Multi-Pollutant Modeling Platform

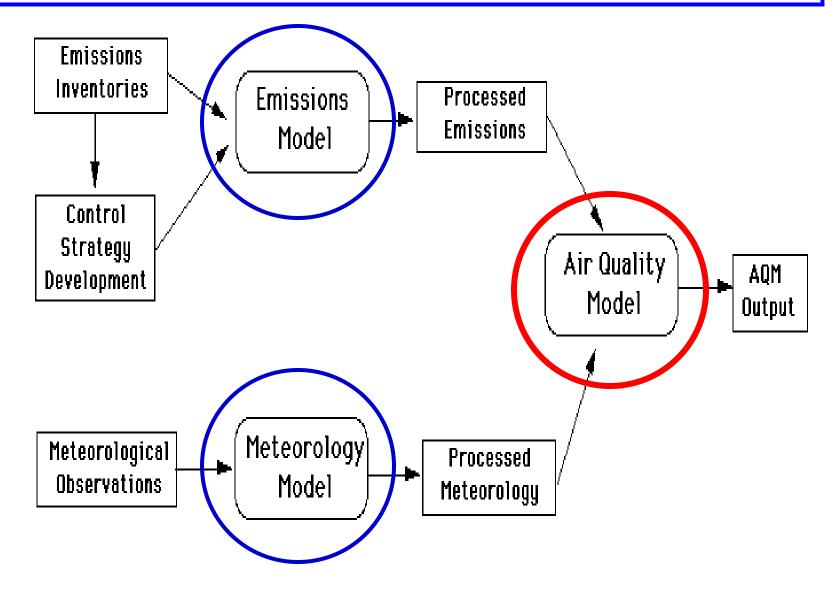
Lunchtime Seminar September 19, 2007

Overview

- What are air quality models?
- How do we use air quality models?
- What is a modeling platform?
- How can this platform be used?

What are air quality models?

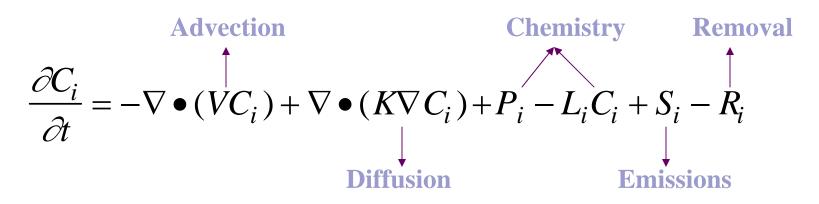
Basic Components of Air Quality Modeling System



Major Atmospheric Processes Simulated in AQ Models

- Chemical Transformations (Gas- & Aqueousphase and Heterogeneous Chemistry)
- Advection (Horizontal & Vertical)
- Diffusion (Horizontal & Vertical)
- Removal Processes (Dry & Wet Deposition)

Species Mass Continuity Equations :



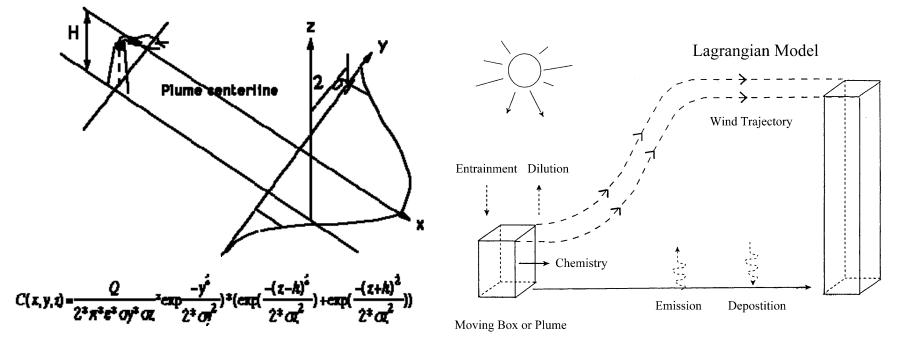
Evolution of Air Quality Models

- **1st-generation AQM** (1970s 1980s)
 - Dispersion Models (e.g., Gaussian Plume Models)
 - □ Photochemical Box Models (e.g. OZIP/EKMA)
- Independent of the second state of the seco
- **3rd-generation AQM** (1990s 2000s)
 - Community-Based "One-Atmosphere" Modeling System (e.g., U.S. EPA's Models-3/CMAQ)

First-Generation Air Quality Models

Gaussian Dispersion Model

Photochemical Box Model

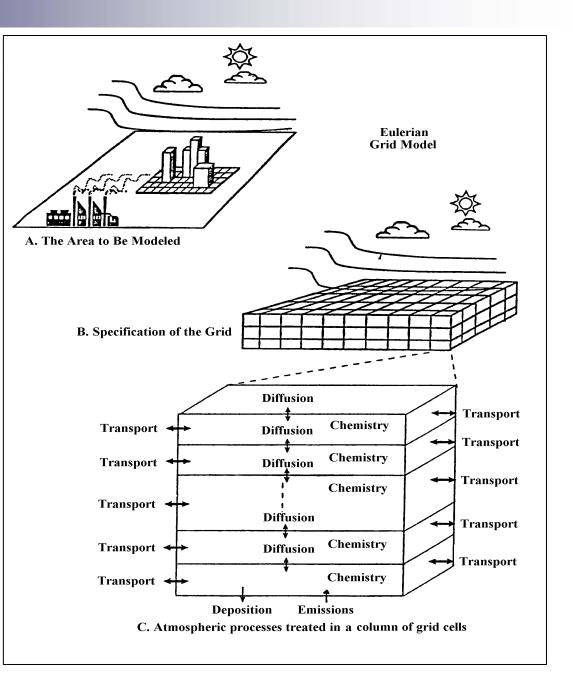


ISC3, CALPUFF, AERMOD (for primary pollutants)

OZIP/EKMA (for ozone)

2nd-Generation Air Quality Models

Photochemical Grid Models: UAM, RADM, REMSAD, ROM



Third-Generation Air Quality Models

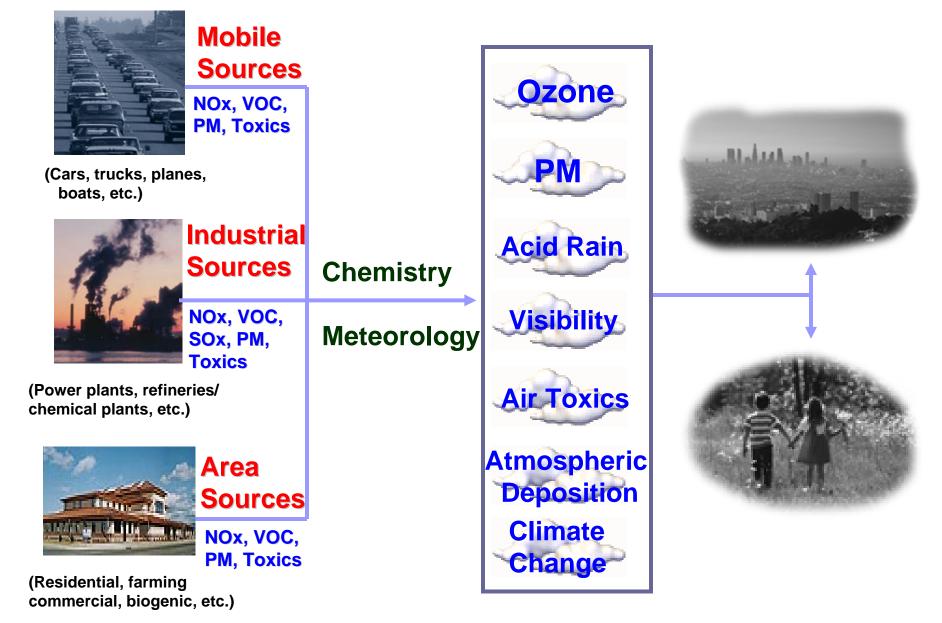
"One-Atmosphere" Modeling

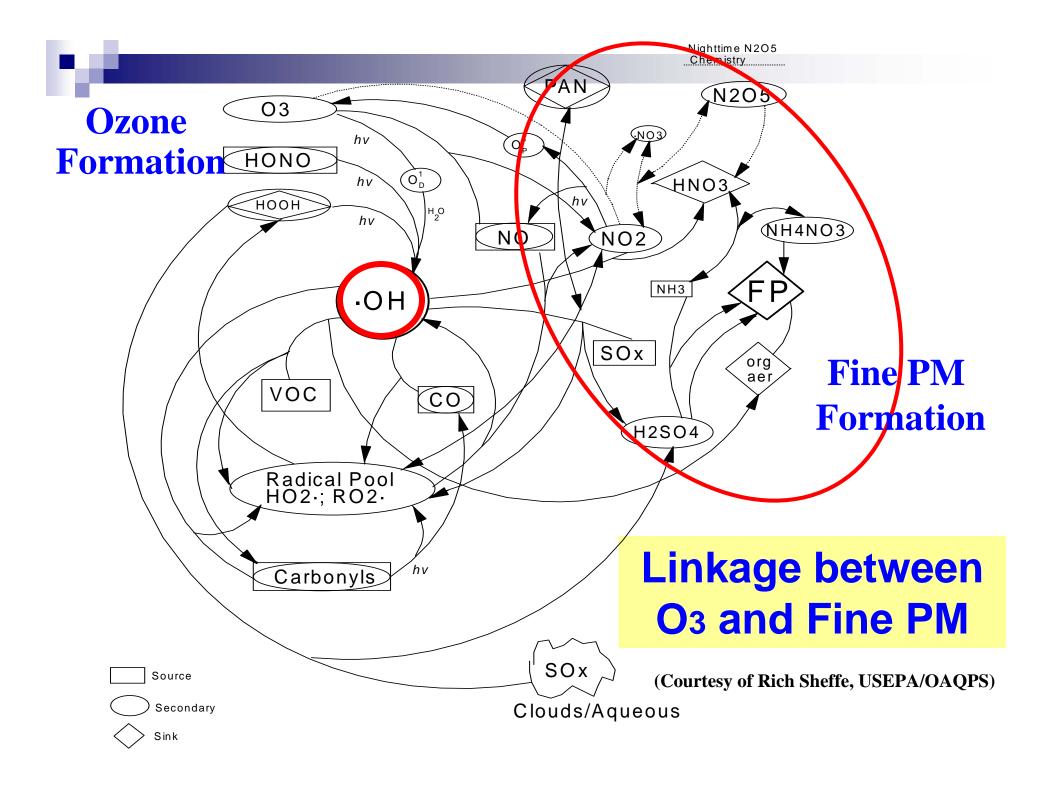
- Multi-pollutant: Ozone, PM, visibility, acid and nutrients deposition, air toxics, etc.
- Multi-scale: International, National, Regional, Local

Advanced Computer Technologies

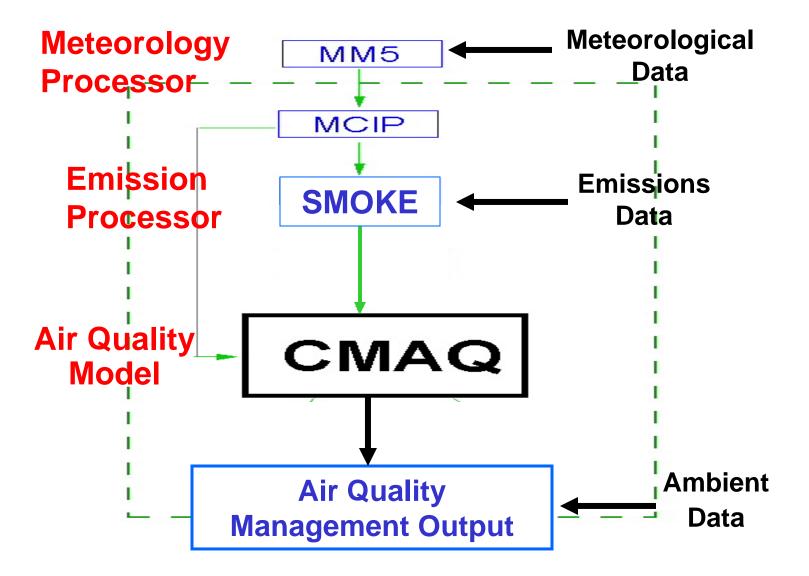
- Fast runtime (highly efficient for parallel & distributed computing) and cross-platform portability (supercomputers to PCs)
- Examples include CAMx and EPA's Community Multi-scale Air Quality (CMAQ) model
 - CMAQ code and documentation available from (http://www.cmascenter.org/)

One-Atmosphere Approach





Air Quality Modeling System



How do we use air quality models?

Why conduct Air Quality Modeling?

Legal and Adminstrative Requirements

- Clean Air Act and Amendments: Can serve as basis or legal justification for Agency action, e.g., OTAQ rules, NOx SIP Call, and CAIR.
- EO 12866 Regulatory Planning and Review: Provide critical inputs to conduct benefits assessment for 'major' rules

Inform Policy Development & Implementation

- NAAQS RIAs: Provides input to identification of "cost-effective" control measures for illustrative demonstration of achieving revised standard(s)
- Provide estimates of contributions to air quality concerns, e.g., CAIR, designations, and future multi-pollutant sector work
- State Implementation Plans (SIPs): Demonstrate attainment of NAAQS based on controls to be implemented by state/local agencies

Communication and Outreach

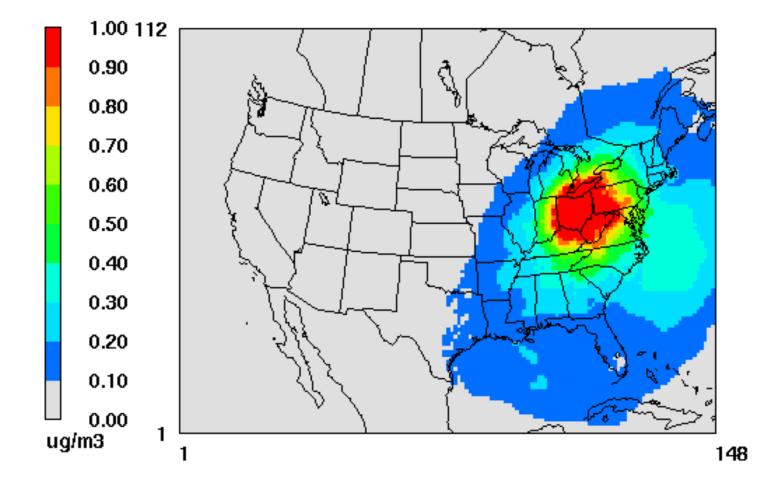
Provides answers to the questions of stakeholders and the public about effectiveness and impacts of actions, e.g., future projections of nonattainment and attainment with regulation.

"Relative Use" of Air Quality Models

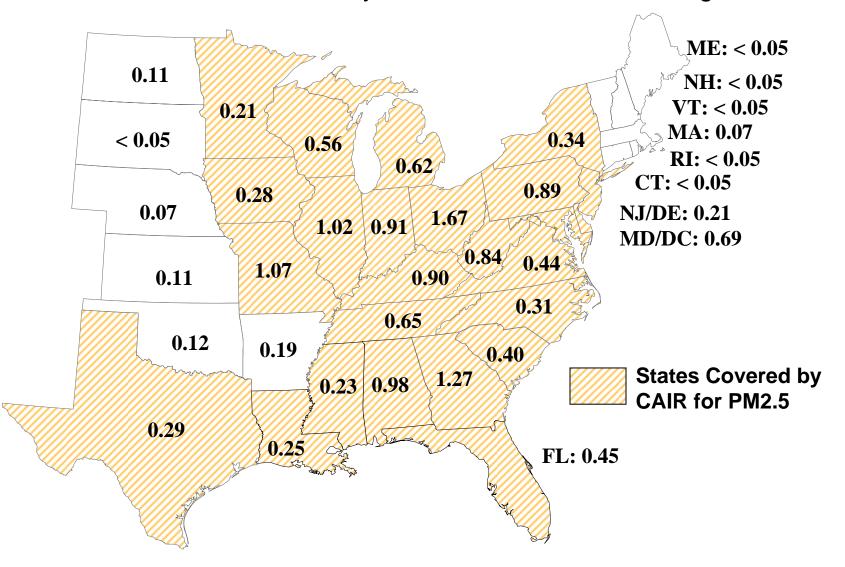
- We use model estimates in a "relative" sense
 - Premise: models are better at predicting relative changes in concentrations than absolute concentrations
- Relative Response Factors (RRF) are calculated by taking the ratio of the model's future to current predictions of ozone or PM2.5 species
 - RRFs are calculated for ozone and for each component of PM2.5 and regional haze

□ Therefore, Future DV = Current DV times RRF

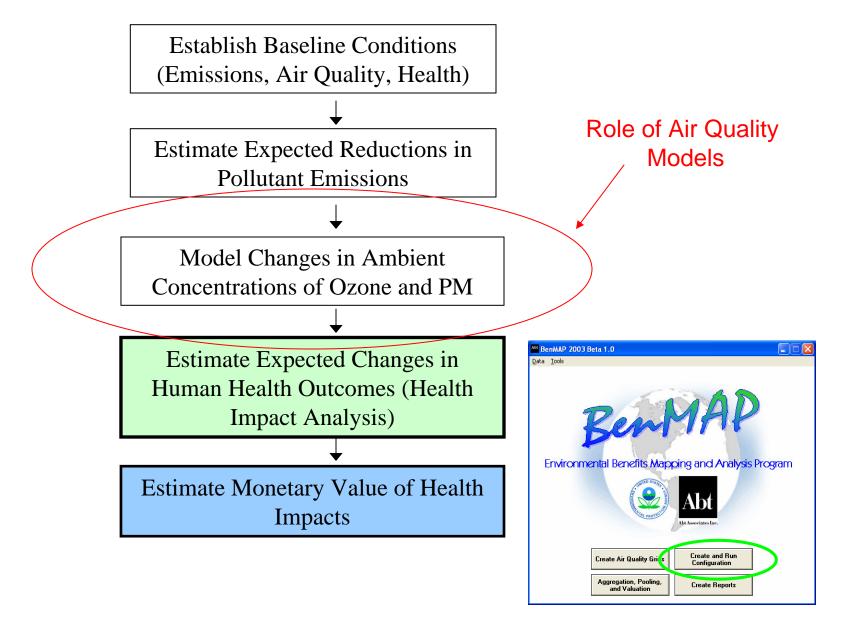
Projected ozone and PM2.5 concentrations are, thereby, "tied" to ambient measurements that provides a more robust and scientifically credible future projection of air quality. Contribution of SO2 & NOx Emissions in Ohio to Annual Avg PM2.5 - Based on Zero-Out Modeling for CAIR -



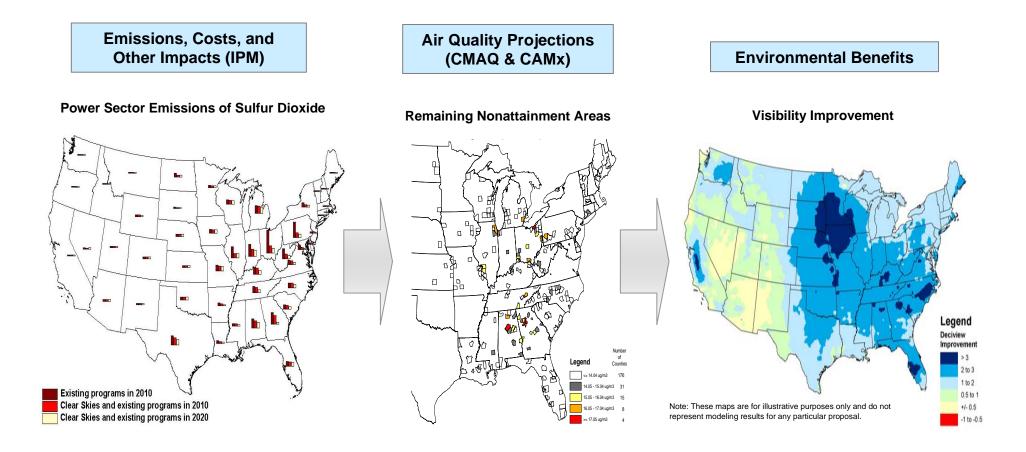
Maximum Contribution (ug/m³) to PM2.5 Nonattainment in Other States - Based on CAIR State-by-State Contribution Modeling -



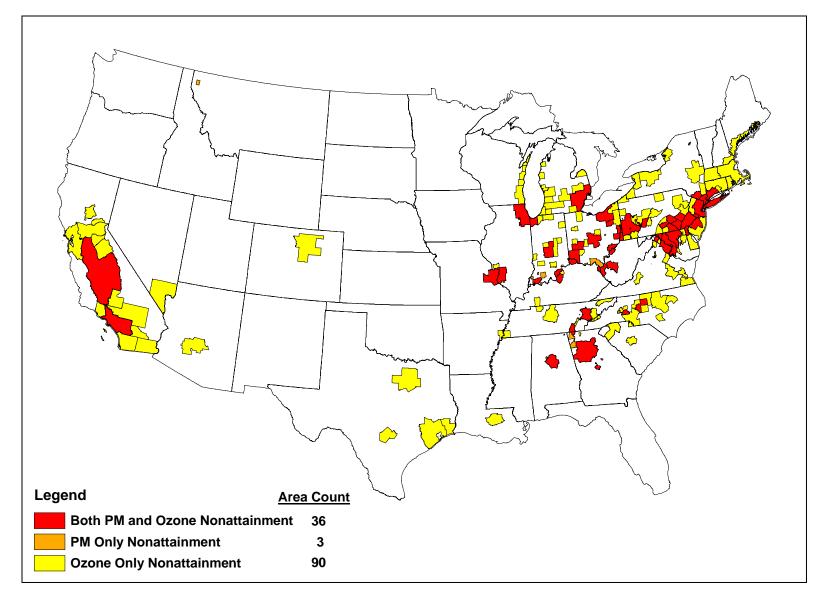
Elements of a Benefits Analysis



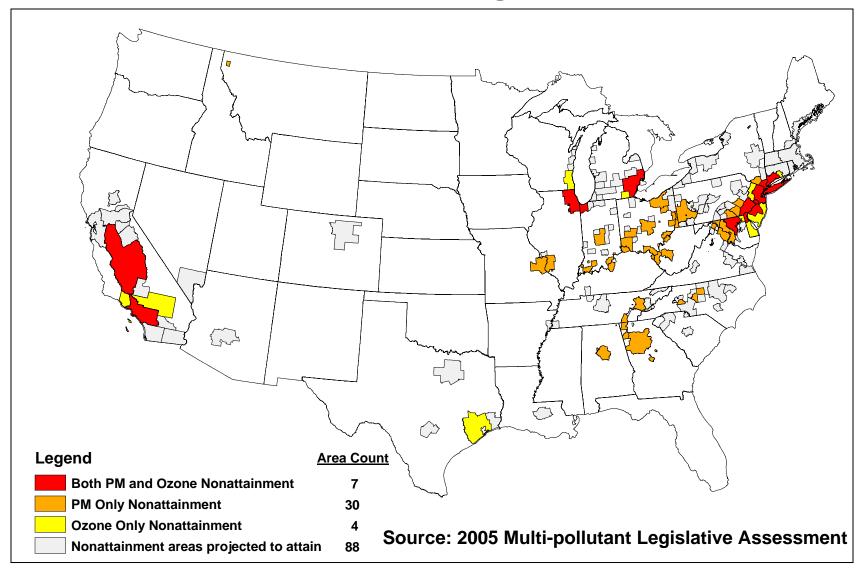
Role of Air Quality Models in Benefits Assessment



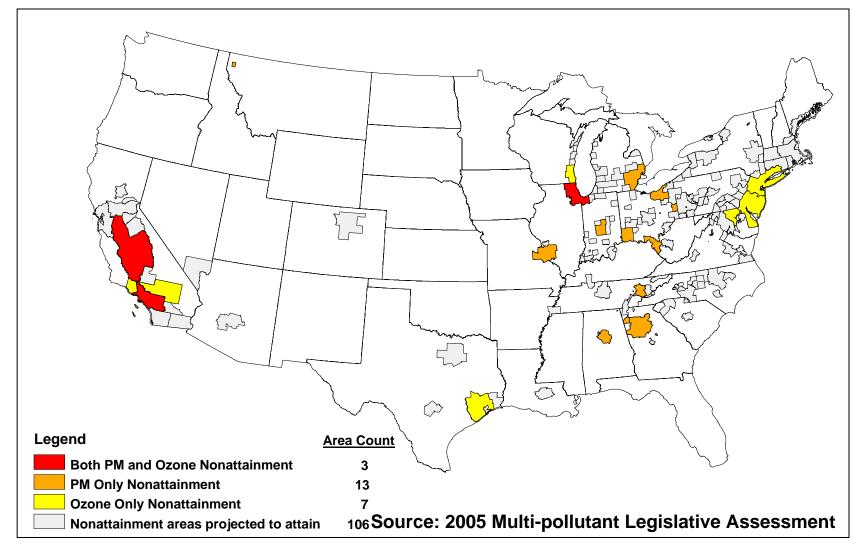
Areas Designated as Nonattainment for 8-Hour Ozone and/or PM2.5



Remaining Areas Projected to Exceed the PM_{2.5} and 8-Hour Ozone Standards in 2020 with Future Baseline Emissions Absent Additional Regional or Local Controls



Remaining Areas Projected to Exceed the PM_{2.5} and 8-Hour Ozone Standards in 2020 with CAIR-CAMR-CAVR Absent Additional Local Controls



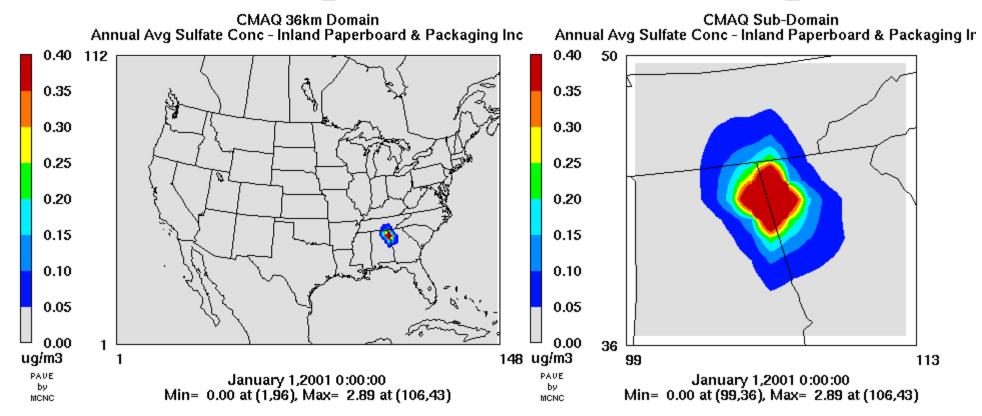
Air Quality Modeling Techniques: Contribution & Control Assessments

- Address source/pollutant "contribution" to air quality concern
 - Sector Zero-Out Modeling
 - Model simulation with "zero-out" of single or all pollutants from sector/sources of interest
 - Modeling Source Apportionment
 - Allows estimation of contributions from different source areas / categories within a single run
- Address relative efficacy of source/pollutant emissions reductions
 - Response Surface Modeling (among others)
 - A statistical "reduced-form" model of a complex air quality model
 - Used in PM NAAQS for control strategy development as part of illustrative attainment of revised standards

Annual Average Contribution to Sulfate: Pulp and Paper Example

ASO4_t2

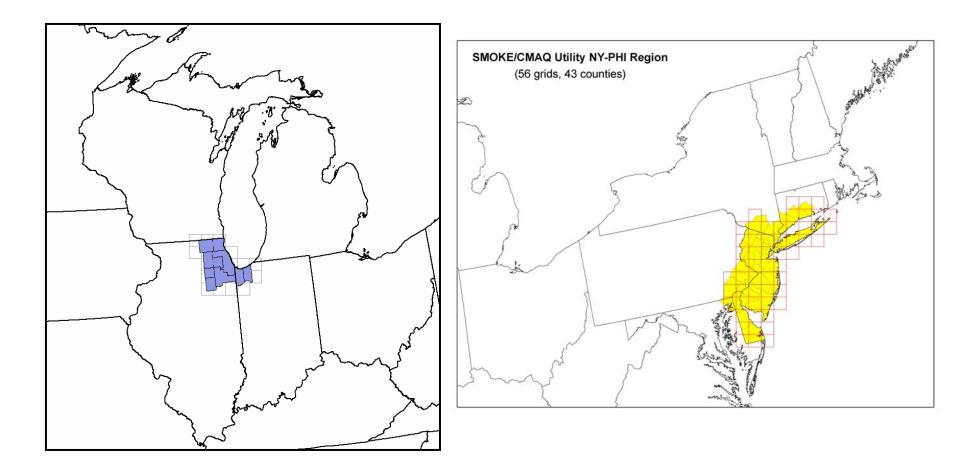
ASO4_t2



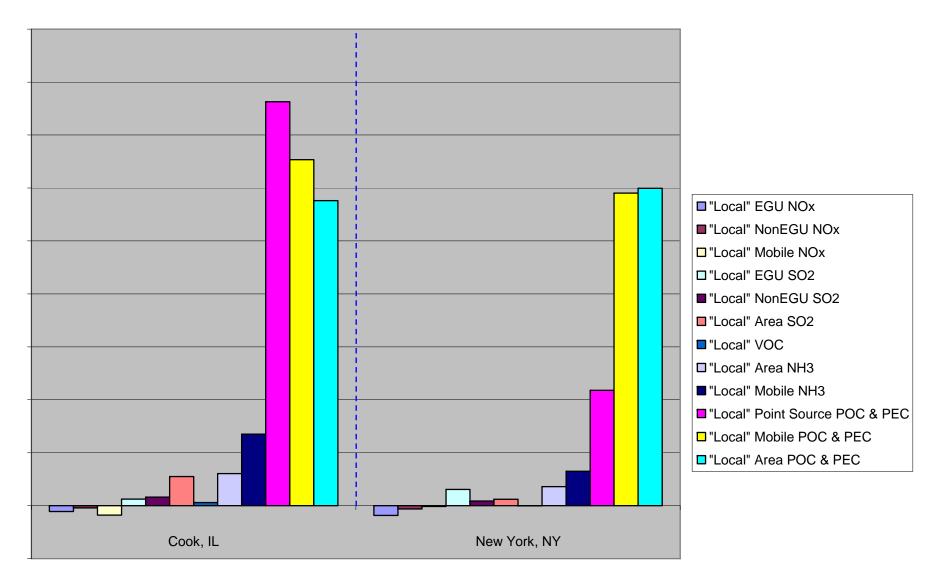
Selected Urban Areas of Focus for PM2.5 Response Surface Modeling

Chicago Urban Area

New York Urban Area



Relative Effectiveness Per Ton of "Local" Emission Reductions Across Sources and Precursor Pollutants



Relative effectiveness per ton in reducing ambient PM2.5 levels is only one factor in determining the appropriateness of controls. Cost effectiveness per microgram is the more complete measure, and reflects both the atmospheric response and costs of the controls.

What is a modeling platform?

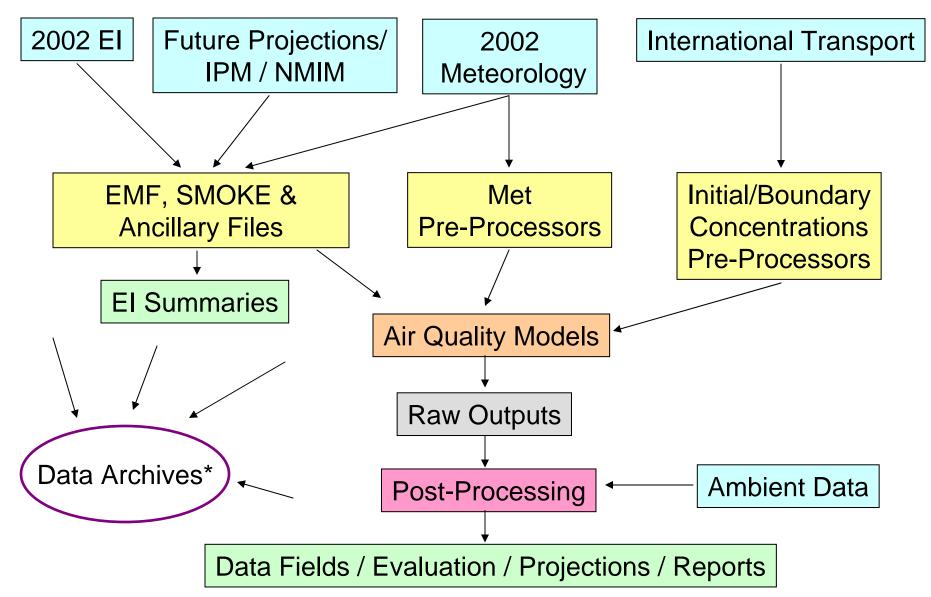
What is a "Modeling Platform"?

- Structured system of connected modelingrelated tools and data that provide a consistent and transparent basis for assessing the air quality response to changes in emissions and/or meteorology
- Currently, there are really two platforms
 - Regulatory Platform: CAPs-only with CMAQ used for regulatory analyses/future year projections
 - Multi-Pollutant Platform: CAPs + HAPs with CMAQ & AERMOD (local scale modeling for Detroit); no future projections for toxics
- Ultimately, certain aspects of these two platforms may merge into a single platform

Benefits of Using 2002 Modeling Platform

- Provide consistency, transparency, and efficient development of baselines for:
 - □ OAR regulatory assessments
 - CMAQ evaluations & research efforts by ORD
 - Accountability efforts across EPA
 - Public health & exposure assessments
- Promote multi-pollutant assessments
 - □ Integrated inventory (criteria and air toxics)
 - "One-atmosphere" CMAQ with AERMOD for selected urban areas
- Provide data and example for others outside of EPA

Modeling Platform Schematic Data Flow Diagram



*Working within OAQPS and with OEI on making modeled data available through RSIG and AirQuest

Components of 2002 MP Modeling Platform

- 2002 National Emissions Inventory (NEI)
 - Criteria and HAPs
- 2002 Meteorological Data
 - □ MM-5 and MCIP v3.1
 - Nationwide 36km
 - □ Separate eastern and western 12km
- Emissions Models, Tools and Ancillary Data
 - Emissions Modeling Framework (EMF)
 - □ SMOKE version 2.3.2, including BEIS3.13 and IPM 3.0
 - Ancillary data updates
- Emissions Projection Methodology
 - Consistent with approach developed for PM NAAQS
- Air quality models
 - □ CMAQ (v4.6.1i): nationwide
 - □ AERMOD (promulgation version w/ dep): Detroit and "other" urban area

2002 National Emissions Inventory

Best integration of CAPs and HAPs to date

Electric Generating Units (EGUs)

- CEM data for SO2 and NOx
- Other pollutants use state or filled-in data
- Mobile Sources
 - On-road mobile from states or NMIM using MOBILE6
 - □ Nonroad mobile from states or NMIM using NONROAD 2005
 - Aircraft, Locomotive, and Marine from national totals subdivided to counties, and state data
- NonEGU stationary point sources from state data
- Nonpoint (area) sources, including agricultural NH₃ from animals and fertilizer
- Wildfires and prescribed burning are (mostly) daily pointsource based data

Projection Method Overview (CAPs only for now)

- EGUs: Updated IPM model
- Stationary sources:
 - Known plant closures
 - National program controls: NOX SIP, Consent Decrees & Settlements, MACT program, Wood Stove changeouts
 - Removed spotty SIP info previously used in 2001 Platform
 - Animal Population growth from DOA/SPPD to project emissions of NH3 from animals

Mobile:

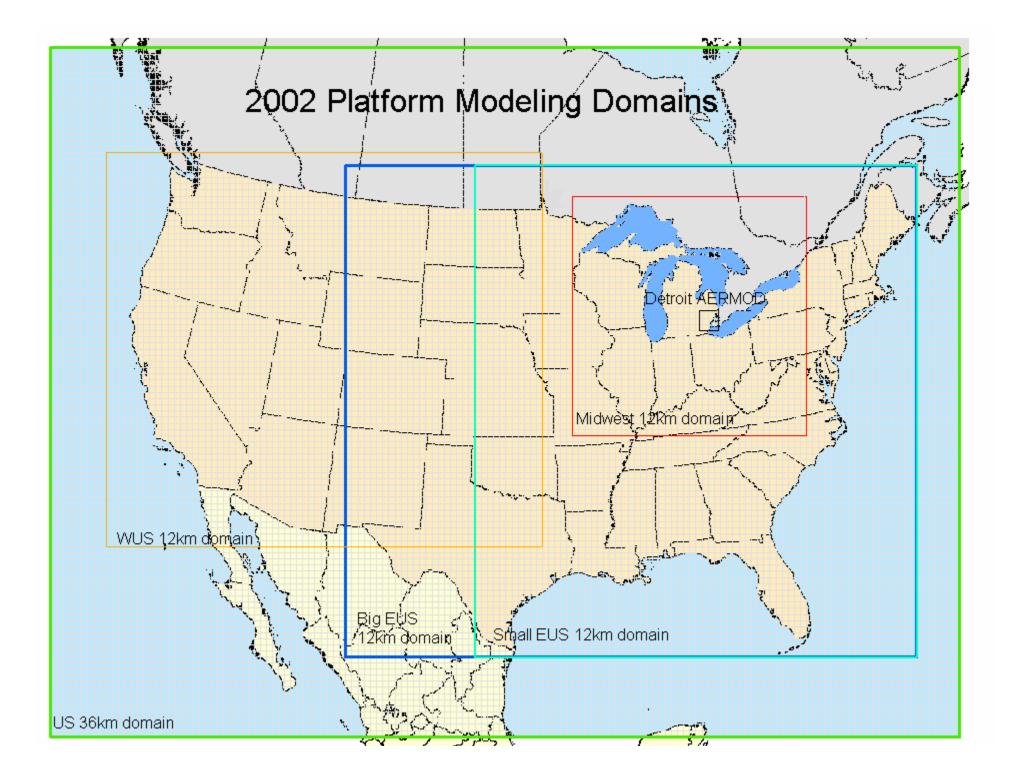
- □ Latest VMT projections in collaboration with OTAQ
- □ Use OTAQ's NMIM to project onroad/nonroad and gas stage 2
- Info on loco/marine from OTAQ
- □ LTO growth for aircraft
- □ Information from OTAQ on gas cans
- Fires: Created new average fire sector

SMOKE Emissions Processing

- Created SMOKE 2.3.2 specifically for platform
- Advanced custom scripts and new approaches
- Ongoing performance improvements for this FY
- Biogenics from BEIS 3.13 with 2002 meteorology
- EGUs: Hourly CEM data for SO2 and NOx (other pollutants follow hourly heat input)

Ancillary data updates

- □ SPECIATE4.1 speciation profiles via EMF's Speciation Tool
- New spatial surrogates vis EMF's Surrogate Tool
- □ New cross-references customized for CAP and CAP/HAP platforms



2002 Meteorological Data

Annual MM-5 Simulations

- □ 36 km US,12 km EUS,12 km WUS (from WRAP)
- Similar configuration as 2001 MM5 (but not identical)
- MM5 data processed via MCIP v3.1 into CMAQ
- Model evaluation indicated similar model performance as the 2001 MM5 simulations
 - Reasonable approximation of the actual meteorology
 - Primary concern: 2-3 deg C underestimation of temperature in the winter months.
 - Journal article fully summarizing evaluation findings will be available in 2008 (as part of CMAS).

Treatment of International Transport (Boundary Condition Concentrations)

- GEOSChem Global Chemistry Transport Model developed at Harvard Univ.
 - □ 2002 simulations of GEOSChem provided via ICAP
 - Domain covers entire globe: 2° x 2° grids and 30 layers up to the Stratosphere
 - Provides Boundary Conditions for CAPs and mercury and some other HAPS (e.g., formaldehyde) for our 36 km CONUS domain
- For toxics not simulated by GEOSChem we used concentrations based on remote measurements and values in the literature via joint effort with AQAG and ORD

Community Multi-Scale Air Quality (CMAQ)

- Photochemical grid model designed to simulate the formation and fate of ozone, oxidant precursors, primary and secondary particles, selected toxics, and deposition
- Latest 'interim' version from ORD is v4.6.1i which includes scientific updates and advancements compared to earlier versions:
 - Integrated "one atmosphere" modeling capabilities including 38 toxic pollutants (see list at end of briefing); ORD plans to include this version in 2008 release of CMAQ
 - Carbon Bond 05 photochemical mechanism with mercury and chlorine chemistry
 - □ Added heterogeneous reaction involving nitrate and added sea salt
 - Improved approach for treating convective mixing
- Next official release will be CMAQ v4.8 with improved SOA mechanism among other improvements

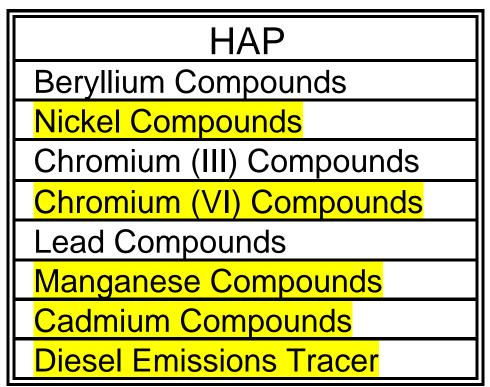
Gas Phase HAPs in CMAQ v4.6.1i

HAP	CAS#
Acrylonitrile	107-13-1
Carbon Tetrachloride	56-23-5
Propylene Dichloride	78-87-5
1,3-dichloropropene	542-75-6
1,1,2,2 - Tetrachloride Ethane	79-34-5
Benzene	71 - 41 - 2
Chloroform	67-66-3
1,2-Dibromomethane	106-93-4
1,2-Dichloromethane	107-06-2
Ethylene Oxide	75-21-8
Methylene Chloride	75-09-2
Perchloroethylene	127-18-4
Trichloroethylene	79-01-6
Vinyl Chloride	7501 -4
Naphthalene	91-20-3
Quinoline	91-22-5
Hydrazine	302-01-2
2,4 <mark>- Toluene Diisocyanate</mark>	584-84-9
Hexamethylene 1,6 -Diisocyanate	822-06-0
Maleic Anhydride	108-31-6
Triethylamine	121 - 44 - 8
1,4-Dichlorobenzene	106-46-7
Total Formaldehyde	50-00-0
Total Acetaldehyde	75-07-0
Total Acrolein	107-02-8
1, 3 -Butadiene	106-99-0
Formaldehyde Emissions Tracer	50-00-0
Acetaldehyde Emissions Tracer	75-07-0
Acrolein Emissions Tracer	107-02-8

НАР	CAS#
toluene	108-88-3
o-xylene	95-47-6
m-xylene	108-38-3
p-xylene	106-42-3
methanol	67-56-1
Hydrochloric acid	7647-01-0
chlorine	7782-55-5

National or Regional Risk driver in NATA 1999

Aerosol Phase HAPs in CMAQ v4.6.1i



National or Regional Risk driver in NATA 1999

Multi-Phase HAPs in CMAQ v4.6.1i

Mercury

AERMOD Modeling: Detroit

- AERMOD is an advanced steady-state plume dispersion model developed by AMS/EPA Regulatory Model Improvement Committee (AERMIC)
- Current draft version will be used
 - □ Includes dry and wet deposition algorithms based on work by ANL
 - Allows multiple urban areas to be defined (will use Detroit MSA and Ann Arbor MSA)
 - New option for varying emissions by hour-of-day and day-of-week (HRDOW7)
- Link-based emissions based on AREA source algorithm with some comparisons to VOLUME source approach
- 2002 meteorological data derived from draft MM5-AERMOD Tool for Detroit

Key Modeling Outputs

- Concentrations of O3, PM2.5 species, mercury, and other toxics
 - Gridded fields used as inputs to BenMap for calculating health benefits of control strategies
- Wet/dry deposition of sulfur, nitrogen (oxidized/reduced), mercury, and toxic species
 - □ Gridded fields used as inputs to Water/Eco models
- Model evaluation and improvement in coordination with ORD
- Projected O3 and PM2.5 design values by monitoring site; used for determining future attainment and residual nonattainment
- Projected visibility at Improve sites in Class I Areas
- CMAQ/AERMOD "Hybrid Approach" providing estimates of fine scale PM2.5 and toxics
- O3 and PM2.5 are used as inputs to "data fusion" for CDC/Phase project

Highlights of 2002 Model Evaluation for CAPs [we can provide separate briefings with details]

- Ozone
 - □ Under predicted for 1-hr and 8-hr daily max. especially O3 > 60 ppb
 - □ Similar to performance for 2001
- Sulfate PM
 - □ Under predicted (~up to 25%) for all seasons in the East and West
 - □ Similar to performance for 2001

Sulfur Dioxide

- □ Over predicted (~35 to >100%) in all seasons in the East and West
- □ Similar to performance for 2001

Nitrate PM

- Over predicted (~30 to > 100%) in the Fall, Winter, and in northern areas of the East in the Spring
- □ Significantly different than performance for 2001

Highlights of 2002 Model Evaluation for CAPs

Organic PM

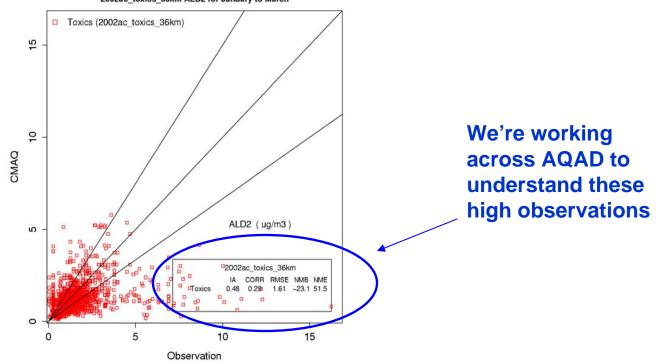
- Over predicted in the North and under predicted in South and West in the Winter
- □ Under predicted in all areas (~25 to 65%) in Fall, Spring, and Summer
- □ Similar to performance for 2001

Elemental Carbon

- Mostly over predicted in urban areas (~45 to >100%) in all seasons in the East and West
- Mostly under predicted in rural areas (0 to >35%) in all seasons in the East and West
- □ Similar to performance for 2001

Multi-Pollutant CMAQ Evaluation: (CAPs + HAPs)

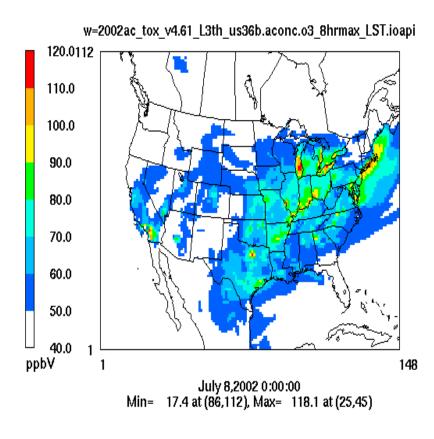
- Conducting 36 km nationwide annual and 12km eastern US annual runs
- Initial modeling results indicate the need to more fully understand ambient toxics data in terms of the proximity of monitors to sources and the sampling time of measurements (example below is for acetaldehyde)

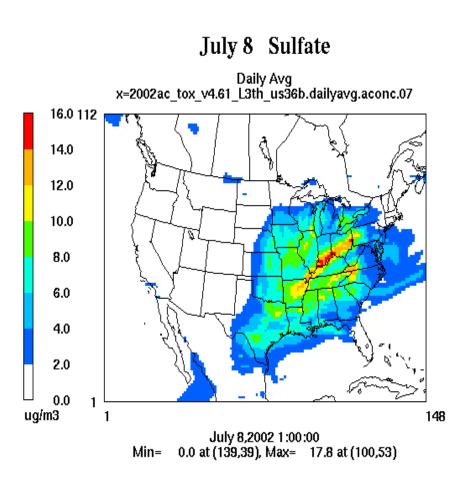


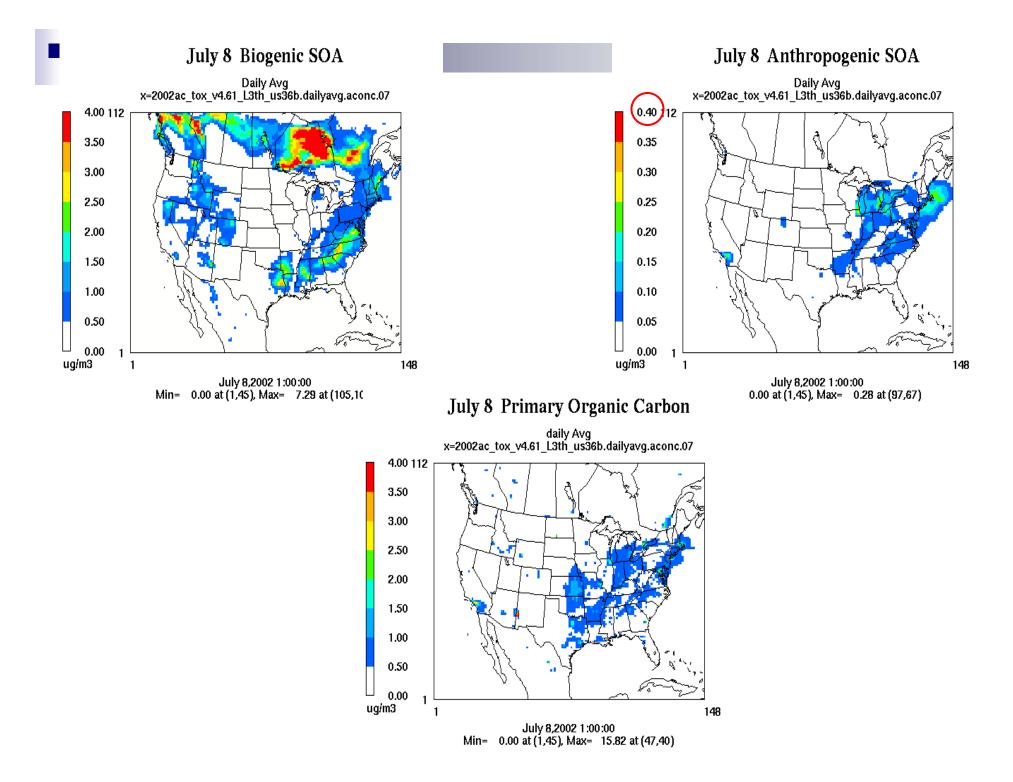
Example of Multi-Pollutant Results

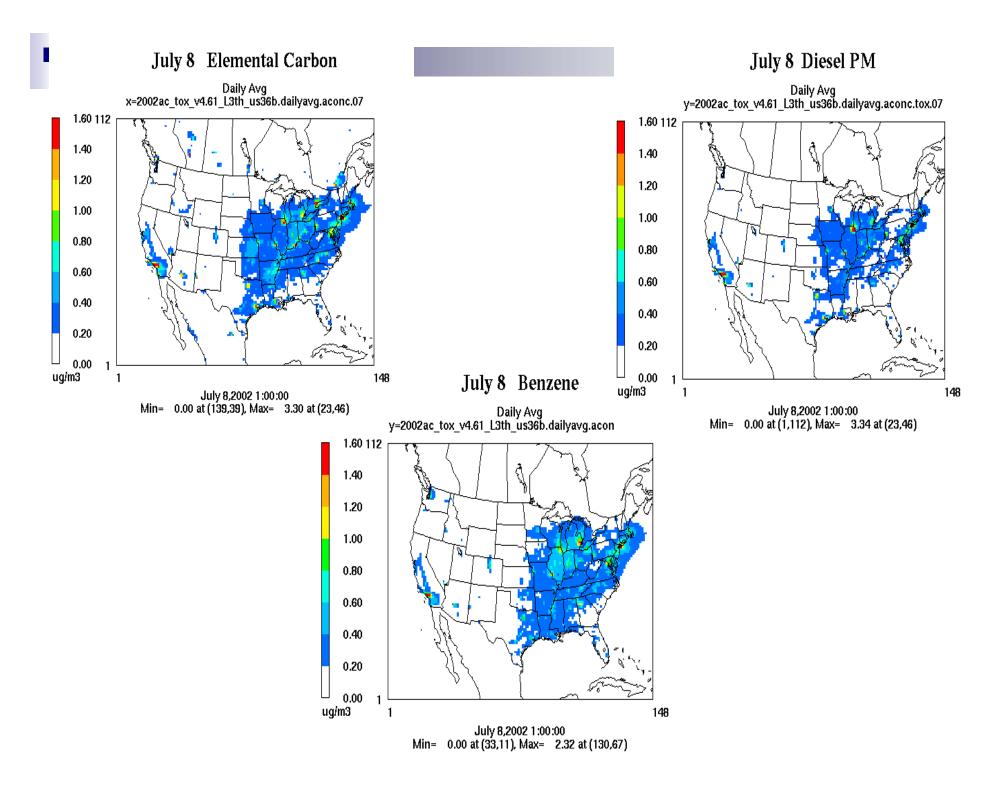
- Spatial Characterization for July 8 -

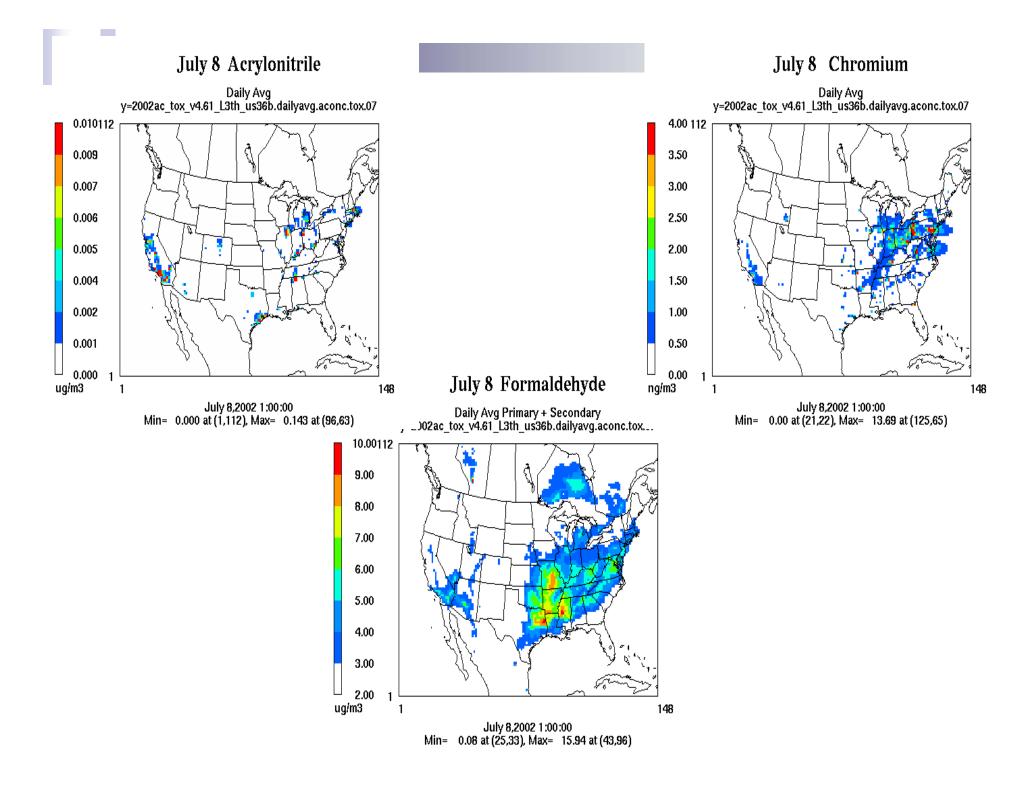
July 8 Daily Max 8-Hr Ozone

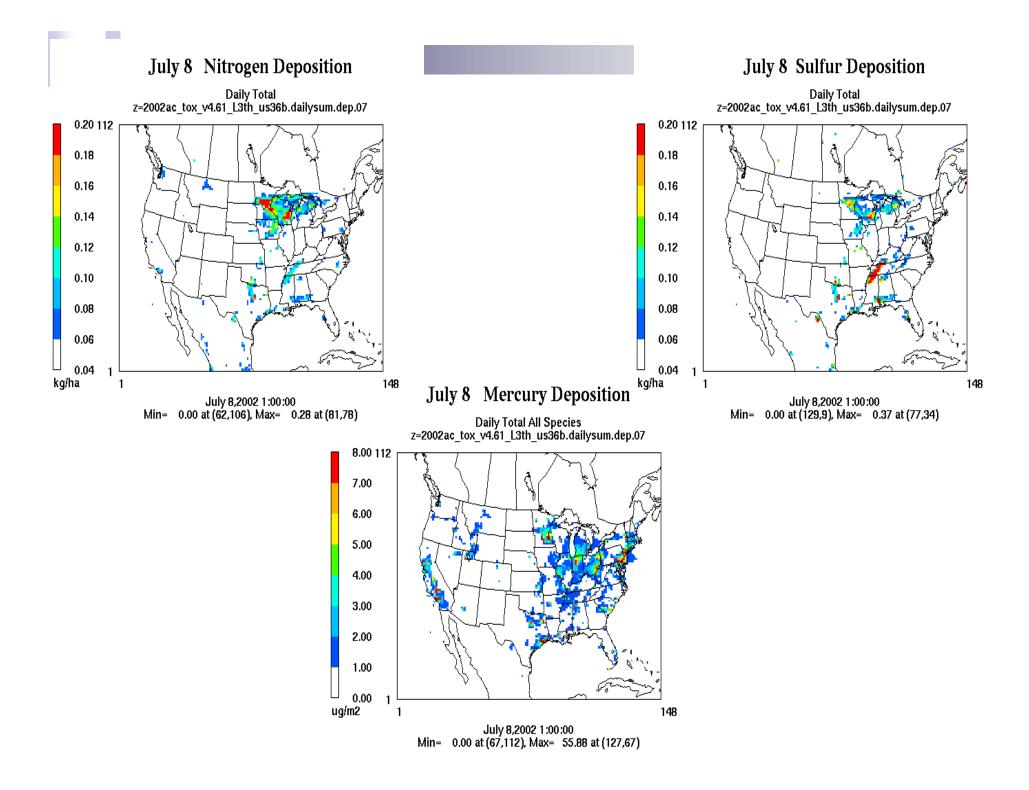












How can this platform be used?

Near-Term Applications using the 2002-based Platform

- O3 NAAQS Final RIA
- OTAQ rules and studies (Loco-Marine, Bond, SECA)
- Accountability/NOx responsiveness
- CDC/PHASE
- Detroit Multi-pollutant Pilot Study (CAPs+HAPs)
- Baltimore Health Indicators Study (CAPs+HAPs) (CDC/Region3/OAQPS/ORD)

Future Applications of Platform

- OTAQ's GHG rule
- Additional Climate Modeling
- NOx/SOx Secondary NAAQS

Risk Assessment and RIA

Sector Modeling for SPPD

Includes source apportionment in CMAQ/CAMx

- PM2.5 Designations/Implementation Rule
- Multi-Pollutant Report (CAPs+HAPs)

Some "Non-traditional" Applications to Highlight

Detroit MP pilot study

Evaluate multi-pollutant platform in local area and inform OAQPS AQMP project & DEARS

DEARS and CDC/PHASE

Improve air quality characterization for health studies and risk/exposure assessments

Climate Modeling

Expand modeling platform to include climate feedbacks and interactions

Comprehensive Air Quality Management Plan: What are we doing for this project?

- Partner with 4 states agencies to integrate the SIP requirements into a comprehensive AQMP
 - □ Assist on technical and policy issues
 - Compare outcomes with the traditional approach
- 3 pilot areas to develop a comprehensive plan
 - \Box New York entire state (Region 2)
 - □ North Carolina entire state (Region 4)
 - The entire state of Illinois combined with St. Louis, MO (Regions 5 and 7)

Project elements: Two parallel efforts

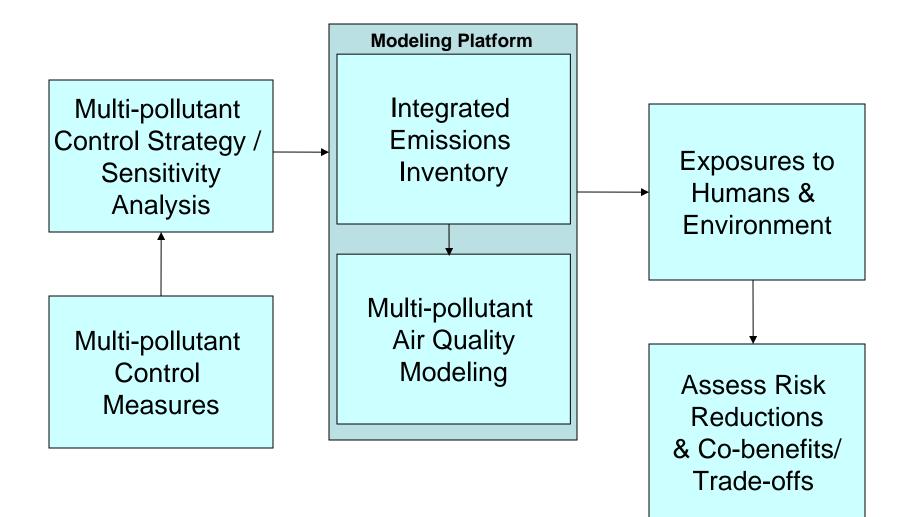
Implement Policy/Outreach Effort (AQPD/OID)

- Defined criteria and selected of partners for pilot studies
- Will work with partners to identify issues to overcome and research potential incentives for areas to promote development of comprehensive AQMPs

Implement Technical Effort (AQAD/HEID/SPPD)

- Complete <u>Detroit analytical work</u> to provide valuable input and insights to selection of partners and design of pilot strategy
- Will provide template for analytical elements of pilot studies and technical input/consultation to partners as needed

Analytical Framework for Multi-pollutant Analysis



Multi-pollutant & Multi-scale

The analytical framework emphasizes two main features:

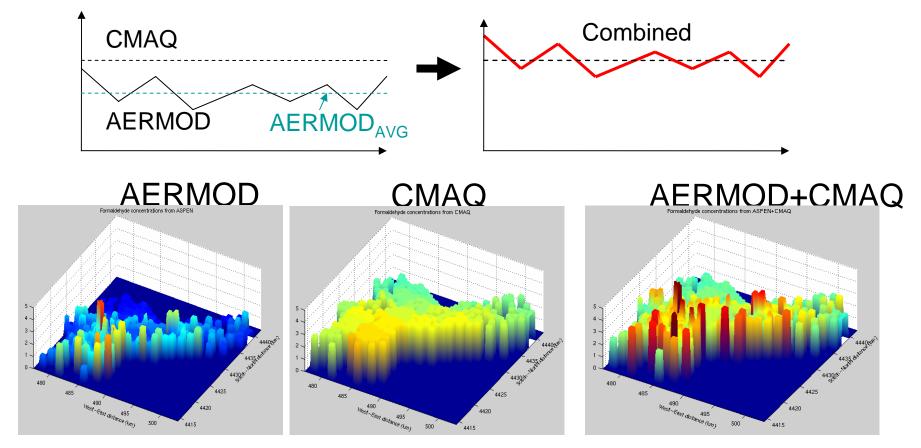
(1) multi-pollutant (integration of HAPS & CAPS), and(2) multi-resolution (regional and local scales).

This provides a challenge for all analytical components:

- Emissions Inventory: include HAPS & CAPS and support regional and local scale modeling
- Control Information: multi-pollutant for implementation into control strategies or sensitivity analyses
- AQ modeling: account for primary & secondary aspects of criteria and toxic pollutants and assess regional and local concentrations and source contributions
- Exposure/risk/benefits assessment: provide information on benefit of pollutant reductions at regional and local scales for criteria and toxic pollutants

Air Quality Modeling: "Hybrid approach"

- Allows preservation of the granular nature of AERMOD while properly treating chemistry/transport offered by CMAQ.
- Generates local gradients incorporating the advantages of both the dispersion and photochemical models into one combined model output (via post-processing techniques)



Detroit Exposure and Aerosol Research Study (DEARS)

- Describe the relationship between concentrations at a central site and residential/personal concentrations
 - PM constituents and Air Toxics
 - PM and Air Toxics from specific sources
- Emphasis placed on understanding impact of:
 - Local sources (mobile and point) on outdoor residential concentrations
 - Housing type and house operation on indoor concentrations
 - Locations and activities on personal exposure



Public Health Air Surveillance Evaluation (PHASE)

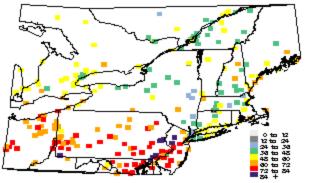
- Exploration among US EPA and CDC, and 3 CDC State Partners: Maine, New York, and Wisconsin
- Provide enhanced, easily accessible air quality information for use in Environmental Health Tracking
 - Model association between air quality and public health, e.g. mortality
 - □ Allow US EPA to measure effectiveness of control programs
- Demonstrate use of spatial prediction using combined sources of data for environmental public health tracking:
 - Ambient air monitoring data (PM_{2.5} and O₃)
 - Air quality numerical model output
 - Satellite data, e.g. MODIS aerosol optical depth

Improve Spatial Prediction with Combined Air Quality Data

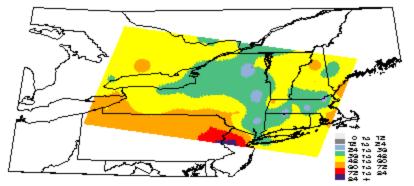
- Issue: Cannot monitor at all locations, but want to know pollution everywhere
 - Typical Solution: use kriging to interpolate air monitoring data, but
 - □ Monitoring data is spatially sparse, some areas have no monitors
 - Use of classical kriging techniques may introduce arbitrarily large prediction errors in these areas
 - New Solution: Consider Combined Prediction Approaches
 - Outcomes:
 - □ Better air quality input for modeling linkages to public health data
 - □ More accurate delineation of pollution non-attainment areas
- What Does the Combined Approach Provide ?
 - Monitoring Data and CMAQ model output can be used simultaneously to predict the pollutant surface
 - Draw on strengths of each data source:
 - □ Give more weight to accurate monitoring data in monitored areas
 - □ Rely on model output in non-monitored areas
 - Model underlying spatial and temporal dependence, and measurement errors of each source

Example spatial surfaces for O3

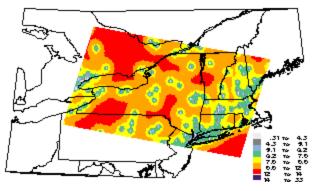
Observed O3 11JUN01



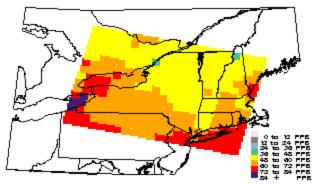
Interpolated O3 11JUN01



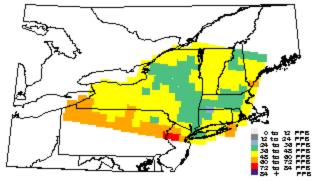
Standard Error O3 11JUN01



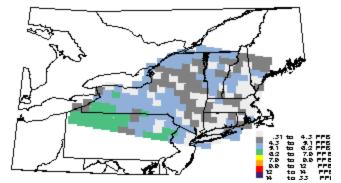
CMAQ O3 IJUN01



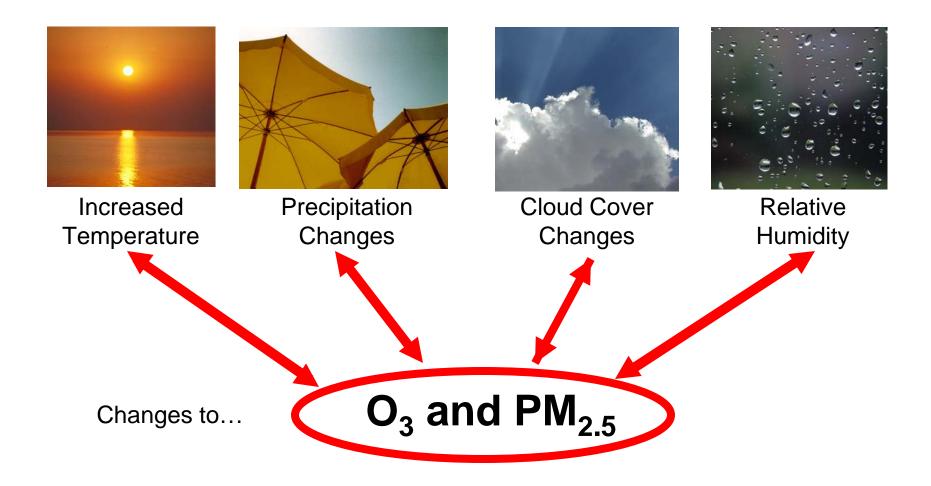
HB Interpolated O3 11JUN01

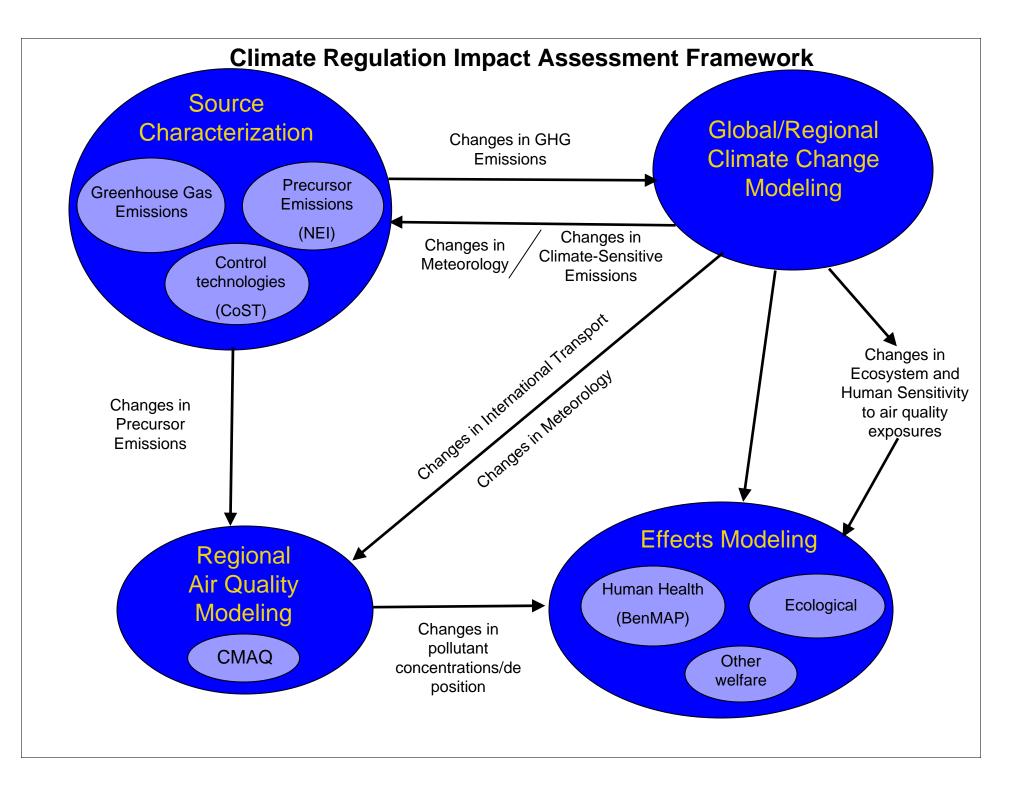


HB Standard Error O3 11JUN01



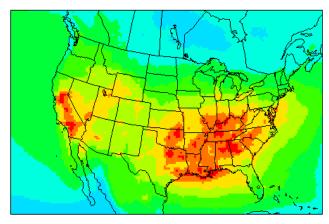
Future Climate Modeling



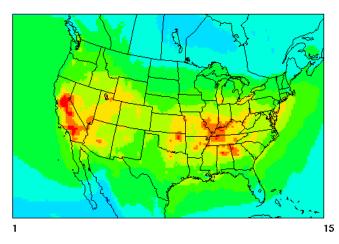


Ozone (8-hr max summer avg.) w/ 2001 Emissions & Current Climate

Summer 2000

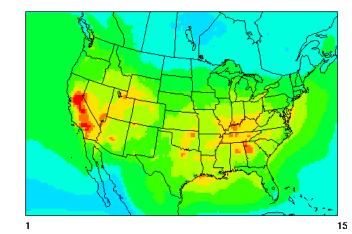


Summer 2002

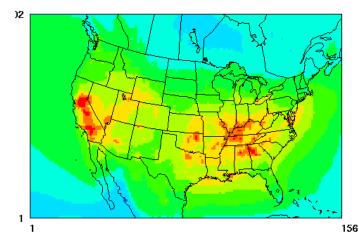


	70.0
	65.0
	60.0
	55.0
	50.0
	45.0
	40.0
	35.0
	30.0
	25.0
p	20.0 pbV
	-

Summer 2001

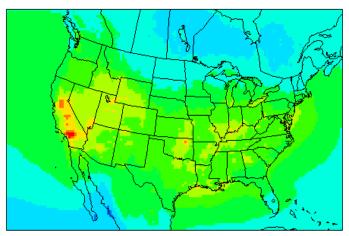


Ensemble (2000-2002)

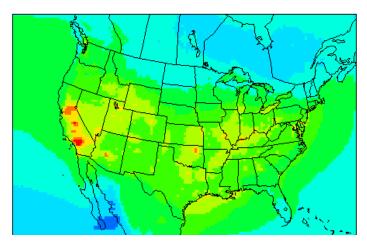


Ozone (8-hr max summer avg., 3-yr ensemble) w/ 2020 Base & CAIR Control Emissions

2020 Base Emissions w/ Current Climate

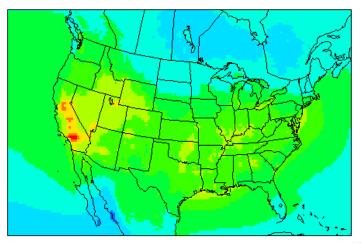


2020 Base Emissions w/ Future Climate

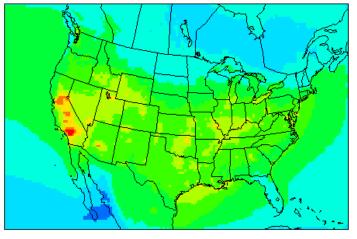


	70.0
	65.0
	60.0
	55.0
	50.0
	45.0
	40.0
	35.0
	30.0
	25.0
	20.0
p	pbV

2020 CAIR Emissions w/ Current Climate



2020 CAIR Emissions w/ Future Climate



Thank you for your time and patience!

Questions?