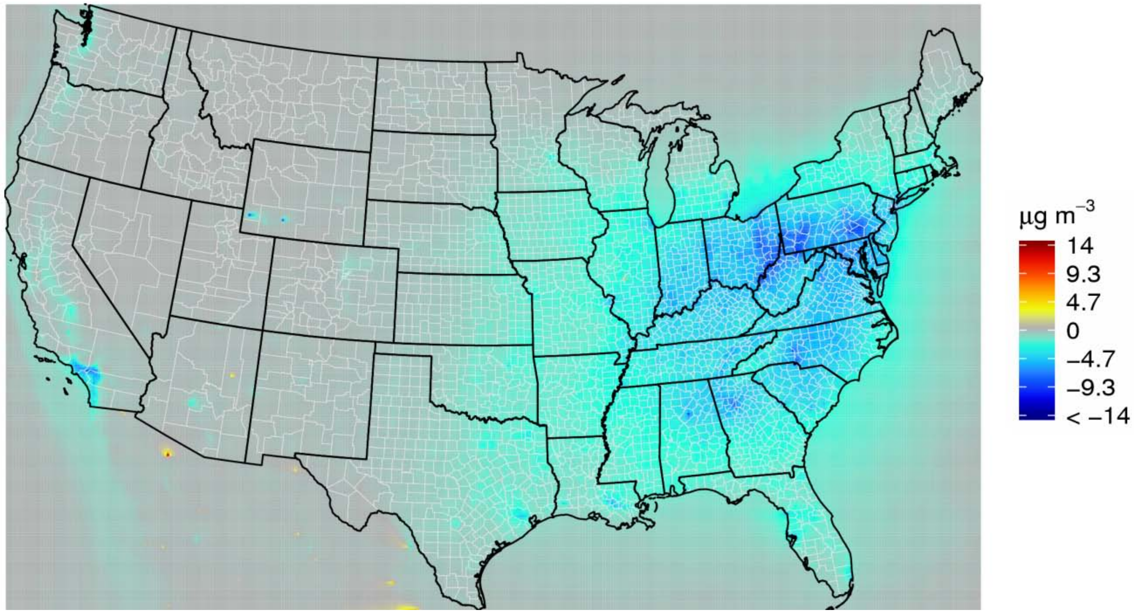


*CMAQ is the "Community Multiscale Air Quality Model"—a community based open-source regional air quality model developed by US EPA (http://www.cmaq-model.org/)

Step 3: Simulate Future-Year Air Quality

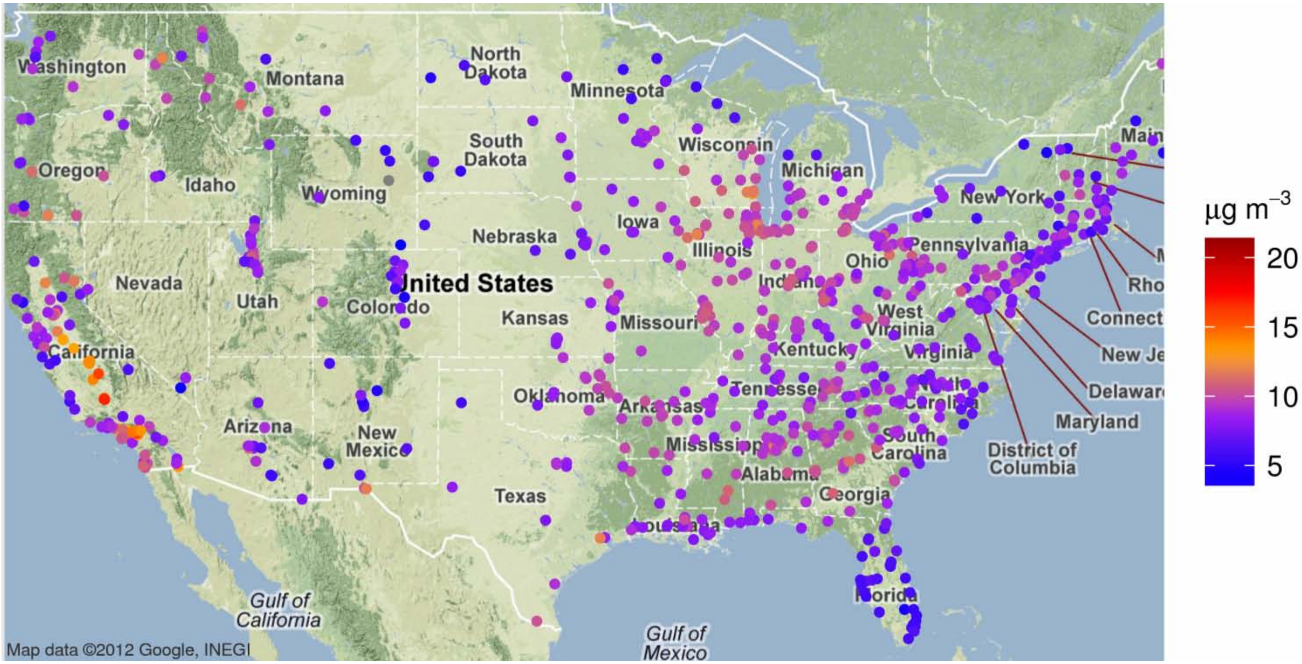
- Create AQ model inputs for 2020 future year
  - Emissions: Project emissions from 2007 based on “on-the-books” rules
  - Meteorology: Same as base-year simulation
  - Boundary AQ: Same as base-year simulation
- Conduct AQ simulation with 2020 emissions using CMAQ

August Average $PM_{2.5}$ Difference (2020 – 2007)



Step 4: Project Base-Year AQ to Future

- Project observation-based AQ value from base to future year
  - Multiply base AQ value by the ratio of modeled concentrations for the base year and the future year*
  - **Future AQ Value = Base AQ Value * (2020 Simulated / 2007 Simulated)**



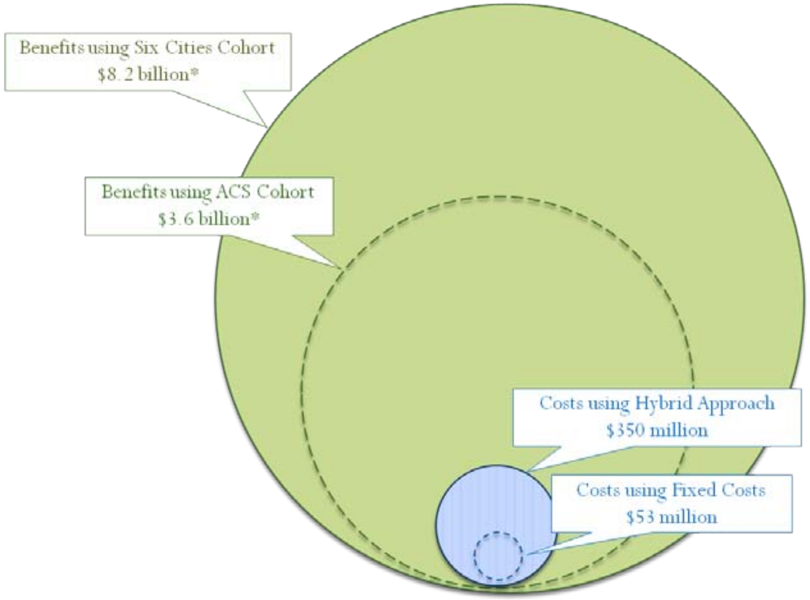
*The projection is performed on speciated basis (i.e., $PM_{2.5}$ components are projected individually using speciated model response)

Step 5: Estimate Future Exceedance Areas

- Some areas exceed the existing standards in projections
  - Two additional CMAQ simulations were conducted to estimate the local response of air quality to reductions in emissions
  - Identified Emissions reductions needed to meet existing standards
- Estimate counties that exceed revised standard after attaining existing standard

Step 6: Estimate Costs/Benefits of Rule

- Estimate additional reductions of emissions required to attain the revised standard level in the future year
- Estimate costs and benefits associated with the emissions reductions needed to attain the revised standard



Considerations in Single-Model Case Study

(I) Use of Models in a Relative Sense

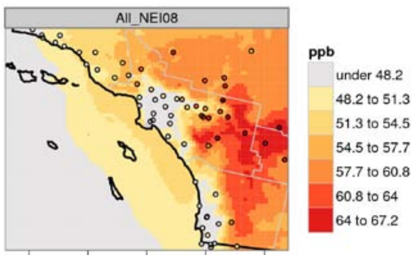
- Future simulated AQ is not directly used as an estimate of future AQ
- Instead, base-year observed AQ is projected to the future using the ratio of future-year to base-year simulated AQ
- Some evidence suggests that this “relative change” approach can be stable across AQ models
  - Hogrefe et. al. (2008; JAWMA):
    - Up to 20 ppb difference in ozone predictions by different AQ models
    - Less than a few ppb difference in projected concentrations between different AQ models
  - Model bias may cancel out to some degree in the ratio calculation

(II) Projections are Not a "Forecast" of the Future

- The base-year AQ value used in projections is based on multi-year averages of observed AQ values
  - Minimize impacts of inter-annual fluctuations in AQ for stable, data-driven projection starting point
- AQ simulations are based on a year with meteorology conducive to pollutant formation
  - Focus AQ management on conditions with pollution episodes
- Same meteorology is used in the base and future year AQ simulations
  - Isolate the impact of emissions changes from meteorology in projection ratios
- Weight-of-evidence analysis is used to corroborate modeled attainment demonstrations in State Implementation Plans
  - Considers observed levels, emissions trends, additional modeling, etc.

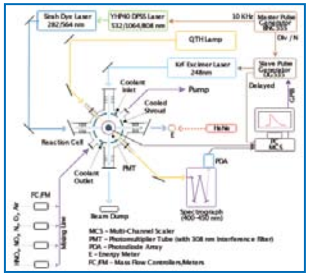
(III) Performance-Based Model Configuration

- Multiple AQ model configurations are possible
- Configure AQ models based on model performance and representation of the state-of-the-science



Mechanisms are incorporated in AQ models and tested with observations

Reaction rates and products are measured in the lab



Chemical mechanisms are developed

Reaction	Rate Constant
1. $NO_2 + h\nu \rightarrow NO + O$	Depends on the light intensity
2. $O + O_2 + M \rightarrow O_3 + M$	$6.0\times10^{-34}\,(T/300)^{-2.3}$ cm^6 molecule^{-2} sec^{-1}
3. $O_3 + NO \rightarrow NO_2 + O_2$	$2.2\times10^{-12}\exp^{(-1430/T)}$ cm^3 molecule^{-1} sec^{-1}
4. $O_3 + h\nu \rightarrow O(^1D) + O_2$	$0.0028k_1$
5. $O(^1D) + M \rightarrow O + M$	2.9×10^{-11} cm^3 molecule^{-1} sec^{-1}
6. $O(^1D) + H_2O \rightarrow 2OH\bullet$	2.2×10^{-10} cm^3 molecule^{-1} sec^{-1}
7. $CO + OH\bullet \rightarrow CO_2 + HO_2\bullet$	2.2×10^{-13} cm^3 molecule^{-1} sec^{-1}
8. $HO_2\bullet + NO \rightarrow NO_2 + OH\bullet$	$3.7\times10^{-12}\exp^{(240/T)}$ cm^3 molecule^{-1} sec^{-1}
9. $OH\bullet + NO_2 \rightarrow HNO_3$	1.1×10^{-11} cm^3 molecule^{-1} sec^{-1}

Parameterizations are tested using smog chambers

Figures adapted from Mollner et al. (2010) Science, 330(6004):646-649 and Rattanavaraha et al. (2011) Atmos. Environ. 45:3848-3855

Considerations in Potential Multiple-Model Studies

(I) How to Define the Scope of the Study?

- The number of the air quality “host” models is limited
  - Two primary models: CMAQ and CAMx
  - Each has certain unique features that may be critical for a given application
- However, the number of potential model configurations and simulations is vast
  - Many choices exist for process modules in each AQ model, global model, and meteorological model; additional choices exist for emissions data
  - Multiple runs are needed for a given application: e.g., base-year, future-year, emissions control, and sensitivity runs
- How to select a limited set of cases for multiple modeling?
  - Current single-model approach selects based on model performance and state-of-the-science

(II) Model Diversity

- Process representations and their limitations are similar across existing AQ models
  - Differences between models is likely small compared with the uncertainty space of interest
  - Unknown physics and chemistry is unknown to all models
  - Unknown future emissions changes will be unknown to all models
- Model diversity might be created by configuring AQ models with older modules or parameterizations
  - Should results based on simulations with low performing configurations be merged with those of high performing configurations?

(III) Legal Interpretations

- If it were possible to identify the true space of uncertainty, what would the legal implications be?
  - Does the Clean Air Act allow a probabilistic assessment or would only the most stringent model result be selected?

(IV) Time Constraints

- AQ modeling time constraints
  - Start Date: driven by the availability of emissions due to need to model a recent base year and account for recent rules in projections
  - End Date: driven by court order or other legal deadline (e.g., for SIPs)
- Approximate dates for RIA case study

Future-year emissions projections available	~August 15th
Future-year "on-the-books" simulation complete	~September 7th
Future-year control and sensitivity runs complete	~October 1st
AQ analysis deadline*	~October 15th

- Insufficient time for an additional simulation (>2 weeks)

** Driven by Dec. 14th court order deadline for rule*

Final Thoughts on Single-Model Approaches

- Select the model configuration based on model performance and representation of the state-of-the-science
- Characterize base-year conditions with observed values
  - Average base-year data as necessary for a stable starting point
- Project AQ to future using ratios of modeled values rather than directly using future concentration predictions
- Continually evaluate model predictions with data and revise parameterizations and model configuration accordingly