

# Air Quality Modeling

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# Overview

- Air Quality Modeling 101
- AQ Modeling for Attainment Demos
- Modeling Guidance for SIP Demos

# EPA/OAQPS

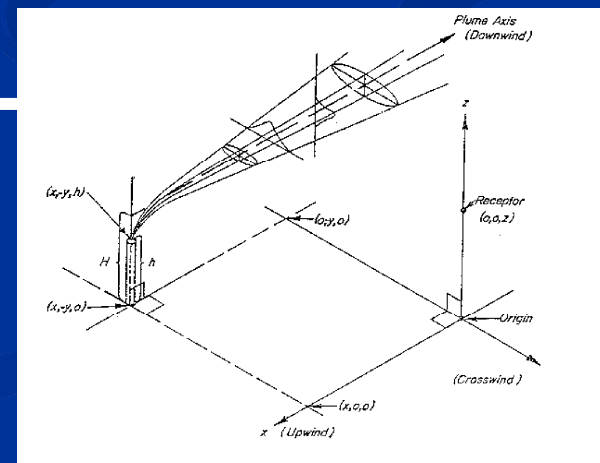
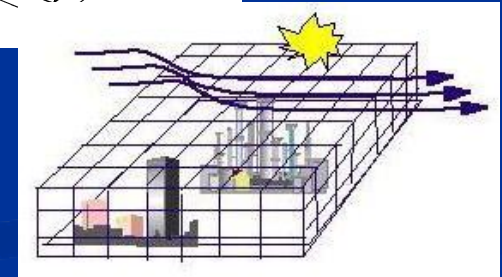
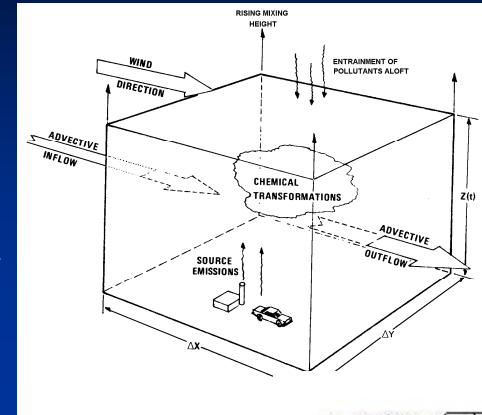
## Air Quality Modeling Group

- Conducts air quality modeling for regulatory and policy assessments
  - e.g., NO<sub>x</sub> SIP Call, Heavy Duty Diesel, Nonroad Rule, Clear Skies, CAIR, CAMR, NAAQS RIAs
- *Provides guidance for the application of air quality models for SIP demonstrations and NSR/PSD permitting*
  - *Appendix W, O<sub>3</sub>/PM/RH Guidance*
- Partners and coordinates w/ others (e.g, ORD, scientific community, etc) on model evaluations and development efforts

# Air Quality Modeling 101

# Air Quality Modeling

- **Photochemical models:** large-scale air quality models that account for chemical and physical atmospheric processes in predicting pollutant concentrations.
  - Can be applied at multiple spatial scales (local, regional/national, and global)
  - Examples include CMAQ, CAMx, REMSAD, UAM, etc
- **Dispersion models:** source-oriented models that characterize atmospheric processes by dispersing a directly emitted pollutant to predict concentrations at selected downwind receptor locations.
  - Typical of permit applications for new sources but can also be run for multiple sources at once (like for NATA risk assessments)
  - Examples include AERMOD, ISC, and ASPEN



# Major Atmospheric Processes Simulated in Air Quality Models

- Chemical transformations (gas- & aqueous-phase and heterogeneous chemistry)
- Advection (horizontal & vertical)
- Diffusion (horizontal & vertical)
- Cloud processes (convection & mixing)
- Emissions (anthropogenic & biogenic)
- Removal Processes (dry & wet Deposition)

## Species Mass Continuity Equations :

$$\frac{\partial C_i}{\partial t} = -\nabla \cdot (VC_i) + \nabla \cdot (K\nabla C_i) + P_i - L_i C_i + S_i - R_i + C_i$$

Diagram illustrating the Species Mass Continuity Equation with process labels:

- Advection** (points to  $-\nabla \cdot (VC_i)$ )
- Diffusion** (points to  $\nabla \cdot (K\nabla C_i)$ )
- Chemistry** (points to  $P_i - L_i C_i$ )
- Emission** (points to  $S_i$ )
- Removal** (points to  $-R_i$ )
- Cloud** (points to  $+C_i$ )

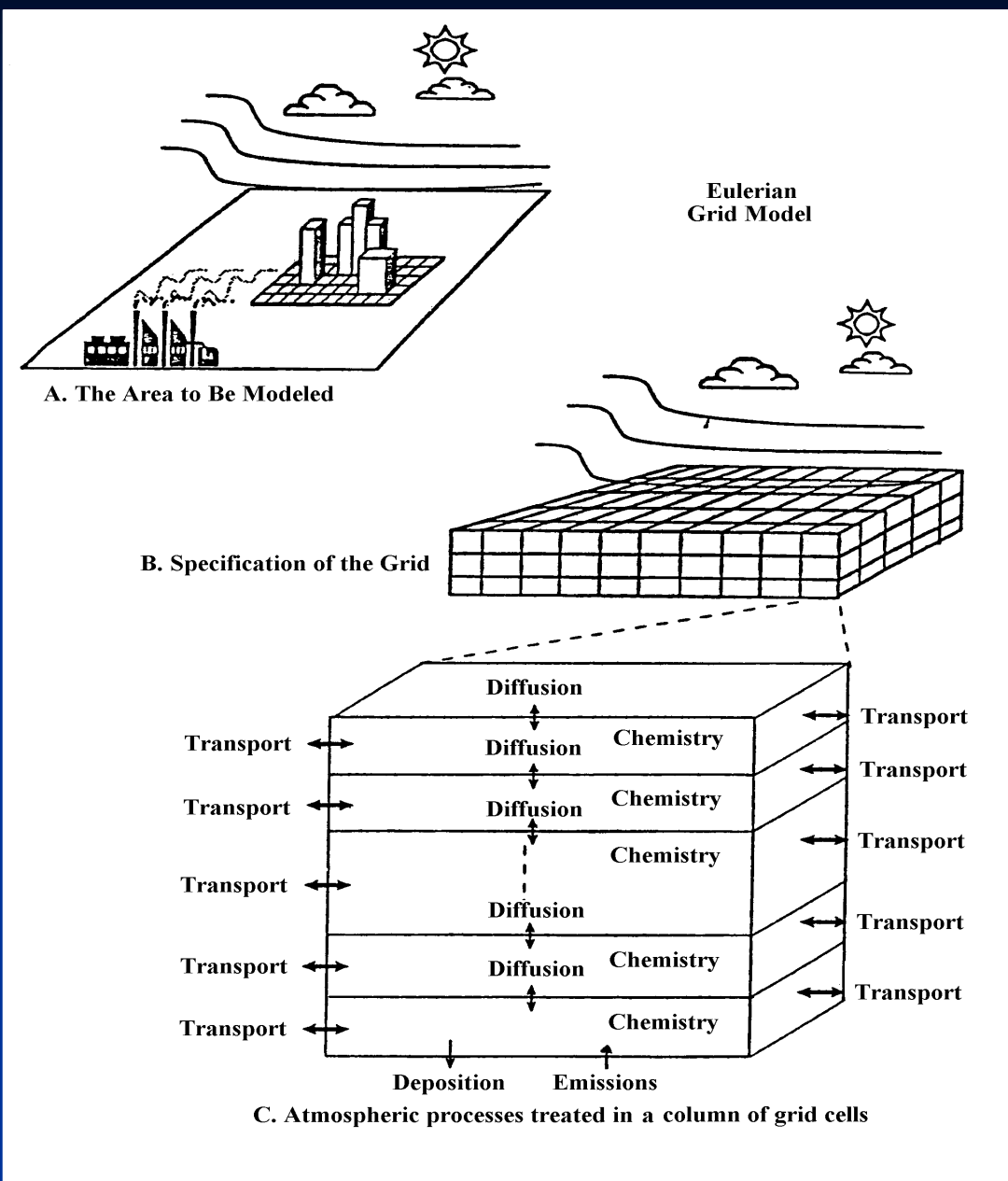
# Photochemical Grid Models:

“2<sup>nd</sup> Generation”

UAM, RADM,  
REMSAD, ROM

“3<sup>rd</sup> Generation”

CMAQ and CAMx



# Example Modeling Domain(s)





# Current 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
  - EPA provides CMAQ code and documentation through the CMAS Center at: <http://www.cmascenter.org/>

# One-Atmosphere Approach



## Mobile Sources

NO<sub>x</sub>, VOC,  
PM, Toxics

(Cars, trucks, planes,  
boats, etc.)



## Industrial Sources

NO<sub>x</sub>, VOC,  
SO<sub>x</sub>, PM,  
Toxics

(Power plants, refineries/  
chemical plants, etc.)



## Area Sources

NO<sub>x</sub>, VOC,  
PM, Toxics

(Residential, farming  
commercial, biogenic, etc.)

Chemistry

Meteorology

Ozone

PM

Acid Rain

Visibility

Air Toxics

Atmospheric  
Deposition

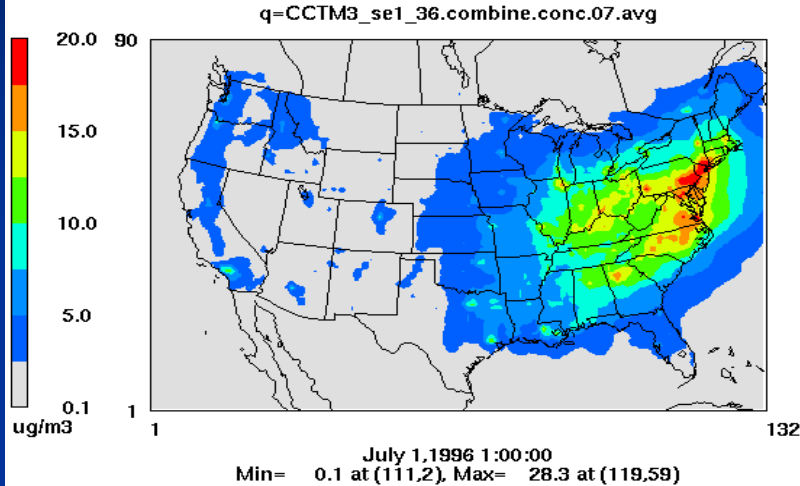
Climate  
Change



# CMAQ "Multi-Pollutant" Modeling

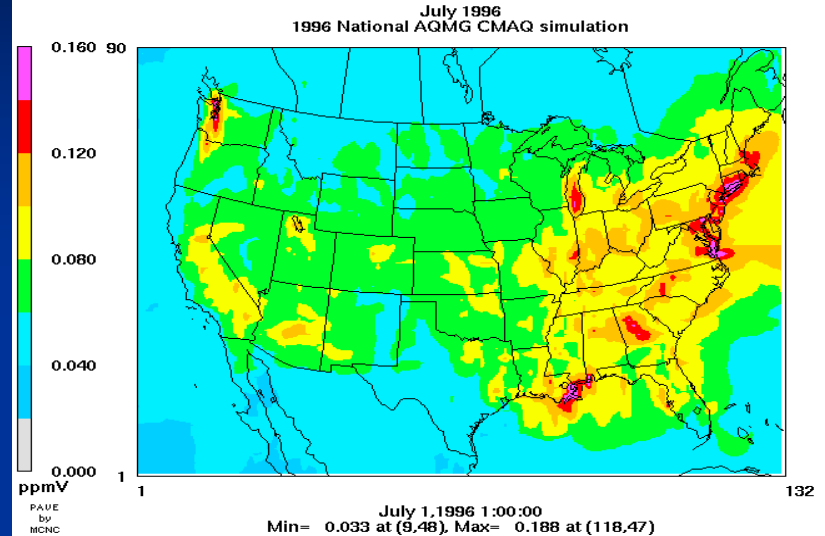
## Annual Avg PM 2.5

Layer 1 PM25q



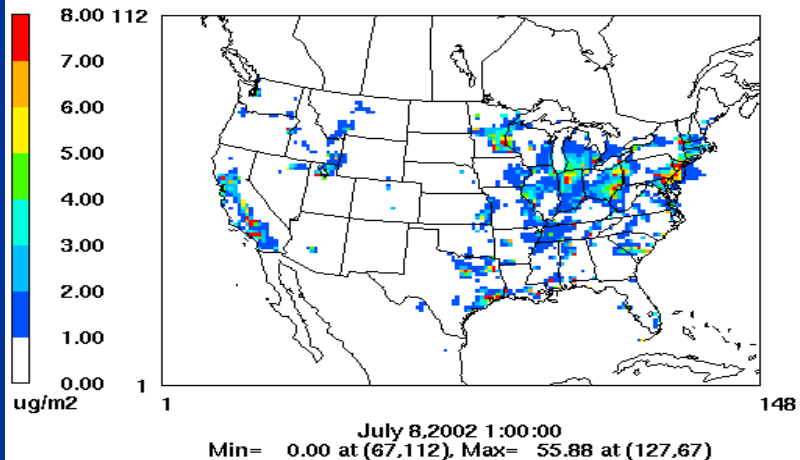
## 8hr Summer Ozone

Monthly Maximum Model Ozone

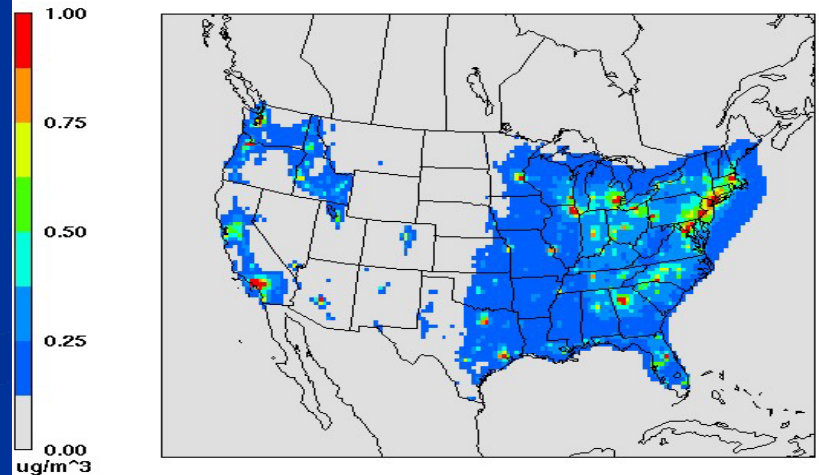


## Annual Hg Deposition

Daily Total All Species  
z=2002ac\_tox\_v4.61\_L3th\_us36b.dailysum.dep.07



## Ann Avg. Benzene



# Air Quality Modeling for SIP Attainment Demonstrations

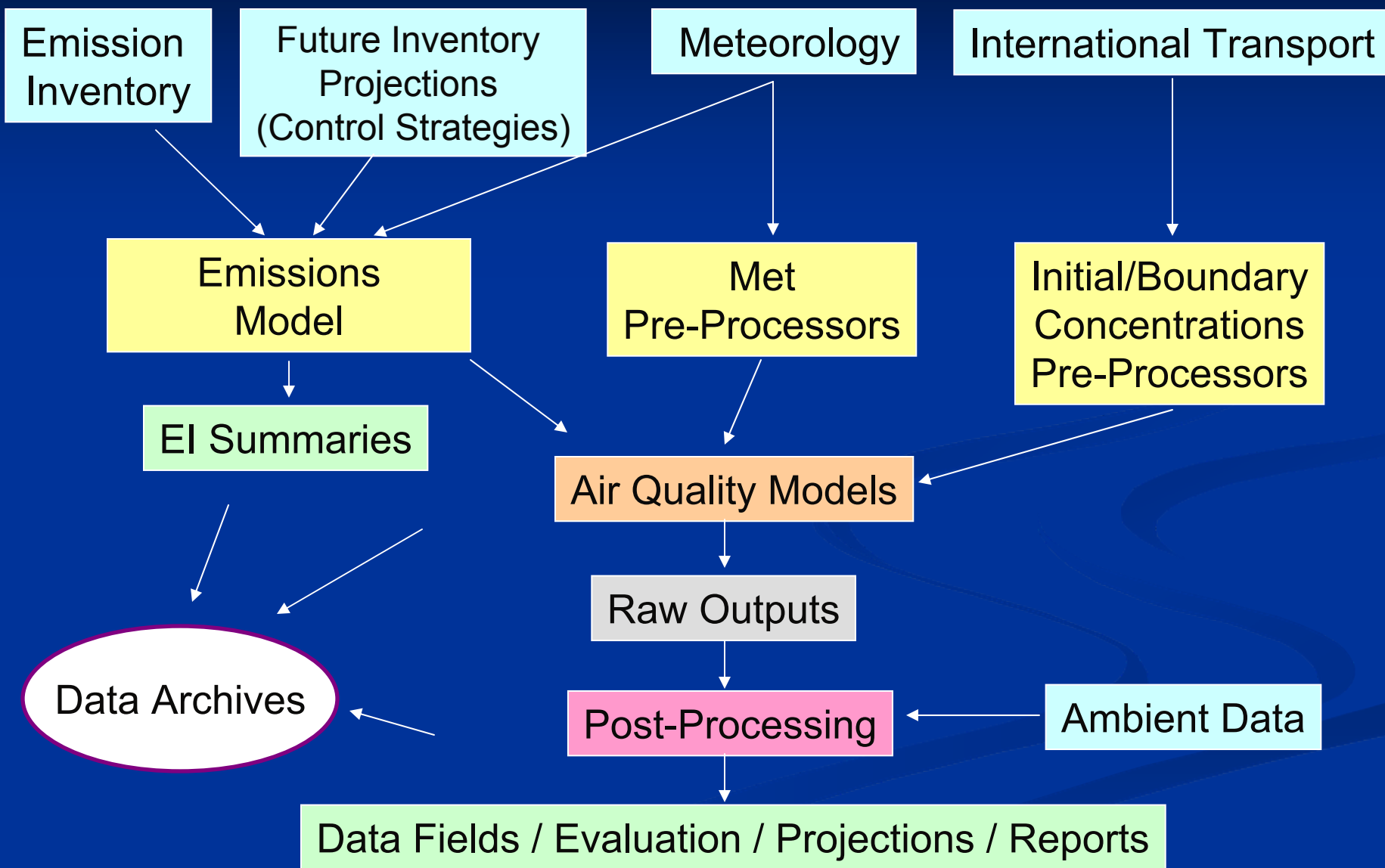
# Why Do We Use Photochemical Grid Models?

- The ultimate goal of photochemical modeling is to assist policy makers in determining the most efficient ways of reaching a future air-quality goal.
  - Models are used to predict the effects of future control strategies
    - Controls necessary for SIP attainment demonstrations (States)
    - Air quality impacts of national rules (EPA)

# Predicting the Future

- Unfortunately, there is no way to verify the accuracy of the model's future year predictions
- Therefore, modelers generally simulate historical periods w/varying meteorological scenarios and assess model performance
  - May be episodes or full year(s)
- The assumption is, if the model can replicate what was done in the past, and is doing so for the right reasons, then it can be used for determinations of predicted future changes in pollutant concentrations

# Modeling Platform Schematic Data Flow Diagram

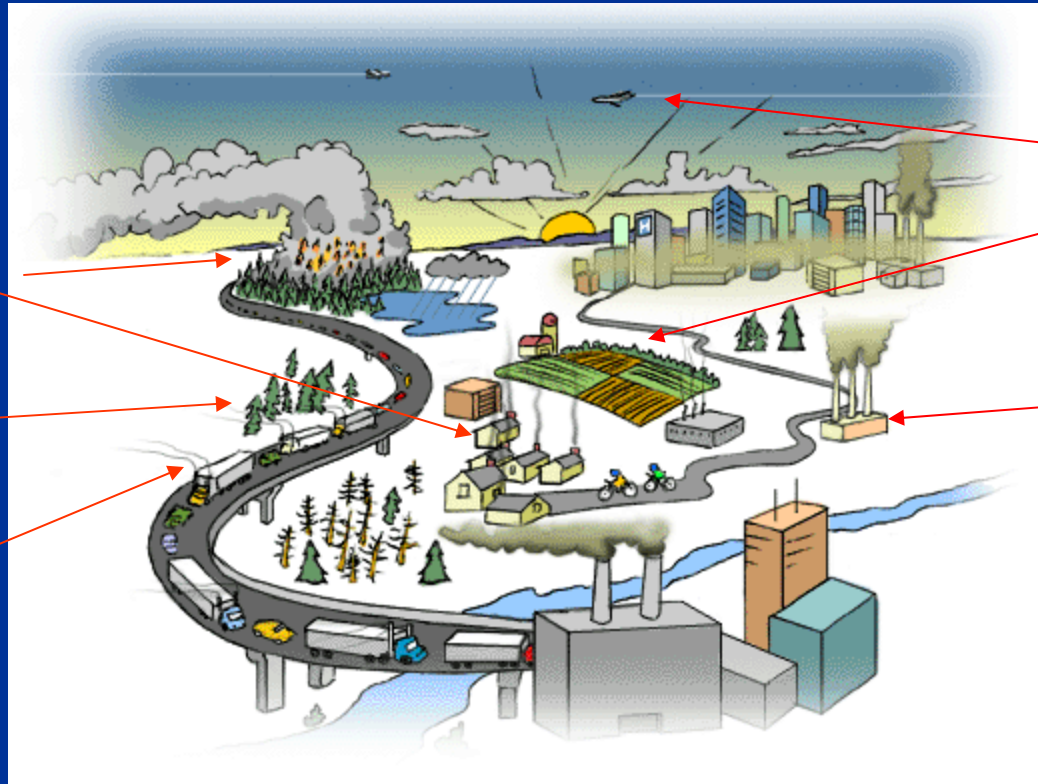


# Model Inputs: Emissions

- Emissions inventory
  - Ozone: Hourly gridded emissions of NO<sub>x</sub>, VOC, and CO
  - PM<sub>2.5</sub>: Hourly gridded emissions of NO<sub>x</sub>, VOC, SO<sub>2</sub>, ammonia, CO, and speciated primary PM
    - Mobile: cars, trucks, buses, etc.
    - Area and Nonroad: industrial equipment, recreational marine, gasoline vapors from refilling, lawn mowers, etc.
    - Point: utilities, refineries, etc.
    - Biogenic: certain tree and plant species emit ozone and PM precursors



# Types of Emissions Sources



ALM

Mobile NonRoad Sources

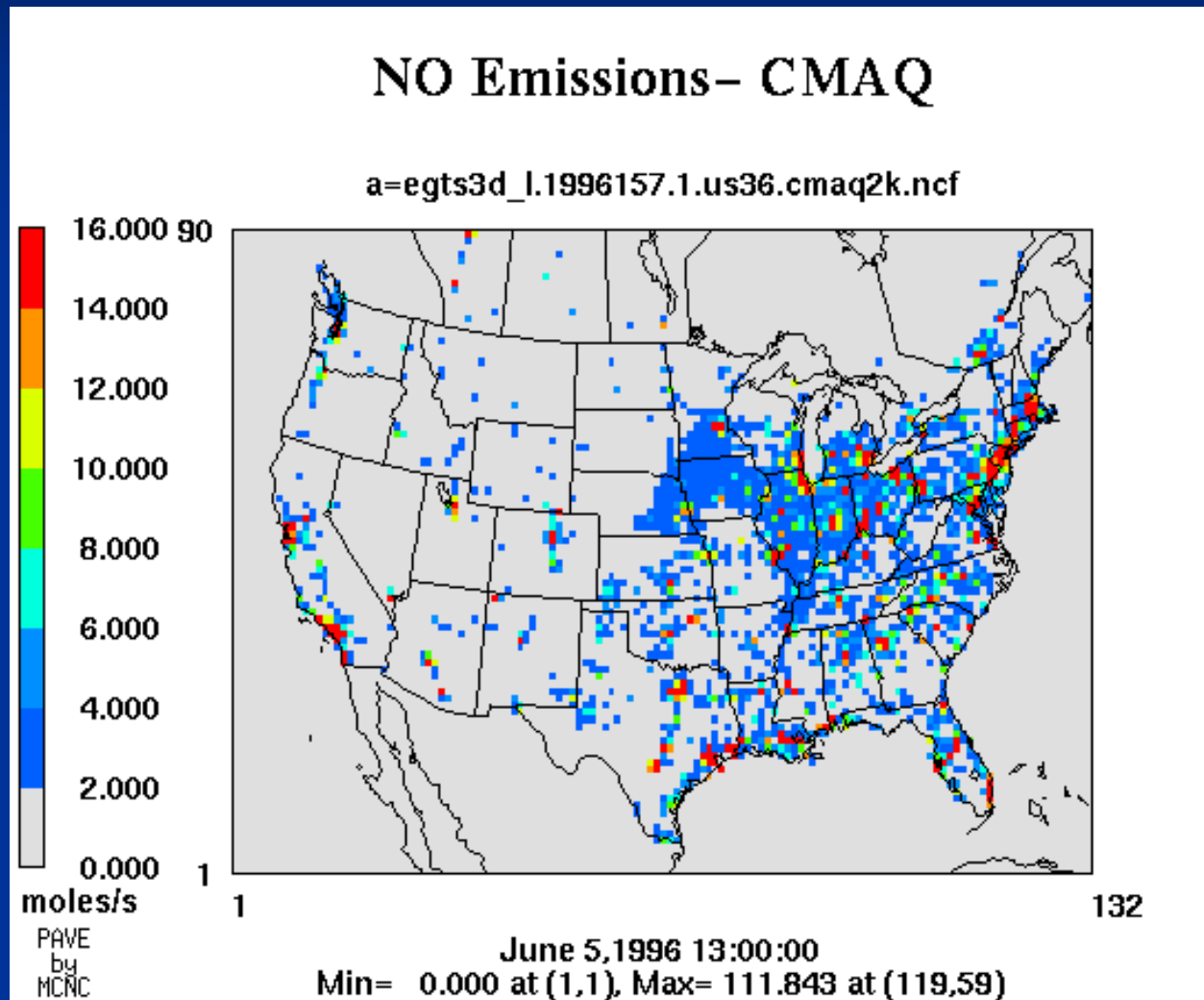
Point Sources

NonPoint Sources

Biogenic Sources

Mobile OnRoad Sources

# Example- Emissions Inputs



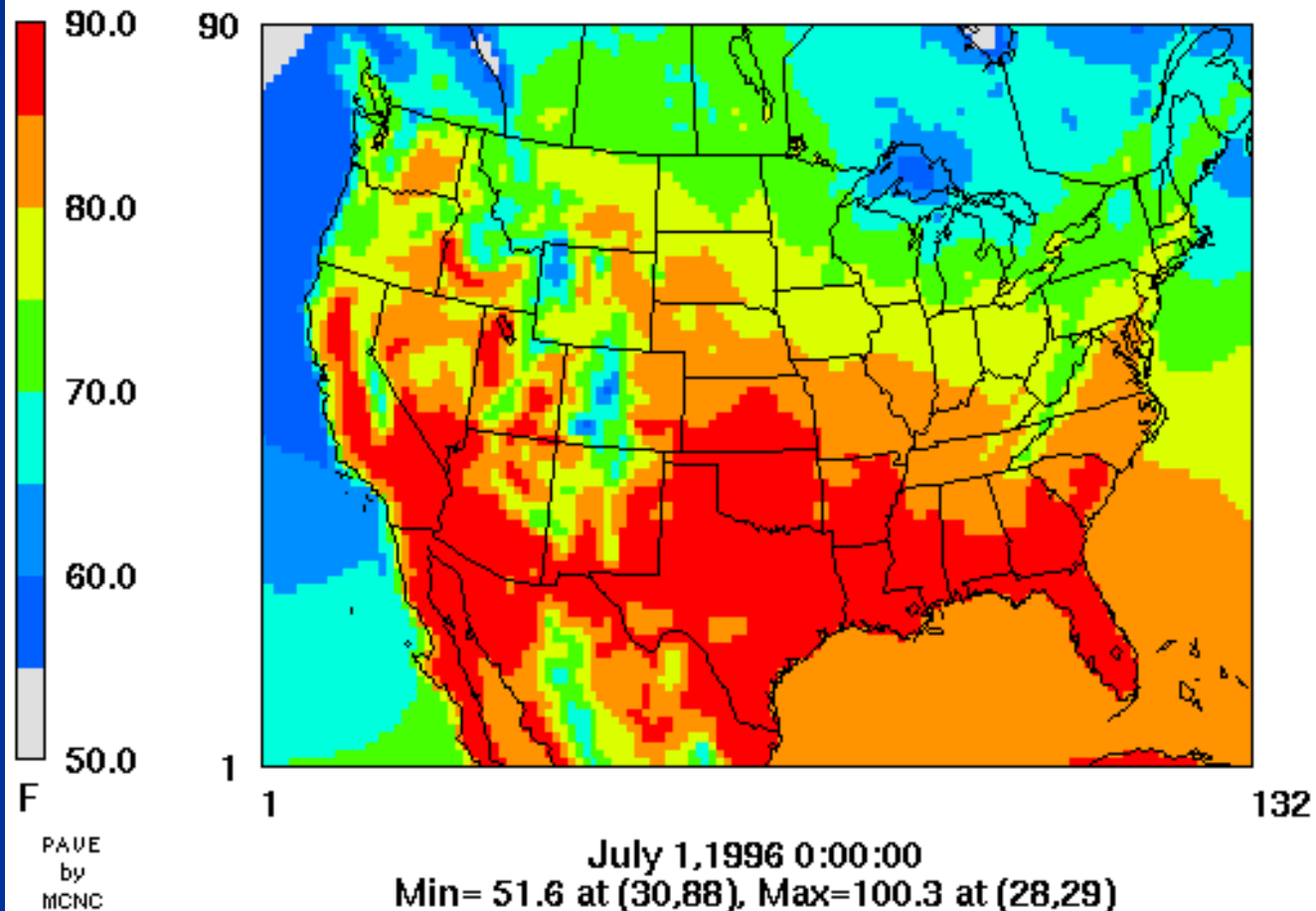
# Model Inputs: Meteorological

- Meteorology
  - Models need many meteorological variables (gridded, hourly) as input to simulate advection, diffusion, deposition, chemical transformation, etc.
    - Wind fields
    - Temperature
    - Moisture
    - Vertical diffusion or Planetary Boundary Layer (PBL) height
- Use gridded data from a meteorological model such as MM5 or WRF
  - More information available at:  
<http://www.epa.gov/ttn/scram/metdataindex.htm>

# Example- Temperature Field

## Average Daily Max Layer 1 Temperature

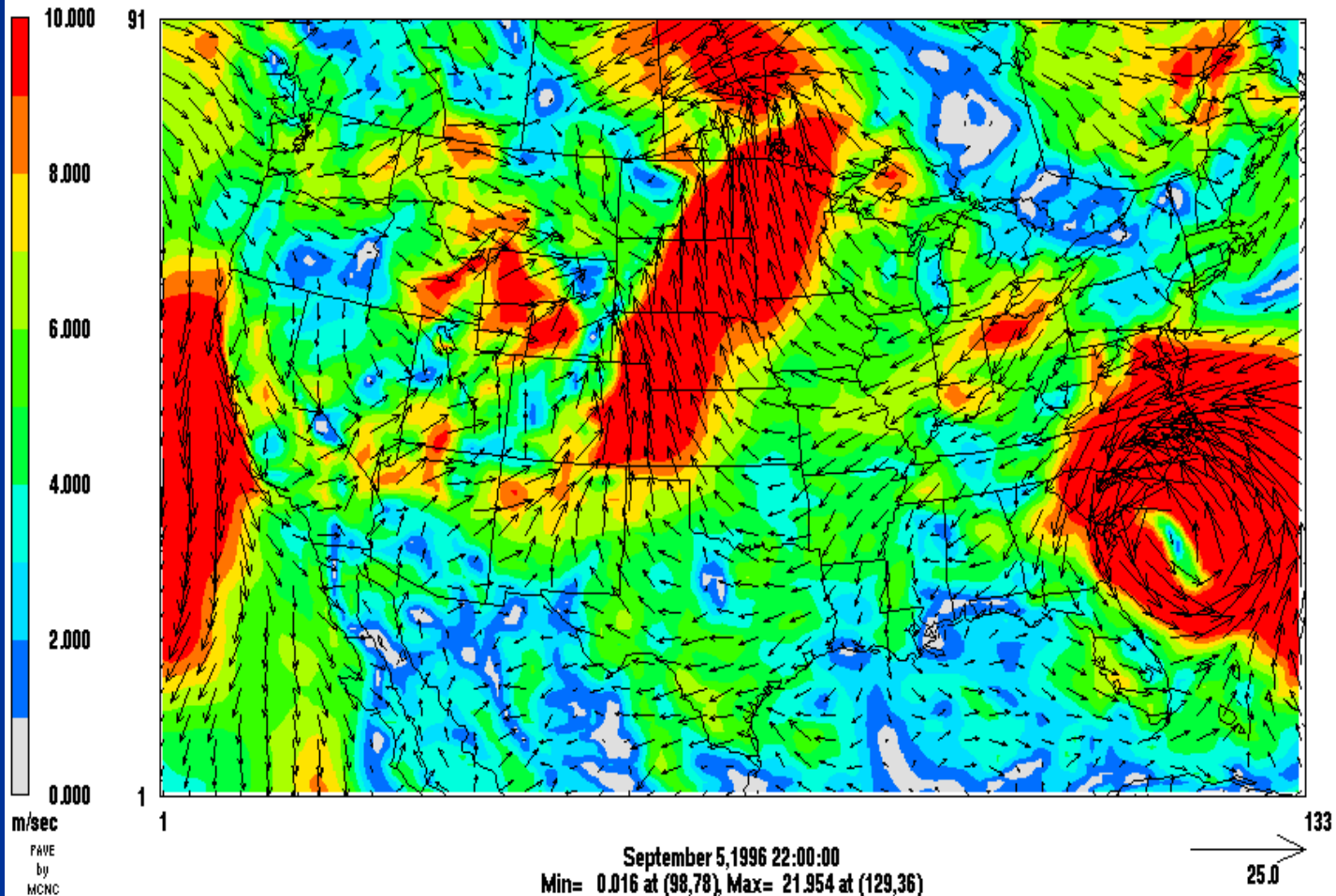
July 1996



# Example- Wind Field

## Mid-Afternoon Wind Field

Layer 1 -- 2200 GMT (1400 PST)  
July 1996 108/36 km MM5 simulation

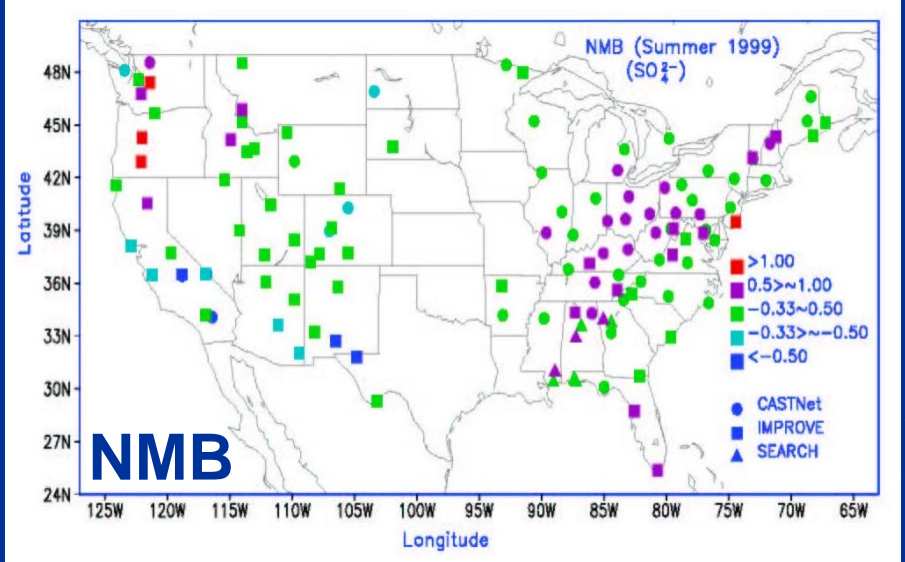
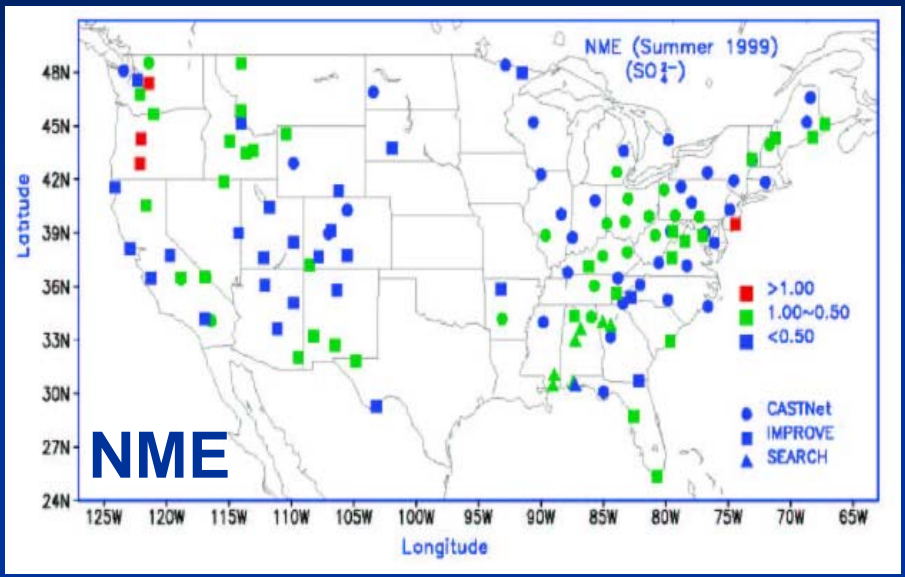


# Model Performance Evaluation

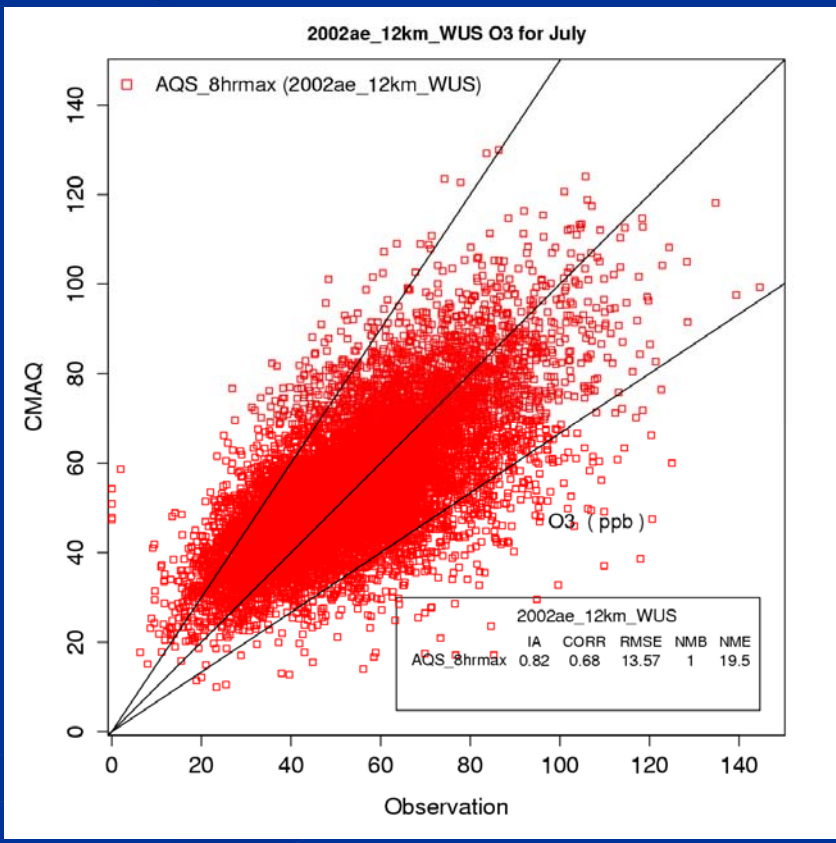
- Operational Evaluation: compare predicted concentrations to observed concentrations
  - Statistics (bias, error, etc.)
  - Scatterplots
  - Time series plots
- If model performance is “acceptable” then the modeling system can be used to predict air quality in the future.

# Example Model Performance Evaluation

Sulfate ( $\mu\text{g m}^{-3}$ ) June 15 – July 16, 1999



## July 2002 Ozone Scatterplot-Daily 8-hr Max



# Future Year Predictions

- Emissions are then projected to a future year and the model is run again (the meteorology is held constant)
  - The difference between the base and future year is the predicted future air quality impacts
  - The model can be run again with alternative future year control strategies



Ozone/PM2.5/  
Regional Haze  
Modeling Guidance  
Summary

# Outline

- SIP modeling requirements
- Summary of SIP modeling guidance for ozone and PM<sub>2.5</sub> attainment demonstrations
- Attainment demonstration software (MATS)

# Attainment Demonstration Requirements

- CAA Section 172(c) requires States with a nonattainment area to submit an attainment demonstration
  - Emissions inventories (base and future years)
  - Adopted control measures
- For PM<sub>2.5</sub>, all States (with nonattainment areas) must submit an attainment demonstration which includes modeling (§51.1007)
  - Photochemical grid modeling and/or local dispersion modeling
- For ozone, moderate and above nonattainment areas are required to submit an attainment demonstration with modeling (§51.908)
  - Photochemical grid modeling

# Ozone/PM2.5/Regional Haze Modeling Guidance

- “Guidance on the use of Models and Other Analyses for Demonstrating Attainment of Air Quality Goals for Ozone, PM2.5, and Regional Haze”
  - “Final” version- April 2007

# What's in the Guidance?

- Part II- Generating Model Results
  - Conceptual description
  - Modeling protocol
  - Selecting a model(s)
  - Choosing days/episodes
  - Selecting domain & spatial resolution
  - Developing met inputs
  - Developing emissions inputs
  - Evaluating model performance/diagnostic analyses

# Conceptual Description/Protocol

- Conceptual description provides an assessment/analysis of the local or regional air quality problem(s)
  - Allows for more informed planning of the modeling demonstration
- Modeling protocol specifies *initial* modeling plans
  - Allows for meaningful comments from stakeholders and/or EPA

# Choosing an Air Quality Model

- There is no “preferred model”
  - Models should meet Appendix W requirements for “alternative models”
- Models should be:
  - Peer reviewed
  - Demonstrated to be applicable to the problem being addressed
  - Adequate data bases should be available to run the model
  - Model should be shown to have performed adequately in the past
  - Source code must be available at no cost (or for reasonable cost)
- Vast majority of States/RPOs have used CMAQ or CAMx for ozone, PM<sub>2.5</sub>, and regional haze modeling
  - CMAQ: <http://cmascenr.org/>
  - CAMx: <http://camx.com/>
  - Use of AERMOD or other dispersion model for local primary PM<sub>2.5</sub> attainment demonstration issues (local area analysis)

# PM2.5 Point Source Modeling

- SIP modeling guidance does not address dispersion modeling of PM2.5 for NSR/PSD
- Guideline on Air Quality Models “Appendix W” addresses requirements for permit modeling
- See [http://www.epa.gov/scram001/guidance\\_permit.htm](http://www.epa.gov/scram001/guidance_permit.htm) for additional resources and links



# Recommendations for “Episode” Selection

- Default recommendations
  - Ozone
    - Model full season or several high ozone episodes
  - Annual PM2.5 NAAQS
    - Model full year or  $\geq 15$  days per quarter
  - 24 Hour NAAQS
    - Model days  $> 35 \text{ ug/m}^3$ \* or “high end of distribution”
    - Model days in each quarter (as appropriate)
  - Regional Haze
    - Model a full year (or more) or at least 10 worst (and best) visibility days at each Class 1 area

\*Guidance revisions to specifically address the  $35 \text{ ug/m}^3$  24-hr PM2.5 NAAQS have not been completed yet.

# Horizontal Resolution

- Ozone  $\leq$  12km resolution
- PM<sub>2.5</sub>  $\leq$  12 km resolution for urban scale modeling
  - $\leq$  36 km for regional modeling
  - Higher resolution may be necessary in areas with high primary PM<sub>2.5</sub> concentration gradients
- Recommend  $\leq$  36 km resolution for regional haze modeling

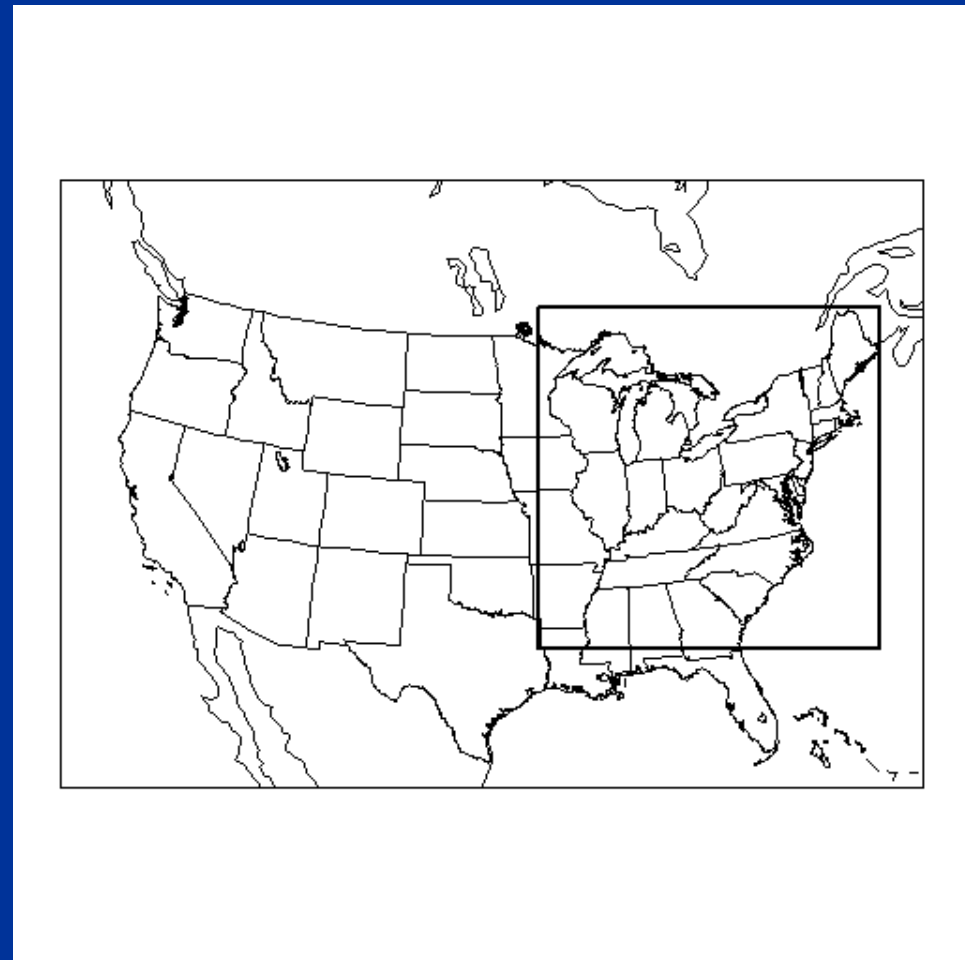
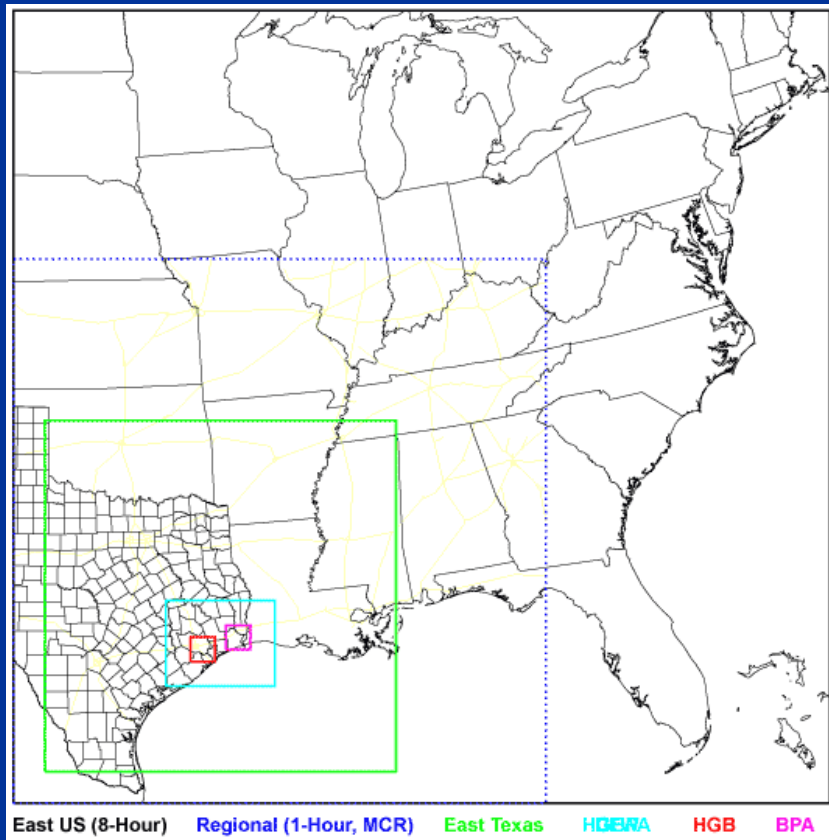
# Modeling Domain

- Photochemical modeling domains are generally large regional domains with nested local domains
  - Large regional domains are needed in most areas of the East and for regional haze
  - Smaller local domains may be sufficient for very local PM<sub>2.5</sub> issues

# Modeling Domain Examples

Houston SIP Modeling Domain  
36/12/4/1 km

OTC SIP Modeling Domain  
36/12 km



# Meteorological Inputs

- MM5 has been the primary met model for air quality modeling over the last 15 years
  - No longer supported by NCAR
- WRF is the replacement model that will be used for most future air quality applications
  - <http://www.wrf-model.org/index.php>
  - More advanced coupled version of WRF and CMAQ is being developed and used in the research community
    - Real-time feedback between met and air quality models

# Emissions Models

- SMOKE and CONCEPT are the main emissions models
  - <http://www.smoke-model.org/index.cfm>
  - <http://www.conceptmodel.org/>
- Additional models are needed to generate certain inventory components
  - Mobile emissions: MOBILE6/MOVES
  - Biogenic emissions: BEIS or MEGAN
- EPA emissions modeling resources
  - <http://www.epa.gov/ttnchie1/emch/index.html>

# Model Evaluation

- Recommendations on various aspects of model evaluation
  - Operational evaluation
    - Statistics
    - Plots/graphs
  - Diagnostic evaluation
    - Indicator species ratios
    - Probing tools (process analysis)
  - Dynamic evaluation
    - Ability of modeling system to replicate historical air quality improvements

# What's in the Guidance? Part 1

- Part I- Using Model Results
  - Modeled Attainment tests
    - 8-hour ozone NAAQS
      - Unmonitored area analysis
    - Annual and 24-hour PM<sub>2.5</sub> NAAQS
      - Unmonitored area analysis
      - Local area analysis (high primary PM<sub>2.5</sub> areas)
    - Regional Haze reasonable progress
  - Supplemental analyses/weight of evidence
  - Activities to support Mid-Course review and future modeling
  - Required documentation



# Modeled Attainment Tests

- All O<sub>3</sub>/PM<sub>2.5</sub>/RH modeled attainment tests 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 PM<sub>2.5</sub> or ozone
  - Ambient concentration \* RRF = Future concentration
- RRFs are calculated for ozone and for each component of PM<sub>2.5</sub> and regional haze

# Speciated Modeled Attainment Test (SMAT)

- The attainment test for PM<sub>2.5</sub> uses separate RRFs for each PM<sub>2.5</sub> species
- Recommend interpolating species concentrations to FRM sites (when necessary)
  - Species concentrations are interpolated to get species fractions at FRM sites
  - FRM values are not interpolated
- Guidance recommends species adjustments based on “SANDWICH” technique (Frank, 2006)

# Speciated PM2.5 Mass Components as defined in SMAT

- $PM2.5_{FRM} = \{ [EC] + [SO4] + [NO3_{FRM}] + [NH4_{FRM}] + [Water] + [OPP] + [OCM_{mb}] + [blank\ mass] \}$ 
  - EC- measured elemental carbon
  - SO4- measured sulfate ion
  - $NO3_{FRM}$ - nitrate retained on the FRM filter
  - $NH4_{FRM}$ - ammonium retained on the FRM filter
  - Water- particle bound water mass attached to sulfate, nitrate, and ammonium
  - OPP-Other Primary Particulate- soil and other inorganic mass
  - $OCM_{mb}$ - organic carbon mass by difference
  - Blank mass- a constant 0.5 ug/m<sup>3</sup> (default) blank mass

# SMAT Components- More detail

- $\text{NO}_3_{\text{FRM}}$  – Retained nitrate
  - Calculated using hourly temperature and relative humidity data
    - EPA has default pre-calculated retained nitrate concentrations
- $\text{NH}_4_{\text{FRM}}$  – Retained ammonium
  - Recommend calculating “indirect” ammonium concentrations using retained nitrate, sulfate, and degree of neutralization of sulfate (DON)
- Particle bound water
  - Recommend using EPA default water equation
    - Two 21 term equations (low acidity and high acidity cases)
- OCMmb- Organic mass by difference
  - Due to uncertainty in OC measurements (positive and negative artifacts), OC is estimated as the difference between measured FRM mass and all other components
  - Guidance recommends setting a “floor” value so that OCM is not unrealistically low

# Model Attainment Test Software (MATS)

- Software has been developed to apply modeled tests
  - Performs ozone, PM<sub>2.5</sub>, and regional haze tests
  - Interpolates ambient data (where necessary) for ozone and PM<sub>2.5</sub> tests
  - Creates “fused” spatial fields for unmonitored area analysis

# MATS

- Provides a consistent set of ambient data for all States to use
  - Ozone and PM<sub>2.5</sub> design values
  - Pre-screened daily average STN and IMPROVE data for PM<sub>2.5</sub> test
  - Official IMPROVE visibility data for regional haze calculations

# Status of MATS

- Current release version (2.2.1) contains ozone, annual PM2.5, and regional haze tests
  - [http://www.epa.gov/scram001/modelingapps\\_mats.htm](http://www.epa.gov/scram001/modelingapps_mats.htm)
- Version with 24-hr PM2.5 test is in beta testing

# Unmonitored Area Analysis (UAA)

- Calculate future year design values in unmonitored areas
  - Uses interpolated ambient design values and model output (fused data)
  - Supplemental analysis to the monitored based tests
  - MATS can create spatial fields needed for the UAA
- Similar tests for ozone and PM<sub>2.5</sub>
- UAA not designed to look for unmonitored PM micro-scale hotspot issues
  - 12 km resolution sufficient for annual PM<sub>2.5</sub>
  - Finer resolution for 24-hr PM<sub>2.5</sub> may be appropriate



# Local Area Analysis

- Focused on evaluating influence of primary PM<sub>2.5</sub> at monitors
  - Test provides a method to examine local primary PM source contributions at FRM monitors
- Local area analysis can use either dispersion model or fine grid Eulerian model (~1km<sup>2</sup>)
- Guidance recommends methods for adding secondary PM components from grid models with primary components from dispersion model

# Base Year Design Value Calculation

- 5 year weighted average design value (ozone, annual and 24-hour PM<sub>2.5</sub> NAAQS)
  - Average of 3 design values centered on the emissions year
  - More stable “anchor point” than a single design value period
  - By design, the center year has the most weight (which is also the emissions year)
  - Consideration should be given to the impact of “extreme” meteorology and/or large emissions changes (during the 5 year period)

# Future Modeling Year(s)

- Future modeling years depend on attainment dates and details contained in the O3 and PM2.5 implementation rules
  - PM2.5- 5 and 10 year deadlines under Subpart 1
  - Ozone- 3, 6, 9, 15, 17, and 20 year deadlines under Subpart 2
  - Generally model a future year which is one year prior to attainment deadline
    - Emissions controls need to be in place in the year or season prior to the deadline

# Weight of Evidence/Supplemental Analyses

- All attainment demonstrations should include “supplemental” analyses to corroborate the modeling results
  - Three main categories of supplemental analyses
    - Modeling
    - Trends
    - Diagnostic analyses
- *Weight of evidence* applies when future design values are “close to” NAAQS (either above or below)

# Weight of Evidence

- Recommended WOE range:
  - Annual PM<sub>2.5</sub> 14.5-15.5 ug/m<sup>3</sup>
  - 24-hour PM<sub>2.5</sub> 62-67\* ug/m<sup>3</sup>
  - 8 hour Ozone 82-87 ppb
- If concentration is >WOE range: “More qualitative results are less likely to support a conclusion differing from the outcome of the modeled attainment test”

\* Guidance will be updated to reflect the 35 ug/m<sup>3</sup> NAAQS

# Next Steps

- Complete guidance revisions in early 2010
  - New PM<sub>2.5</sub> and ozone NAAQS
  - Miscellaneous updates
- Release MATS with 24-hr PM<sub>2.5</sub> test