MARAMA Webinar on :

Introduction to Air Quality Modeling

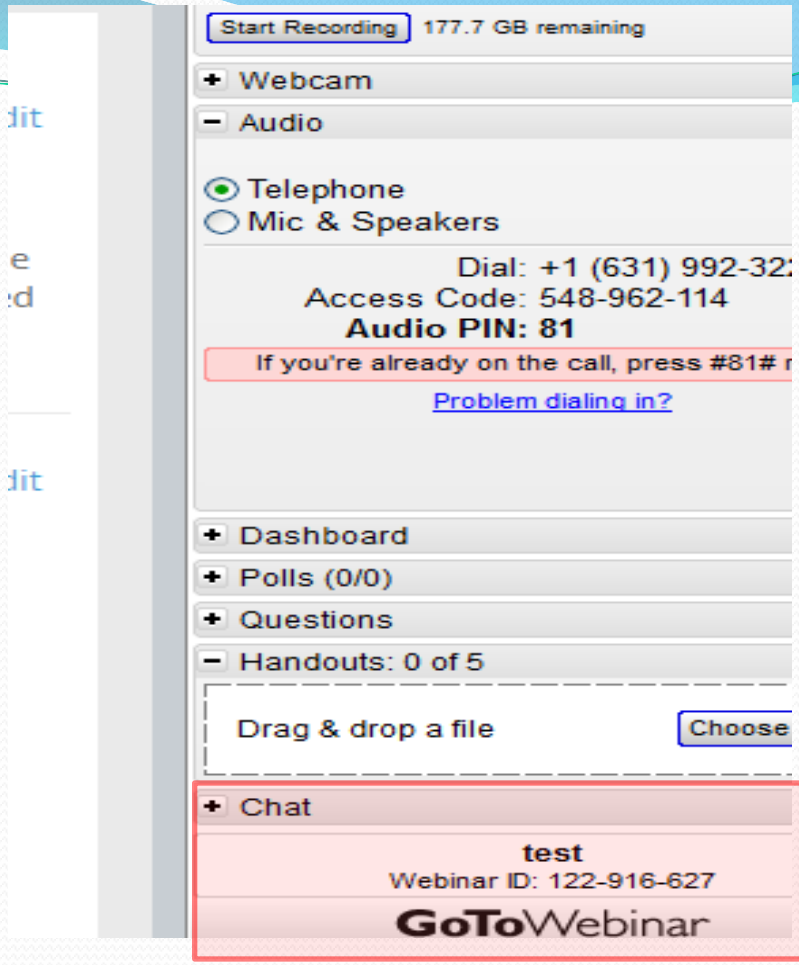
Presented by Julie McDill, P.E.

August 17, 2016

MARAMA

Mid-Atlantic Regional Air Management Association, Inc.

Q & A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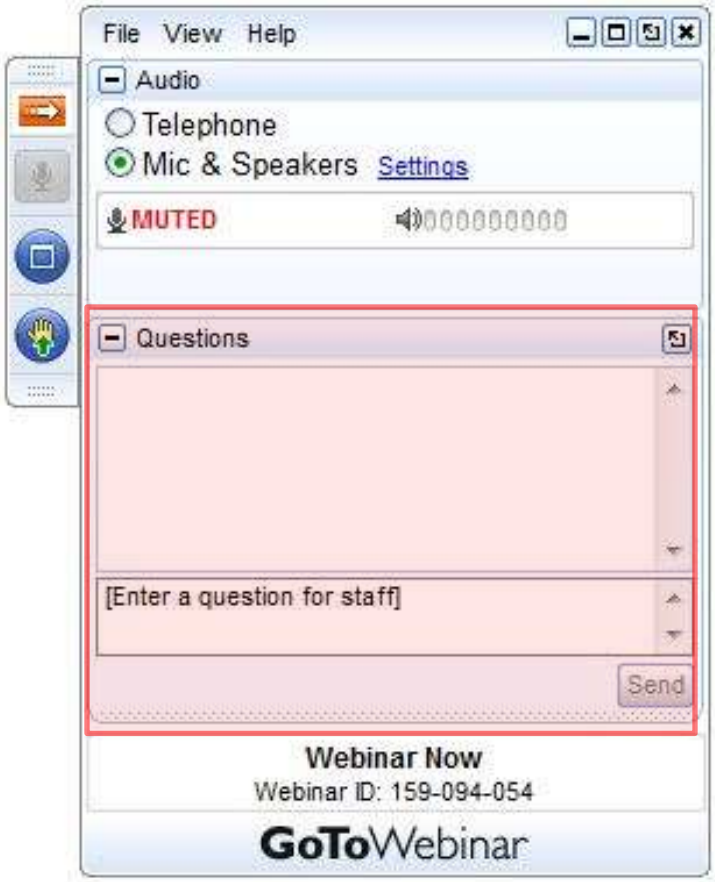
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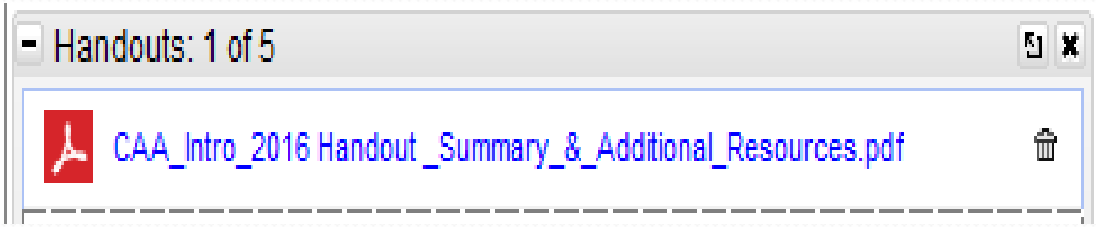
Handouts: 1 of 5
CAA_Intro_2016 Handout _Summary_&_Additional_Resources.pdf

Introduction to Air Quality Modeling Agenda

- **Part 1 – Some Types of Models**
- **Part 2 – Setting up Regional Air Quality Models**
- **Part 3 – Emissions Inventories for Regional Modeling**
- **Part 4 – More about Using Models for SIPs .**

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Learning Objectives

The participant will be able to:

1. Correctly use *model names and acronyms* in discussion or written materials
2. Identify the *types of modeling needed* to address a variety of air quality issues
3. Identify *photochemical grid models* for SIP planning
4. Identify *dispersion models* for point source analysis
5. Define *source apportionment modeling* and *receptor modeling* and their role in identifying source contribution to air pollution
6. Identify the step to develop an *emissions inventory*
7. Recognize & understand the purpose of *meteorological models*
8. *Find more information* when needed.

Which of these learning objectives are the most important to you? (Please answer in chat box.)

Let's check

- How much do you think you understand about air quality modeling?
  - A. I'm an expert
  - B. Somewhat familiar with how models are used
  - C. Novice

Webinar Overview

- Part 1 – Some Types of Models
- Part 2 – Setting up Regional Air Quality Models
- Part 3 – Emissions Inventories for Regional Modeling
- Part 4 – More about Using Models for SIPs

What are Models?

Tools to represent our understanding of how the world works and predict the effect of changes. Two general types:

- Physical
- Mathematical

Part I – Some Types of Air Quality Models

- Receptor models
- Photochemical models
- Dispersion models
- Trajectory models
- Emissions models

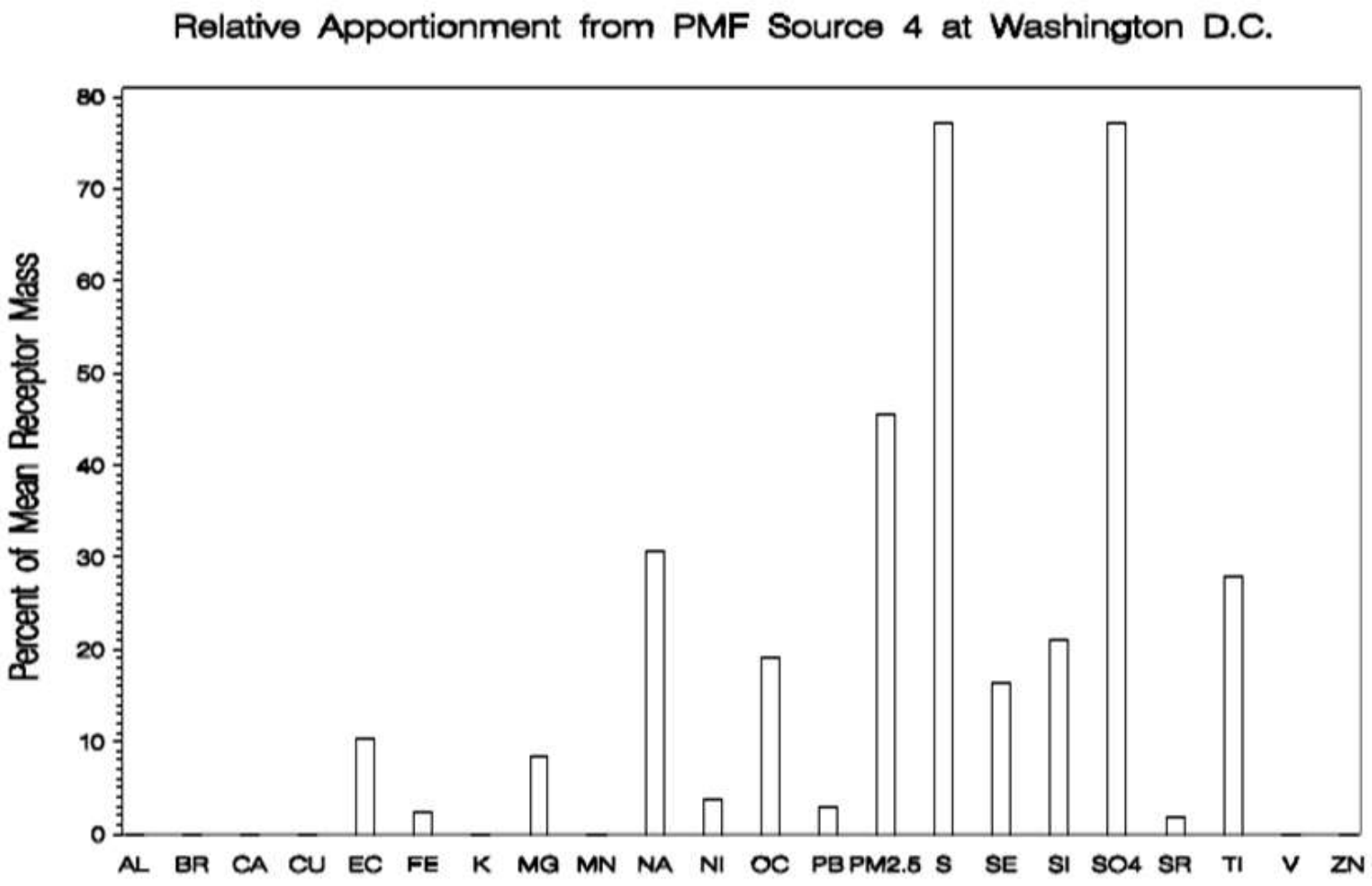
Types of Mathematical Models

- Statistical models
  - E.g., Forecast air quality based on current conditions as compared to past experience
  - E.g., Receptor modeling
- Air quality models – Representation of physical processes
  - Lagrangian models
  - Eulerian models

Example of a Statistical Model

- Receptor Modeling
  - Statistical analysis and qualitative interpretation of air quality data and source characteristics
  - Factor analysis of measured air quality data
    - Uses multiple regression analysis to define “factors”
    - Factors characterized by similar groups of chemicals
    - Compares “factors” to emissions patterns from likely sources

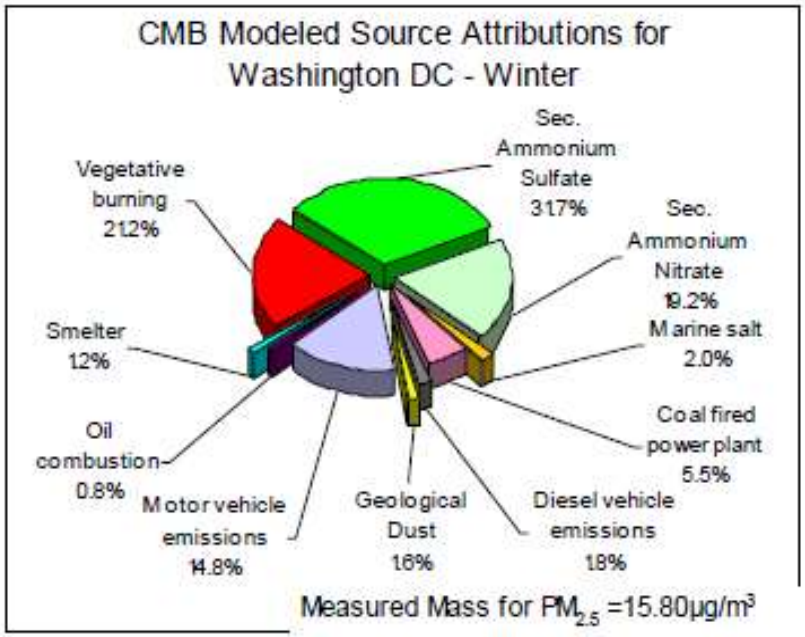
Sample analysis of chemicals

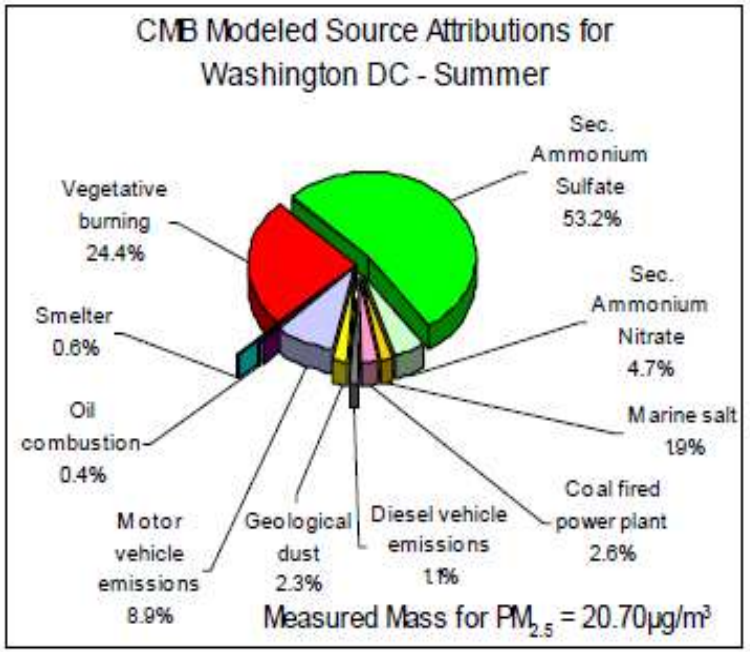


More on Receptor Modeling

- **Purpose:** Identify likely sources of air pollution based on chemicals present at a source and receptor (an air quality monitor).
- **Input data needed:** Best with long-term data sets of chemical constituents (e.g. constituents of $PM_{2.5}$) both in the air and from sources.
- **Models:** PMF, UNMIX, CMB
- **Limitations:** Analyzes the past. Does not predict the future. Qualitative analysis.

Source Apportionment Sample Results





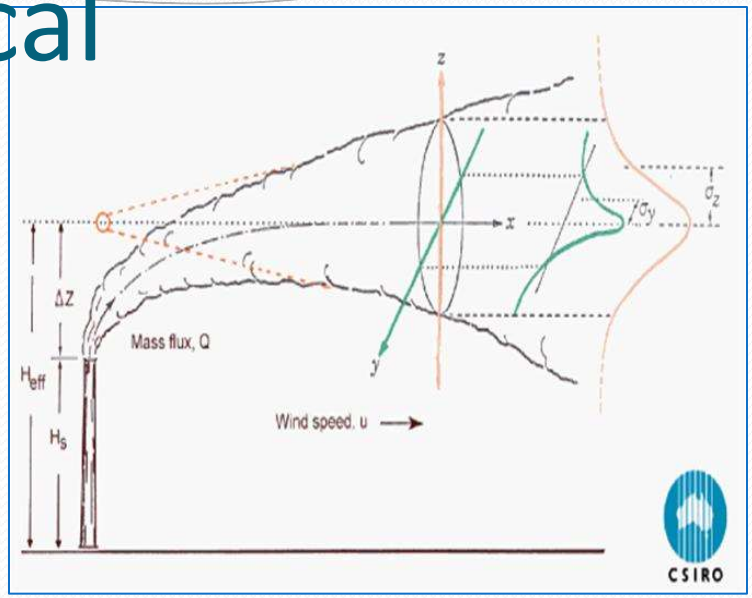
Source: *Source Apportionment Analysis of Air Quality Monitoring Data: Phase II*. Prepared by DRI for MARAMA, 2005

Types of Mathematical Models

- Statistical models
  - E.g., Forecast air quality based on current conditions as compared to past experience
  - E.g., Receptor modeling
- Air quality models
  - Lagrangian models
  - Eulerian models

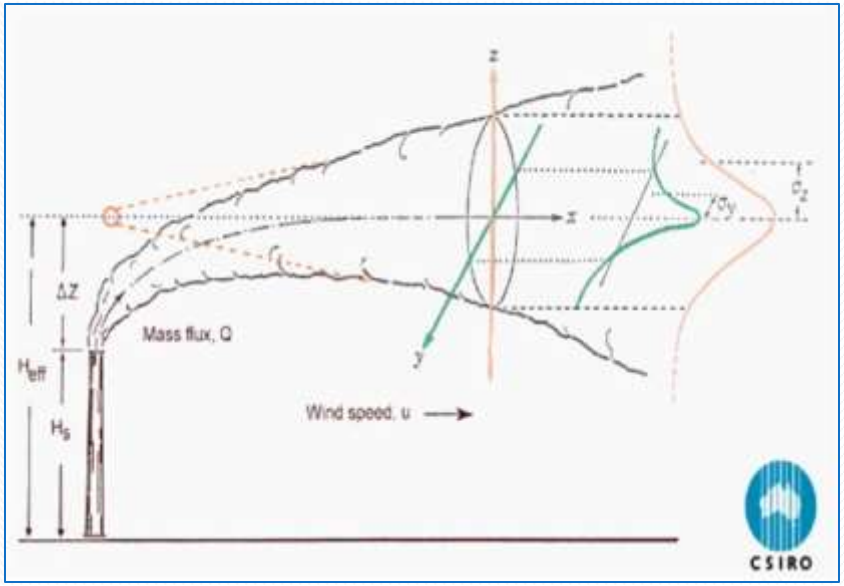
Types of mathematical air quality models

- *Lagrangian models* simulate dispersion or reactions in parcels of air that move along with the wind trajectory – mathematical representation of physics.
- *Eulerian* approaches divide the problem domain into fixed grid cells. Various methods are then used to solve equations over the full domain. Heavier emphasis on chemistry than physics



Which models use which math?

- *Lagrangian models*
  - Dispersion models
  - Trajectory models
- *Eulerian*
  - Photochemical grid models

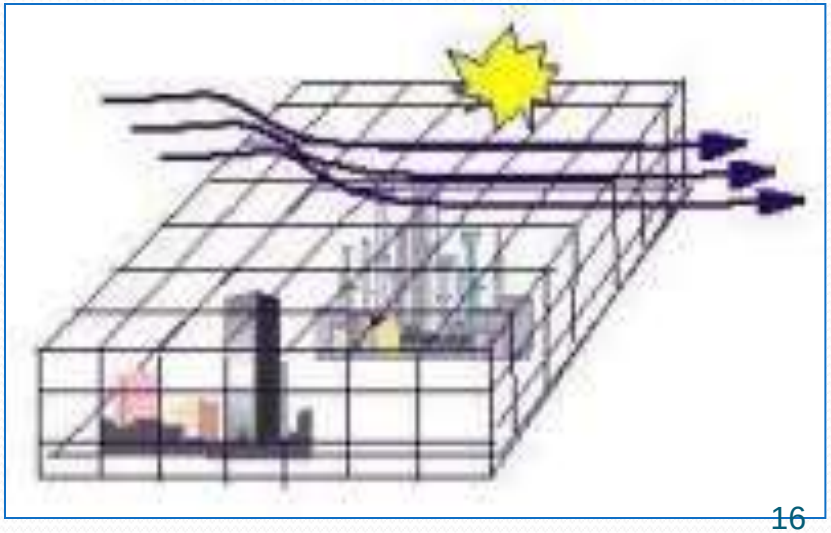


Let's explore each of these:

Dispersion models

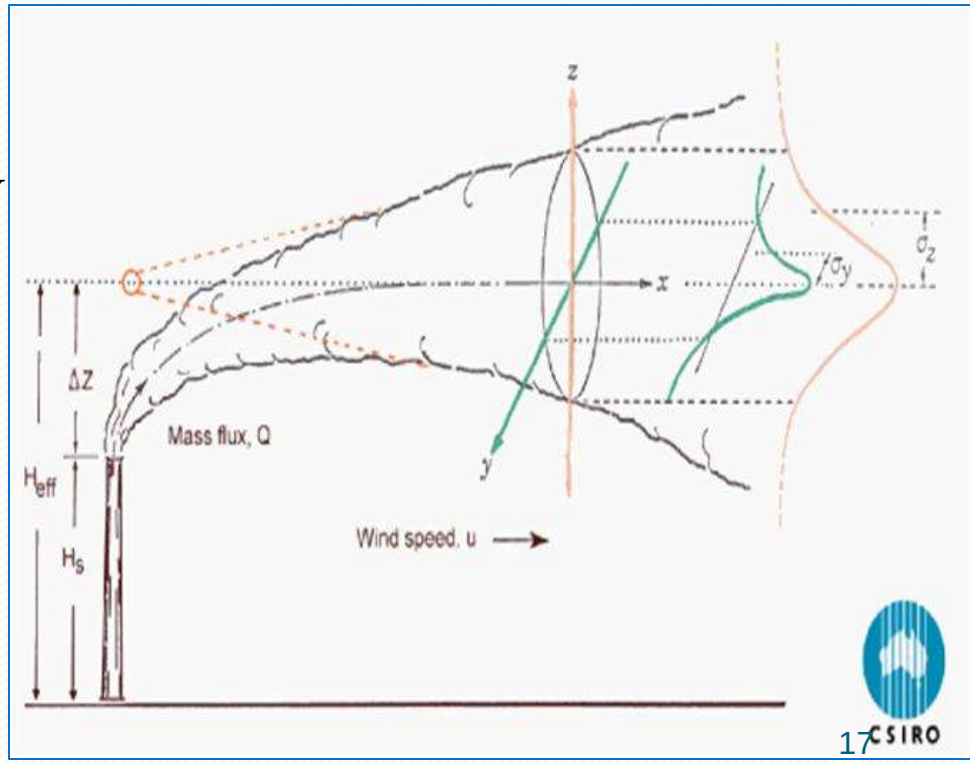
Trajectory models

Photochemical grid models



What is dispersion modeling?

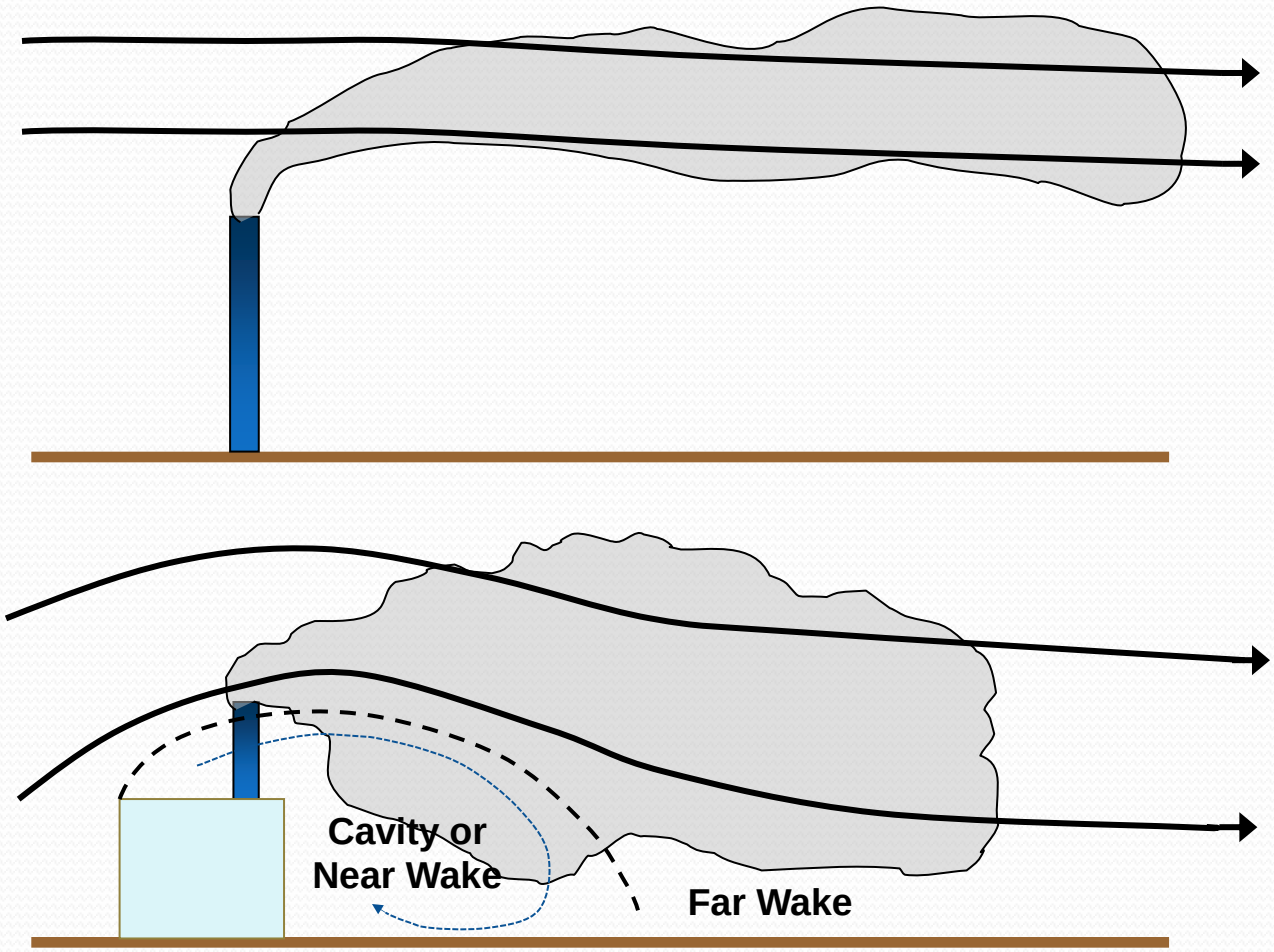
- Lagrangian Model
- Purpose: Estimate the effect of
  - local sources
  - local atmosphere
  - pollutants not affected by chemical transformation
- Examples: AERMOD, CALPUFF



What can dispersion models do that other models cannot?

- Represent effect of terrain & buildings on plume
- Detailed characterization of fundamental boundary layer parameters

Building Influences / Downwash



Atmospheric Boundary Layer

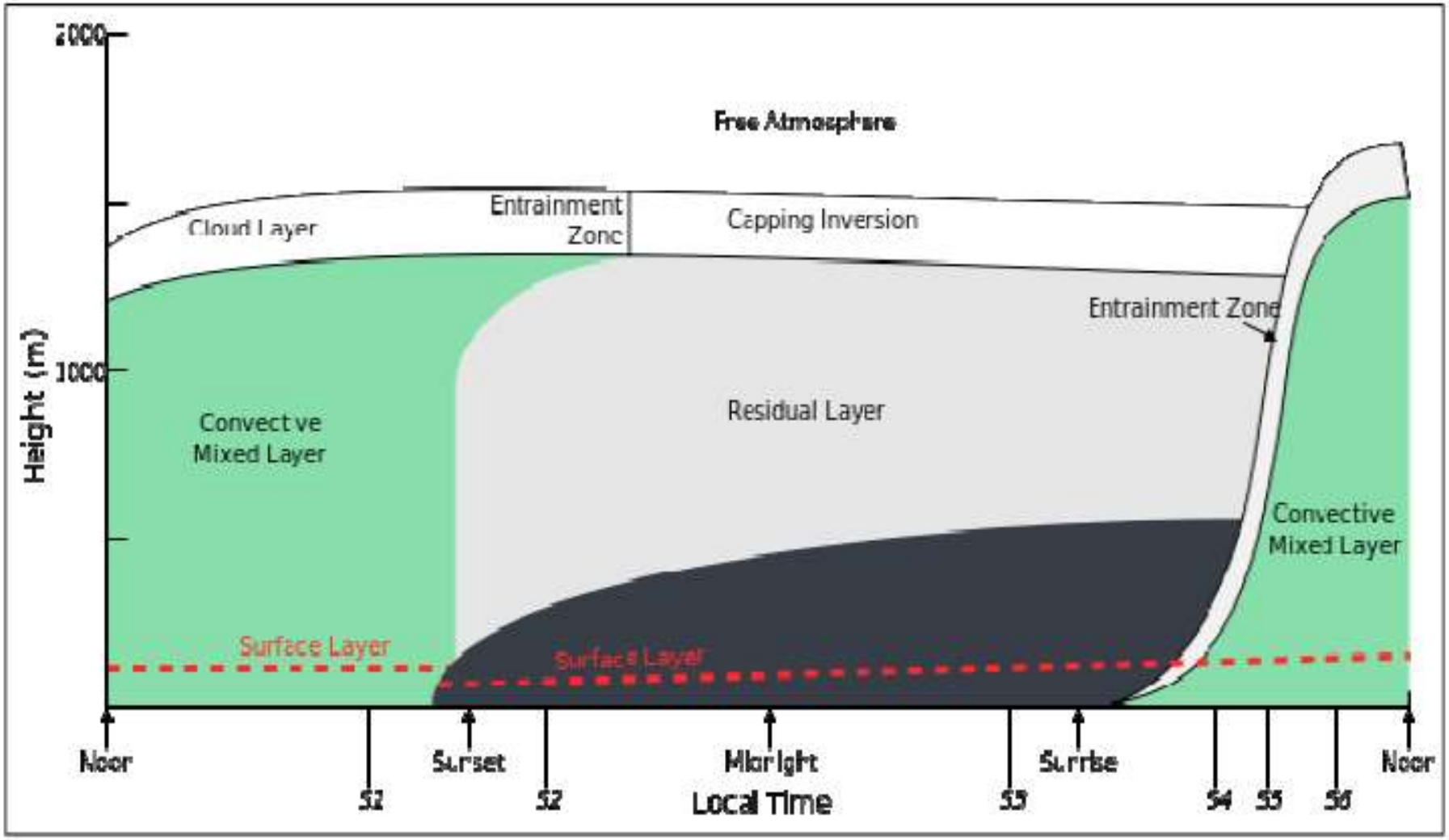


Figure 3. Atmospheric boundary layer structure (NikNaks, 2012 based on Stull, 1988).

AERMOD Primary & Ancillary Programs

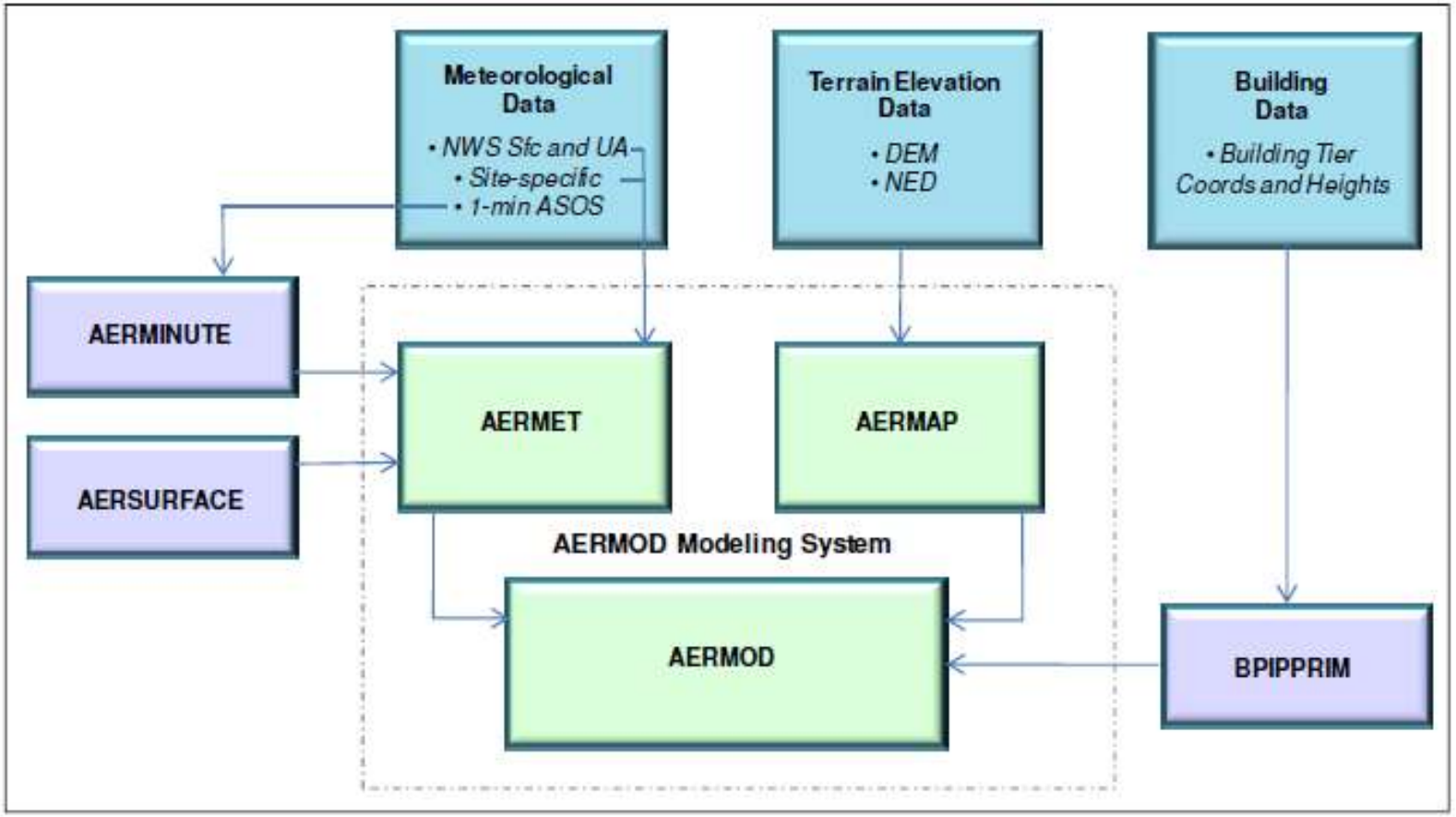
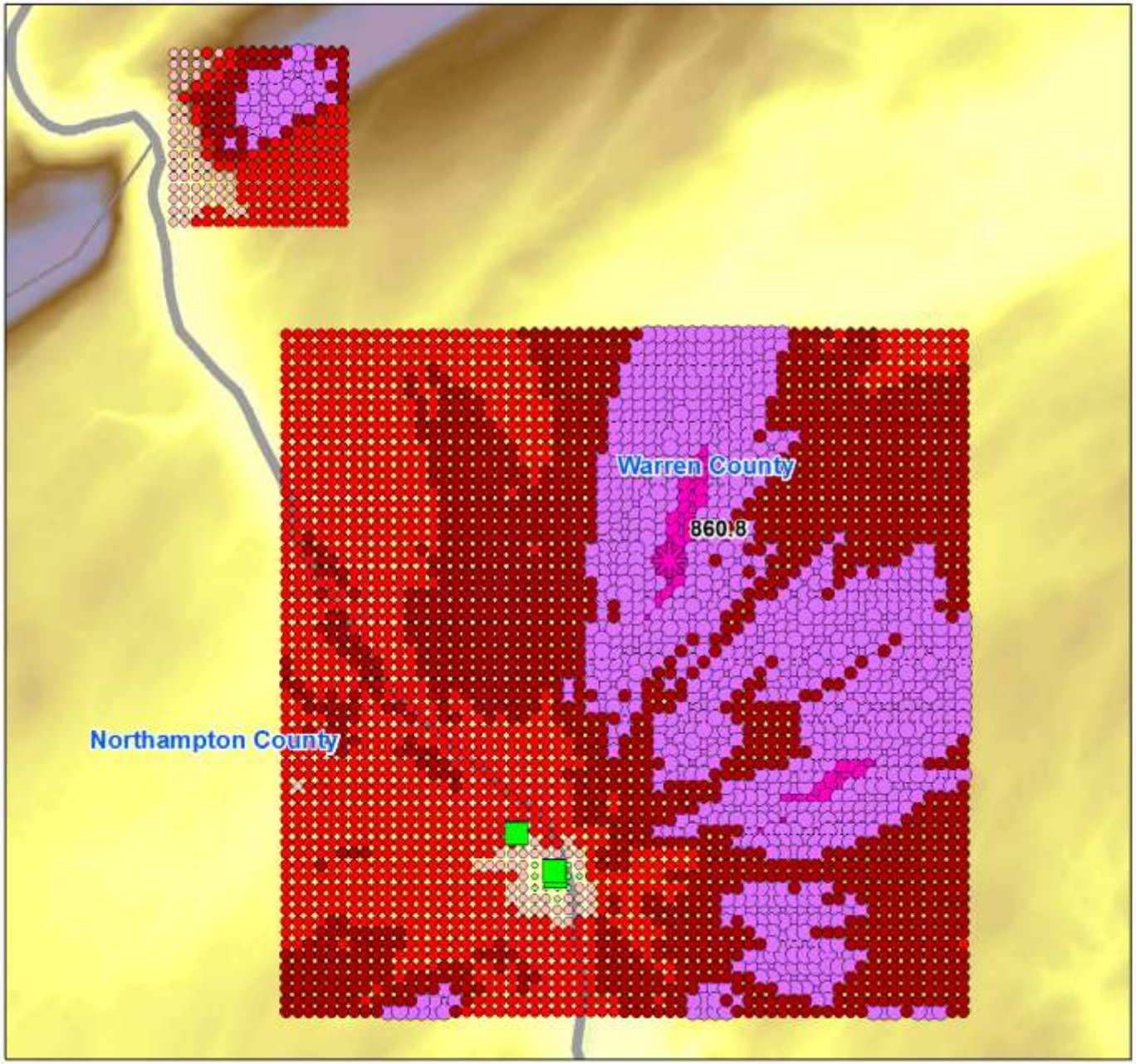


Figure 9. AERMOD primary and ancillary programs.

AERMOD Analysis - NJ 126 - Run 1 (100-meter Grid) - PGS 1, 2 & 5 at Allowable Rates



Legend

N
W
E
S

Model Peak Run 1

PGS Units 1, 2 & 5

Fine Grid Receptors

Run 1 All, 4th High 1-Hour

- < 196.2 ug/m3
- 196.2 - 350 ug/m3
- 350 - 500 ug/m3
- 500 - 650 ug/m3
- 650 - 800 ug/m3
- > 800 ug/m3

NED 1/3 Arc Elevation

Meter

High : 703.472

Low : -0.610803

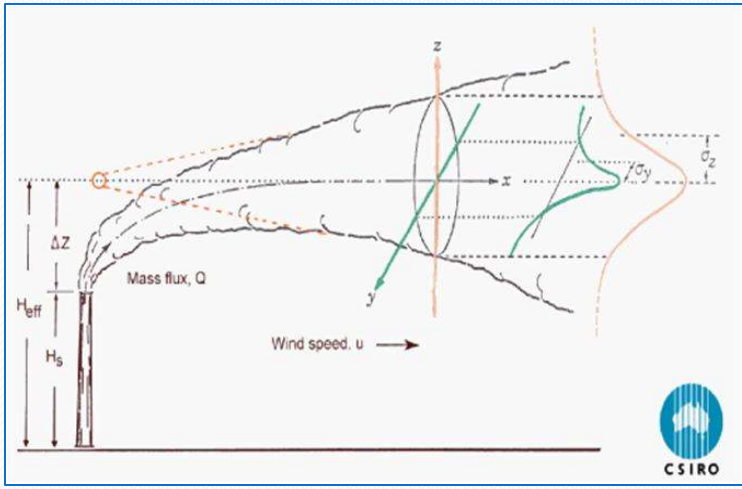
0 1.5 3 6 Kilometers

EPA United States

What is trajectory modeling?

- Purpose: Compute the location of an air parcel in the time before it arrived at a specific location. Used to help identify source regions contributing to pollution at a given location.
- Examples: HYSPLIT
- Trajectory modeling vs dispersion modeling

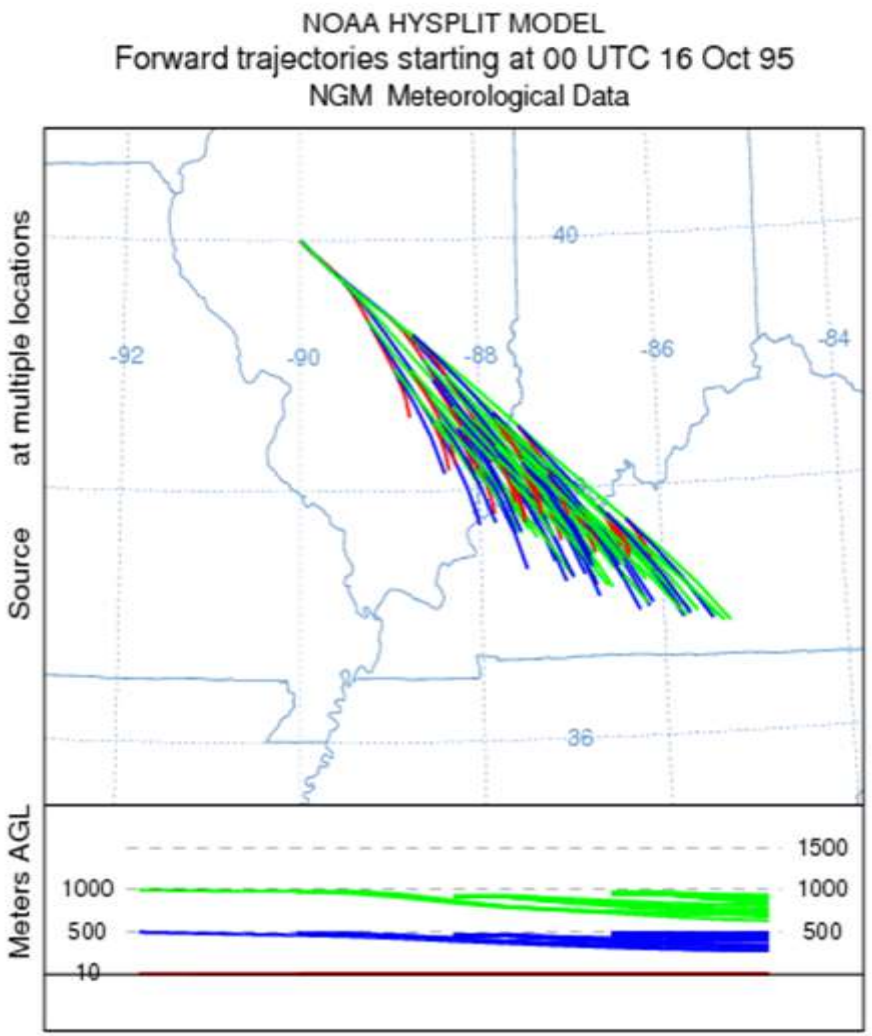
  Trajectory modeling doesn't involve emissions and concentrations—just wind direction and speed.



Dispersion modeling

Trajectory Modeling

NOAA HYbrid Single-Particle Lagrangian Integrated Trajectory Model (HYSPLIT)



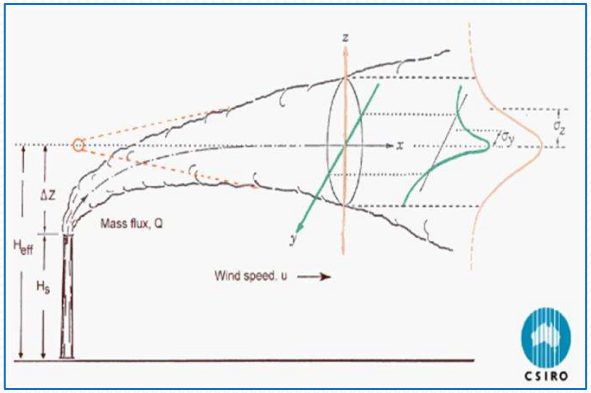
- Uses meteorological forecast fields from regional or global models to predict advection, stability and dispersion
- Can be run at varying heights
- Can be run forward (where will a particle go from a source)
- Can also calculate back trajectories (where did a particle come from)
- This picture shows forward trajectories

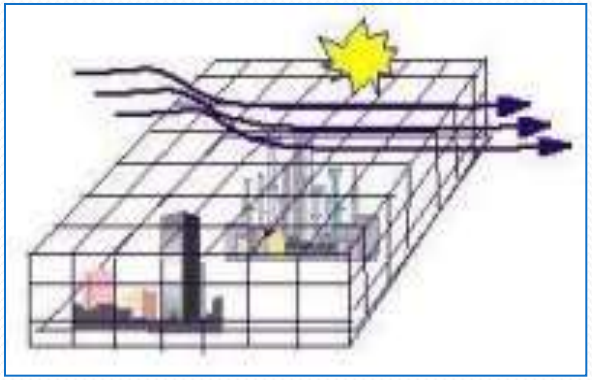
48-Hour Backward Trajectories for Acadia National Park

Start Height = 200 m. Best Days are Blue, Worst Days are Red

Now lets review photochemical grid models

- *Lagrangian models*
  - Dispersion models
  - Trajectory models
- *Eulerian*
  - Photochemical grid models





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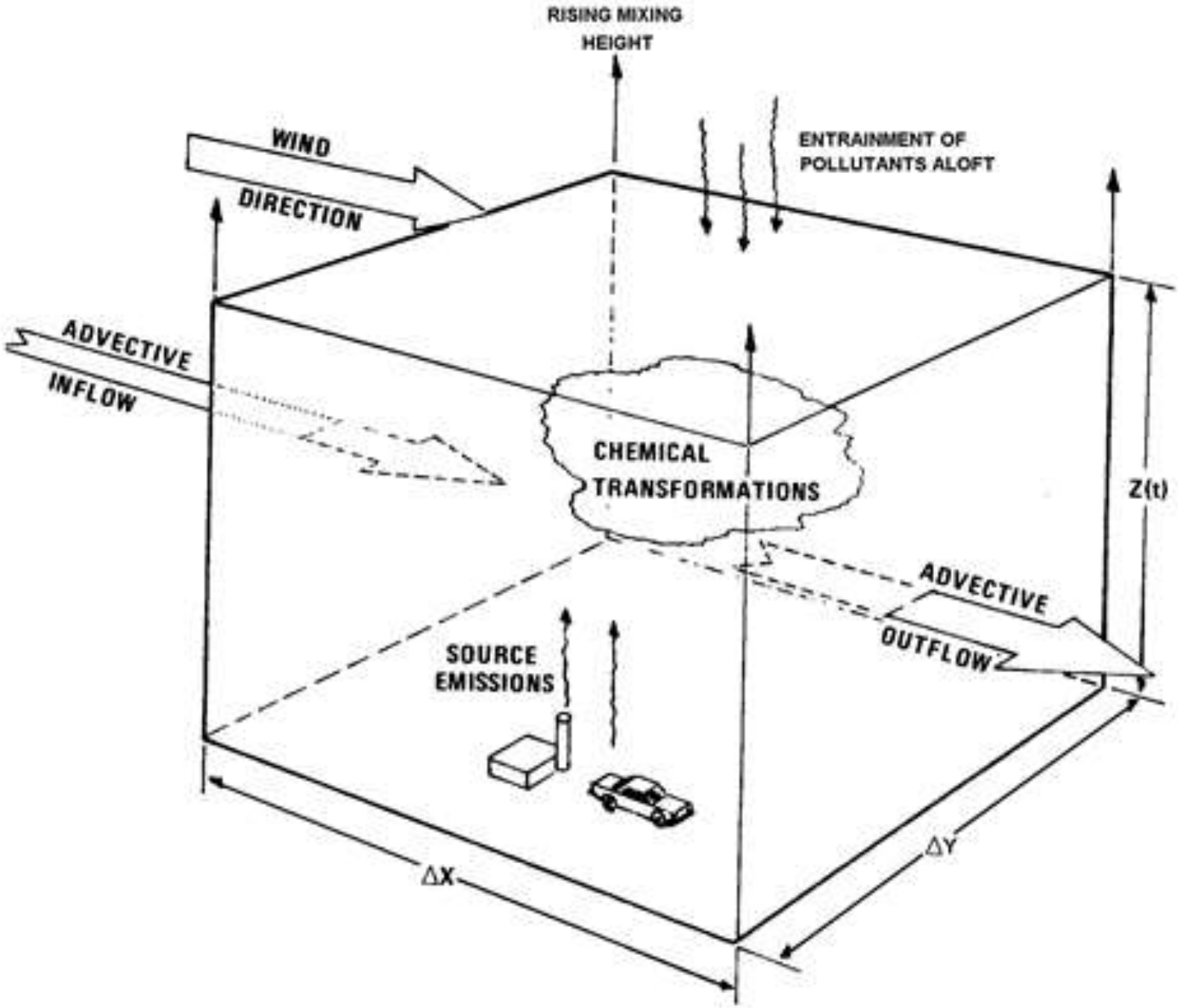
Dispersion models

Trajectory models

Photochemical grid models


RISING MIXING HEIGHT
WIND DIRECTION
ENTRAINMENT OF POLLUTANTS ALOFT
ADVECTIVE INFLOW
CHEMICAL TRANSFORMATIONS
Z(t)
ADVECTIVE OUTFLOW
SOURCE EMISSIONS
ΔX
ΔY

Photochemical Grid Modeling

- Purpose: Estimate formation ozone and reactive particulate matter in the atmosphere.
  - Secondary air pollutants formed downwind.
- Predict long range transport and atmospheric chemical transformations over hundreds and even thousands of miles.
- Examples: CMAQ, CAMx
- Related terminology: CB05 is the set of equations that represent atmospheric chemistry inside the photochemical model.

Comparing the Purposes of Various Types of Models

	Model type	Pollutants involved
PM SIP	Receptor, Dispersion, Photochemical	PM2.5, SO_2, NO_X, CO, Ammonia, a variety of other species.
Ozone SIP	Photochemical	VOC, NO_X, CO
Haze SIP	Receptor, Dispersion, Photochemical	All of the above
Conformity	Emissions	NO_X and CO, and PM
Source permitting	Dispersion	Source specific
NO_X 1 hour attainment demonstration	Dispersion	NO_X
SO_2 1 hour attainment demonstration	Dispersion	SO_2

Part 1 - Quiz

- Which type of models are primarily used to analyze the impacts of a single source?
  A. Dispersion models
  B. Regional air quality models

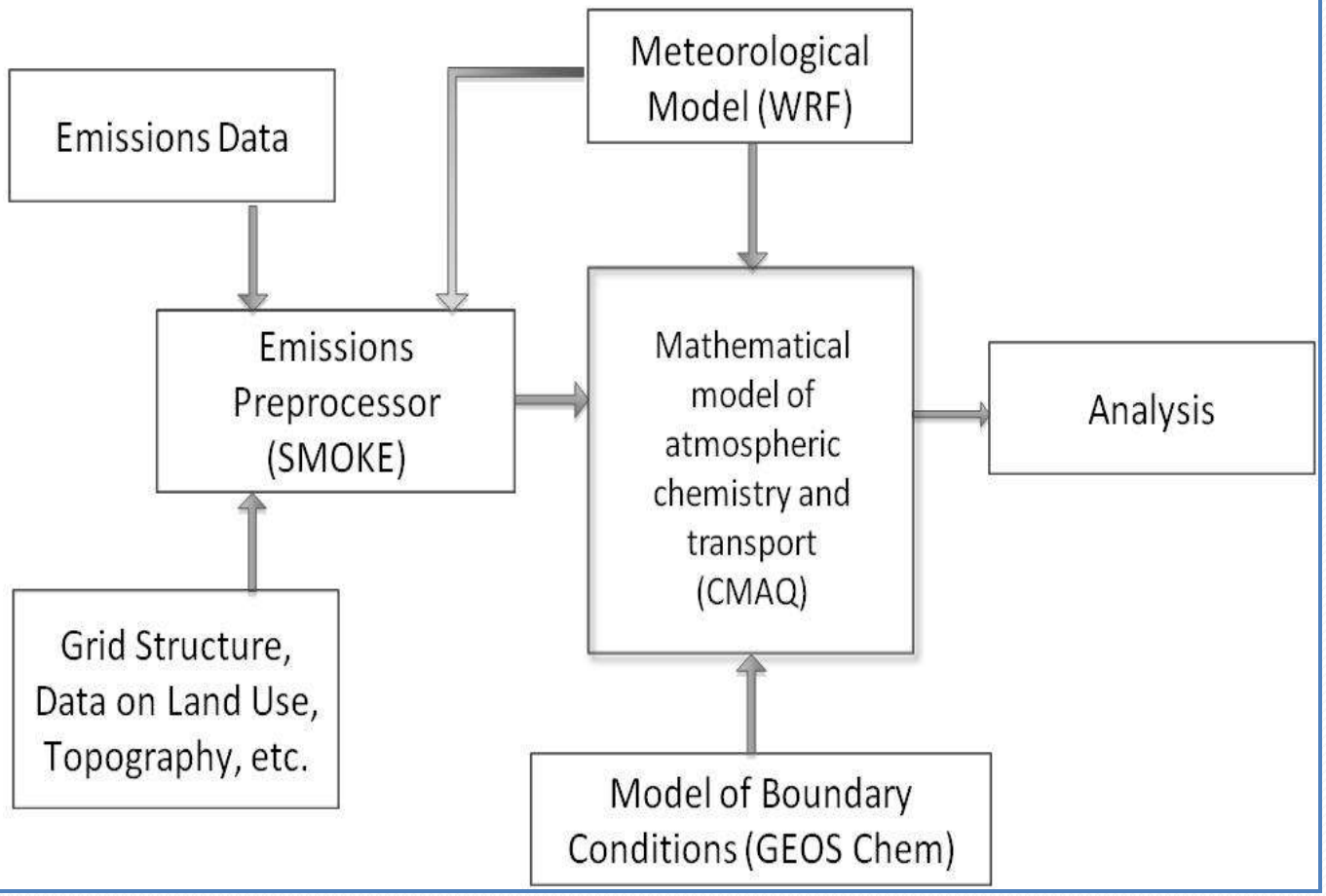
Part 1 - Quiz

- Which model is primarily used for regional air quality modeling?
  A. CMAQ
  B. AERMOD

Moving on…

- Part 1 – Some Types of Models
- Part 2 – Setting up Regional Air Quality Models
- Part 3 – Emissions Inventories for Regional Modeling
- Part 4 – More about Using Models for SIPs

Basic Photochemical Air Quality Model Diagram

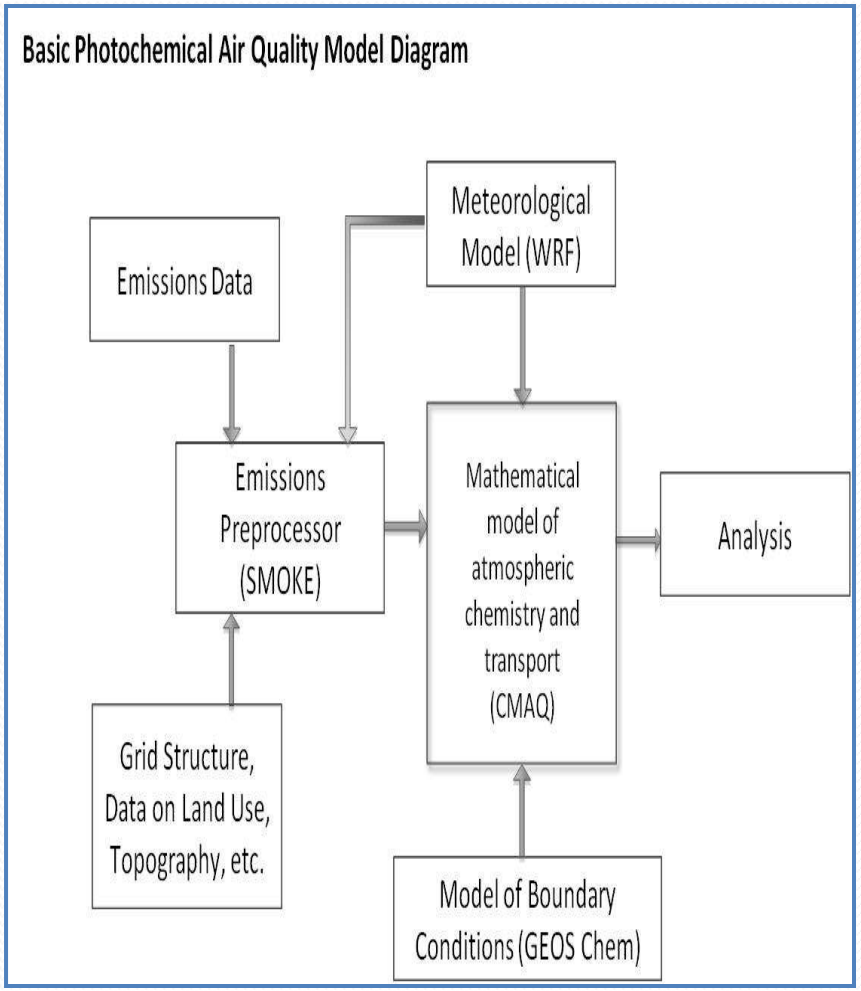


Who does photochemical modeling?

- Ozone Transport Region:
  - New York State DEC
  - Virginia DEQ
  - New Jersey DEP
  - University of Marland
- Southeast (including VA, WV, Region IV)
  - Southeastern Modeling, Analysis, and Planning Project (SEMAP) coordinated by SESARM
- Midwest - LADCO

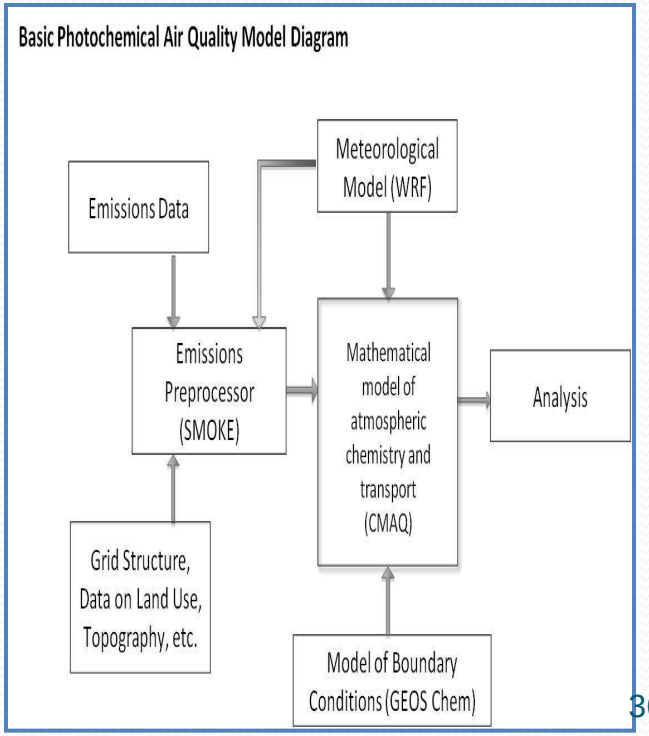
Setting up Regional Air Quality Models

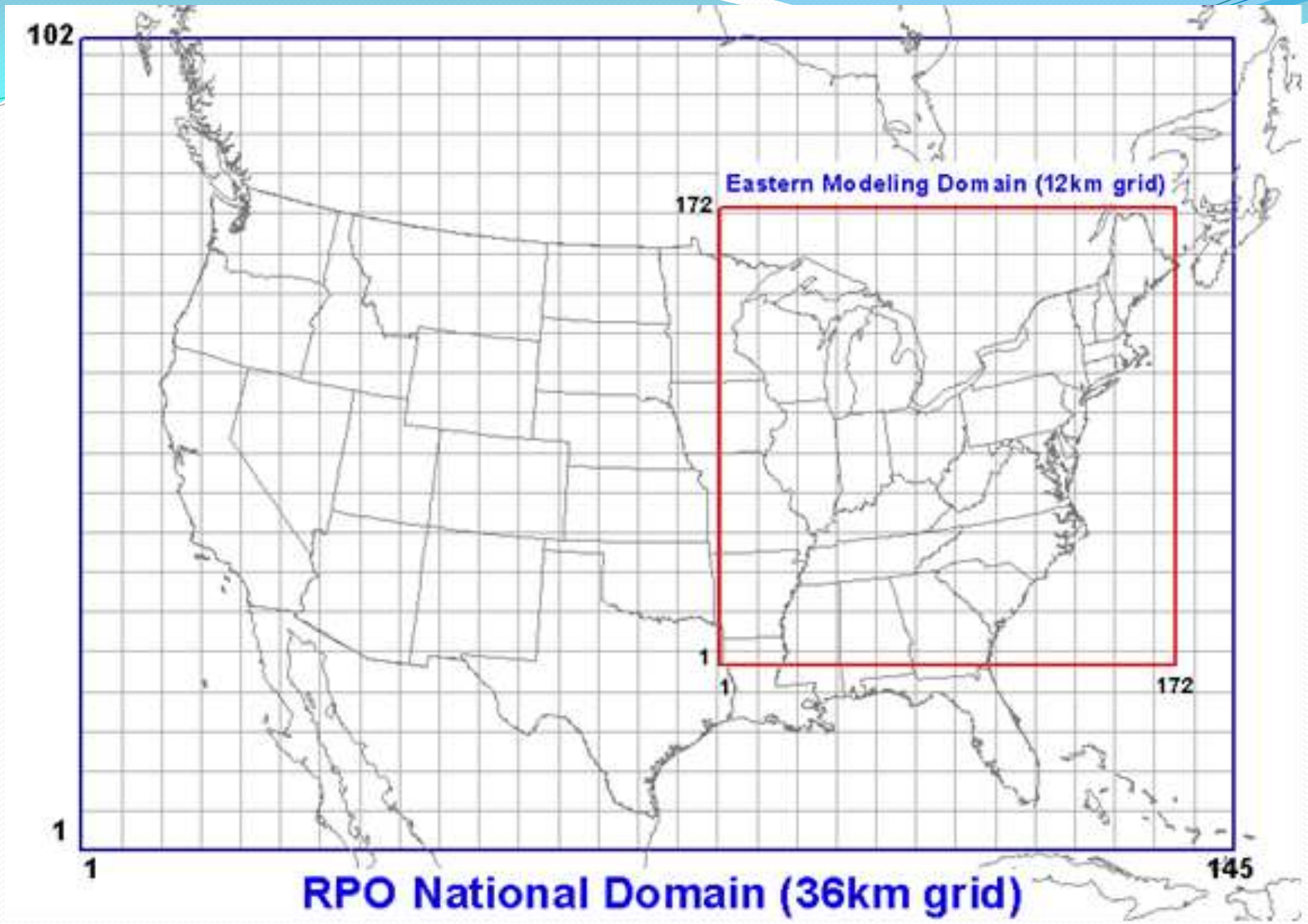
- Modeling Domain
- Boundary Conditions
- Grid Structure
- Meteorological Model
- Pre-processing/post-processing
- Emissions Inventory



The Modeling Domain

- The size and nature of the domain depends on the purpose of the modeling project
  - For *source permitting*, screening modeling is used to define the area of potential impact, and there are requirements for including sources within specific distances
  - For *regional air quality modeling*, geographic features that influence transport patterns and the location of major sources are considered in defining the modeling domain

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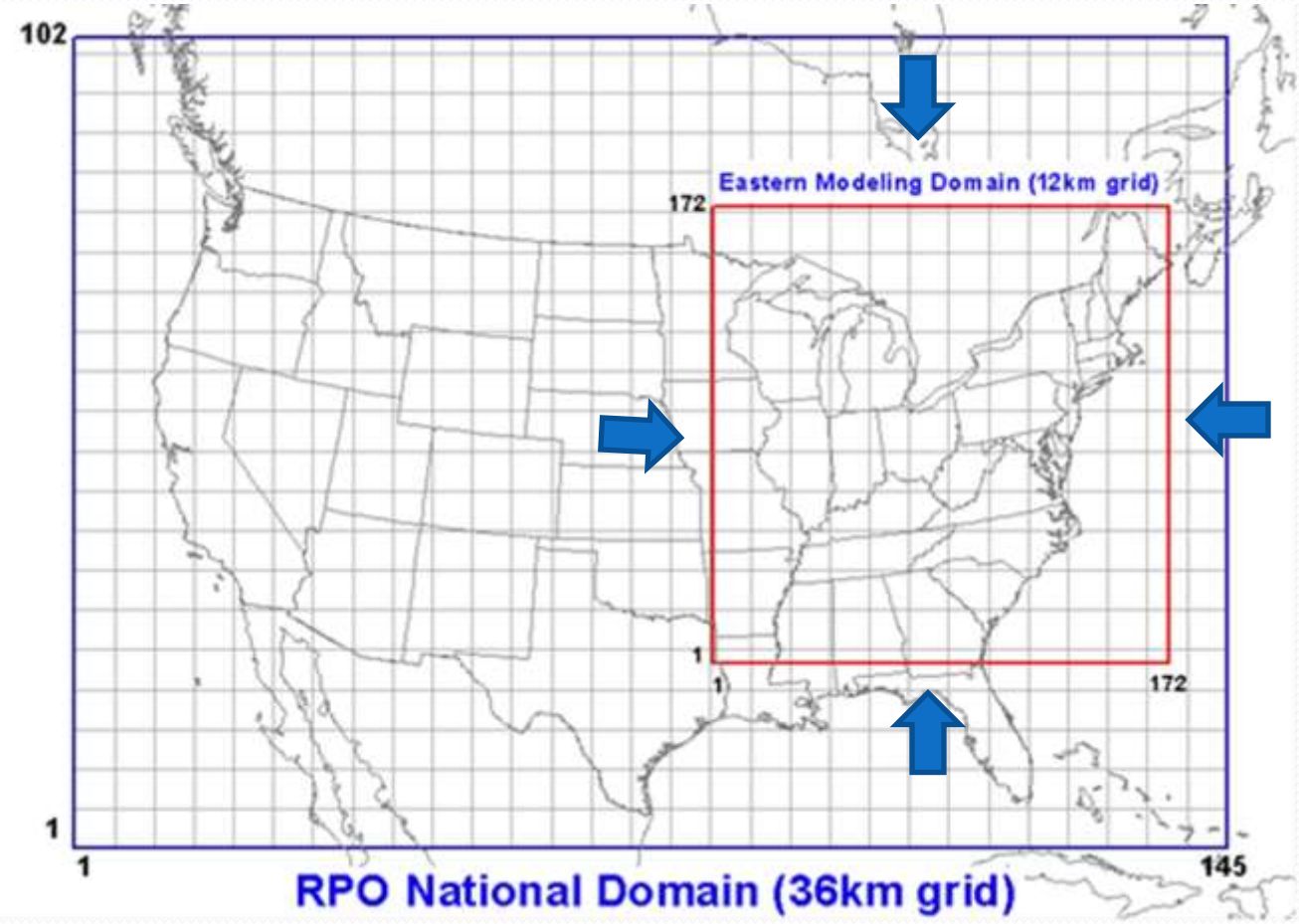
Eastern Modeling Domain (12km grid)
172
1
1
172
1
1
145
RPO National Domain (36km grid)

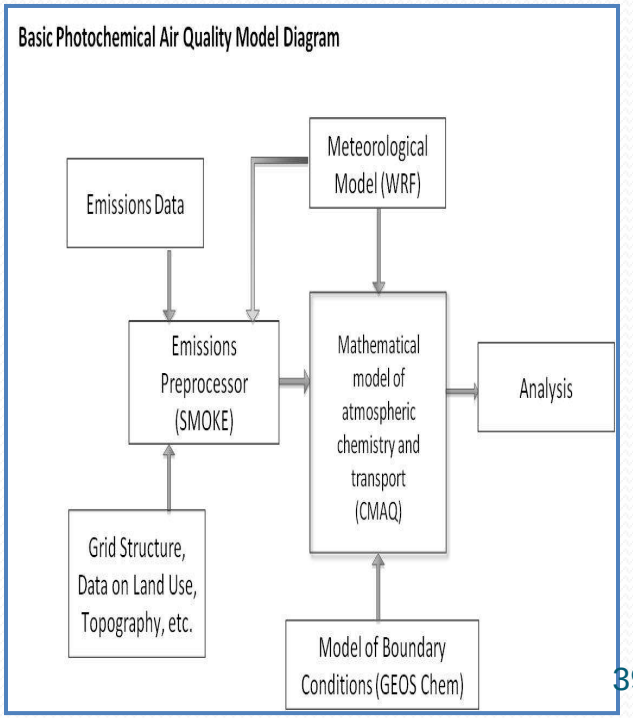
Boundary Conditions



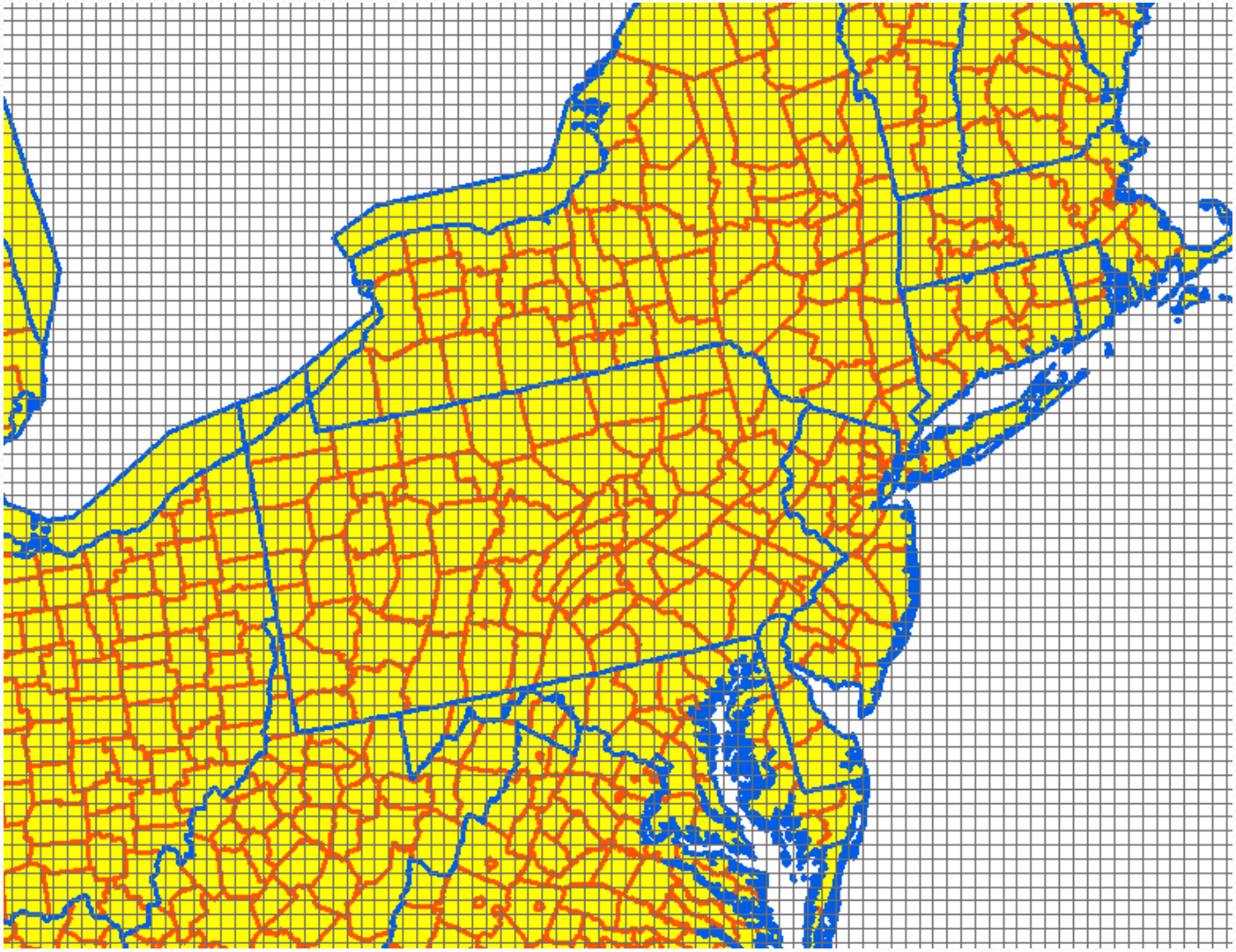
Modeling the national domain provides information about air quality at the boundaries of the Eastern Modeling Domain

The importance of grid and domain size

- Grid and domain size both influence the time and computer resources needed to run photochemical grid models
- Grid size controls the level of detail required in input and available in output for analysis

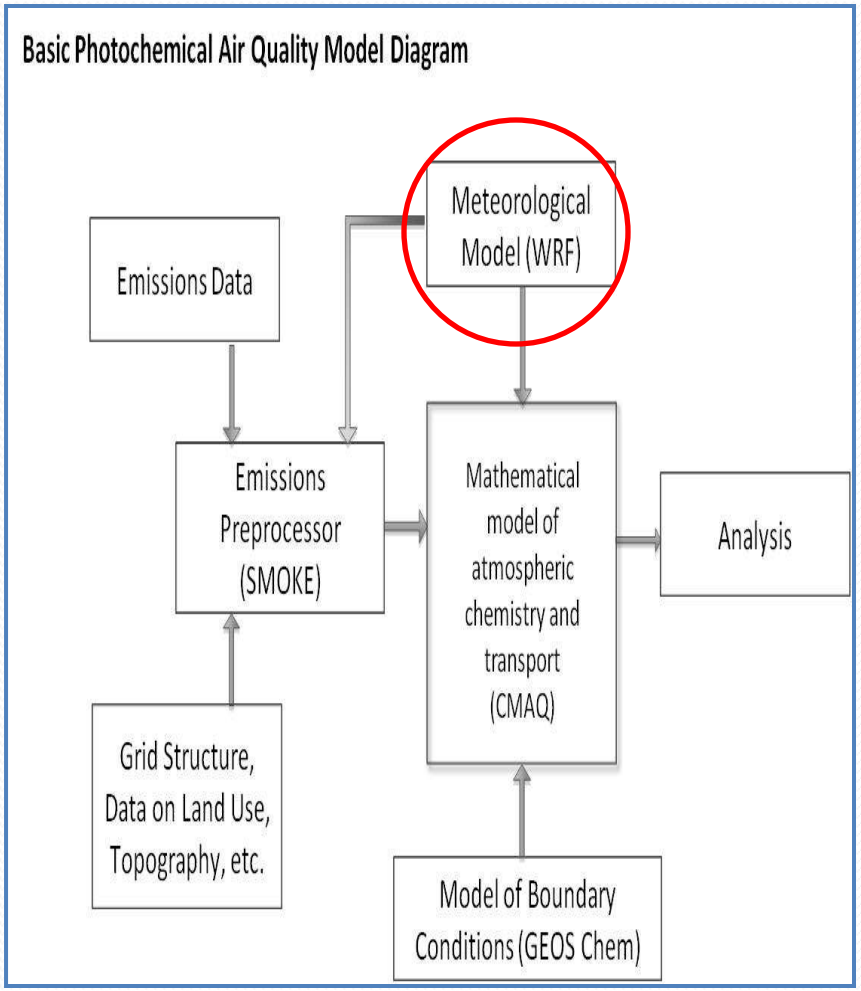


Comparing 12 km Grid to Counties



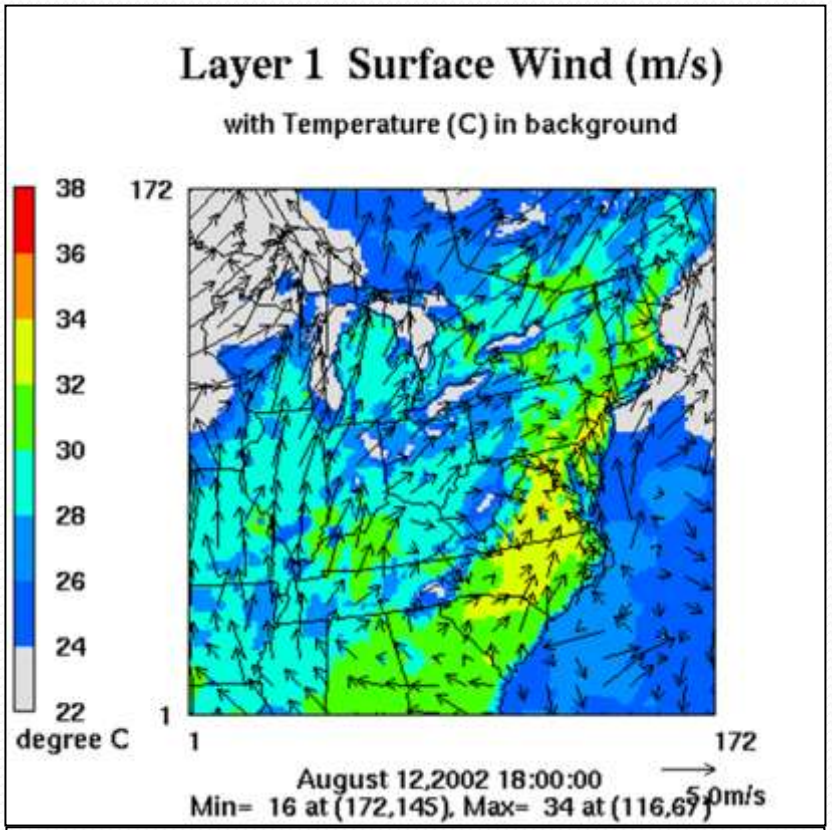
Setting up Regional Air Quality Models

- Modeling Domain
- Boundary Conditions
- Grid Structure
- **Meteorological Model**
- Pre-processing/post-processing
- Emissions Inventory



What are Meteorological Models?

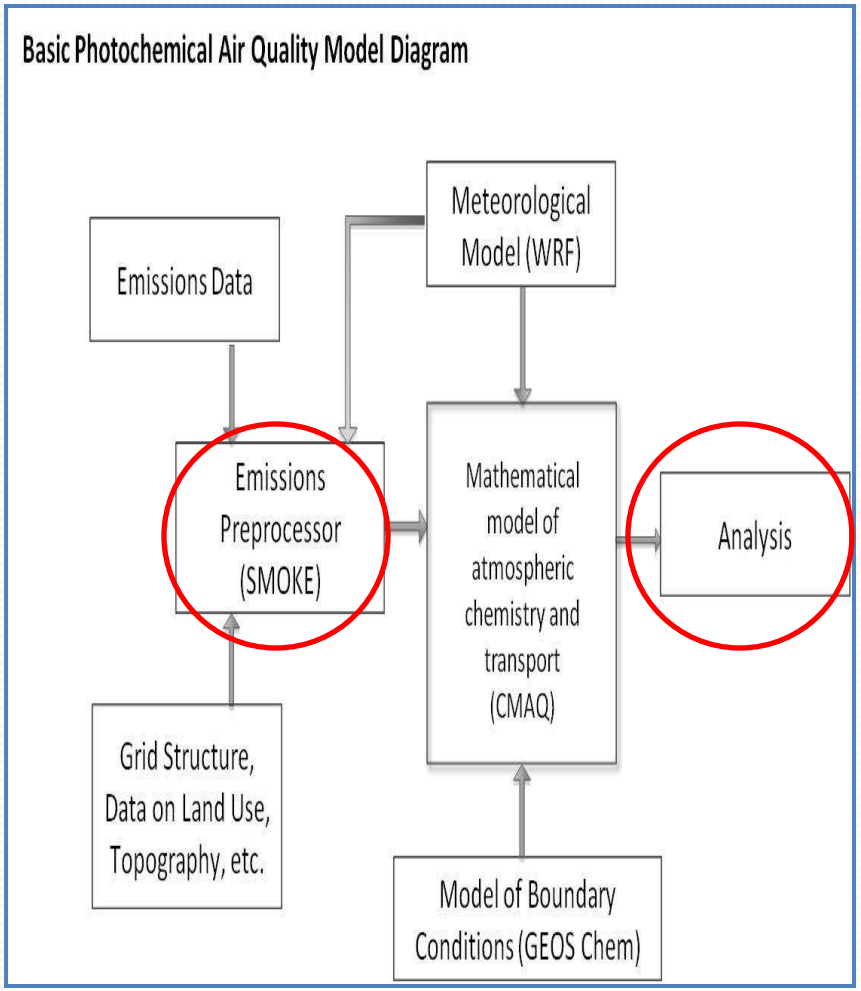
- These models provide wind, humidity, temperature, and other information for each grid cell in a photochemical modeling domain.
- The models start from measured data, but they make various assumptions to generate wind fields for the entire domain.
- Examples: WRF, MM5



Example: Winds and temperatures from MM5 for 2002

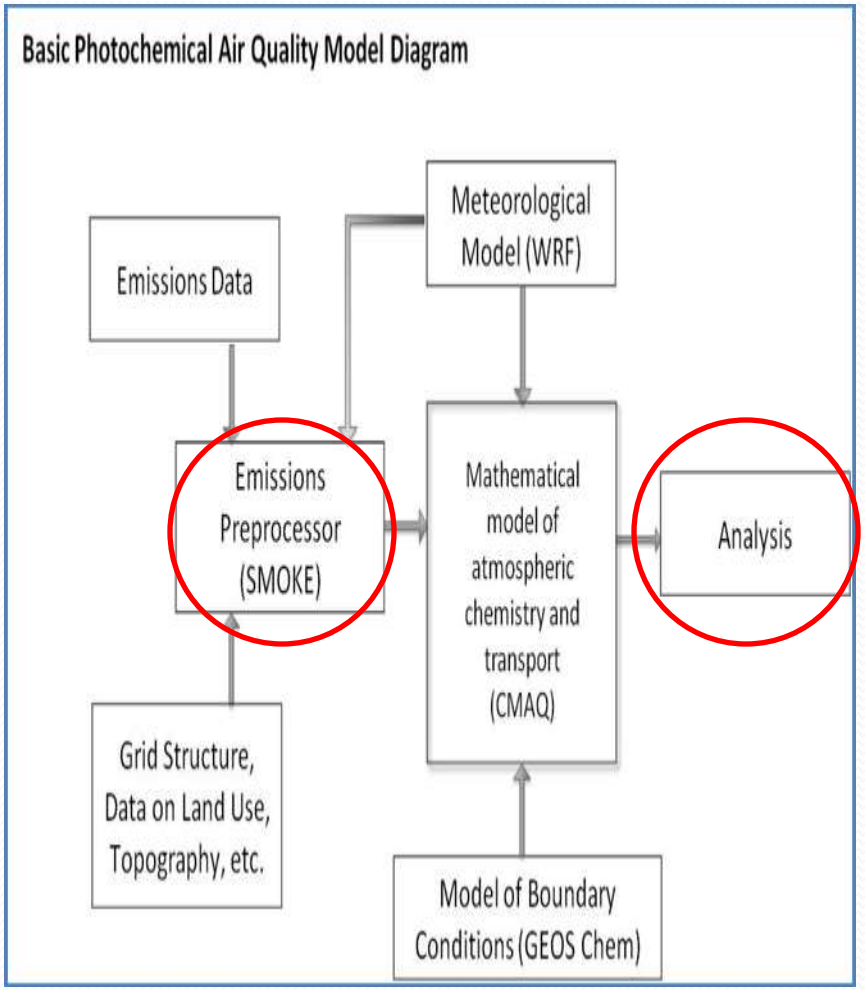
Setting up Regional Air Quality Models

- Modeling Domain
- Boundary Conditions
- Grid Structure
- Meteorological Model
- **Pre-processing/post-processing**
- Emissions Inventory



Pre-processing & Post-processing

- Purpose: Prepare data for use (model or user)
- Preprocessors include SMOKE, CONCEPT
- Post-processors include GIS-based mapping programs



Preprocessor Example: SMOKE

- Purpose: to create gridded, hourly emissions data for use in photochemical models.
- Input data: spatial characteristics such as
  - land use,
  - meteorological data,
  - emissions data by county and for particular points,
  - grid definition

Part 2 - Quiz

- What type of model is the SMOKE model?
  A. Pre-processor
  B. Post-processor
  C. Dispersion

Part 2 - Quiz

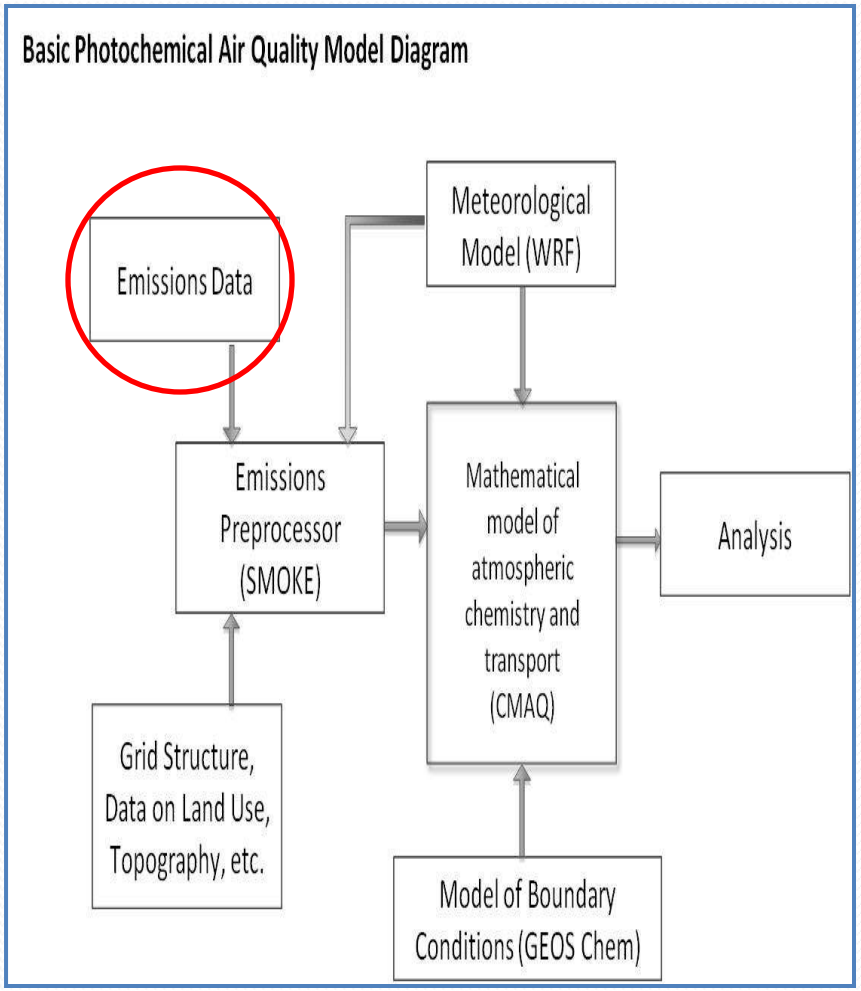
- What is the purpose of the meteorological model?
  A. Interpret weather data to generate wind and other weather characteristics for each grid cell in the modeling domain
  B. Predict the weather for a future year

And our next topic is…

- Part 1 – Some Types of Models
- Part 2 – Setting up Regional Air Quality Models
- Part 3 – Emissions Inventories for Regional Modeling
- Part 4 – More about Using Models for SIPs

Setting up Regional Air Quality Models

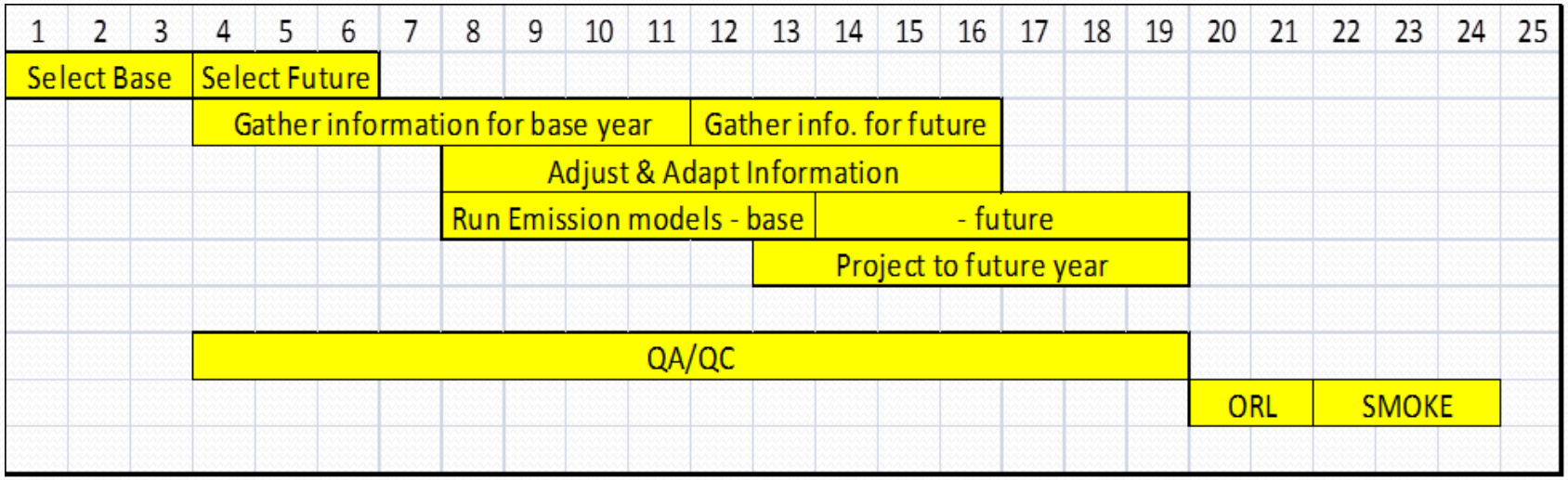
- Modeling Domain
- Boundary Conditions
- Grid Structure
- Meteorological Model
- Pre-processing/post-processing
- **Emissions Inventory**



Emissions Inventory Steps

- Select years
- Gather information (activity, emissions)
- Adjust and adapt information
- Run emissions models
- Project future years
- Convert annual data files to required input format
- Run model to create gridded hourly data for model input for each year

Rough Schedule for Creating a Modeling Inventory



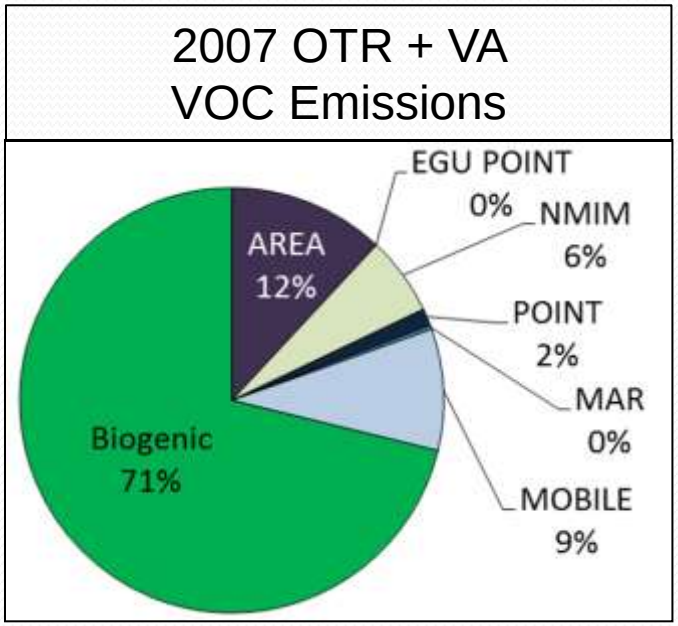
Allow approximately 2 years.

What are emissions models?

- Emissions models are complex sets of equations and steps to produce emission estimates
- Examples:
  - BEIS/MEGAN (biogenic emissions)
  - MOVES (on-road mobile sources)
  - NMIM/NONROAD (non-road mobile sources)
  - IPM (electricity generating units)
  - ERTAC EGU (electricity generating units)

Emissions Models – Biogenic Emissions

- Purpose:
  - Estimate emissions from natural sources
- Basis:
  - Spatial data on vegetation and land use
  - Environmental conditions such as solar radiation and temperature
- Examples:
  - BEIS
  - MEGAN



The MOVES Emissions Model

- MOVES stands for
  - MOtor Vehicle Emissions Simulator
- MOVES estimates emissions from
  - Cars, trucks, motor cycles
- MOVES scales: national, county, or project
- MOVES can be used for
  - Criteria pollutants
  - Some toxic air pollutants
  - Greenhouse gases

More about MOVES

- Input Data needed
  - Vehicle types & age distribution
  - Vehicle miles traveled – monthly, daily, hourly
  - Road type, ramp fraction, average speed
  - Fuel supply & formulation by month
  - I/M program, NLEV, CalLev, Stage II efficiencies
  - Meteorology
- MOVES stores information in MySQL databases

2 MOVES Modes

Emissions Inventory Mode

Emissions Rate Mode

(We'll go over each mode briefly)

2 MOVES Modes

Emissions Inventory Mode

- Quantifies emissions (national, county, project)
  - Format not suitable for use with regional air quality model—just county-wide totals, not gridded hourly emissions
- Used to prepare activity data
  - Converts VMT and Vehicle Population from MOVES input format to SCC format needed for SMOKE model

Emissions Rate Mode

2 MOVES Modes

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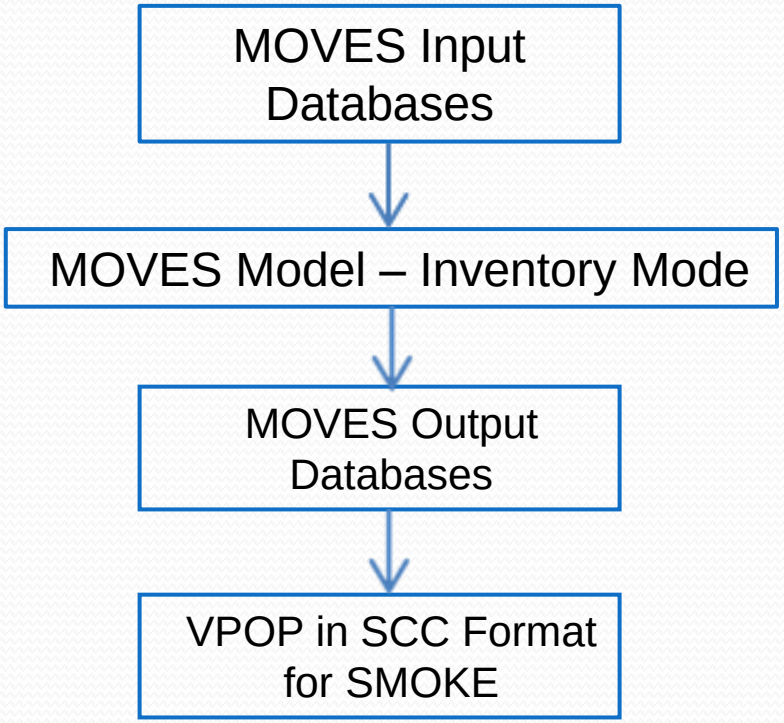
Emissions Rate Mode

- Produces emission rates
  - Rate per distance (on-road) (by temperature and speed)
  - Rate per vehicle (start-up, idling) (by fuel, temperature, time of day)
  - Rate per profile (vapor venting when parked) (by fuel, temperature, time of day)
- Used with vehicle population data and VMT data as input to SMOKE

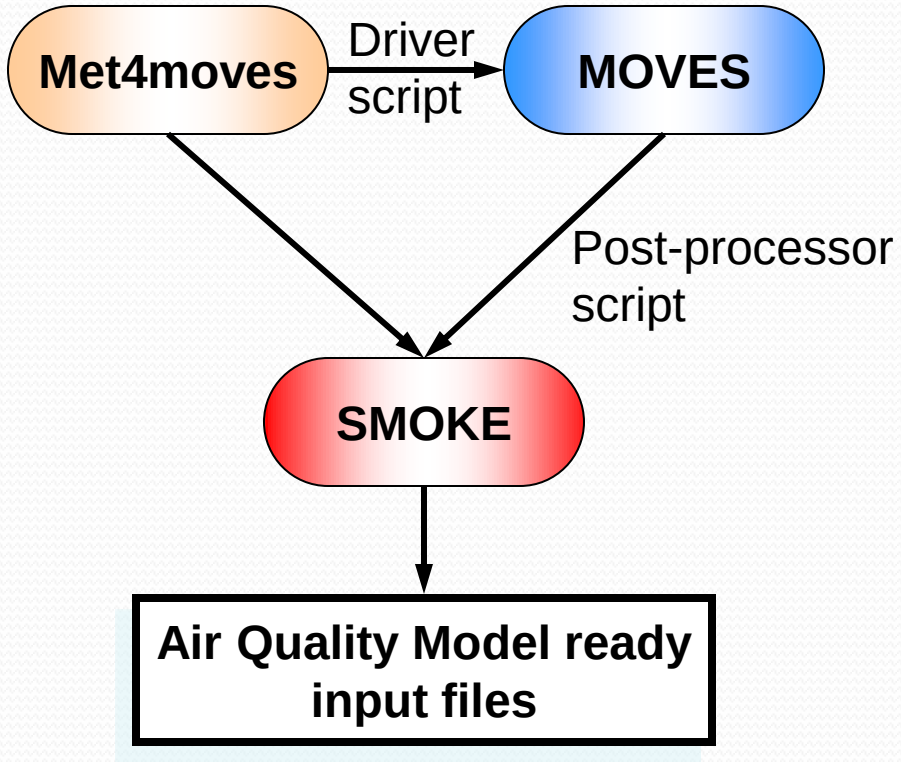
Run MOVES in Inventory Mode



- Purpose: Convert VMT and VPOP to SCC Format for SMOKE Processing
- Inventory mode provides activity data
- Look up table mode provides emission factors

SMOKE-MOVES System

- Met4MOVES:
  - Meteorological data preprocessor
  - Provides temperatures and humidity
  - Driver script sets up MOVES emission rate runs
- MOVES:
  - Reformat activity data
  - Create emissions factors
  - Post-processing script converts output into format needed by SMOKE
- SMOKE:
  - Applies the emission factors to the activity data to compute grid-cell emissions



SMOKE/MOVES - Strategies to reduce run time

- Group counties:
  - Similar fuel, I/M, vehicle type & age, meteorology
  - A single “representative county” is run and results are used for all counties in the group
- Fuel months – just 2 types
  - Summer & winter
- Limit temperature ranges to those typical for an area

Part 3 - Quiz

- What are two emissions models used to estimate biogenic and mobile source emissions? (type in text)

Part 3 - Quiz

- For which geographic area does MOVES estimate emissions?
  A. County
  B. Region
  C. Grid cell

Almost there…

- Part 1 – Some Types of Models
- Part 2 – Setting up Regional Air Quality Models
- Part 3 – Emissions Inventories for Regional Modeling
- Part 4 – More about Using Models for SIPs

Questions to ponder:

1. What is sensitivity modeling?
2. In regional modeling, how can we tell what sources are causing the model to predict violations?
3. If the model is run for only one year, how can you compare that to a three-year design value?
4. What is a Weight of Evidence demonstration?

Sensitivity modeling can show effects of changing emissions

- **Purpose:** understand the effect of changing input variables—how important is a parameter to modeled air quality?
- **Example:** How much will air quality improve if emissions are reduced by 20%?
- Distinguished from final or "SIP quality" runs that use emissions defined by adopted rules and meet model evaluation criteria

Who is contributing?

- "Source apportionment" means deciding how much of a predicted concentration to apportion to a specific source, a geographic area, or a type of source
- Tools for source apportionment include
  - Dispersion modeling
  - Receptor modeling
  - Photochemical grid modeling

Some photochemical models can be used for source apportionment

- Purpose: to identify culpability for modeled concentrations by analyzing model inputs and results
- This requires use of specific model tools
  - CMAQ: PPTM and OPTM
  - CAMx: PSAT and OSAT
- Can be used to identify contributions from source regions, source types, or specific sources
- Was used by NESCAUM in regional haze modeling

Attainment modeling follows EPA guidance

- Modeled attainment test: using an air quality model to show that future air quality will meet NAAQS
  - How do we deal with uncertainty in model?
  - Attainment is measured in terms of the *design value*, which in the case of ozone is a three-year average.
  - How can we convert modeling into a 3-year average

Relative Reduction Factor

- Relative Reduction Factor (RRF):
  - For each specific monitoring site (nearby grids)
  - Compare *future modeled* air quality to *base year modeled* air quality at the site: ratio Future:Base
- The RRF is multiplied times the *measured* air quality at the site to predict future air quality.
  - Usually multiplied times the 3-year design value

Models can be part of a Weight of Evidence demonstration

- When the modeled attainment test is not passed or narrowly passes,
- EPA's guidance on the use of additional corroborative analyses to support the attainment demonstration.
- This is called a weight of evidence demonstration (WOE).

What provides Weight of Evidence?

- Using a variety of tools
  - Air quality trends
  - Emissions trends
  - Chemical transport model(s)
  - Dispersion model
  - Receptor model
- "All models are wrong, some models are useful." – (Quote from statistician George Box)

Example: MANE-VU Used Many Models & Tools

- Ambient data analysis (Identify key pollutants)
- Receptor modeling (Identify source types)
- Trajectory modeling (Identify source regions)
- Dispersion modeling (Identify 167 sources)
- Emissions data analysis (Evaluate control effectiveness, evaluate model results)
- CMAQ modeling (Set progress targets)

Part 4 - Quiz

- Which would be completed first, sensitivity modeling or an attainment demonstration?
  A. Sensitivity modeling
  B. Attainment demonstration

Part 4 - Quiz

- What does RRF mean?
  A. Resource Recovery Facility
  B. Relative Reduction Factor
  C. Really Rare Function

Where to find More Information

- EPA TTN website
  http://www.epa.gov/ttn/scram

  (TTN = Technology Transfer Center)
  (SCRAM = Support Center for Regulatory Air Models)

- EPA's Air Pollution Training Institute
  https://www.apti-learn.net

- University of North Carolina Community Modeling and Analysis System Center (CMAS)
  https://www.cmascenter.org/

Current Topics in Modeling

- AERMOD – what has prompted improvements?
  - Use of AERMOD to demonstrate attainment of 1 Hr SO2 and NO_X NAAQS has prompted improvements
  - Incorporation of better wind speed data
- CMAQ & CAMX
  - Updates to land use data
  - Improved Chemistry

Key Topics Covered

- Terminology and basic concepts
- Types of models and how they are used
- Photochemical modeling vs. dispersion modeling
- Source apportionment modeling and receptor modeling
- Emissions modeling, particularly with MOVES
- Use of models in SIPs

Recap: Learning Objectives

1. Correctly use *model names and acronyms* in discussion or written materials
2. Identify the *types of modeling needed* to address a variety of air quality issues
3. Identify *photochemical grid models* for SIP planning
4. Identify *dispersion models* for point source analysis
5. Define *source apportionment modeling* and *receptor modeling* and their role in identifying source contribution to air pollution
6. Identify the step to develop an *emissions inventory*
7. Recognize & understand the purpose of *meteorological models*
8. *Find more information* when needed.

Upcoming Training Opportunities

NACT 200 Series: November 1-4, 2016 in Richmond, VA

- November 1, 2016 – NACT 221: Continuous Emissions Monitoring
- November 2, 2016 – NACT 285: Landfill Gas Control Facilities
- November 3, 2016 – NACT 272: Stationary Gas Turbines & Power Plants
- November 4, 2016 – NACT 284: Volatile Organic Compound Control Devices

15th Annual CMAS Conference: October 24-26, 2016, UNC-Chapel Hill

Visit MARAMA's website for more information:

http://www.marama.org/training-center/event-schedule

Last Words

- **Webinar On-Line Evaluation**

  https://www.surveymonkey.com/r/Modeling2016

  This link will also be forwarded to registered participants via email following the webinar.

  Provide names and head count on the evaluation

- **Certificates of attendance**

  Available to MARAMA agency attendees that complete the on-line evaluation and answer 5 of the 7 survey questions correctly.

- **Feedback?** Send to training@marama.org

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