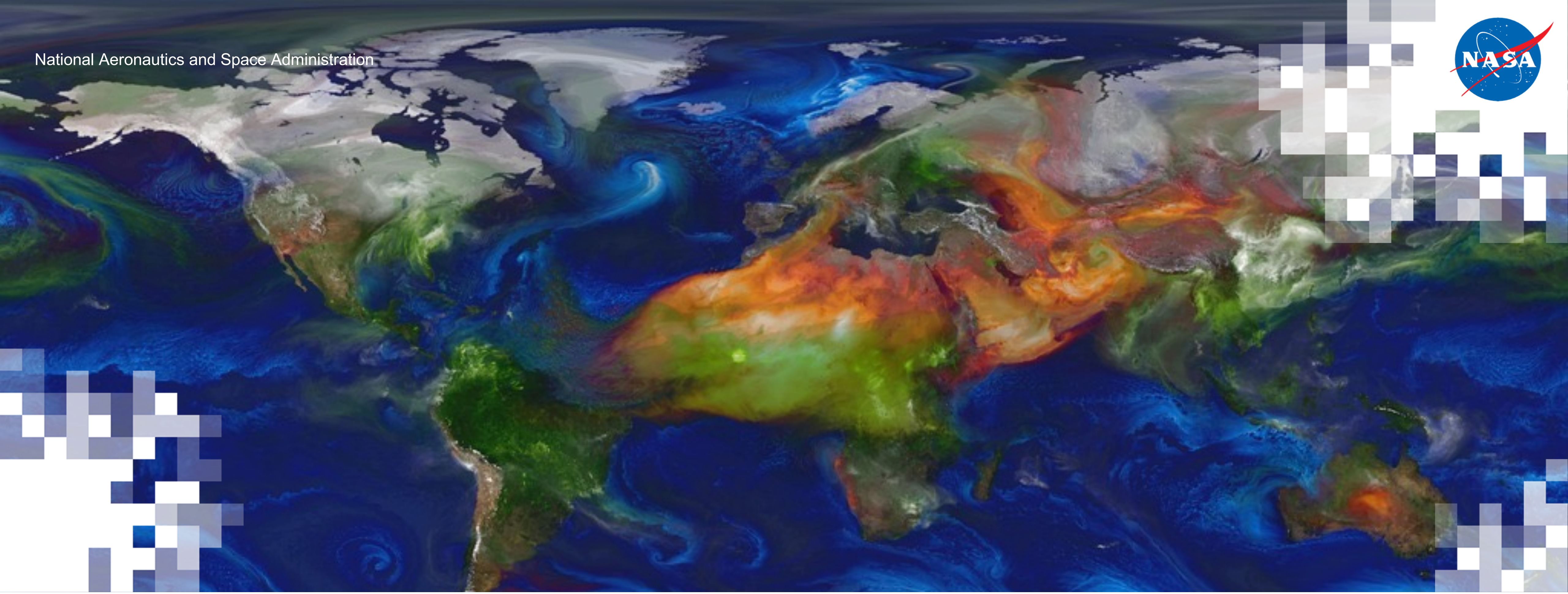
National Aeronautics and Space Administration



# Introduction to Air Quality Forecasting

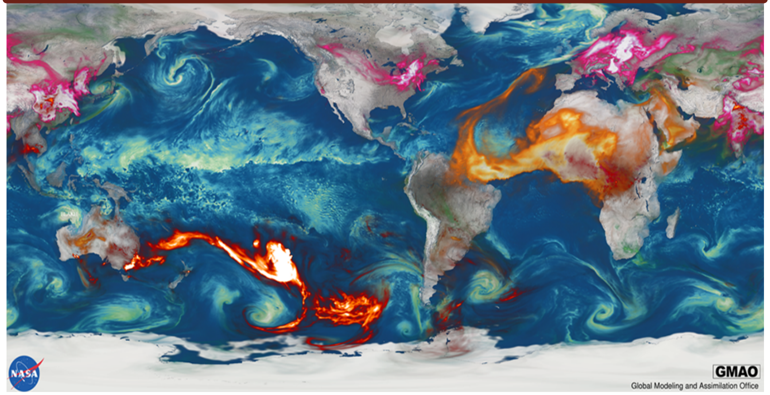
Pawan Gupta & Melanie Follette-Cook

September 23, 2021

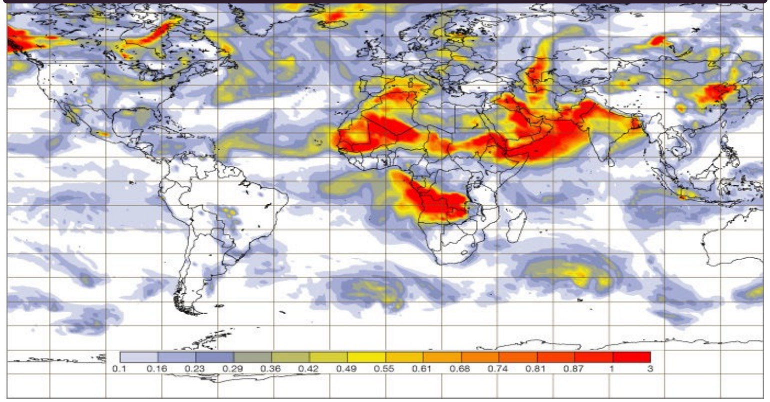
# Webinar Agenda

## Part 1:
## Air Quality (AQ) Basics

## Part 2:
## NASA GEOS Model



## Part 3:
## ECMWF CAMS Model



# Learning Objectives

**By the end of this training, attendees will understand:**

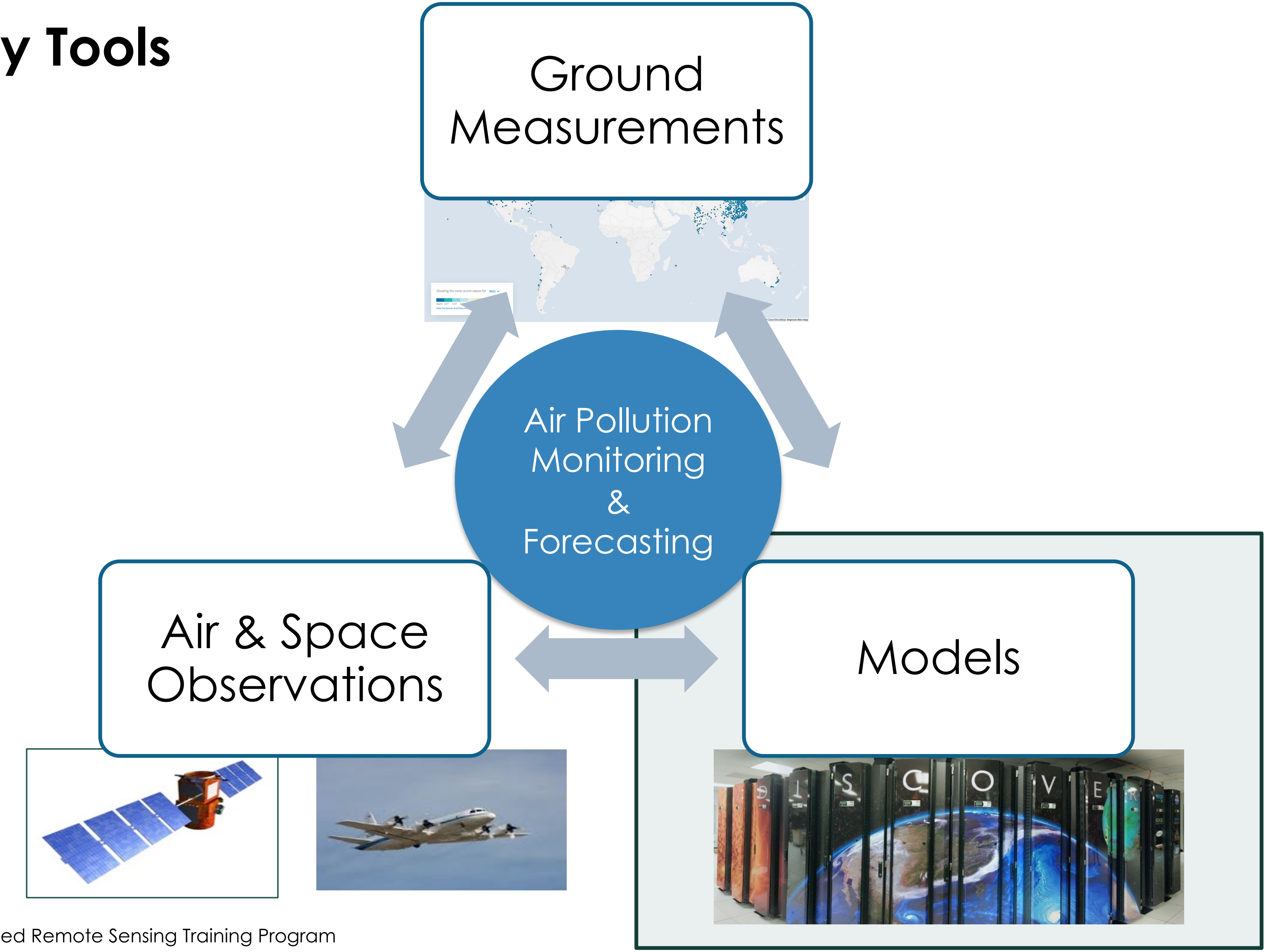
- The science behind AQ forecasting and parallels to weather forecasting
- Various methods to forecast air quality
- Model components such as emissions, boundary conditions, and initialization
- Regional AQ models for offline and online use

# Air Pollution

- Contamination of the atmosphere by gases, liquids, or solids
- Has serious affects on human health and the biosphere, reduces visibility, and damages materials
- Major Pollutants:
  - Ozone ($O_3$)
  - Particulate Matter (PM, Particles)
  - Lead
  - Carbon Monoxide (CO)
  - Nitrogen Dioxide ($NO_2$)
  - Sulfur Dioxide ($SO_2$)
  - Toxic Compounds (e.g., Lead)

https://climatekids.nasa.gov/air-pollution/

# Air Quality Tools



Ground Measurements

Air Pollution Monitoring & Forecasting

Air & Space Observations

Models

# Air Quality Forecasting

- Provides the public with air quality information in advance, similar to weather forecasting
- Helps people make daily lifestyle decisions to protect public health
- Allows people to take precautionary measures to avoid or limit their exposure to unhealthy levels of pollution
- Many communities use forecasts for initiating air quality “action” or “awareness” days, which seek voluntary participation from the public to reduce pollution and improve local air quality.

Yeehaw! Sky’s hat is green, which means the air is safe and clean for all Texans. Get outside and enjoy our beautiful state!

Sky’s hat is yellow, which means you can still play outside. However, you might want to avoid too much activity if you are extra sensitive to air pollution.

Uh oh! Looks like Sky’s hat is orange today, which means you might want to avoid too much time outside, especially if you are sensitive to air pollution.

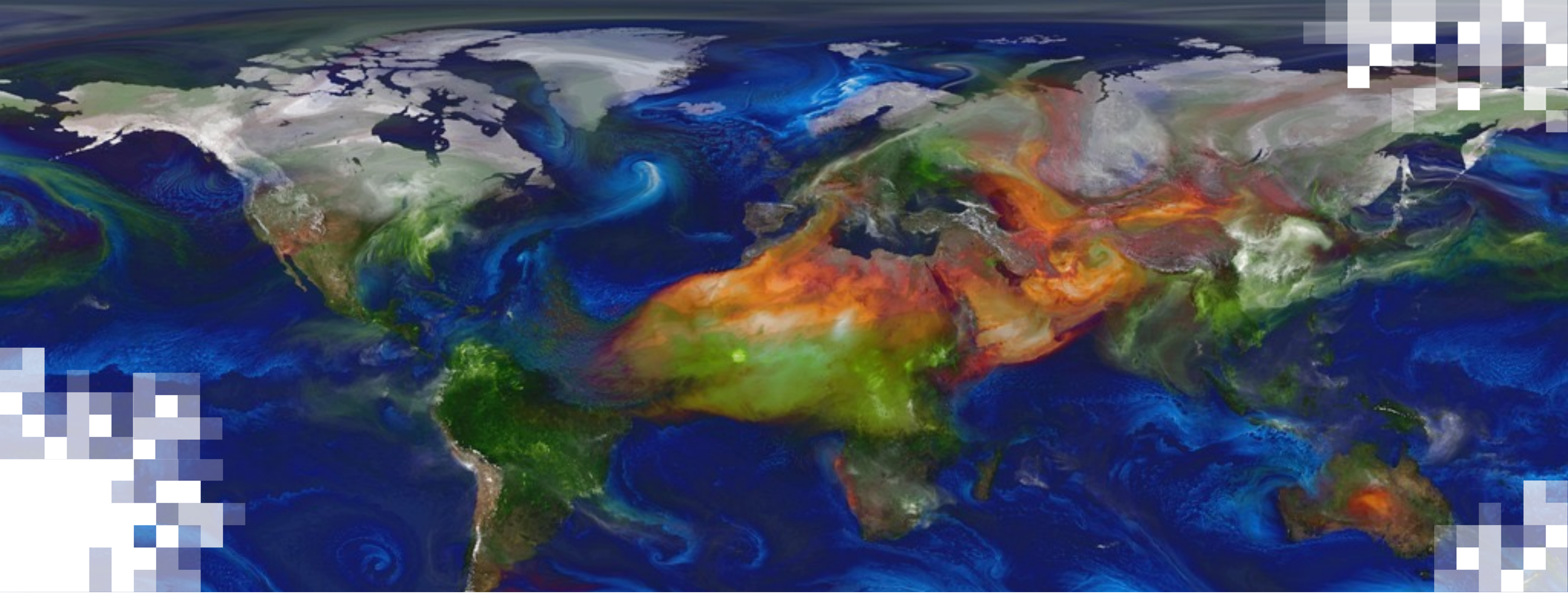
Yikes! Sky’s hat is red, which means all Texans should avoid spending too much time outside today. Maybe play outside in the morning or evening, when it is cooler.

Sky’s hat is purple today, which means the air is very unhealthy for all Texans. Find fun activities and games to play inside today!

https://takecareoftexas.org/kids/what-is-air-quality

# What determines ambient pollution concentrations?

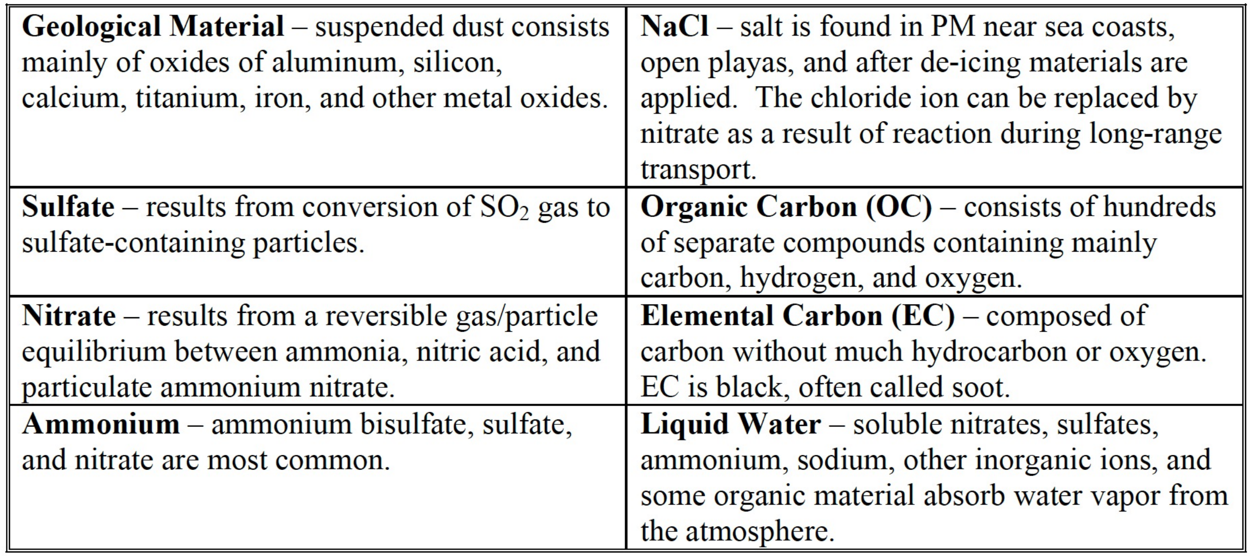
Changes in emissions do not necessarily translate into changes in pollution concentration at the surface due to other factors such as atmospheric processes and meteorology.



# Particulate Matter

# Particulate Matter

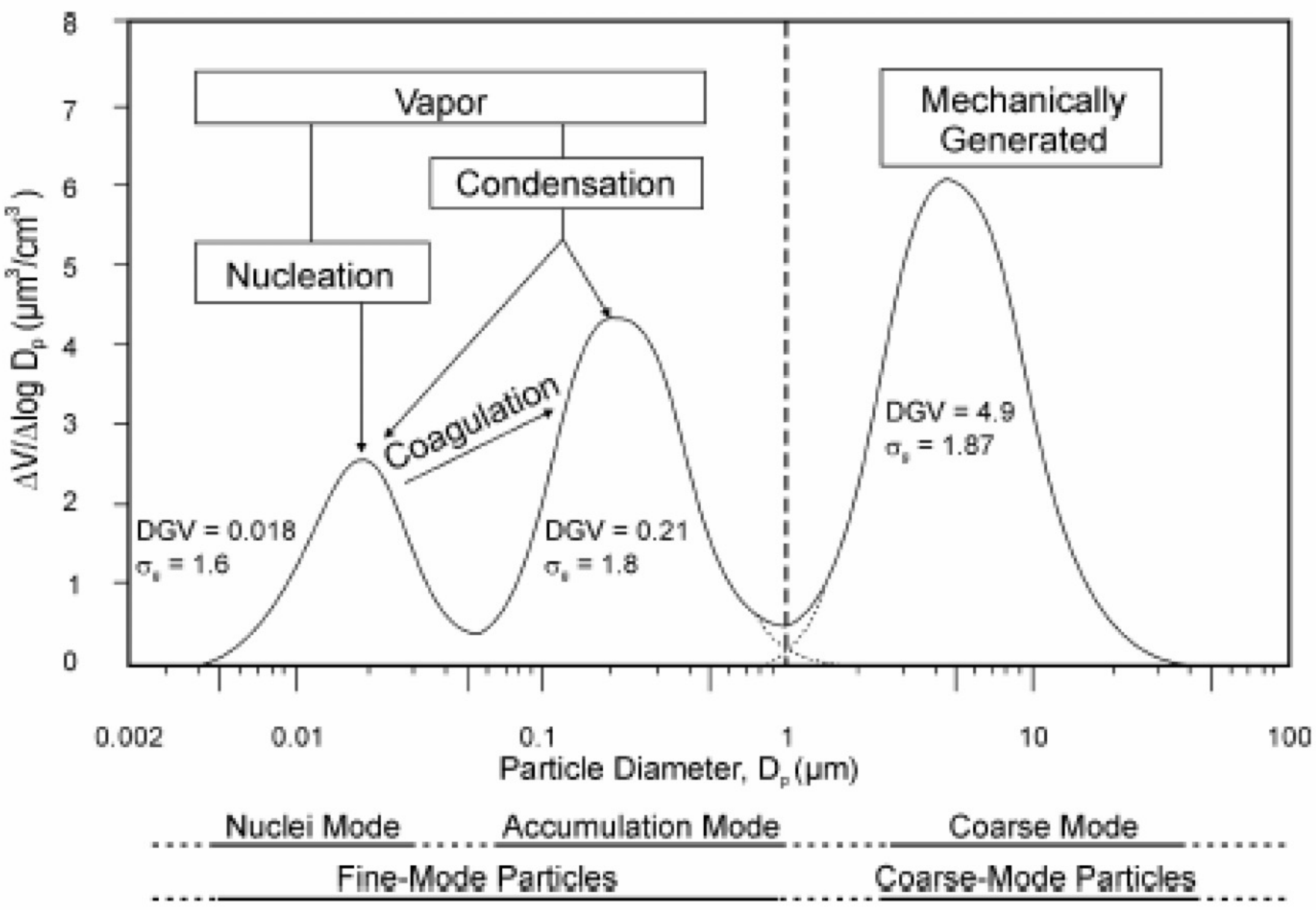
- Not a specific chemical entity, but a mixture of particles of different sizes, shapes, compositions, and chemical, physical, and thermodynamic properties.
- PM is directly emitted (primary particles) and created in the atmosphere as secondary particles by gas-to-particle conversion.
- Primary – If it exists in the same chemical composition as it was emitted in the atmosphere
- Secondary – Formed in the atmosphere by chemical reactions



| | |
|---|---|
| **Geological Material** – suspended dust consists mainly of oxides of aluminum, silicon, calcium, titanium, iron, and other metal oxides. | **NaCl** – salt is found in PM near sea coasts, open playas, and after de-icing materials are applied. The chloride ion can be replaced by nitrate as a result of reaction during long-range transport. |
| **Sulfate** – results from conversion of $SO_2$ gas to sulfate-containing particles. | **Organic Carbon (OC)** – consists of hundreds of separate compounds containing mainly carbon, hydrogen, and oxygen. |
| **Nitrate** – results from a reversible gas/particle equilibrium between ammonia, nitric acid, and particulate ammonium nitrate. | **Elemental Carbon (EC)** – composed of carbon without much hydrocarbon or oxygen. EC is black, often called soot. |
| **Ammonium** – ammonium bisulfate, sulfate, and nitrate are most common. | **Liquid Water** – soluble nitrates, sulfates, ammonium, sodium, other inorganic ions, and some organic material absorb water vapor from the atmosphere. |

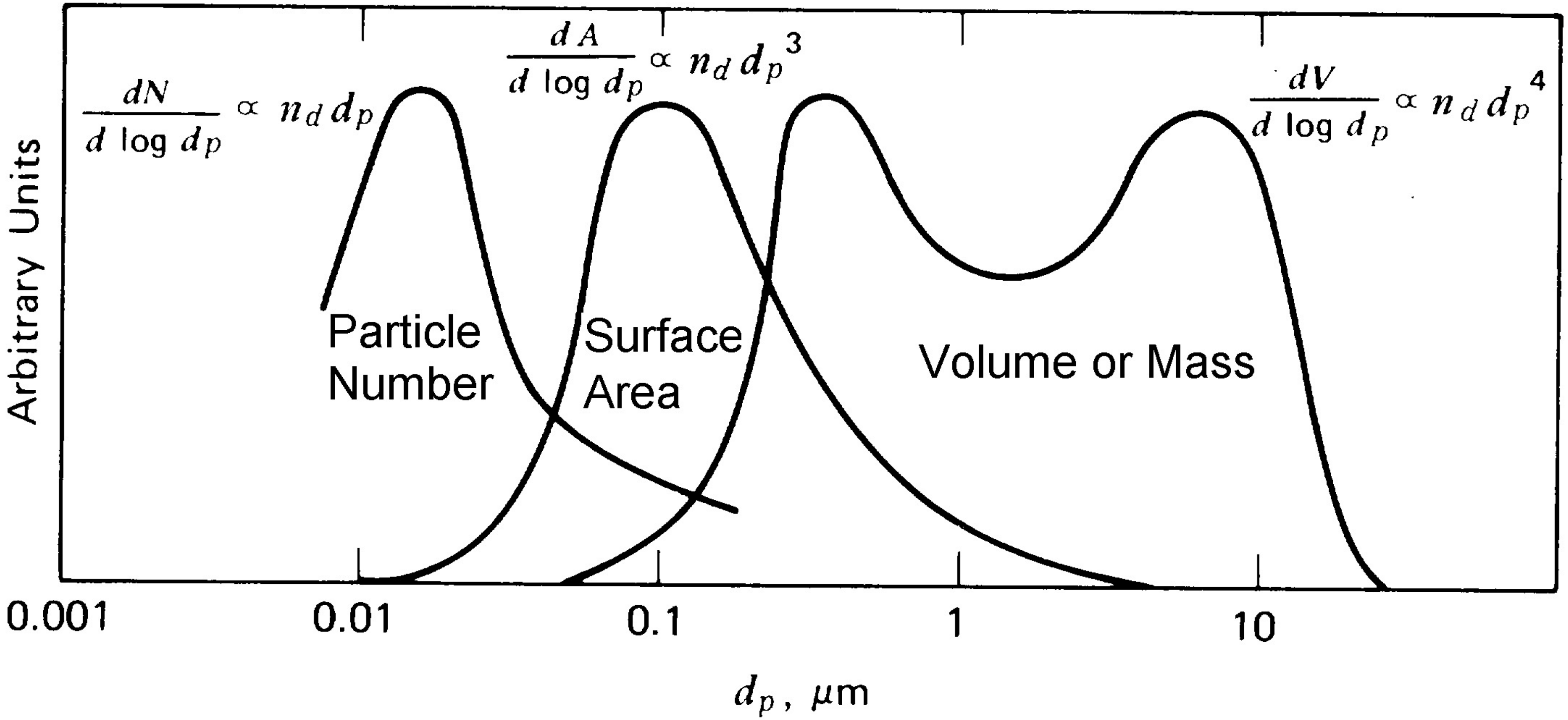
# Particle Formation

- Chemical processes can either form new particles or add layers to existing particles.
- Depends on concentration of precursors, solar radiation, temperature, RH, interaction medium
- Form in the atmosphere through chemical reactions involving:
  - $O_2$, $H_2O$, $O_3$
  - NOx, $SO_2$, $NH_3$, VOCs



**Volume Size Distribution**

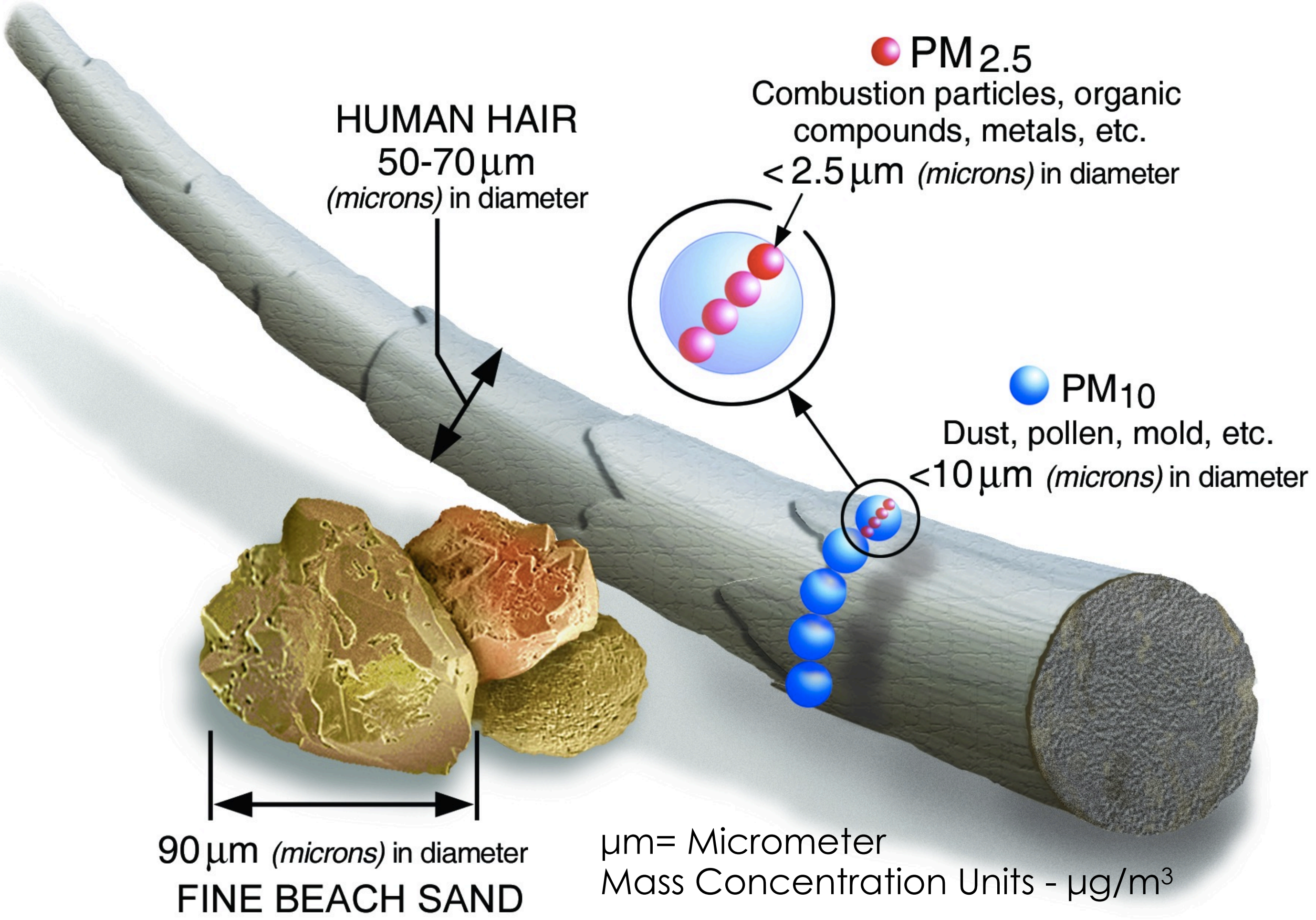
# Particle Distribution



Dominating particle size range varies by type of measurements (i.e., number, area, or volume).

# $PM_{2.5}$

- Particles with a size range of 0.1-2.5 µm can last days to weeks in the atmosphere (i.e., their lifetime).
- Particles in this size range can penetrate deep into human lungs.
- They are also very efficient light scatterers at visible wavelengths.
- Thus, $PM_{2.5}$ is very important to investigate for its impact on human health, visibility, and climate.

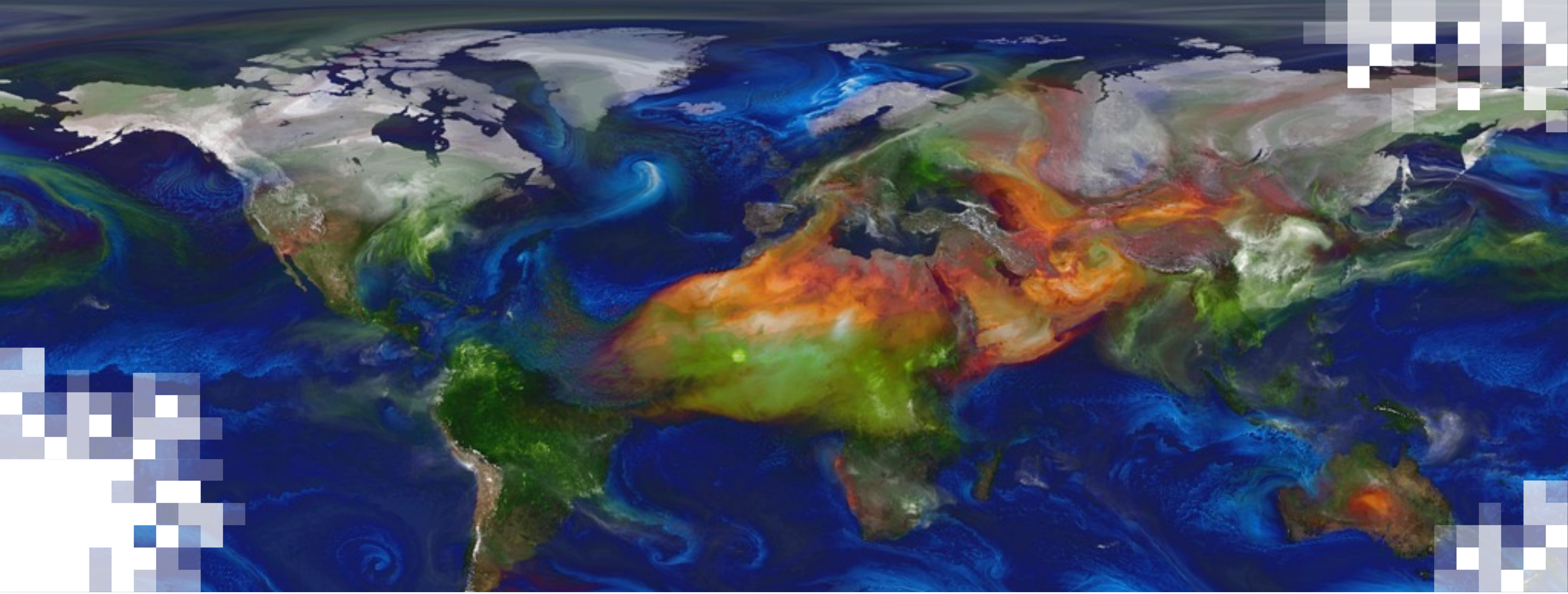


µm= Micrometer
Mass Concentration Units - µg/$m^3$

Image Credit: U.S. EPA

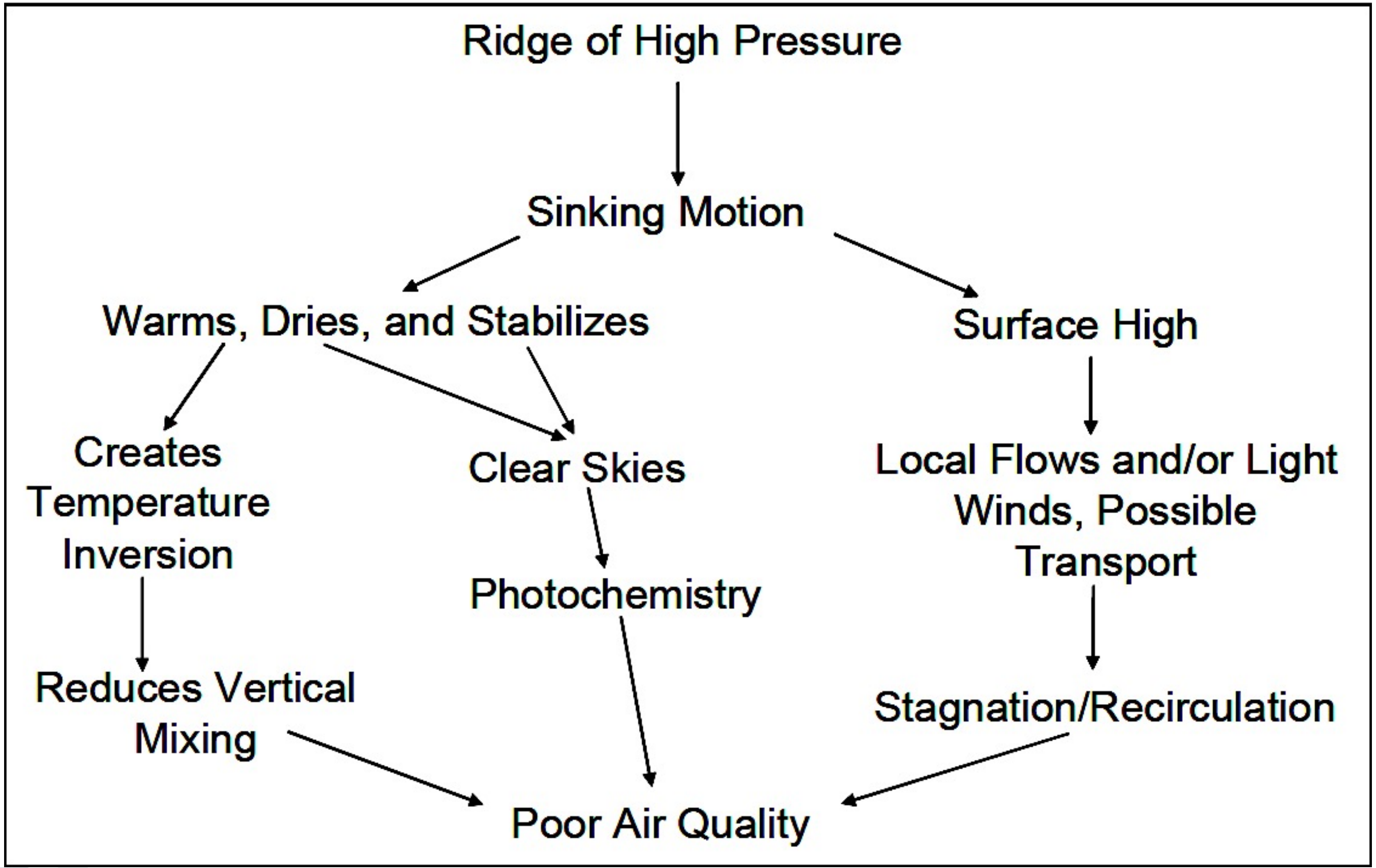
# $PM_{2.5}$ Monitoring

- Historically measured using filter-based samplers and averaged for 24-hrs or longer
- Federal reference method using Teflon filter to collect the samples
- Continuous monitoring of $PM_{2.5}$ & $PM_{10}$ began in 1999 (FRM).
  - BAM (Beta Attenuation Monitor) – An optical method
  - TEOM (Tapered Element Oscillating Microbalance) - Inertial mass measurement method
- Chemical composition is still largely measured using filter-based methods
- Some continuous monitoring of chemical composition done using Aethalometers and Nephelometers
- Low-cost sensor monitoring



# Meteorology

# Air Quality and Meteorology



Ridge of High Pressure

Sinking Motion

Warms, Dries, and Stabilizes

Surface High

Creates Temperature Inversion

Clear Skies

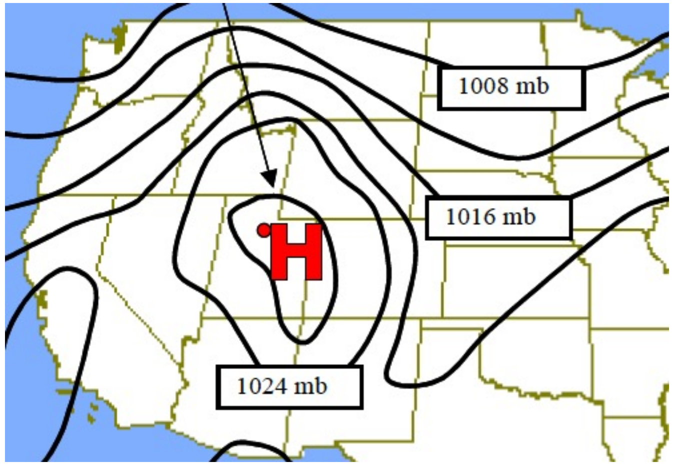
Local Flows and/or Light Winds, Possible Transport

Photochemistry

Reduces Vertical Mixing

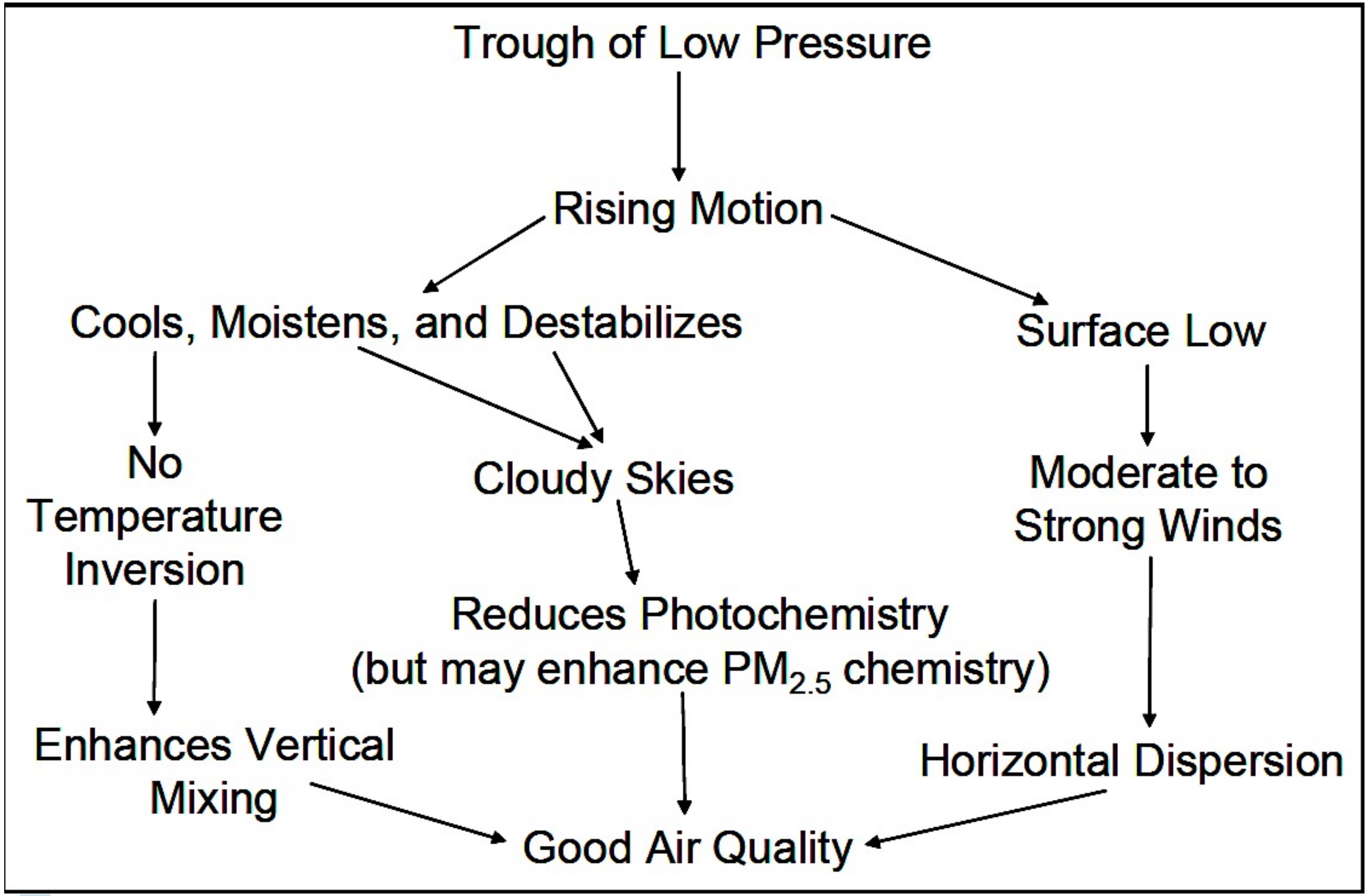
Stagnation/Recirculation

Poor Air Quality



Weather patterns influence the air quality even under constant emissions. Therefore, weather-related measurements can be critical in modeling air quality.

# Air Quality and Meteorology



Trough of Low Pressure

Rising Motion

Cools, Moistens, and Destabilizes

Surface Low

No Temperature Inversion

Cloudy Skies

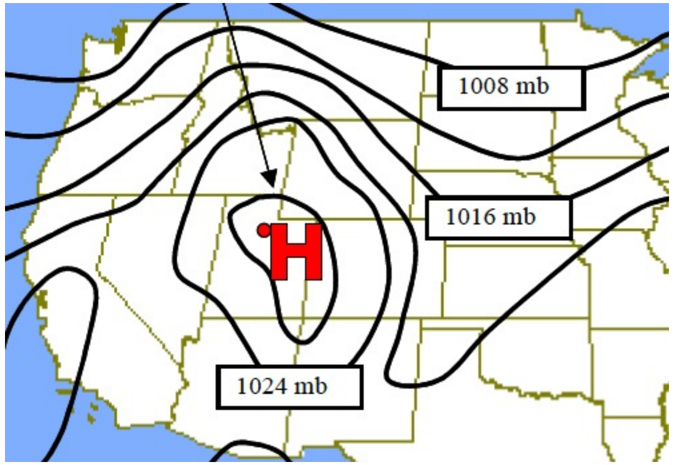
Moderate to Strong Winds

Reduces Photochemistry (but may enhance $PM_{2.5}$ chemistry)

Enhances Vertical Mixing

Horizontal Dispersion

Good Air Quality



Weather patterns influence the air quality even under constant emissions. Therefore, weather-related measurements can be critical in modeling air quality.

# Winds

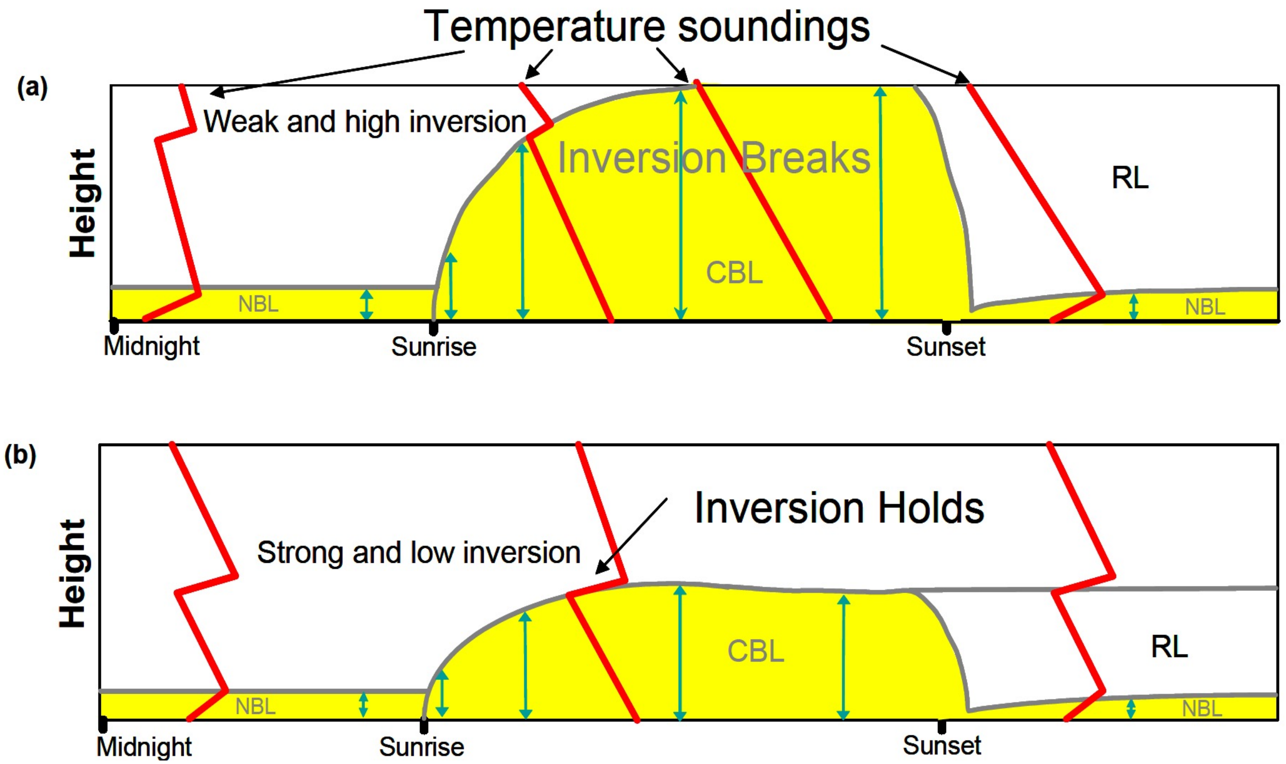
- Emissions from some natural sources can be impacted (i.e., dust, sea salt, etc.).
- Chemistry – Stronger winds can disperse pollution, diluting concentrations and making less favorable for secondary chemistry
- Concentration – Strong winds disperse pollution, leading to lower concentrations, and weak winds can help the accumulation of pollution in one place. Transport by wind can also either increase or decrease pollution at a given place depending on wind direction and location of source.
- Example – Smoke/Dust Transport

Tracking the smoke from the 2019 agricultural fires in India and Pakistan with the NASA/GMAO GEOS model

15 October 00:00z

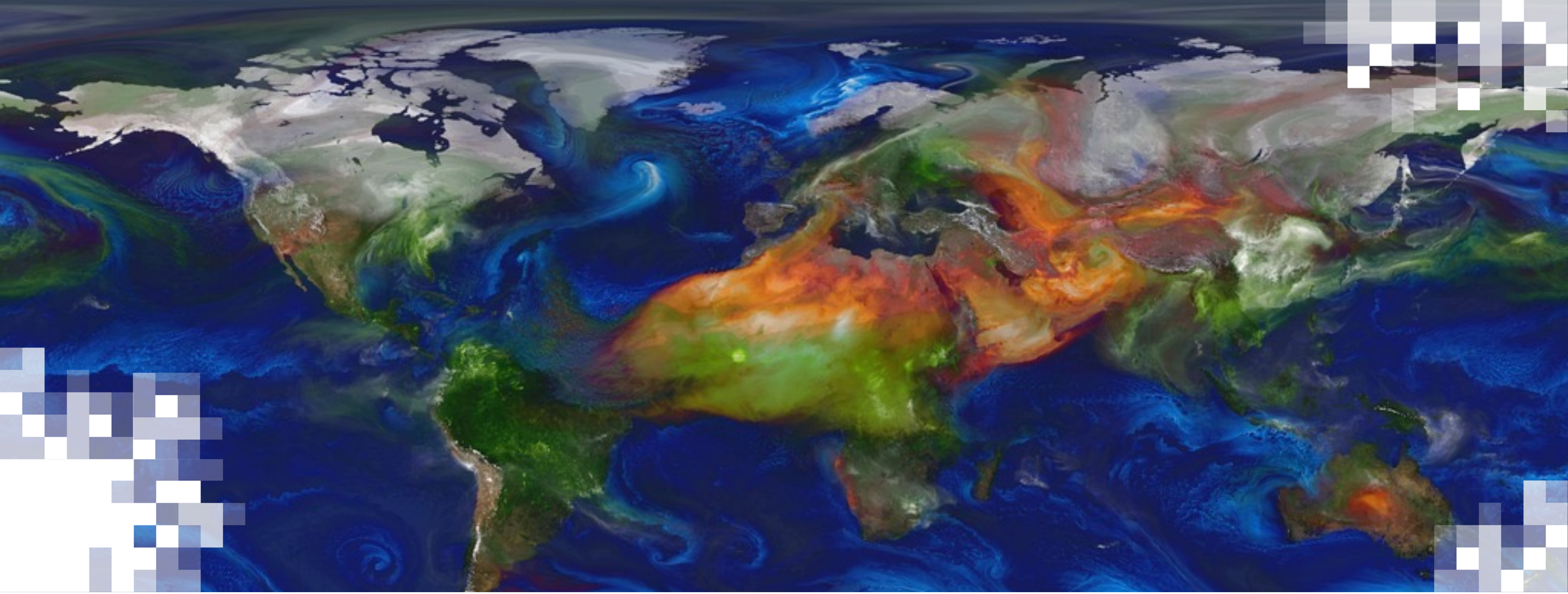
# Temperature

- **Emissions:**
  - Certain emissions can be enhanced or suppressed.
- **Chemistry:**
  - Low temperature and inversion can reduce vertical mixing -> increasing concentration of precursors -> more secondary pollution
- **Concentration:**
  - Low Temperature -> inversion -> lower mixing layer height -> accumulation of participles -> increased concentration at surface
  - High Temperature -> inversion breaks -> higher mixing layer height -> dispersion of particles -> decreased concentration at surface



# Rain, Moisture, Clouds

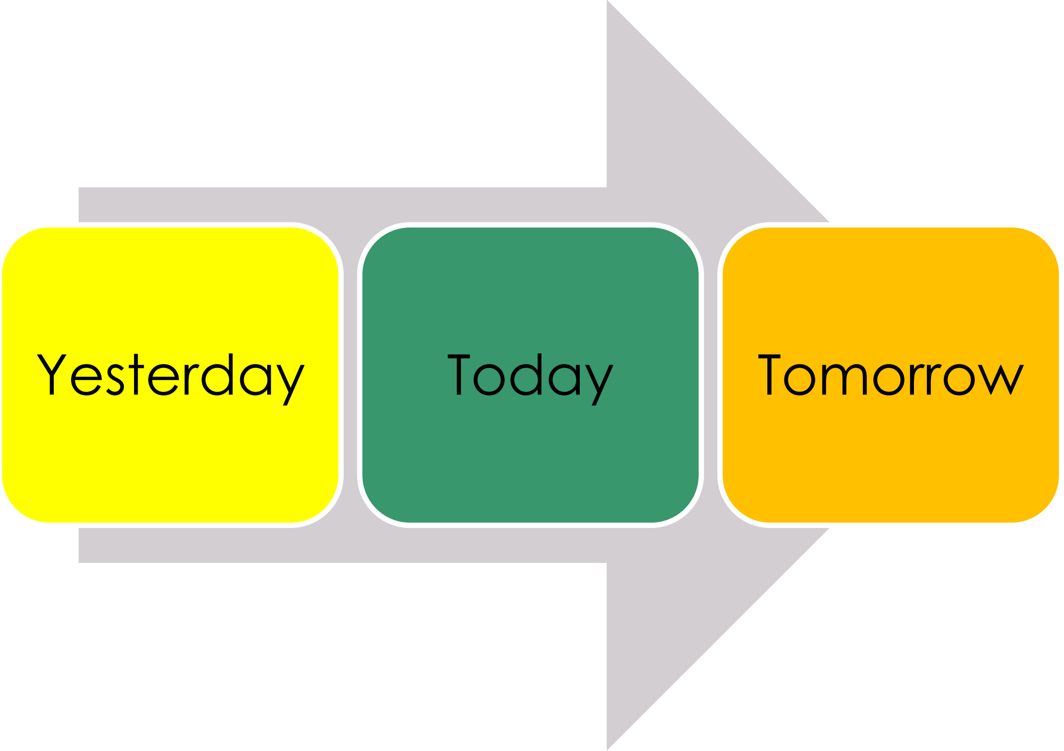
- **Rain:**
  - Can remove pre-cursor and PM
  - Can suppress certain emissions such as dust
- **Clouds:**
  - Cloudy conditions can reduce formation of secondary particles due to reduced photochemistry
  - But chemical reaction on/inside cloud particles can be enhanced
- **Moisture:**
  - Higher soil moisture can suppress emissions such as dust
  - Atmospheric moisture (higher water vapor) can enhance production of secondary particles



# Air Quality Forecasting

# AQ Forecasting Purpose

- Notify public of potential health risks
- Air quality episodic action control program
  - Prescribed burning
  - Action days -> no burn day, no lawn mowing, driving restrictions, etc.
- Schedule specific monitoring programs (field campaigns, etc.)
- Each of these purposes have specific forecasting needs which vary in accuracy and spatial and temporal scales.



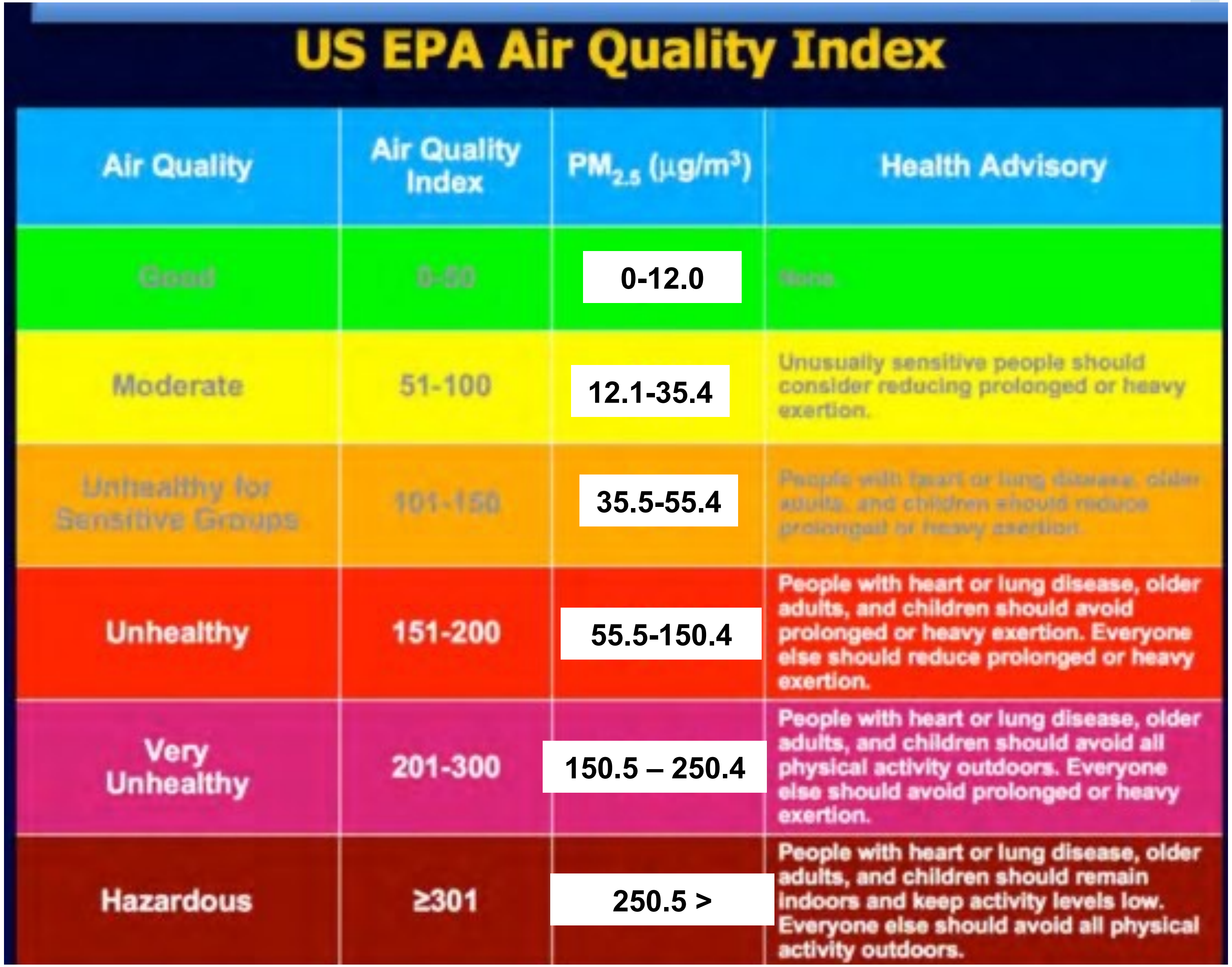
Yesterday

Today

Tomorrow

# AQ Forecasting

- AQI Forecasting
- Concentration Forecasting



US EPA Air Quality Index

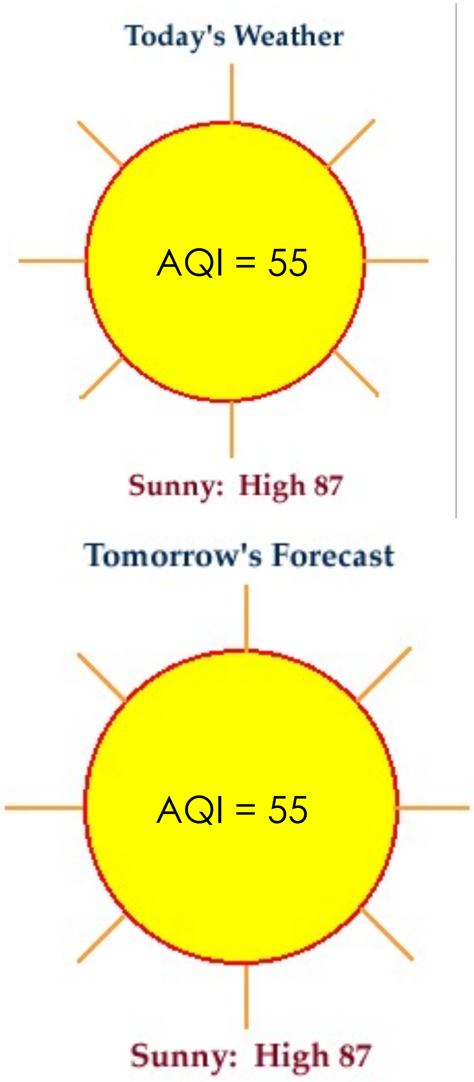
| Air Quality | Air Quality Index | $PM_{2.5}$ (µg/m$^3$) | Health Advisory |
|---|---|---|---|
| Good | 0-50 | 0-12.0 | None |
| Moderate | 51-100 | 12.1-35.4 | Unusually sensitive people should consider reducing prolonged or heavy exertion. |
| Unhealthy for Sensitive Groups | 101-150 | 35.5-55.4 | People with heart or lung disease, older adults, and children should reduce prolonged or heavy exertion. |
| Unhealthy | 151-200 | 55.5-150.4 | People with heart or lung disease, older adults, and children should avoid prolonged or heavy exertion. Everyone else should reduce prolonged or heavy exertion. |
| Very Unhealthy | 201-300 | 150.5 – 250.4 | People with heart or lung disease, older adults, and children should avoid all physical activity outdoors. Everyone else should avoid prolonged or heavy exertion. |
| Hazardous | ≥301 | 250.5 > | People with heart or lung disease, older adults, and children should remain indoors and keep activity levels low. Everyone else should avoid all physical activity outdoors. |

# Air Quality Forecasting Methods

- Persistence
- Climatology
- Criteria
- CART
- Regression
- AI/Machine Learning
- Deterministic/Physical

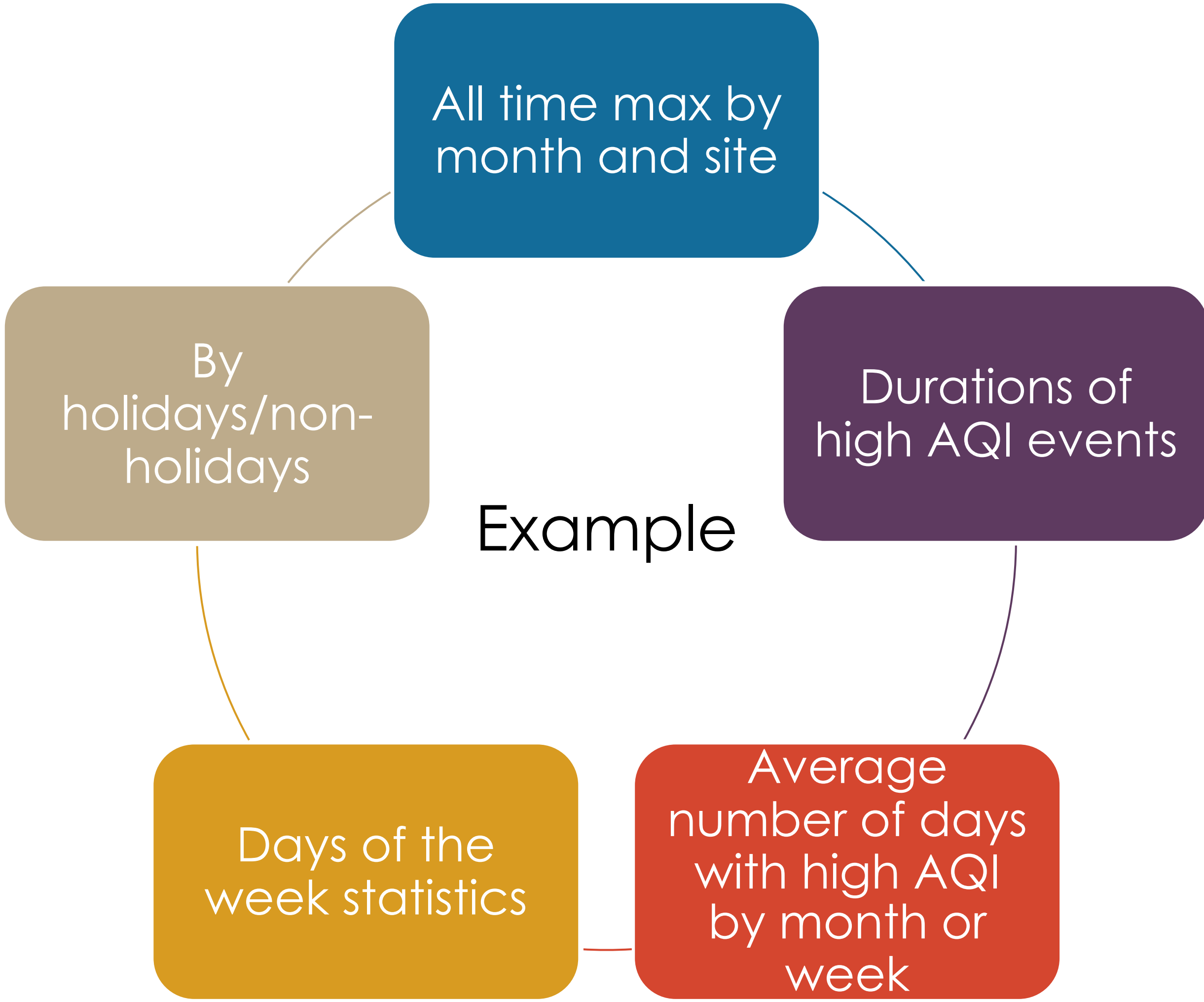
# Air Quality Forecasting Methods

- **Persistence –**
  - Tomorrow’s concentration will be the same as today’s or yesterday’s
  - Often used as a starting point and to help guidance for other forecasting methods
  - It can also serve as a baseline to compare other methods
  - Should not be used as stand-alone method
  - Works well in areas with less pollution variability
  - Works in areas with persistent weather and air quality conditions for several days
  - High uncertainties
  - Cannot predict beginning and end of an air quality event
  - Only requires data from measurements
  - Minimal software and expertise required



# Air Quality Forecasting Methods

- **Climatology –**
  - Uses average and extreme conditions at a given location
  - Air quality is highly dependent on weather patterns, and when they repeat, air quality patterns do as well.
  - Required to prepare data for multiple years
  - Data quality control and change in emissions should be known
  - The climatological values act as a bound and a guide to the air quality forecast.
  - Not a stand-alone method but a tool to support other methods
  - Minimal software and expertise required



All time max by month and site

Durations of high AQI events

Average number of days with high AQI by month or week

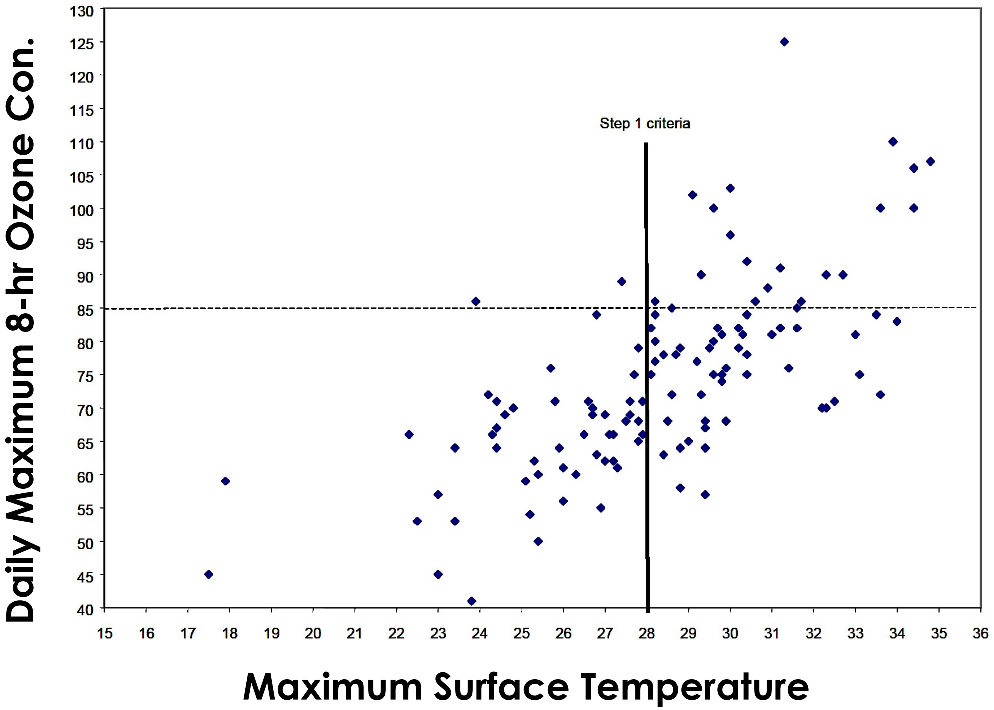
Days of the week statistics

By holidays/non-holidays

Example

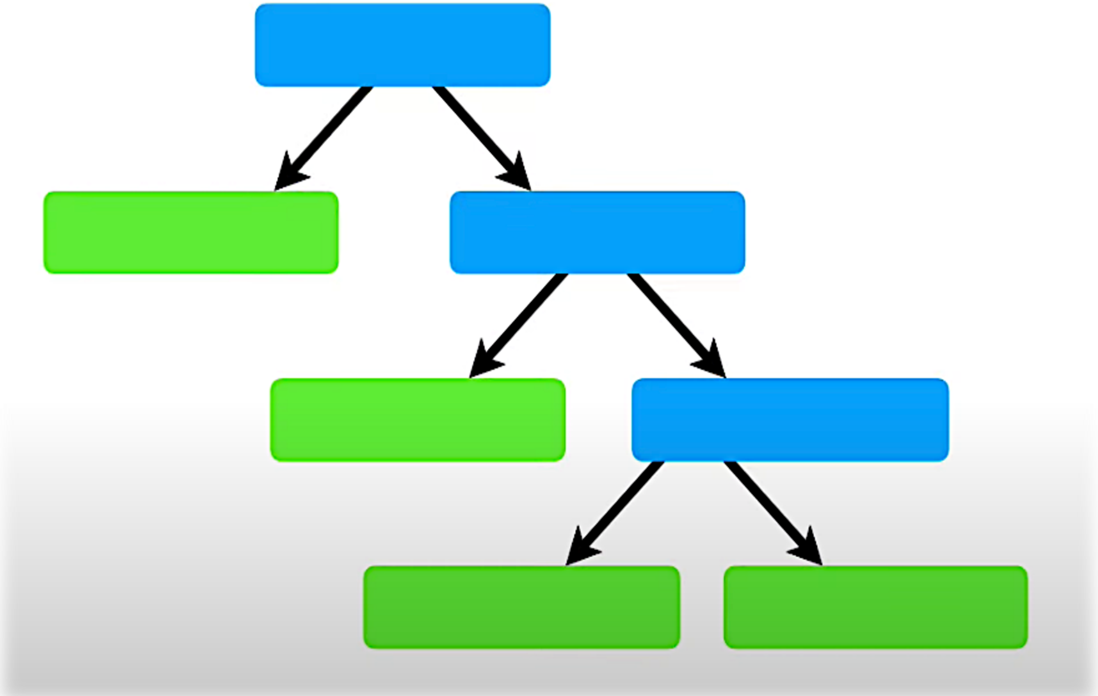
# Air Quality Forecasting Methods

- **Criteria –**
  - Also called 'rule of thumb'
  - Uses a threshold value of either meteorological or air quality variables or both
  - Example, shallow boundary layer often associated with high $PM_{2.5}$ concentration
  - Good method to forecast an exceedance, non-exceedance, or pollution in a particular AQI category range rather than an exact concentration
  - Need knowledge of physical and chemical processes that can influence pollution concentration
  - Can be used as a primary forecasting method, but also with other methods
  - Easy to use and relatively simple to develop
  - Can also be revised easily as more data becomes available



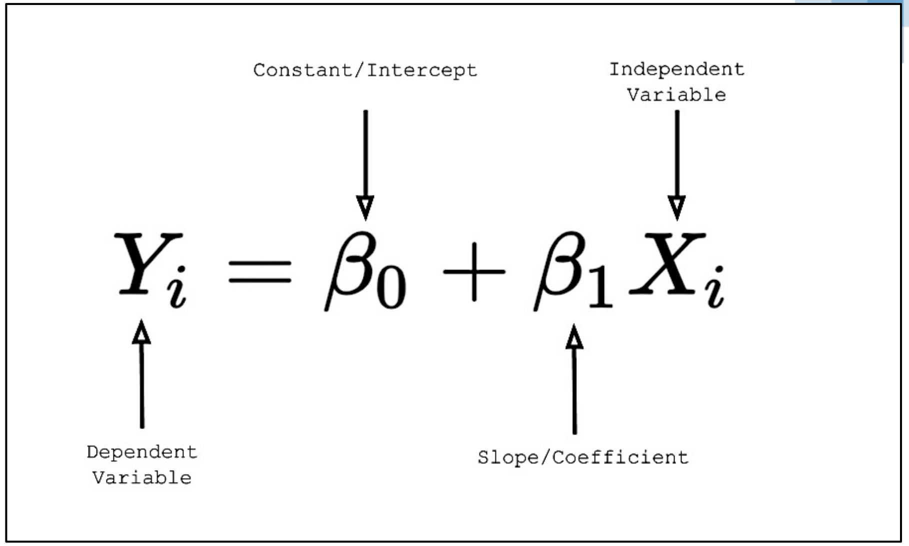
# Air Quality Forecasting Methods

- **Classification and Regression Tree (CART) –**
  - Statistical method, it divides data into distinct groups or clusters
  - Iterative method to develop regression tree
  - Uses multiple meteorological and other variables (day of the week, etc.) as inputs
  - Uses software to create CART data using multiple years of data
  - Uncertainties in input variables can have larger impacts on PM2.5
  - May not be able to predict under unusual emission patterns (e.g., fires, dust)



# Air Quality Forecasting Methods

- **Regression Equations/AI/ML –**
  - Statistical method, it is based on relationship between input (met) and output ($PM_{2.5}$) parameters
  - Regression equation often uses weather forecasts (i.e., T, W, RH, etc.) as input and predicts $PM_{2.5}$
  - Understanding of physical and chemical process and associated parameters is required
  - Statistical software to fit regression model between input and output
  - Independent model verification required
  - Over-fitting can be a problem
  - Tends to predict mean better than the extremes (high and lows) of the distribution
  - Often underpredicts the high concentrations and overpredicts the low concentrations
  - AI/ML algorithms learn patterns and train on input data to predict outputs



Constant/Intercept

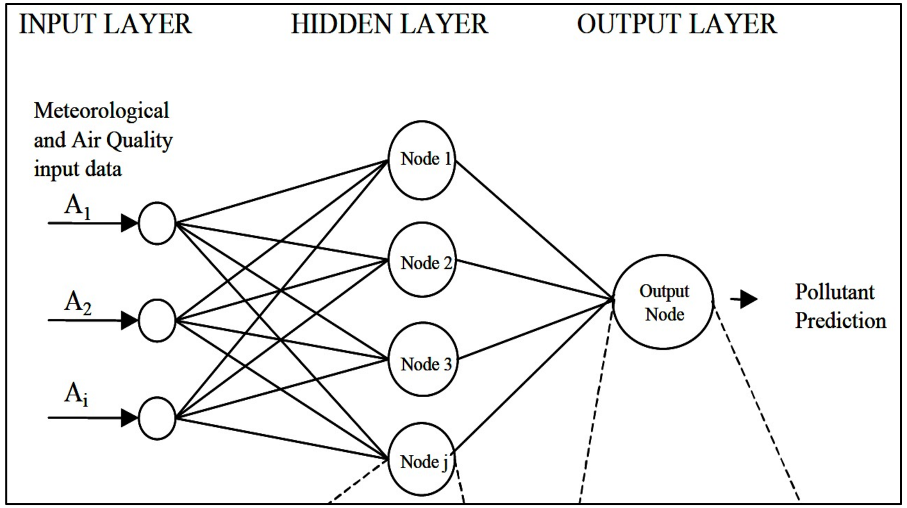
Independent Variable

$$Y_i = \beta_0 + \beta_1 X_i$$

Dependent Variable

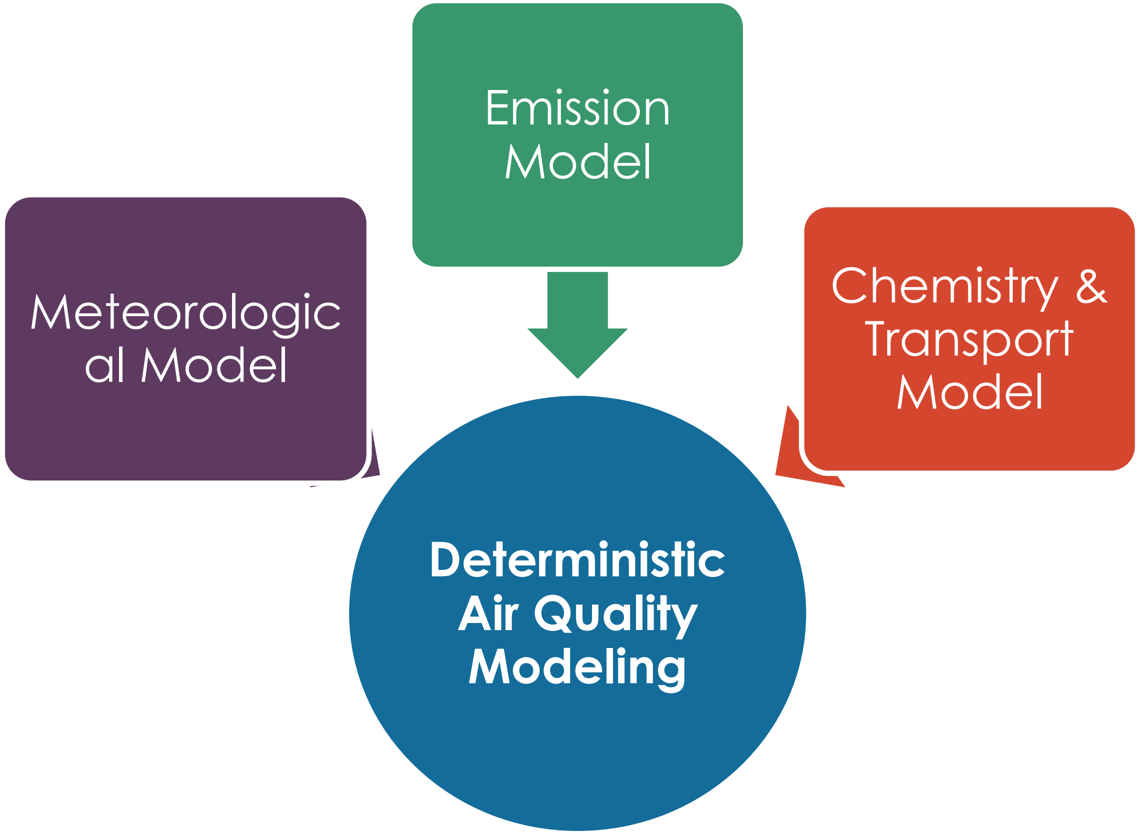
Slope/Coefficient

$$Y = b_0 + b_1x_1 + b_2x_2 + .... + b_nx_n$$



# Air Quality Forecasting Methods

- **Deterministic Air Quality Modeling –**
  - Mathematically represents the processes that affect air quality
  - A system of models that work together to simulate the emission, transport, diffusion, transformation, and removal of air pollution
  - Historically used to simulate future scenarios of air pollution for change in emissions or change in climate
  - Simple 1-D to 3-D models
  - Requires years of development and in-depth expertise on air quality processes and access to emission datasets with high-end computing resources



Emission Model

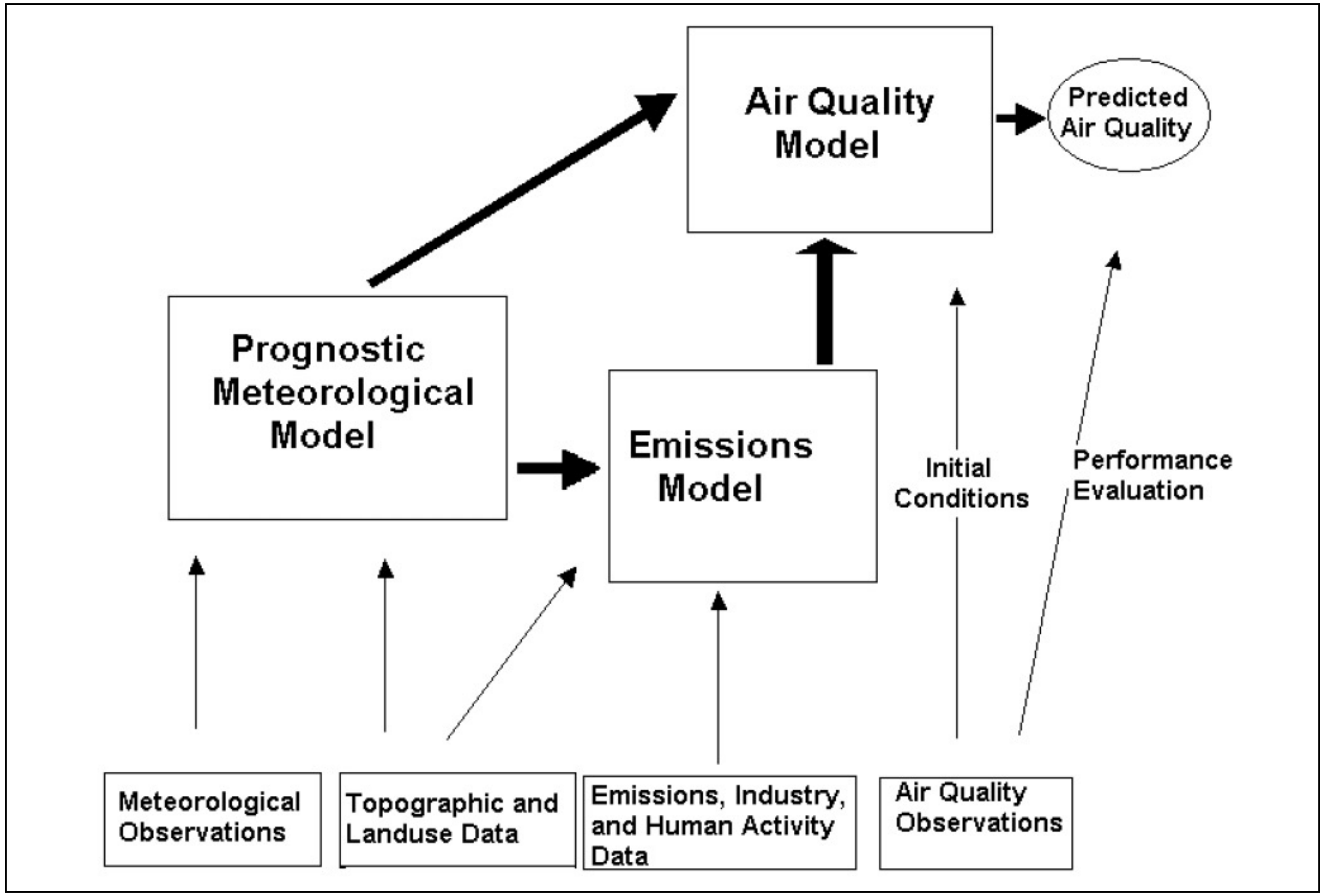
Meteorological Model

Chemistry & Transport Model

**Deterministic Air Quality Modeling**

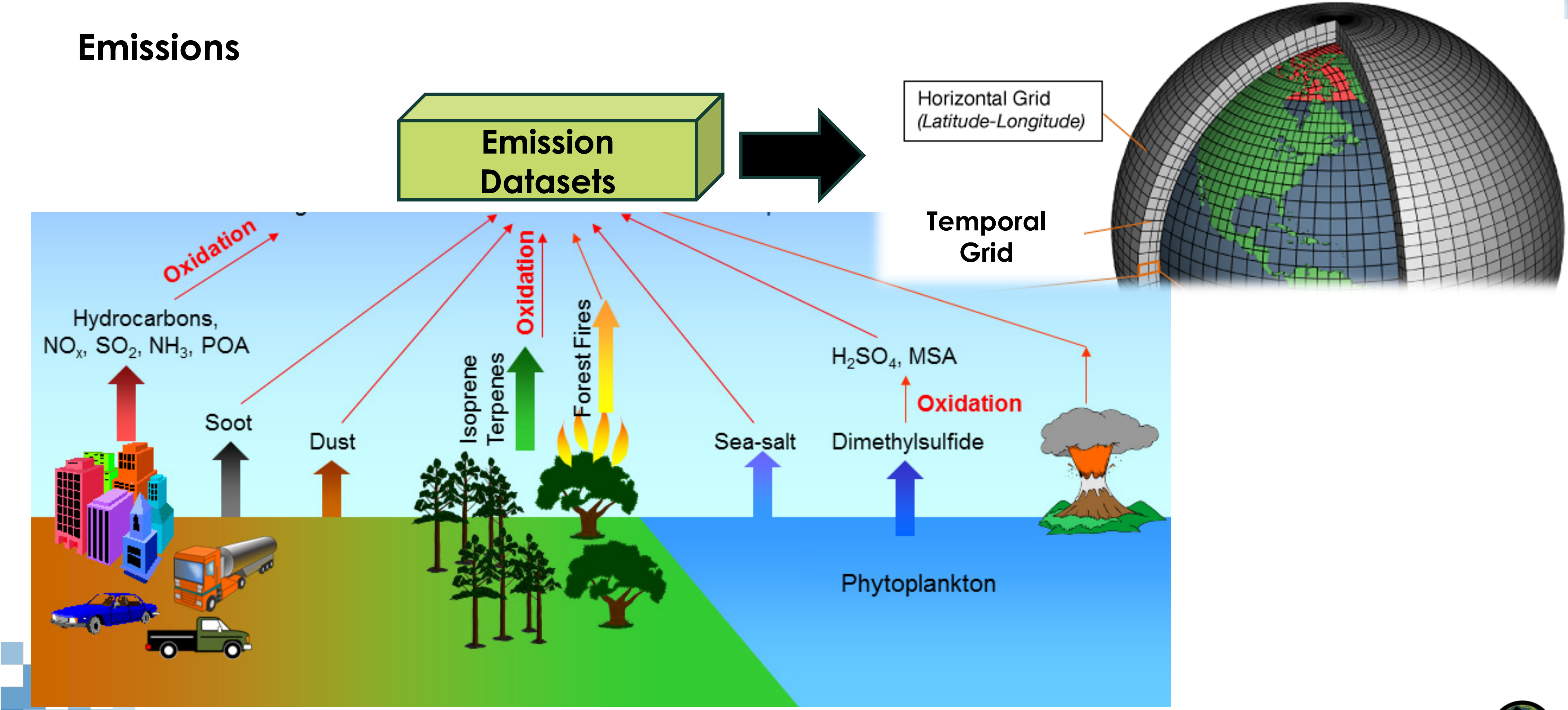
# Deterministic Air Quality Modeling

- Prognostic meteorology models solve fundamental equations to simulate atmospheric behavior.
- Some candidate mesoscale models are MM5, RAMS, & WRF.
- Emission models help estimate emissions at the spatial and temporal scale required for AQ models.
- AQ models are either Lagrangian (trajectory) or Eulerian (grid-based calculations).



# Deterministic Air Quality Modeling

## Emissions

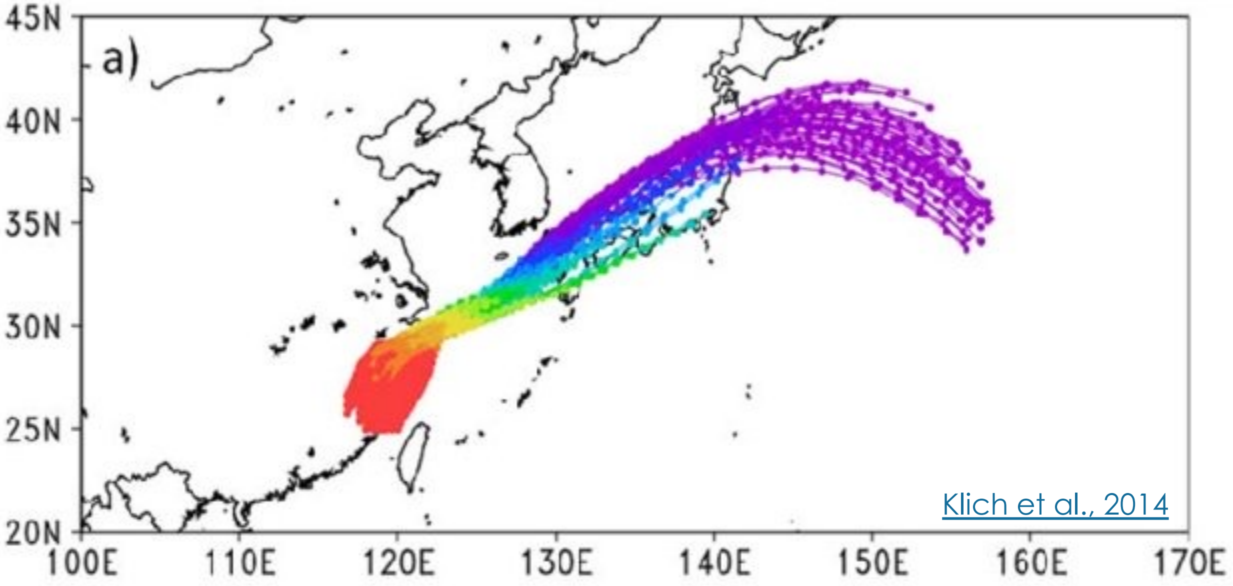


https://www.bnl.gov/newsroom/news.php?a=26257

# Deterministic Air Quality Modeling

## AQ Models – Lagrangian

- Follow individual air parcels over time using the meteorological data to transport and diffuse the pollutants. It may also include chemical transformations.
- Example - The Hybrid Single-Particle Lagrangian Integrated Trajectories with a generalized nonlinear Chemistry Module (HY-SPLIT CheM)
- It is good when number of emissions sources are limited, but not suited for a large number of sources

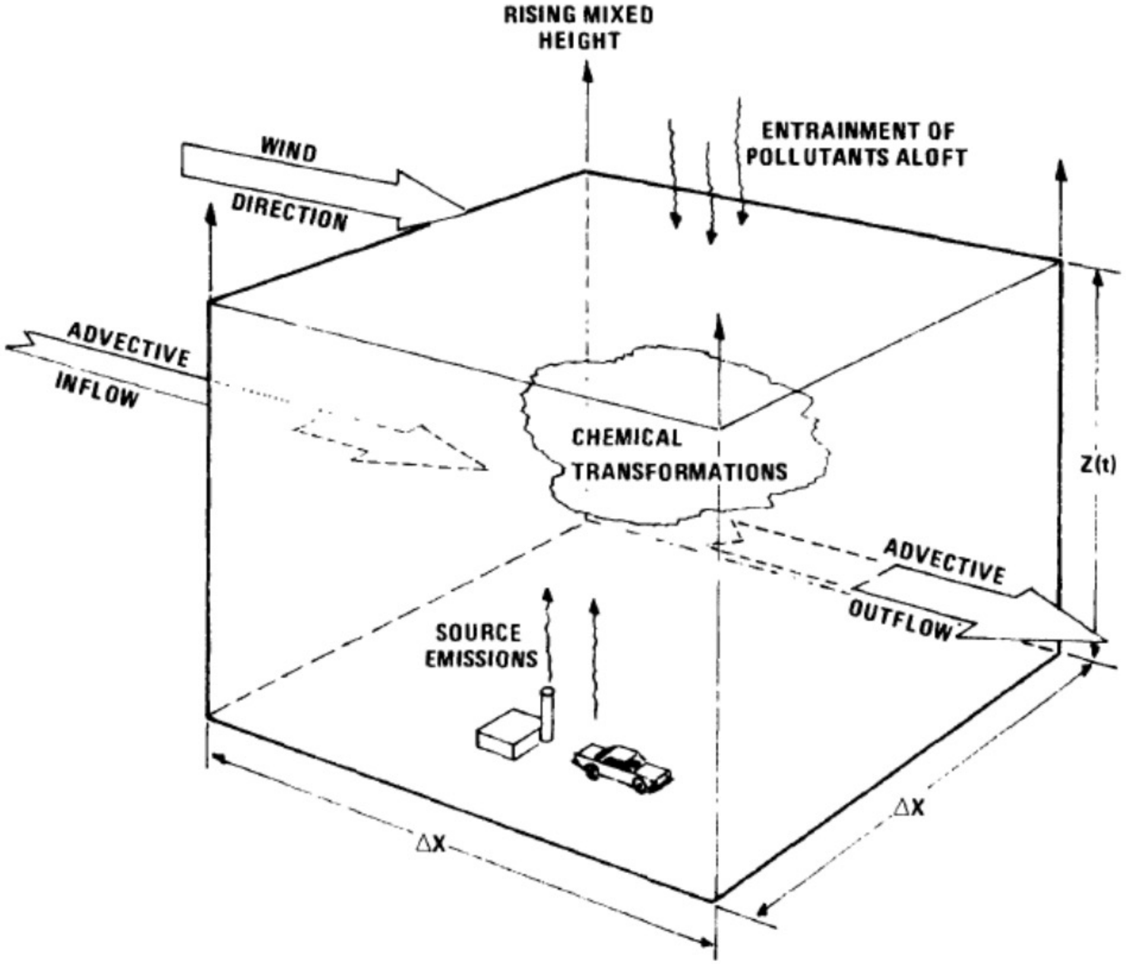


Klich et al., 2014

# Deterministic Air Quality Modeling

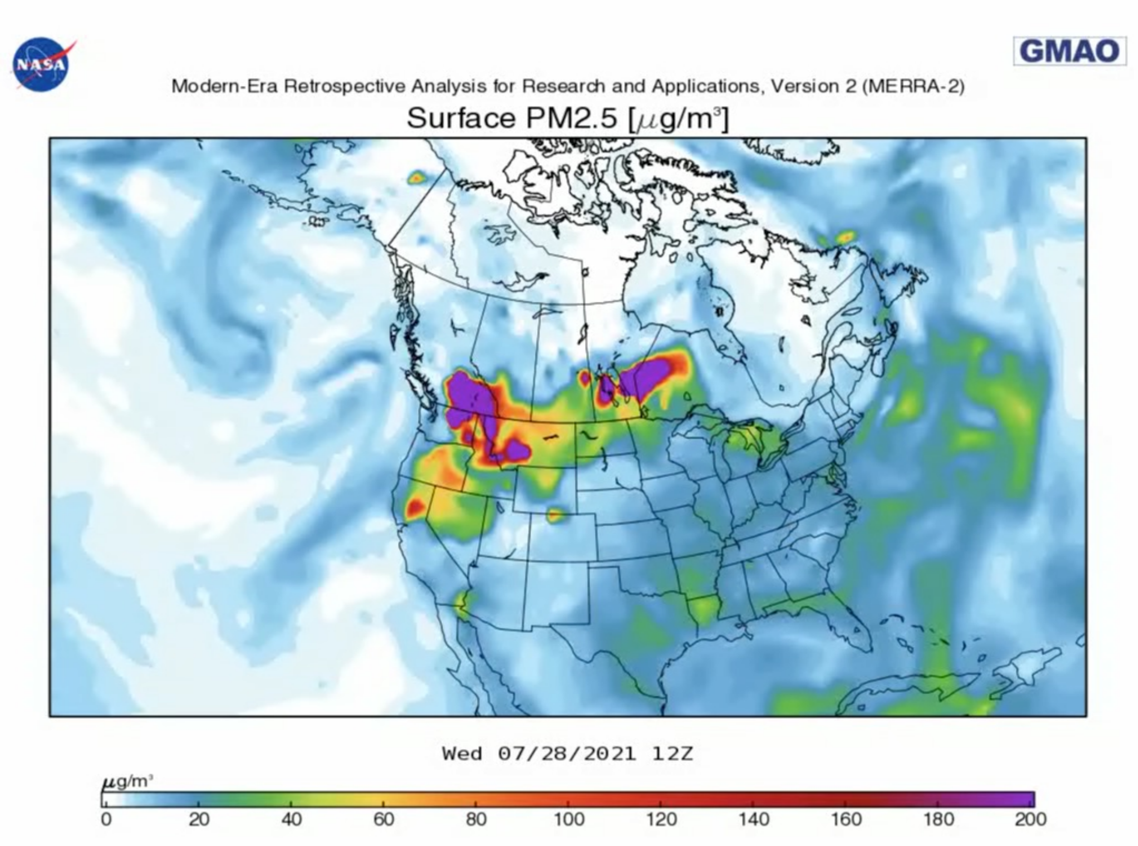
## AQ Models – Eulerian

- Solve the chemical transformation equations in a grid cell and pollutants are exchanged between cells
- Can produce 3D concentration fields for many pollutants
- Requires high-end computing resources
- Models have both vertical (number of levels) and horizontal resolutions (size of grid on Earth's surface)
- Smaller grid -> higher resolution -> higher computational power -> often higher accuracies
- Examples – CMAQ, WRF-Chem



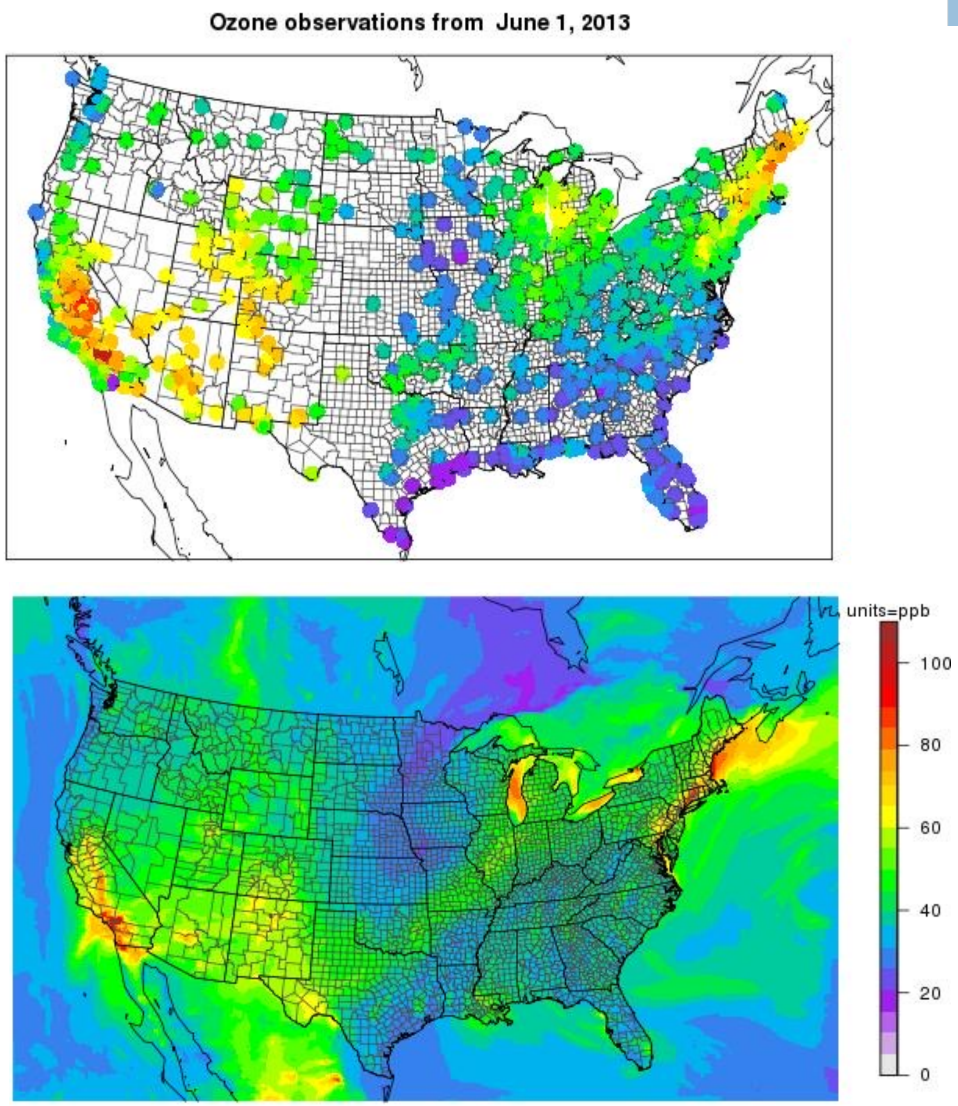
# Air Quality Models – Strengths

- 3D AQ models are phenomenologically based, simulating the physical and chemical processes that result in the formation and destruction of air pollutants.
- Can forecast for a large geographic area, irrespective of ground measurements
- Spatial and temporal patterns can be analyzed by mapping outputs
- More suitable for operational regional and global air quality forecasting and alerting the public (parallel to weather forecasts)
- Can be used to assess the importance of local emission sources or long-range transport



# Air Quality Models - Limitations

- AQ forecasting accuracies depend on the ability of meteorological models to forecast conditions with sufficient accuracy.
- Out of date, coarser-resolution, and uncertain emissions inventories can also be a source of uncertainty.
- Spatial scales of model forecasts become important when comparing and assessing the forecast with ground observations
- Requires expertise in both development and running models for operational AQ forecasting
- Large amount of data to handle



# Understanding Forecasting Needs

- Who will use the forecasts?
- What should the length and frequency of the forecast be?
- Timing of forecast initialization
- How frequently should the forecasts be revised?
- Accuracy requirements or level of tolerance
- Forecast the AQI category or specific pollutant concentrations?

# Assessing the Forecasts – Numerical

- **Accuracy –**
  - Mean closeness between forecast and observed value

Forecast Observation

$$A = \frac{1}{N}\left(\sum_{1}^{N}\left|f - o\right|\right)$$

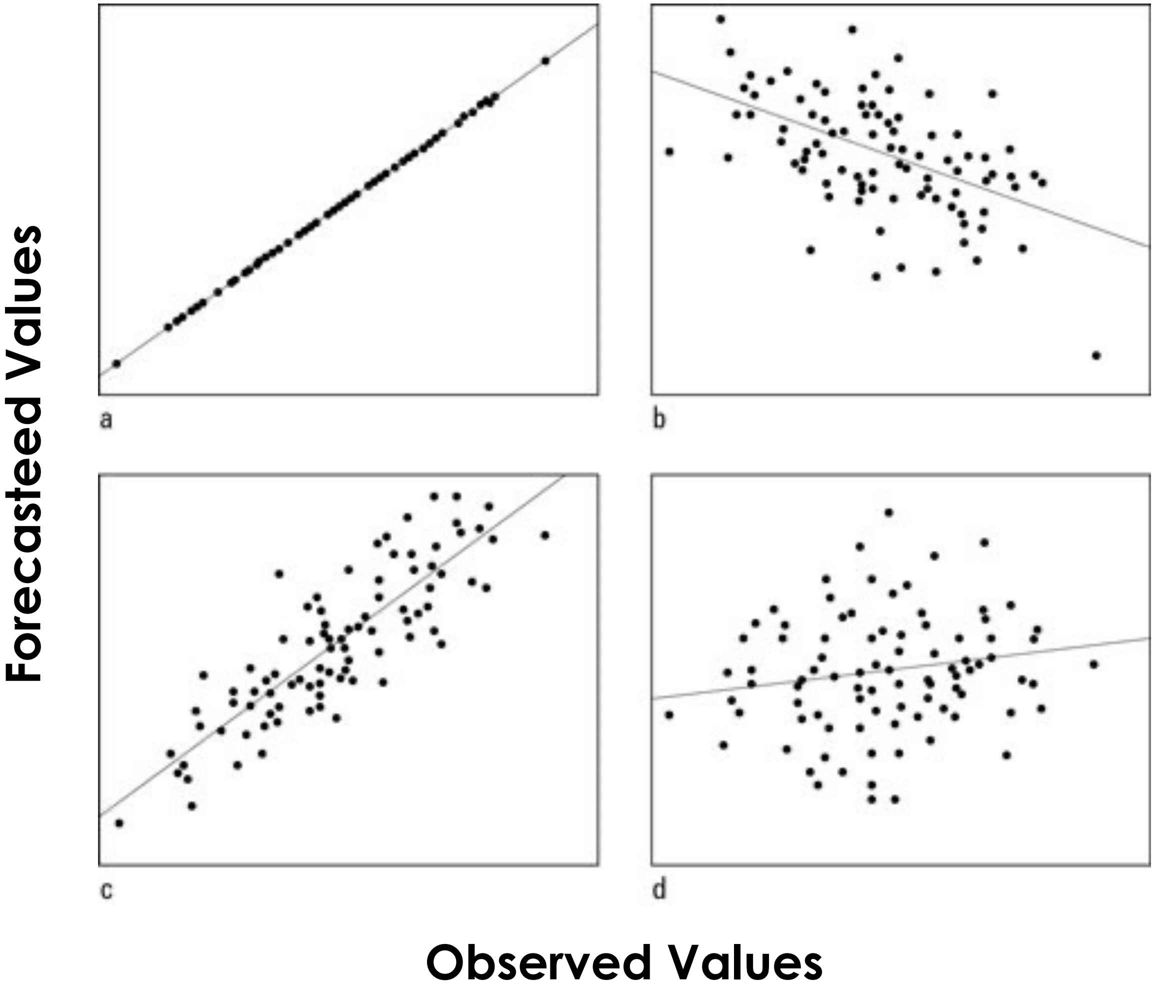
Number of Data Points

- **Bias –**
  - On average, an indicator of under- or over-estimation by forecast

$$B = \frac{1}{N}\left(\sum_{1}^{N}\left(f - o\right)\right)$$

# Assessing the Forecasts - Numerical

- **Correlation –**
  - Degree of relationship between forecast and observed value



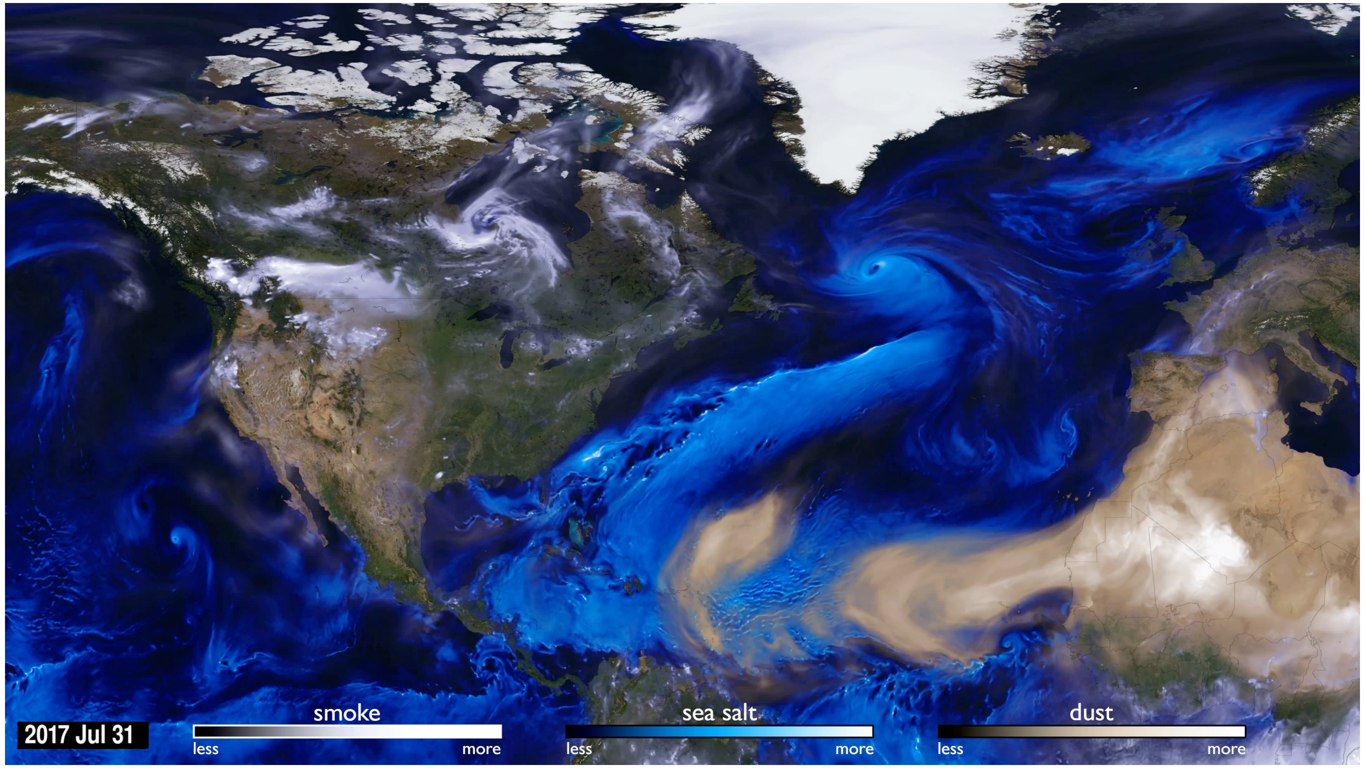
- **Categorical** →

Forecasted

| Observed | Good | Moderate | Unhealthy for Sensitive Groups | Unhealthy |
|---|---|---|---|---|
| Good | k | l | m | n |
| Moderate | o | p | q | r |
| Unhealthy for Sensitive Groups | s | t | u | v |
| Unhealthy | w | x | y | z |

# Role of Satellite Data in AQ Forecasting

- **Emissions:**
  - Biomass burning emissions
  - Dust emissions
  - Volcanic emissions
  - Anthropogenic emissions
- **Boundary Conditions:**
  - Boundary condition outside model domain
- **Data Assimilation:**
  - Inform/initialize the model using latest satellite observations
  - AOD assimilation
- **Inter-Comparison/Validation:**
  - Compare spatial and temporal pattern from model and satellite



# Satellite Based Fire Emissions: Quick Guide

| | GFED4s | FINN | QFED | GFAS | FEER |
|---|---|---|---|---|---|
| Product | Burned Area, Active Fire Counts | Active Fire Counts | FRP | FRP | FRP |
| Time Period | 1997 - Present | 2002 - Present | 2000 - Present | 2003 - Present | 2003 - Present |
| Resolution | 0.25° | 1 km | 0.1° | 0.1° | 0.1° |
| Reference | Giglio et al. (2013); Randerson et al. (2012); Van der werf et al. (2017) | Wiedinmyer et al. (2011) | Darmenov and Da Silva (2015) | Kaiser et al. (2012) | Ichoku and Ellison (2014) |
| Website | https://www.globalfiredata.org/ | https://www2.acom.ucar.edu/modeling/finn-fire-inventory-ncar | https://portal.nccs.nasa.gov/datashare/iesa/aerosol/emissions/QFED/v2.5r1/ | https://atmosphere.copernicus.eu/global-fire-emissions | https://feer.gsfc.nasa.gov/ |

# The Community Multiscale Air Quality Modeling System (CMAQ)

https://www.epa.gov/cmaq

- An open-source Eulerian model by US EPA to simulate air quality
- Used by a wide range of researchers around the globe, including agencies such as EPA, NWS, & CDC
- Uses coupled mathematical representations of actual chemical and physical processes to simulate air quality

**Learn about CMAQ**

- CMAQ Models
- Overview of Science Processes
- Publications and Peer Review
- CMAQ Fact Sheet
- CMAQ Impact Statement

**CMAQ Applications**

- EPA Mission Support
- Evaluation Studies
- Human Exposure to Pollutants
- Ecosystems and Air Quality
- Emerging Applications

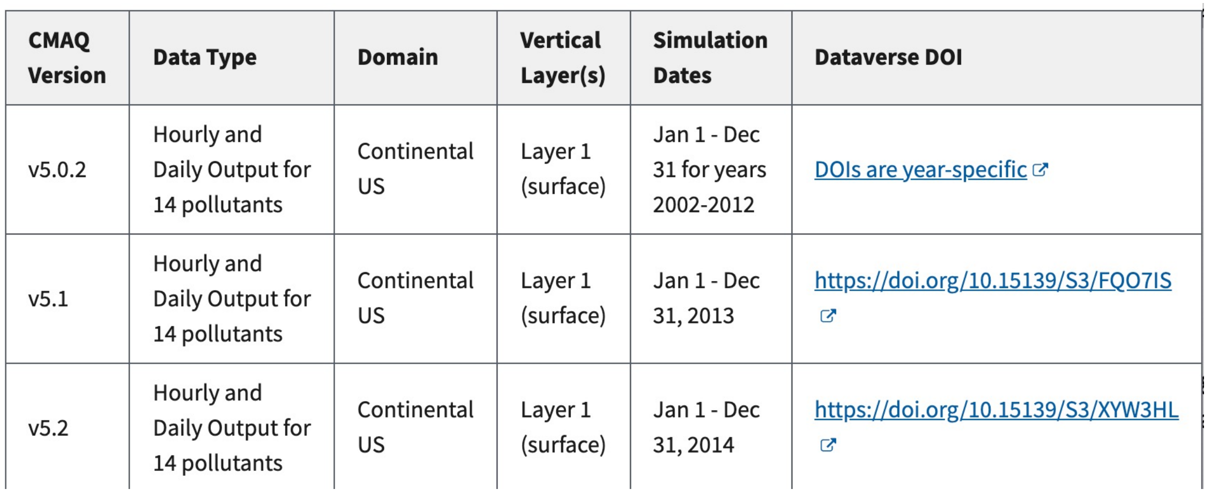
**Download CMAQ**

- Model Source Code
- Documentation
- Model Inputs and Test Case Data
- Resources/Utilities for Model Users

**CMAQ Research**

**CMAQ Community**

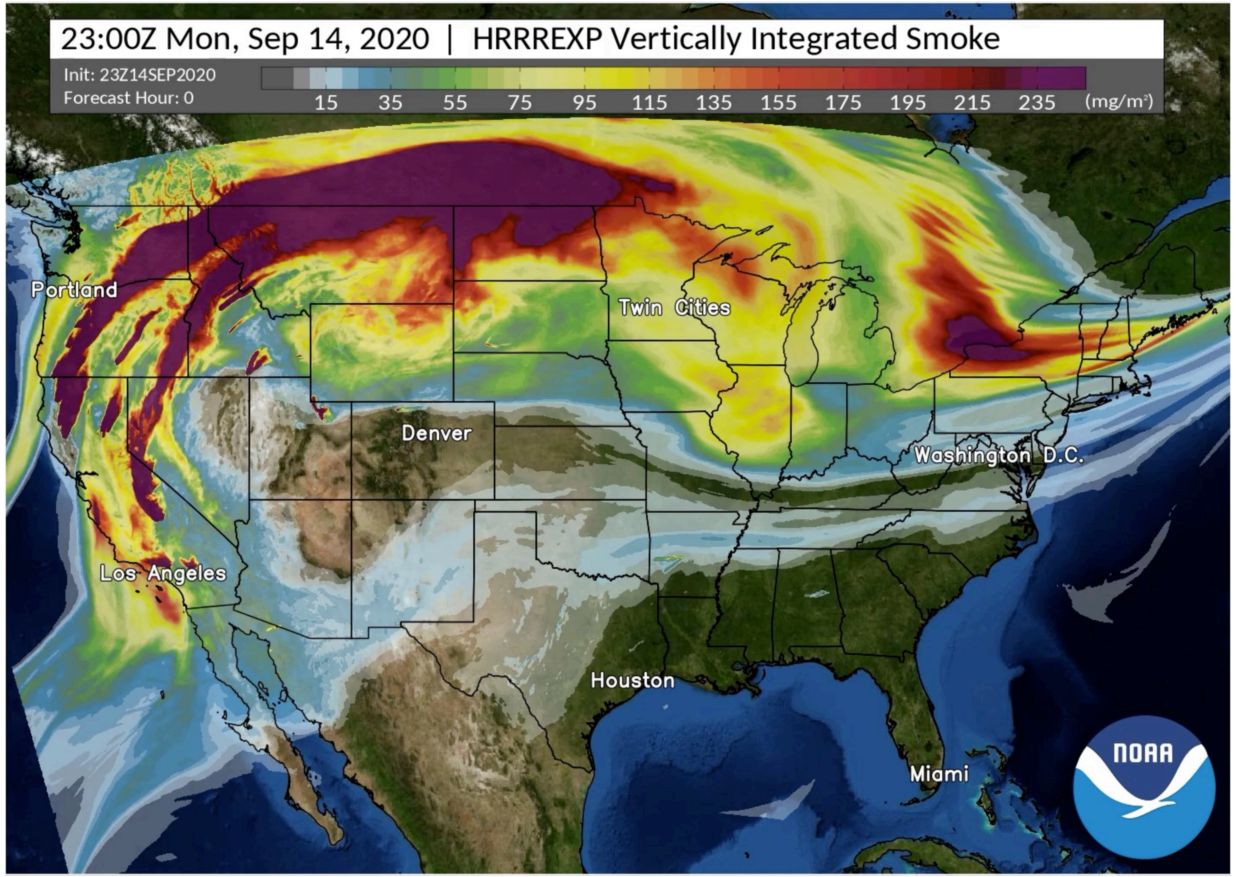
**CMAQ Output**



| CMAQ Version | Data Type | Domain | Vertical Layer(s) | Simulation Dates | Dataverse DOI |
|---|---|---|---|---|---|
| v5.0.2 | Hourly and Daily Output for 14 pollutants | Continental US | Layer 1 (surface) | Jan 1 - Dec 31 for years 2002-2012 | DOIs are year-specific |
| v5.1 | Hourly and Daily Output for 14 pollutants | Continental US | Layer 1 (surface) | Jan 1 - Dec 31, 2013 | https://doi.org/10.15139/S3/FQO7IS |
| v5.2 | Hourly and Daily Output for 14 pollutants | Continental US | Layer 1 (surface) | Jan 1 - Dec 31, 2014 | https://doi.org/10.15139/S3/XYW3HL |

# WRF-Chem

- Weather Research and Forecasting (WRF) model coupled with Chemistry (Chem)
- Can be used for regional-scale air quality, field program analysis, and interactions between clouds and chemistry
- Development lead by NOAA but larger community contributes significantly
- Some forecasts can be accessed from - [https://ruc.noaa.gov/wrf/wrf-chem/](https://ruc.noaa.gov/wrf/wrf-chem/)



# References

- **Guidelines for Developing an Air Quality (Ozone and PM2.5) Forecasting Program, EPA-456/R-03-002, June 2003 – Materials presented in this session were based on this document.**
- National Research Council (1991) – Explains how tropospheric ozone forms and provides details about ozone chemistry.
- Seinfeld and Pandis (1998) – Provides a basic overview of atmospheric chemistry (ozone and PM2.5) and describes how meteorology affects atmospheric chemistry.
- Wallace and Hobbs (1977) – Provides general meteorological information about weather maps, atmospheric stability, and atmospheric motions from the synoptic-scale to the local-scale.
- Wilks (1995) – Describes statistical techniques and how these can be applied to meteorological data. Many of the techniques discussed can also be applied to air quality.

# Thank You!