Air Quality Modeling

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Overview

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

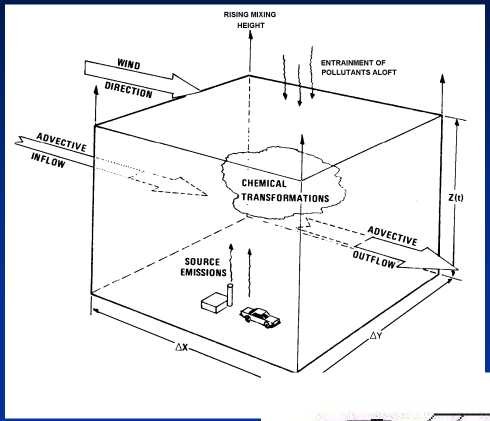
EPA/OAQPS
Air Quality Modeling Group

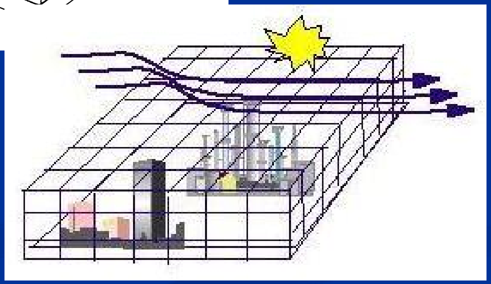
- Conducts air quality modeling for regulatory and policy assessments
  - e.g., NOx SIP Call, Heavy Duty Diesel, Nonroad Rule, Clear Skies, CAIR, CAMR, NAAQS RIAs
- *Provides guidance for the application of air quality models for SIP demonstrations and NSR/PSD permitting*
  - *Appendix W, O3/PM/RH Guidance*
- Partners and coordinates w/ others (e.g, ORD, scientific community, etc) on model evaluations and development efforts

Air Quality Modeling 101

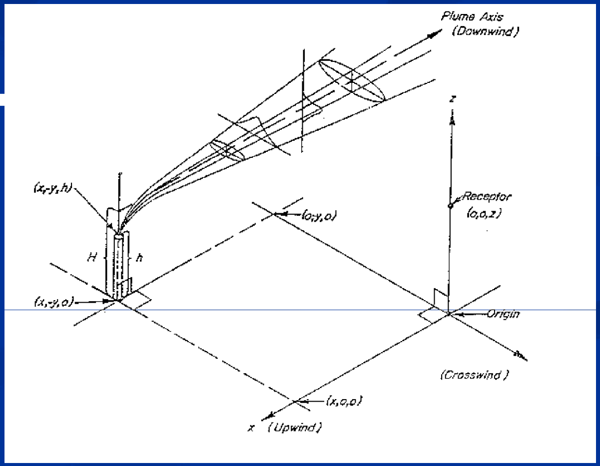
Air Quality Modeling

- **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 :

$$\frac{\partial C_i}{\partial t} = -\overbrace{\nabla \bullet (VC_i)}^{\textbf{Advection}} + \underbrace{\nabla \bullet (K\nabla C_i)}_{\textbf{Diffusion}} + \overbrace{P_i - L_i C_i}^{\textbf{Chemistry}} + \underbrace{S_i}_{\textbf{Emission}} - \overbrace{R_i}^{\textbf{Removal}} + \underbrace{C_i}_{\textbf{Cloud}}$$

Photochemical Grid Models:

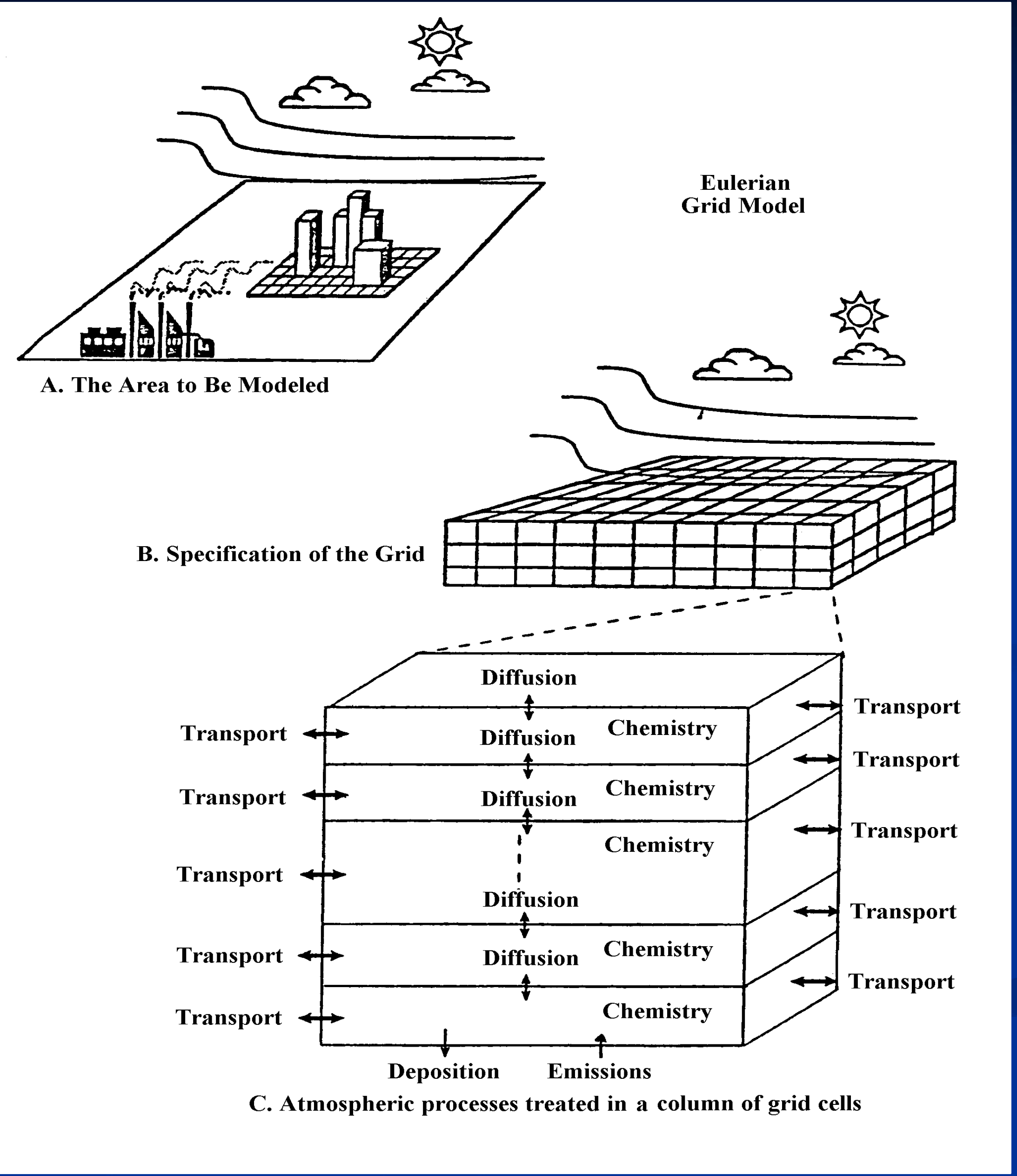
“2nd Generation”

UAM, RADM,

REMSAD, ROM

“3rd Generation”

CMAQ and CAMx



Example Modeling Domain(s)

12 km West

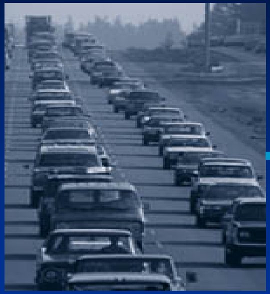
12 km East

36 km
CONUS

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

NOx, VOC, PM, Toxics

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

Industrial Sources

NOx, VOC, SOx, PM, Toxics

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

Area Sources

NOx, VOC, PM, Toxics

(Residential, farming commercial, biogenic, etc.)

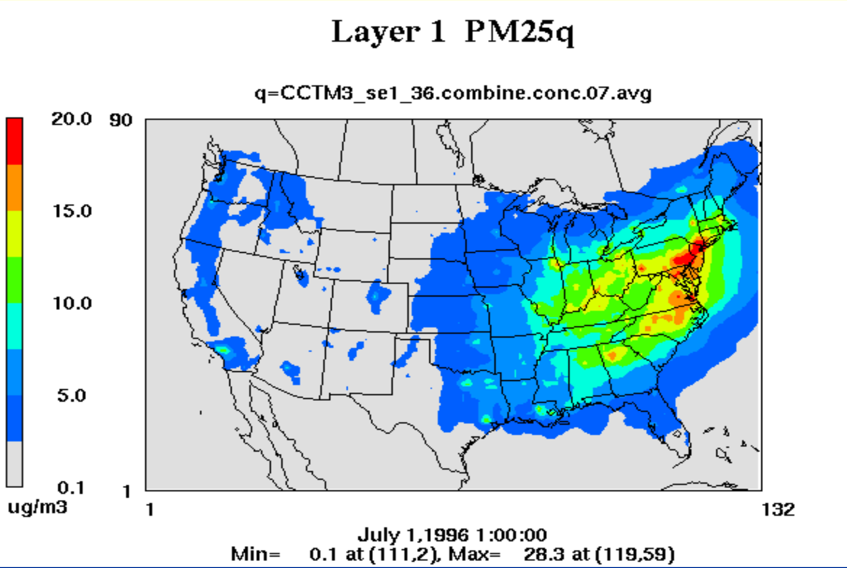
Chemistry

Meteorology

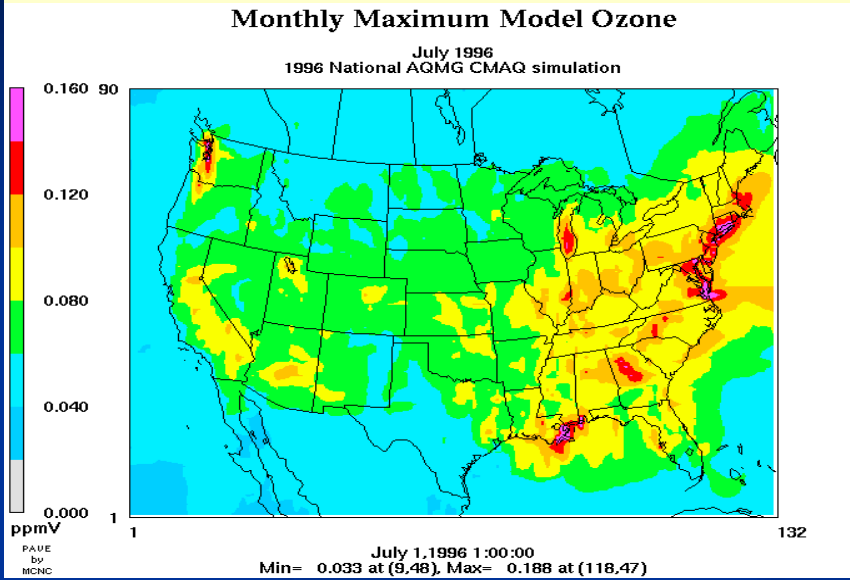
- Ozone
- PM
- Acid Rain
- Visibility
- Air Toxics
- Atmospheric Deposition
- Climate Change

CMAQ “Multi-Pollutant” Modeling

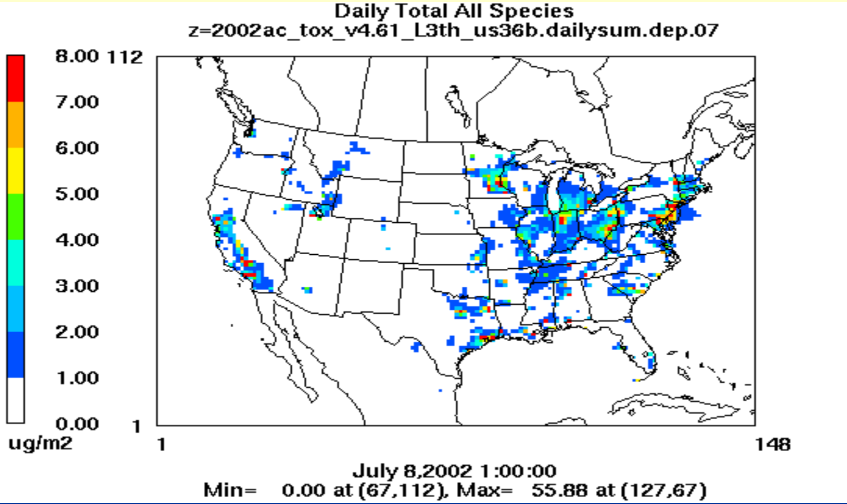
Annual Avg PM 2.5



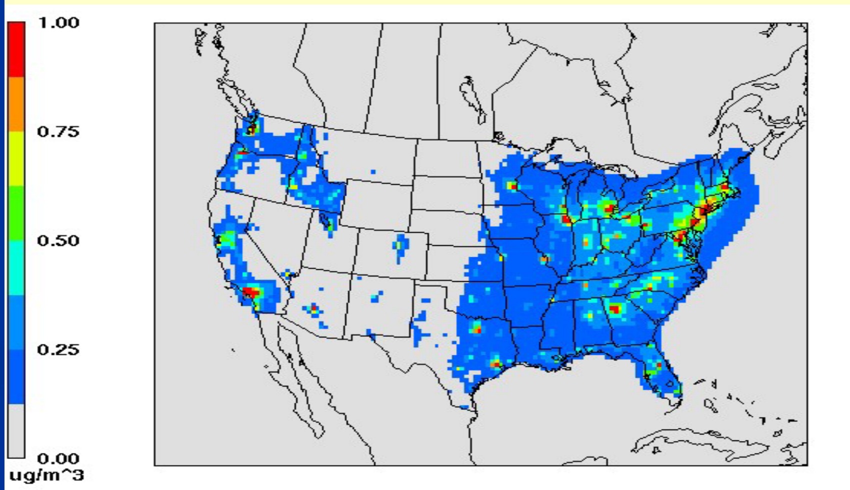
8hr Summer Ozone



Annual Hg Deposition



Ann Avg. Benzene



Air Quality Modeling for SIP Attainment Demonstrations

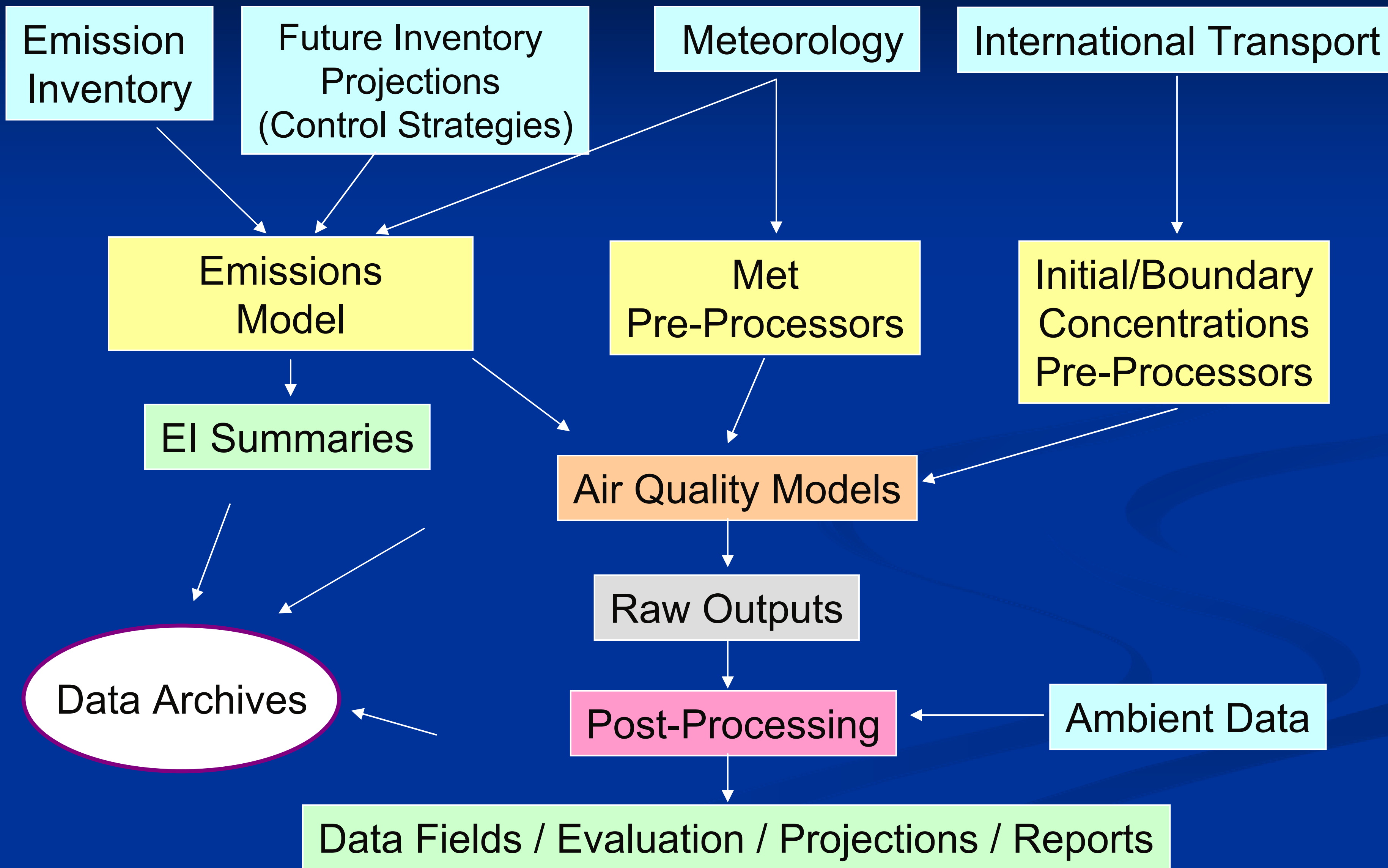
Why Do We Use Photochemical Grid Models?

- 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

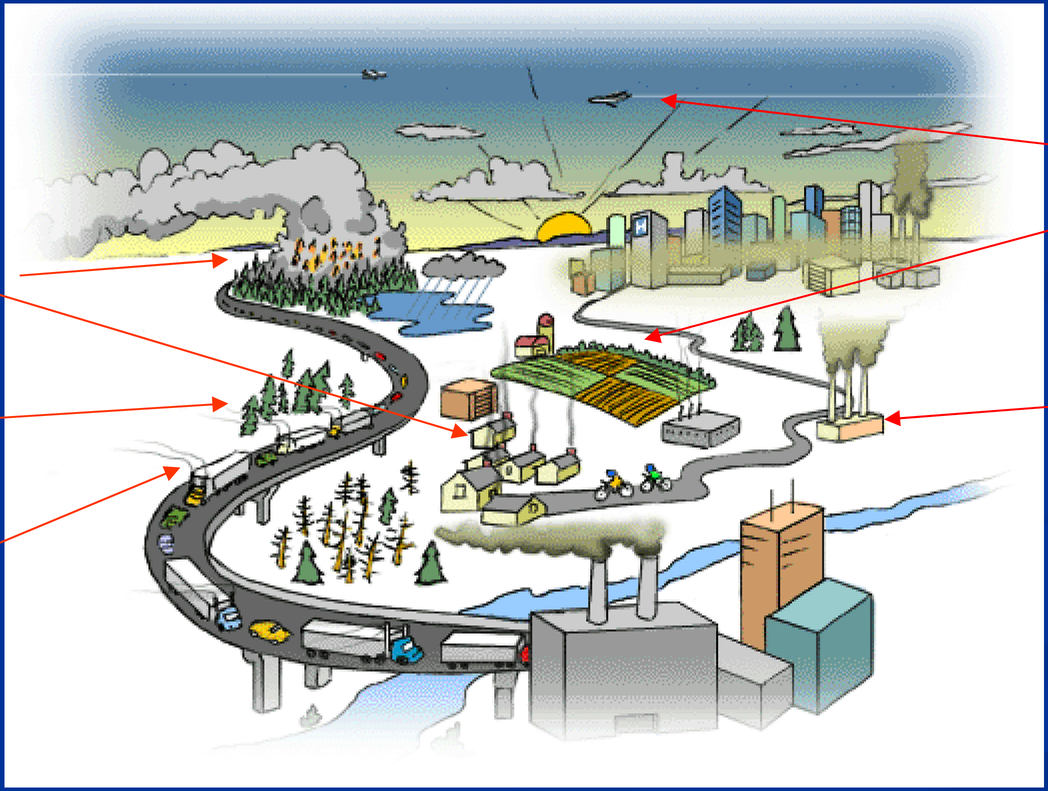
Modeling Platform Schematic Data Flow Diagram



Model Inputs: Emissions

- Emissions inventory
  - Ozone: Hourly gridded emissions of NOx, VOC, and CO
  - PM2.5: Hourly gridded emissions of NOx, VOC, SO2, 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

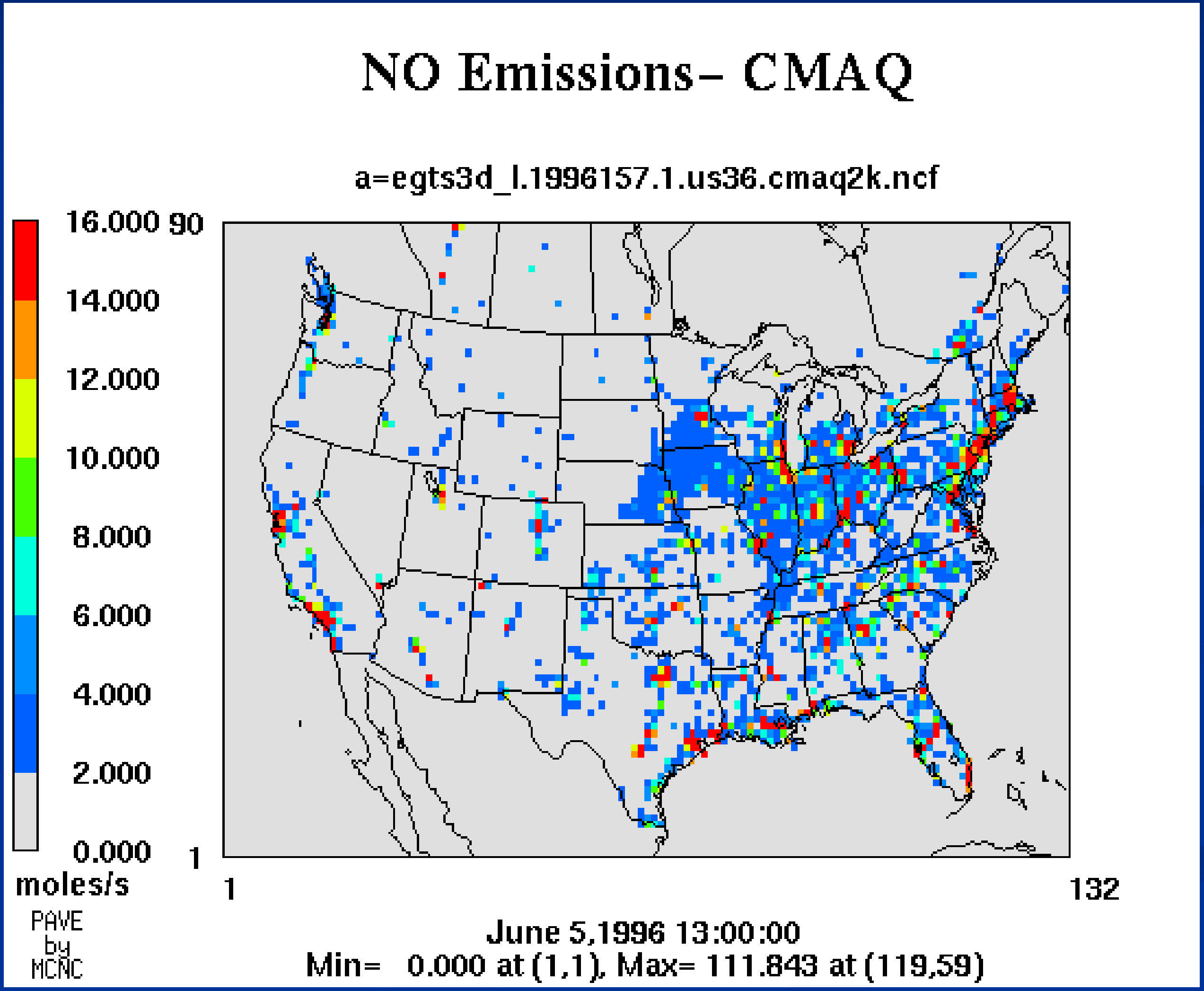
NonPoint Sources

Biogenic Sources

Point Sources

Mobile OnRoad Sources

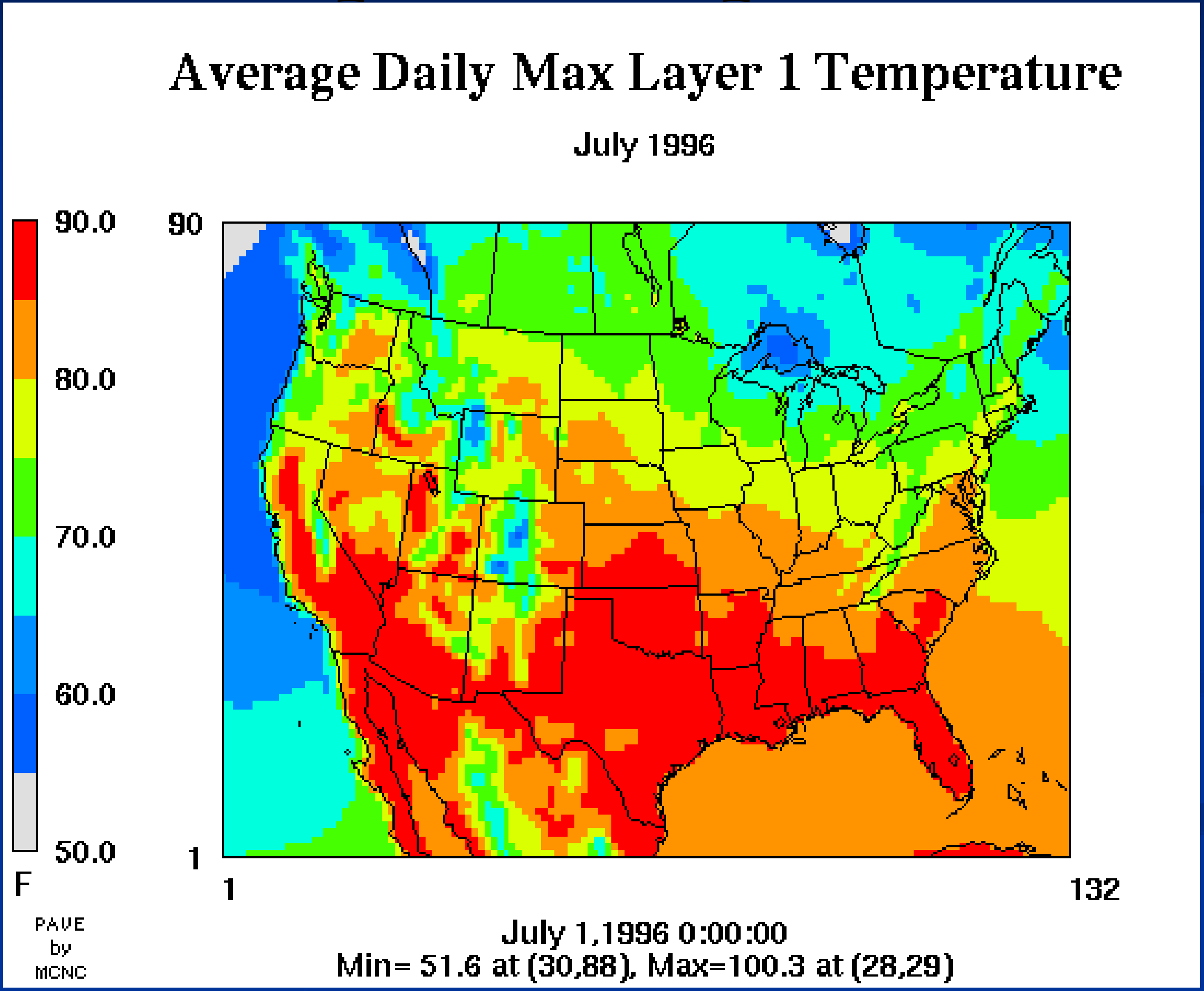
Example- Emissions Inputs



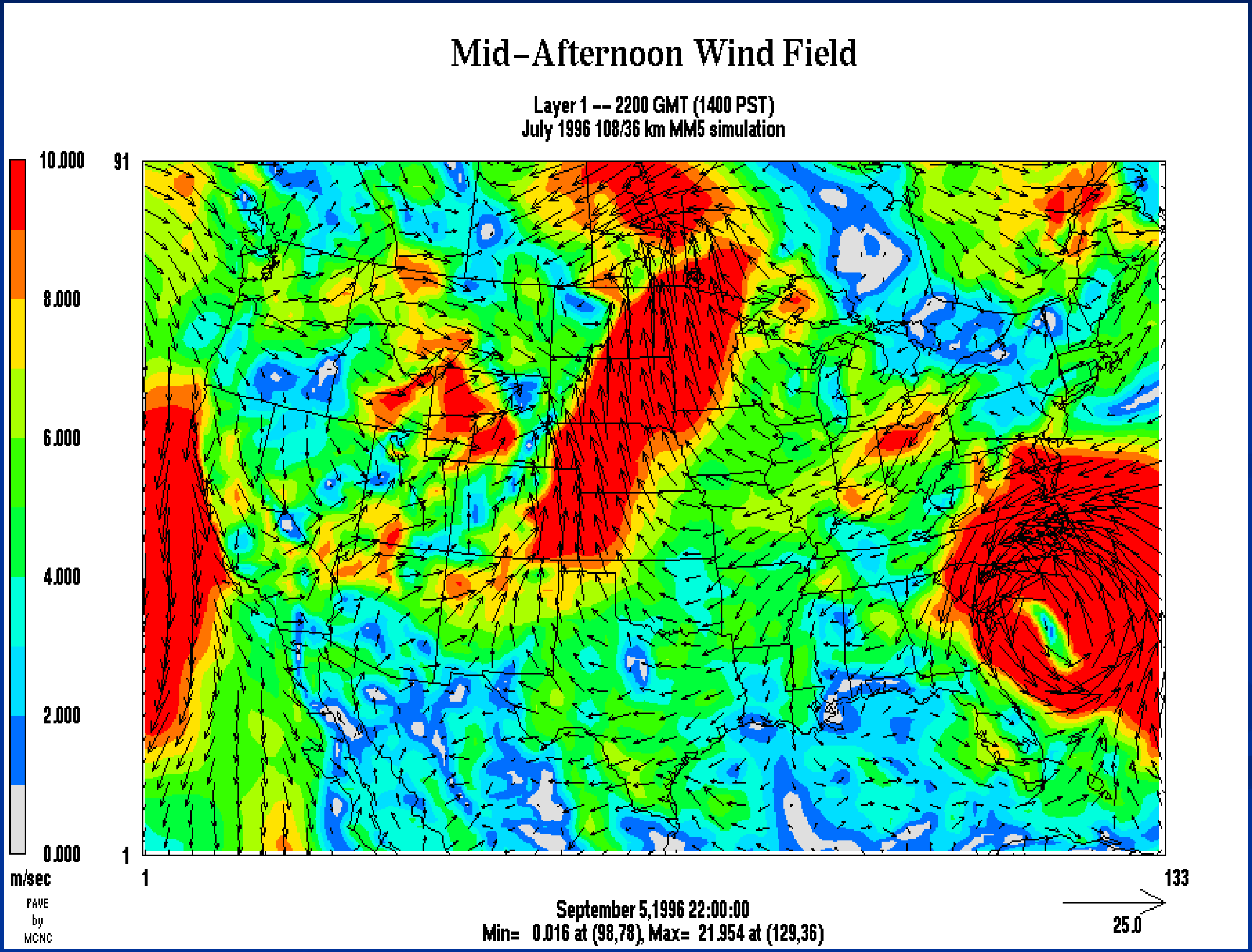
Model Inputs: Meteorological

- 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



Example- Wind Field

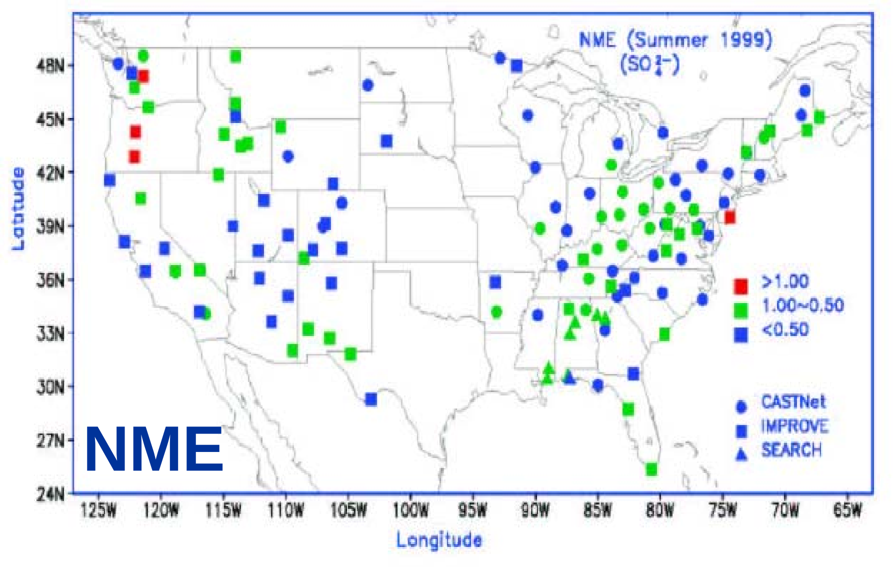


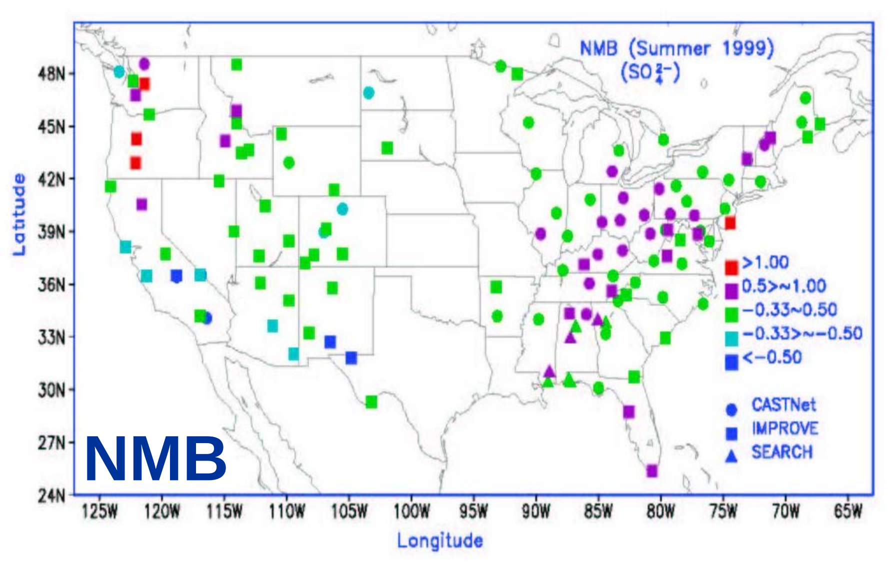
Model Performance Evaluation

- 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.

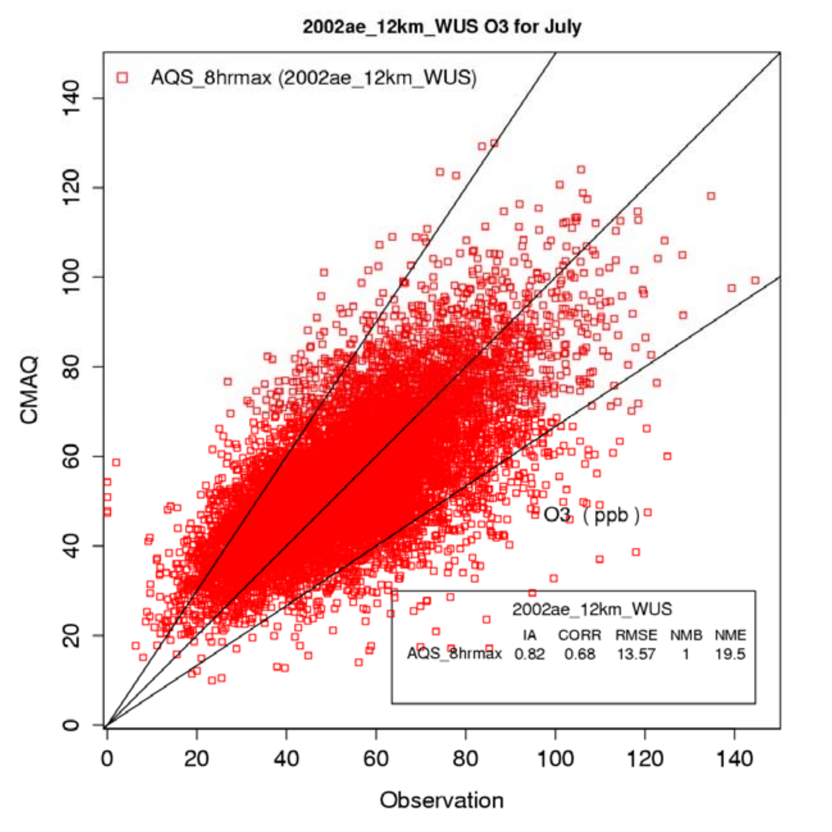
Example Model Performance Evaluation

Sulfate (μg 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 PM2.5 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 PM2.5, 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, PM2.5, and regional haze modeling
    - CMAQ: http://cmascenter.org/
    - CAMx: http://camx.com/
  - Use of AERMOD or other dispersion model for local primary PM2.5 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 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 >= 15 days per quarter
  - 24 Hour NAAQS
    - Model days > 35 ug/m3* 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 ug/m3 24-hr PM2.5 NAAQS have not been completed yet.

Horizontal Resolution

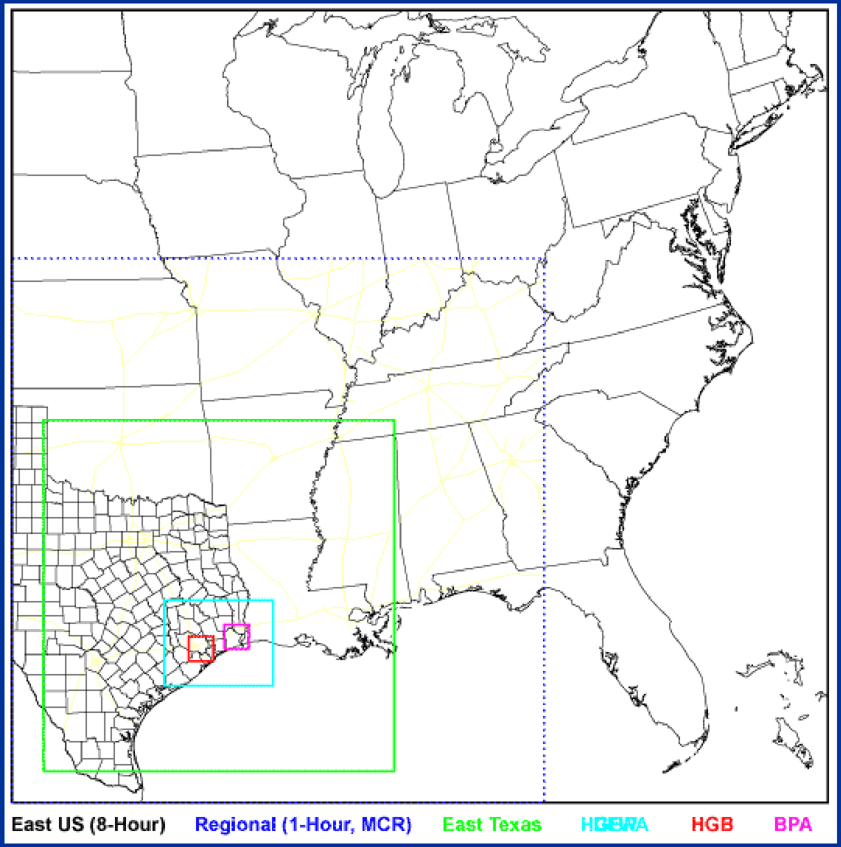
- Ozone <= 12km resolution
- PM2.5 <= 12 km resolution for urban scale modeling
  - <= 36 km for regional modeling
  - Higher resolution may be necessary in areas with high primary PM2.5 concentration gradients
- Recommend <= 36 km resolution for regional haze modeling

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 PM2.5 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 PM2.5 NAAQS
      - Unmonitored area analysis
      - Local area analysis (high primary PM2.5 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 O3/PM2.5/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 PM2.5 or ozone
  - Ambient concentration * RRF = Future concentration
- RRFs are calculated for ozone and for each component of PM2.5 and regional haze

Speciated Modeled Attainment Test (SMAT)

- The attainment test for PM2.5 uses separate RRFs for each PM2.5 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] + [OCMmb] + [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/m3 (default) blank mass

SMAT Components- More detail

- $NO3_{FRM}$ – Retained nitrate
  - Calculated using hourly temperature and relative humidity data
    - EPA has default pre-calculated retained nitrate concentrations
- $NH4_{FRM}$- 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, PM2.5, and regional haze tests
  - Interpolates ambient data (where necessary) for ozone and PM2.5 tests
  - Creates “fused” spatial fields for unmonitored area analysis

MATS

- Provides a consistent set of ambient data for all States to use
  - Ozone and PM2.5 design values
  - Pre-screened daily average STN and IMPROVE data for PM2.5 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
- 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 PM2.5
- UAA not designed to look for unmonitored PM micro-scale hotspot issues
  - 12 km resolution sufficient for annual PM2.5
  - Finer resolution for 24-hr PM2.5 may be appropriate

Local Area Analysis

- Focused on evaluating influence of primary PM2.5 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?)
- 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 PM2.5 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 PM2.5 14.5-15.5 ug/m3
  - 24-hour PM2.5 62-67* ug/m3
  - 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/m3 NAAQS

Next Steps

- Complete guidance revisions in early 2010
  - New PM2.5 and ozone NAAQS
  - Miscellaneous updates
- Release MATS with 24-hr PM2.5 test