

# Atmospheric Issues - Chemical Releases

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# Topics

1. Emissions of chemical into the atmosphere
2. Atmospheric transport, diffusion and deposition
3. Chemical reactions
4. Air quality management
5. The role of **computer models**

# 1. Chemical Releases

- Anthropogenic (“man-made”), e.g., power plants
  - Industrial activities, e.g., from stacks
  - Urban activities, e.g., heating
  - Transportation, e.g., cars and trucks
- Natural, e.g., volcanoes
  
- Planned, e.g., regular industrial production
- Unplanned, e.g., accidental releases
  
- Traditional (“criteria”) chemicals, e.g., SO<sub>2</sub>, CO, O<sub>3</sub>
- Air Toxics, e.g., benzene
  
- Primary emissions (e.g., NO, CO)
- Secondary chemicals (e.g., O<sub>3</sub> and a fraction of PM<sub>2.5</sub>)

# Air Pollution



Natural

Manufactured











# Adverse Effects

The World Health Organization states that 2.4 million people die each year from causes directly attributable to air pollution, with 1.5 million of these deaths attributable to indoor air pollution.

[http://www.who.int/entity/quantifying\\_ehimpacts/countryprofilesebd.xls](http://www.who.int/entity/quantifying_ehimpacts/countryprofilesebd.xls)

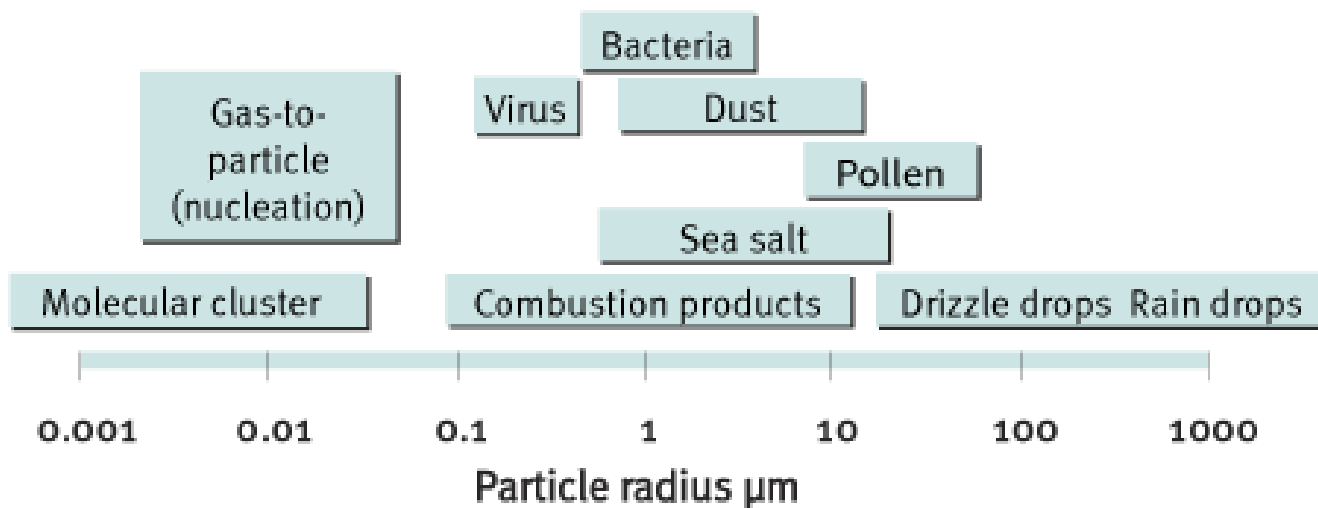
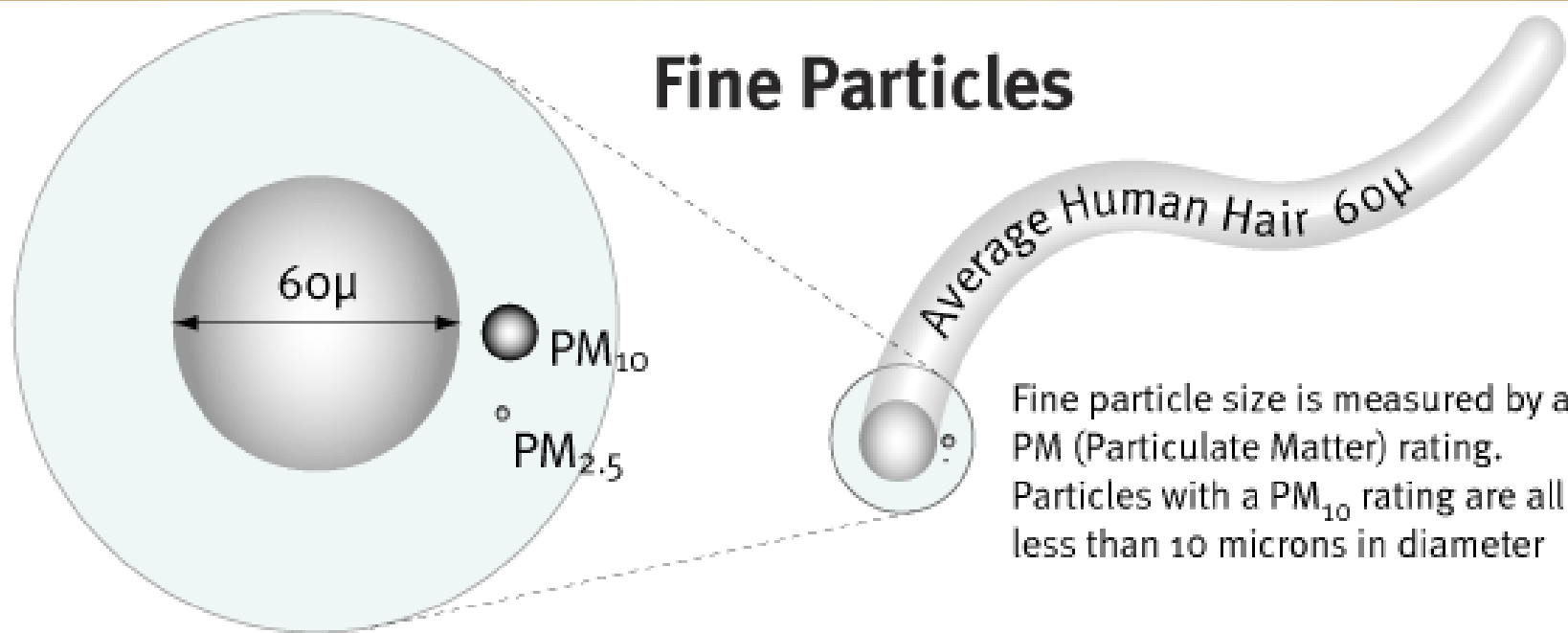
## 2. Atmospheric Transport, Diffusion and Deposition

- Pollutants carried by the wind (Meteorology)
- Diffused by atmospheric turbulence (Meteorology)
- Deposited at the ground by dry and wet processes
- [transport.pdf](#)

# 3. Chemical Reactions

- Creation of urban smog
  - Ozone
  - Photochemical smog
  - [urban chemistry.pdf](#)
- Long range transport of urban and industrial plumes
  - Secondary PM<sub>2.5</sub>
    - SO<sub>2</sub> → sulfates
    - NO<sub>x</sub> → nitrates
    - VOC → organic particles
  - Acidic deposition

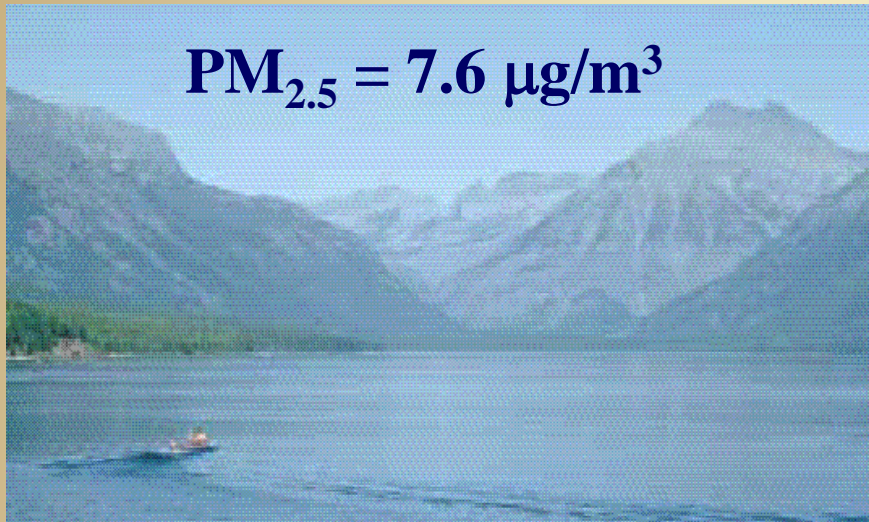
# Fine Particles



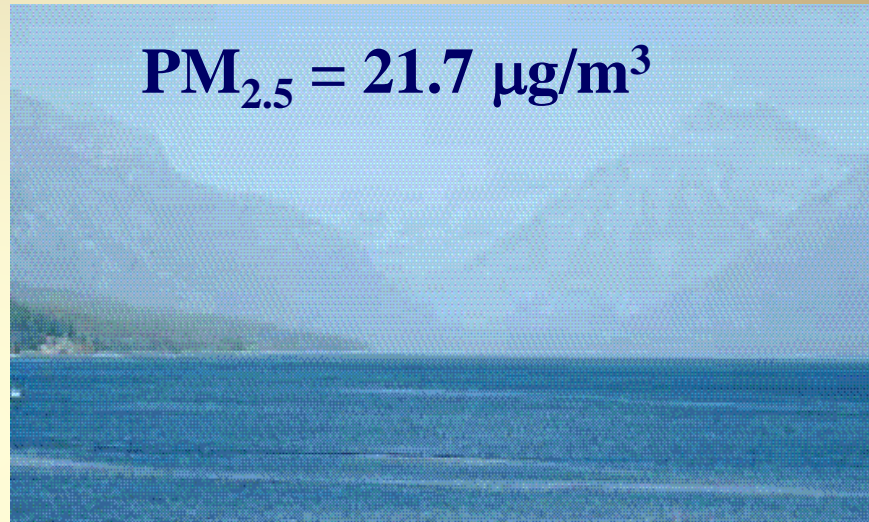
# Particles and Visibility

(Photos below generated by computer simulation)

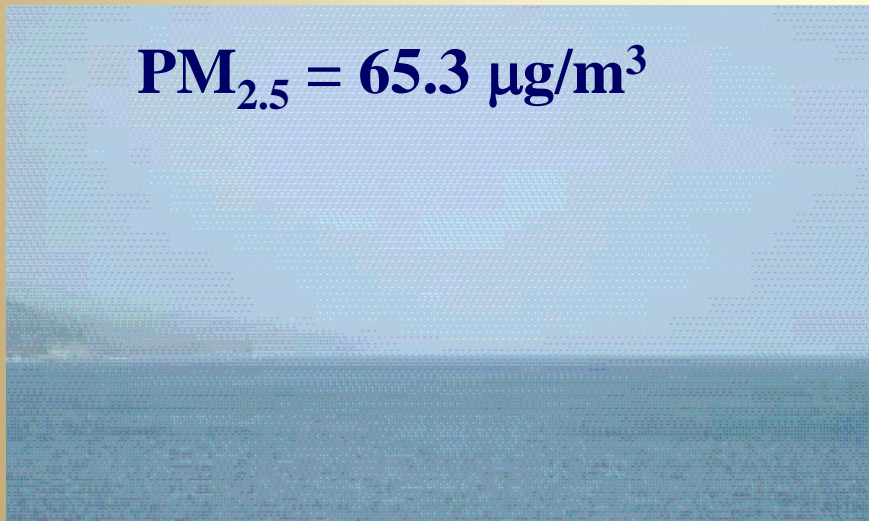
$PM_{2.5} = 7.6 \mu\text{g}/\text{m}^3$



$PM_{2.5} = 21.7 \mu\text{g}/\text{m}^3$



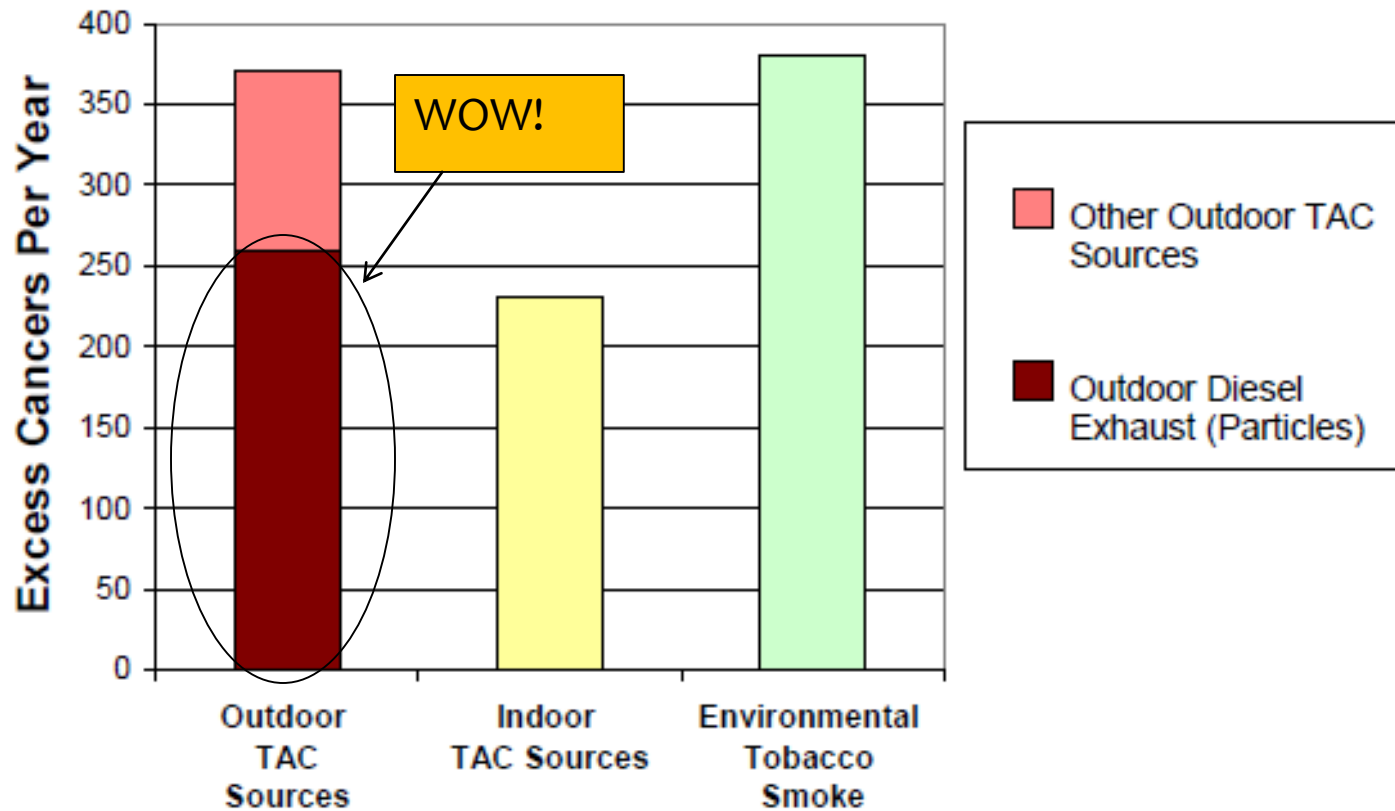
$PM_{2.5} = 65.3 \mu\text{g}/\text{m}^3$



# Diesel Particulate Matter (DPM)

- A particularly dangerous portion of PM<sub>2.5</sub>
- Comprised mostly of
  - Soot (“elemental carbon”)
  - Many different forms of “organic carbon”
- Sources: Diesel fueled engines (stationary and mobile)
  - Heavy-duty trucks
  - Construction equipment
  - Others ...

**Figure ES-2:  
Estimated Potential Cancer Burden from Air Toxics  
in California by Source**



Note: TAC = “Toxic Air Contaminant”, which is comprised of many air pollutants that are toxic  
<http://www.arb.ca.gov/research/apr/reports/l3041.pdf>

# 4. How do we Manage Air Pollution?

- “Routine” management at local level
  - To achieve pre-defined air quality goals
  - To protect human health and the environment
- Emergency management
  - Emergency preparedness
  - Emergency response
- Large scale issues
  - Long-range pollution within a country
  - Trans-boundary pollution
  - Global issues
- **Computer modeling** is the key tool, e.g., in the US ...



# Air Quality Management

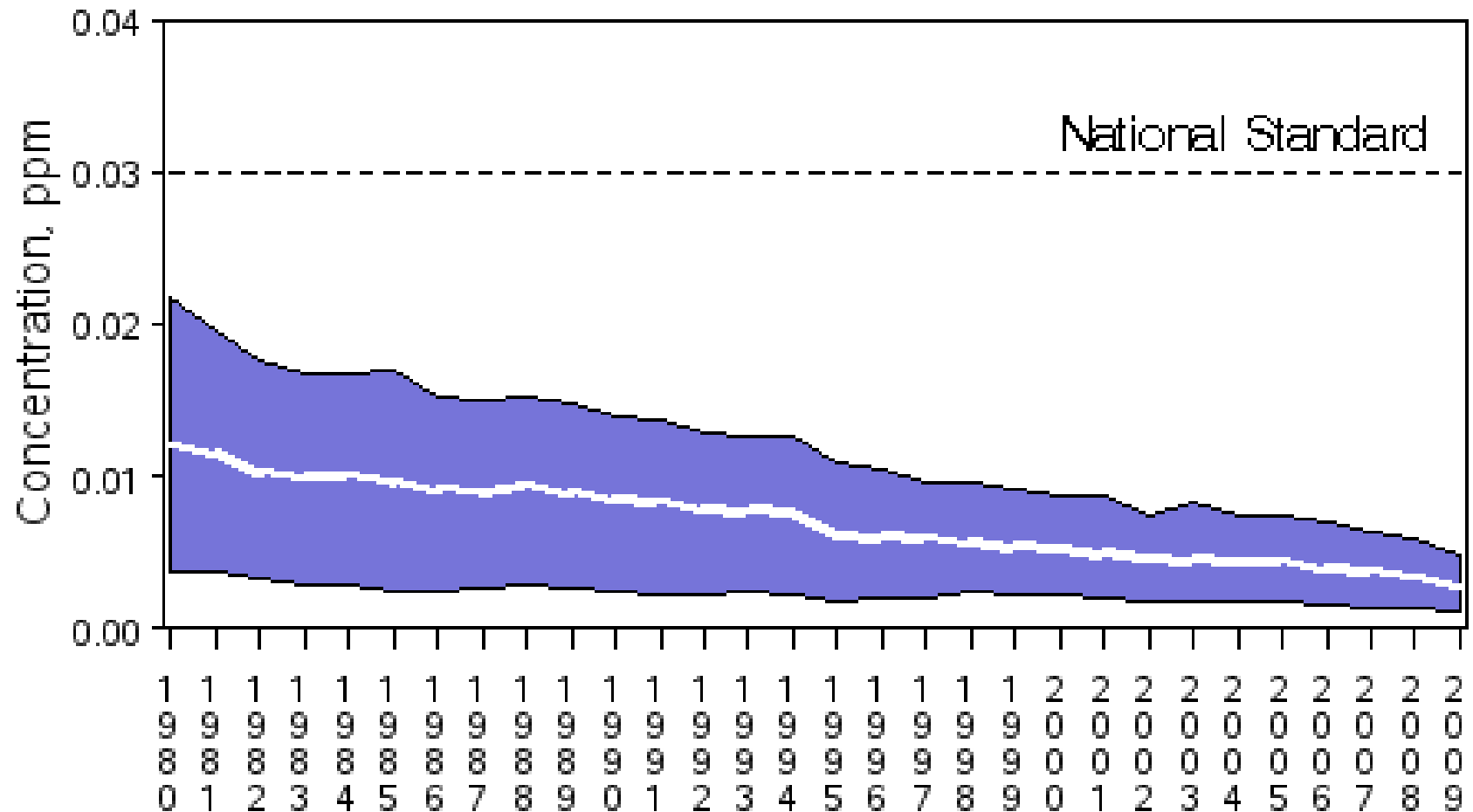
The US EPA Approach



# SO2 Air Quality, 1980 - 2009

(Based on Annual Arithmetic Average)

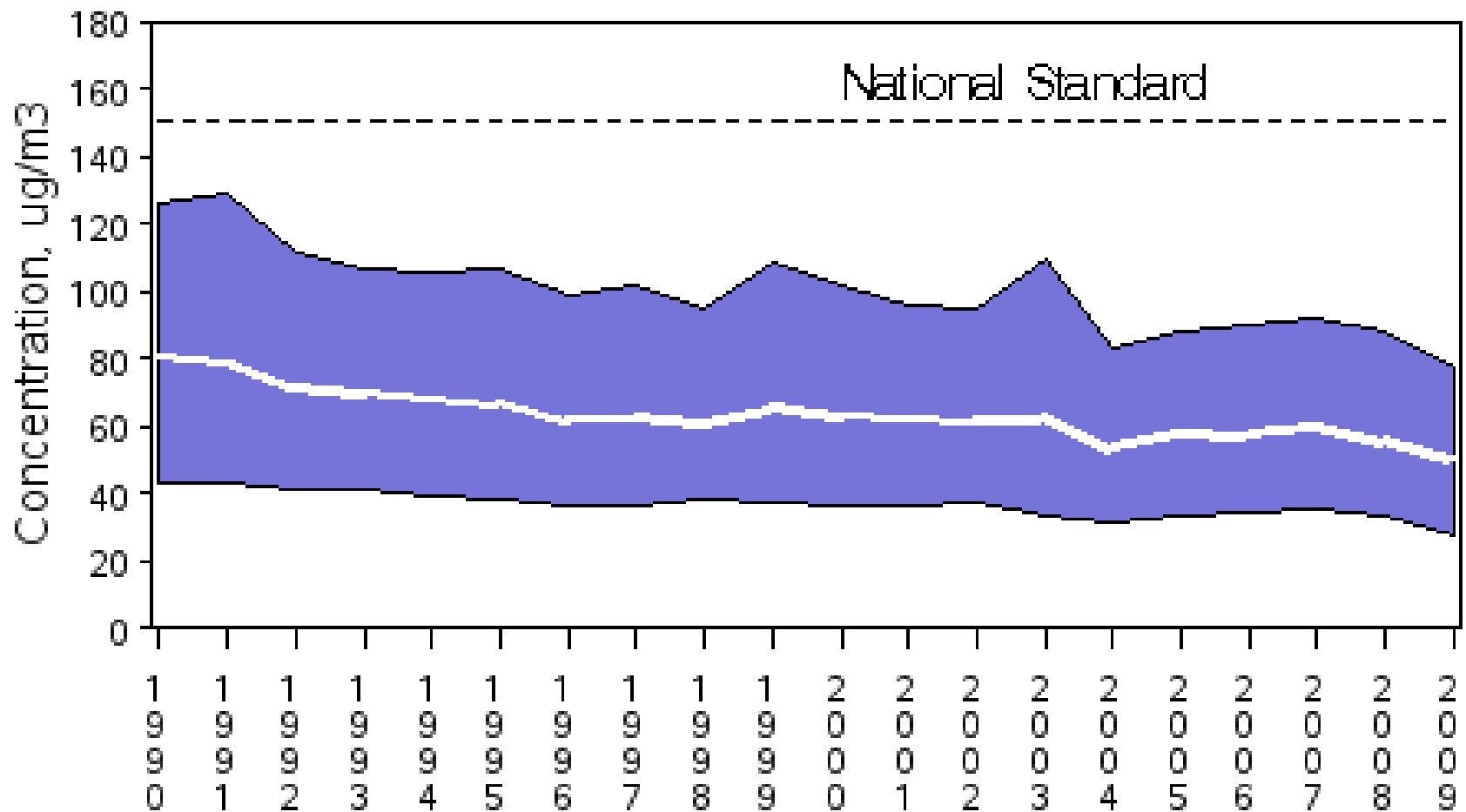
National Trend based on 134 Sites



1980 to 2009 : 76% decrease in National Average

# PM10 Air Quality, 1990 - 2009

(Based on Annual 2nd Maximum 24-Hour Average)  
National Trend based on 310 Sites

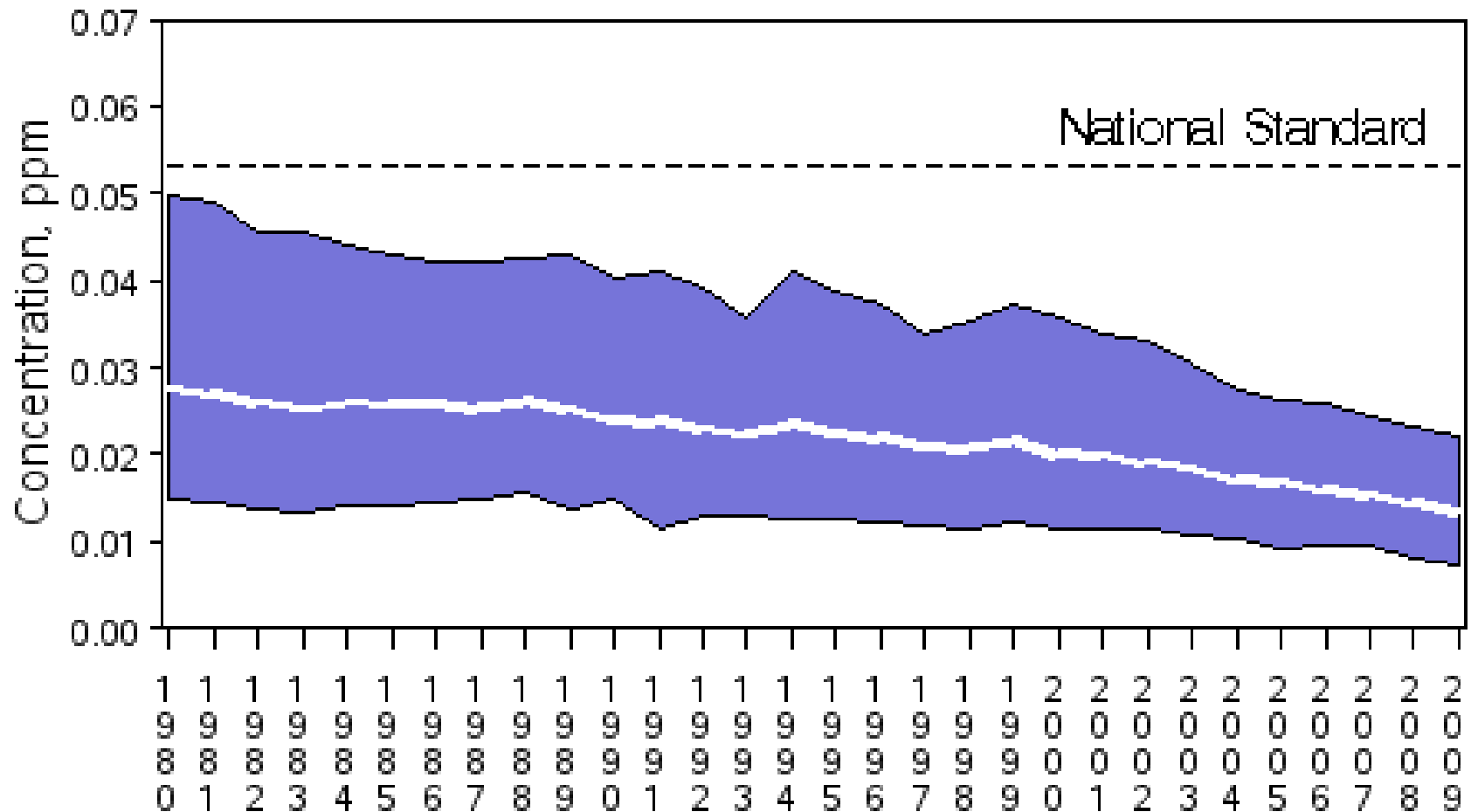


1990 to 2009 : 38% decrease in National Average

# NO2 Air Quality, 1980 - 2009

(Based on Annual Arithmetic Average)

National Trend based on 81 Sites

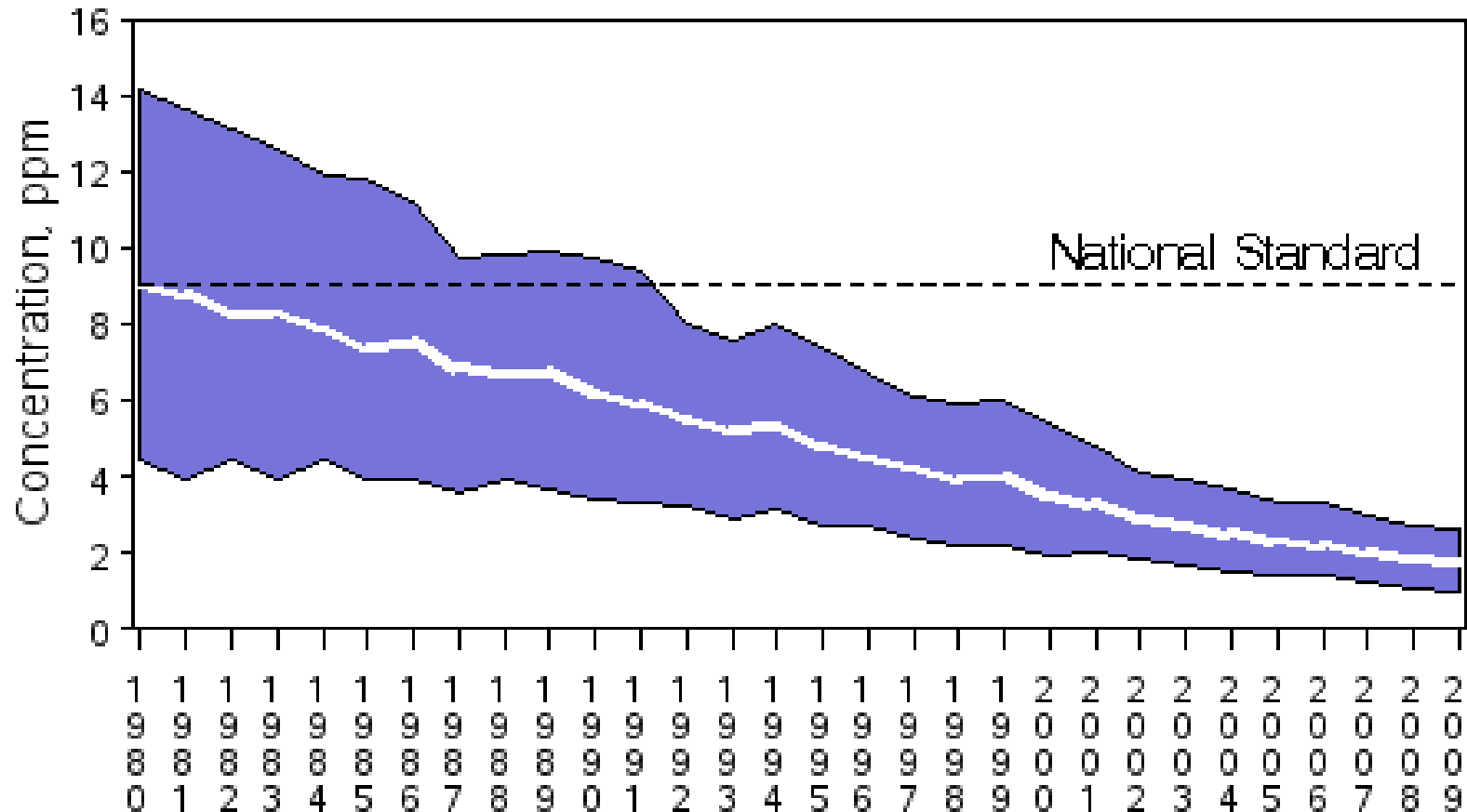


1980 to 2009 : 48% decrease in National Average

# CO Air Quality, 1980 - 2009

(Based on Annual 2nd Maximum 8-hour Average)

National Trend based on 114 Sites

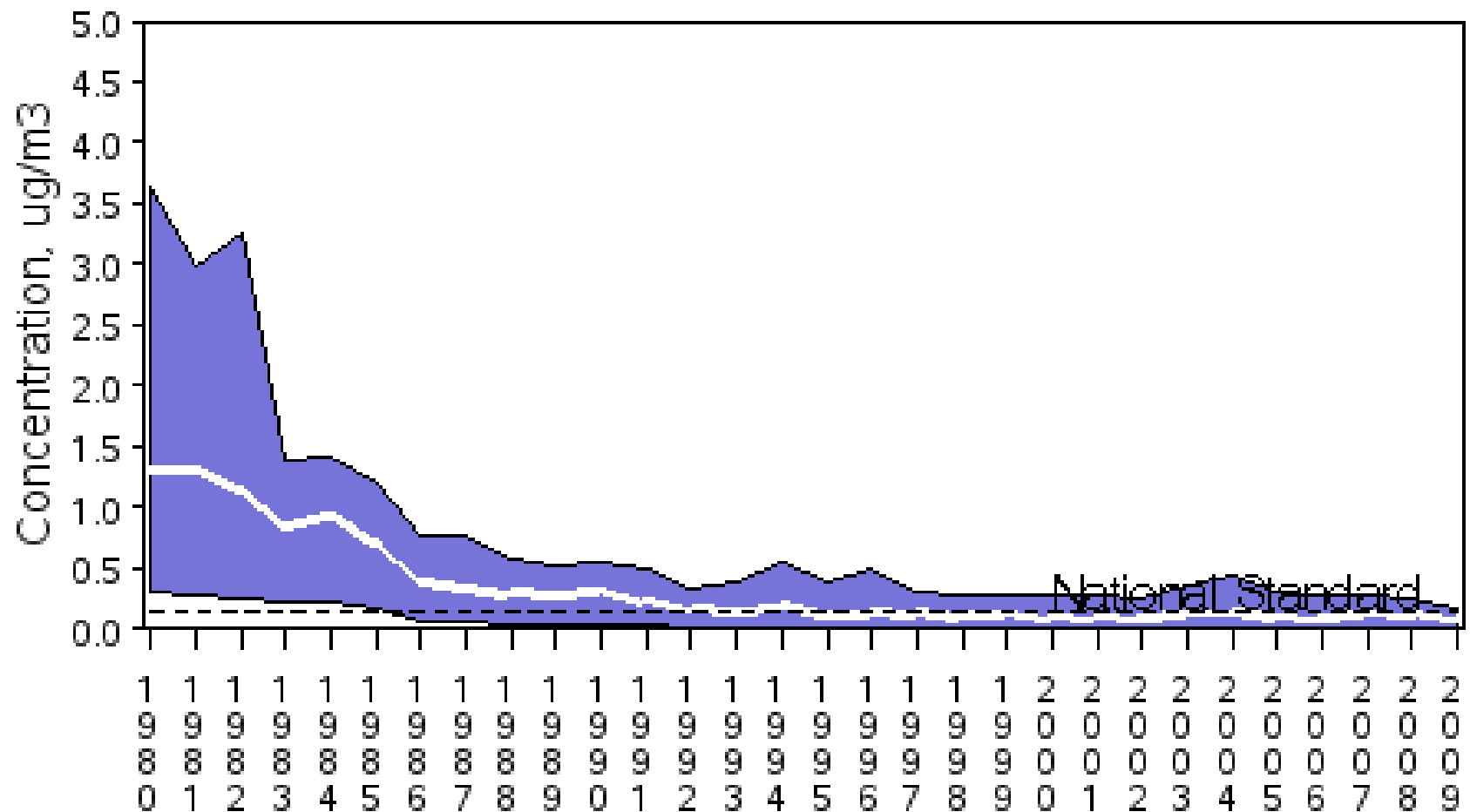


1980 to 2009 : 80% decrease in National Average

# Lead Air Quality, 1980 - 2009

(Based on Annual Maximum 3-Month Average)

National Trend based on 20 Sites

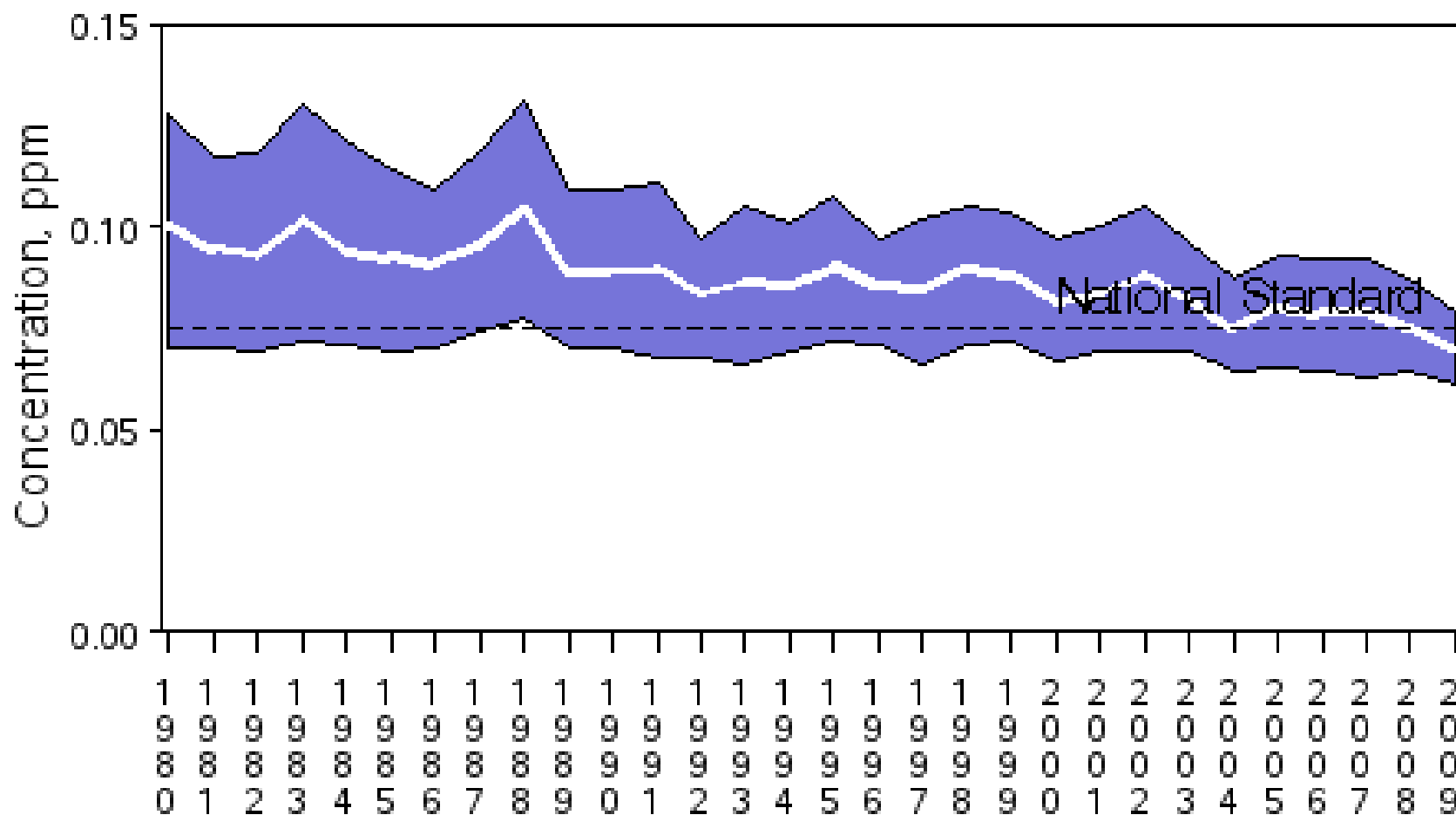


1980 to 2009 : 93% decrease in National Average

# Ozone Air Quality, 1980 - 2009

(Based on Annual 4th Maximum 8-Hour Average)

National Trend based on 255 Sites

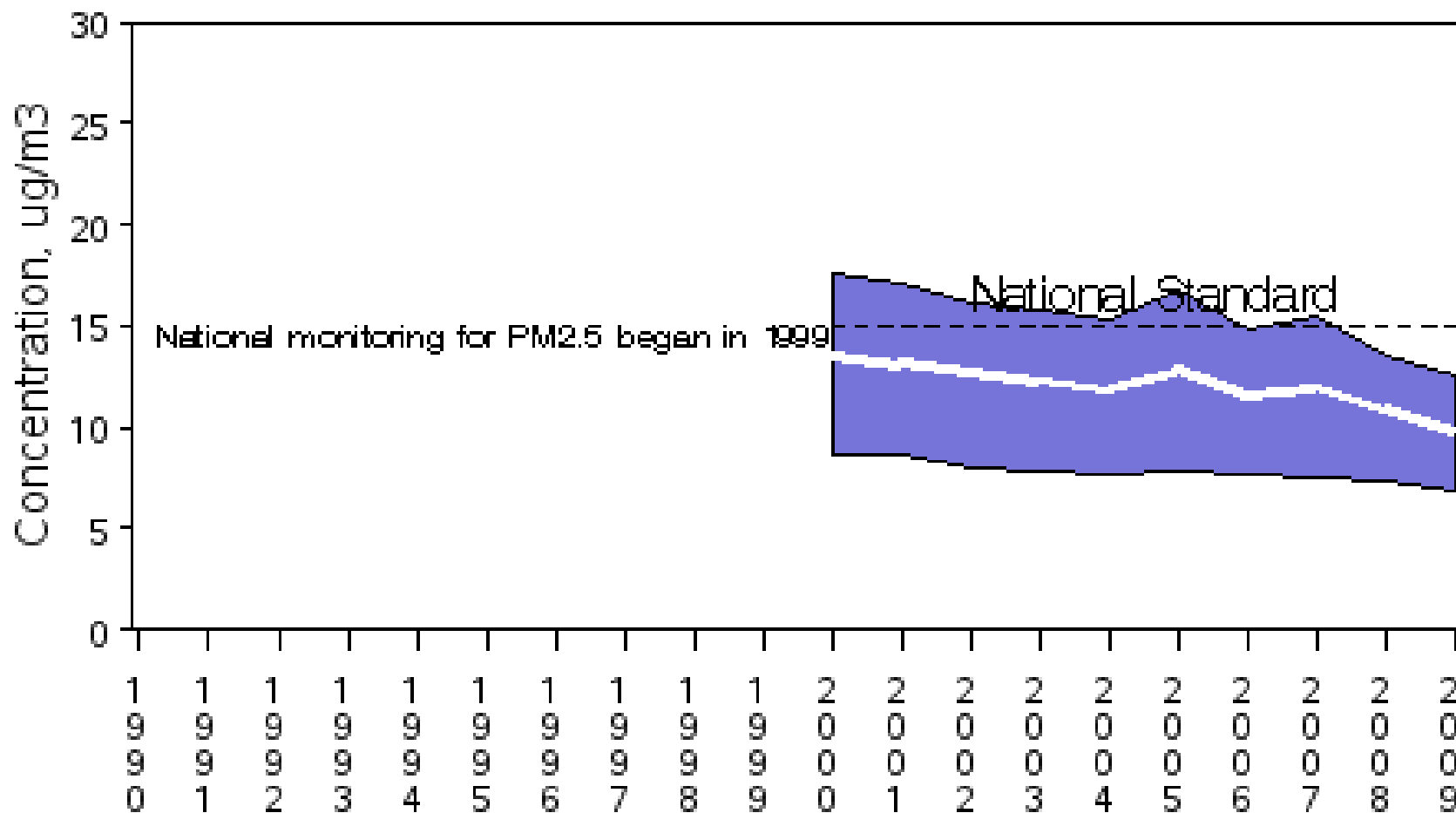


1980 to 2009 : 30% decrease in National Average

# PM2.5 Air Quality, 2000 - 2009

(Based on Seasonally-Weighted Annual Average)

National Trend based on 724 Sites



2000 to 2009 : 27% decrease in National Average



# Los Angeles (1950s)



# The Los Angeles Case

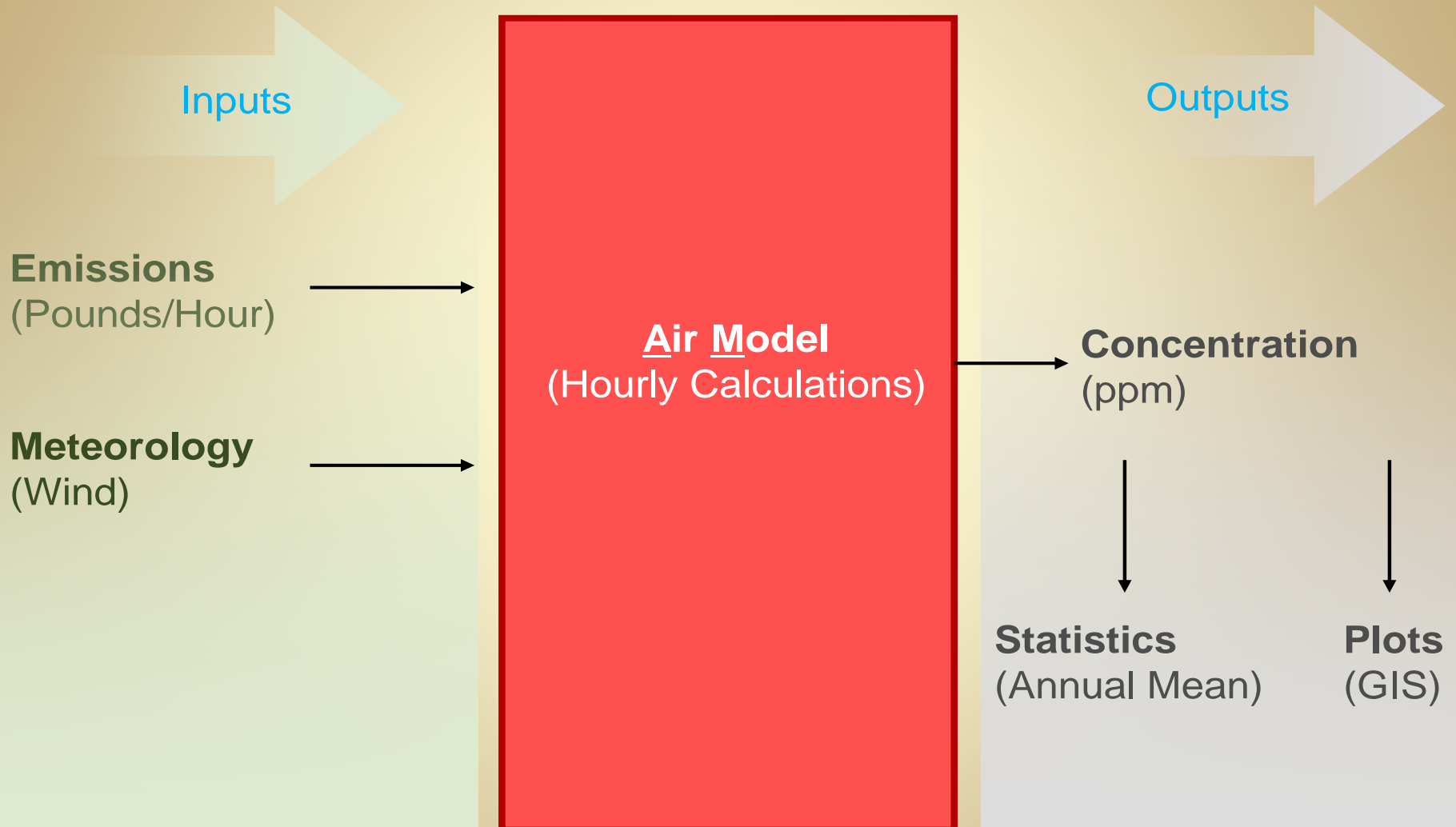
# More on Air Quality Management



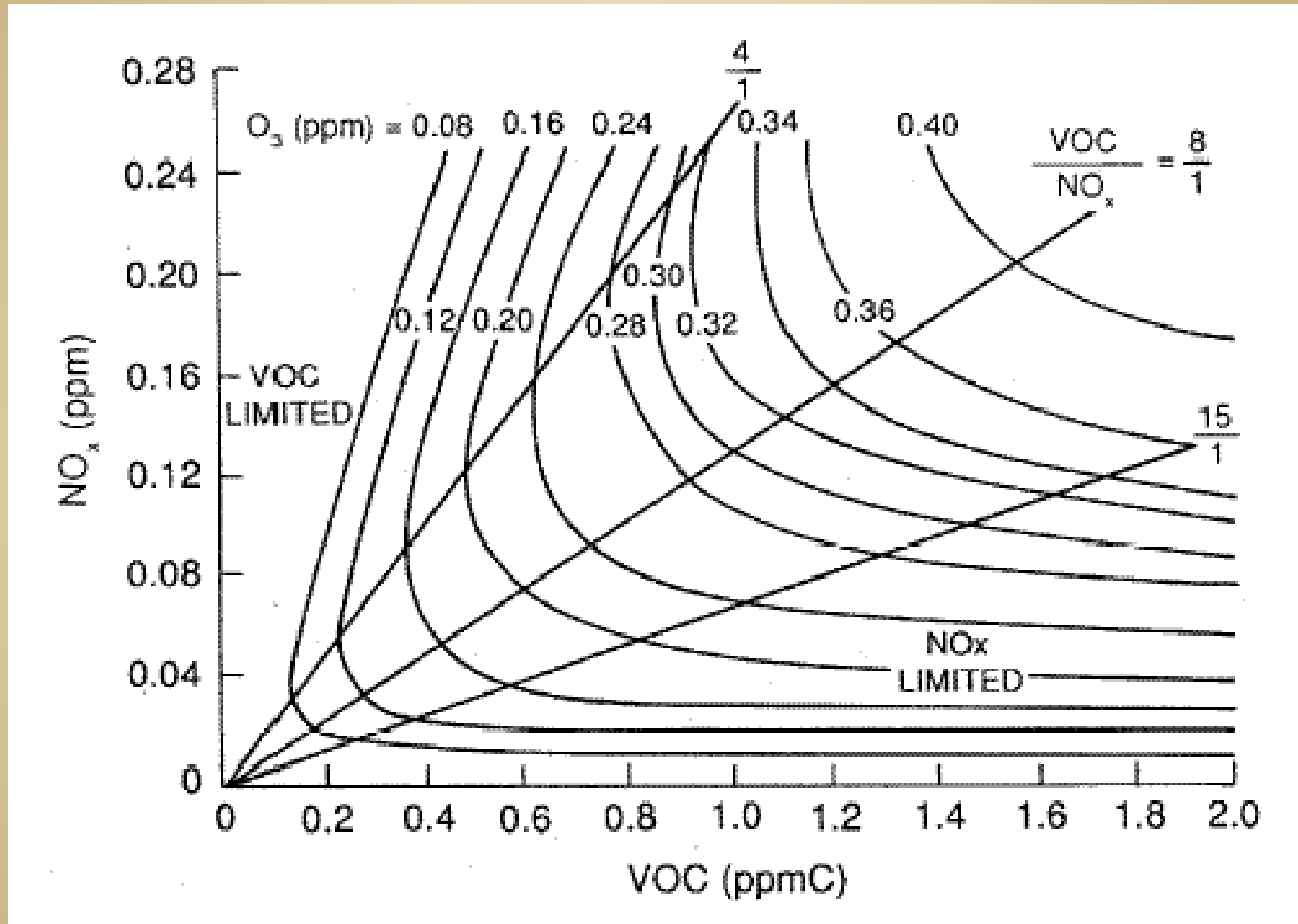
# 5. Air Quality Modeling

- Air Quality modeling is the mathematical simulation/prediction of ambient concentrations/depositions of air pollution, based on measured/calculated inputs.
- Air quality modeling is the necessary substitute for ubiquitous air quality monitoring, which is impossible.
- More importantly:
  - measurements cannot distinguish between the contributions of different emissions. Models can.
  - Models can simulate the past, present, and future air pollution
  - Models incorporate best deterministic/statistical science

# Air Modeling Methodology



# Challenge: Non-Linearity (e.g. Ozone)



Empirical kinetic modeling approach (EKMA) diagram. SOURCE: NRC 1991, adapted from Dodge 1977.

# Modeling for air quality management purposes

- Two broad categories:
  - dispersion modeling - used to predict ambient concentrations
  - receptor-based (or source apportionment) models - use ambient data to determine the sources.
- Other categorization:
  - on the required model inputs (i.e., meteorological data);
  - on the spatial scale (global; regional-to-continental; local-to-regional; local);
  - on the temporal scale (episodic models, long-term models);
  - on the treatment of the transport equations (Eulerian, Lagrangian models);
  - on the treatment of various processes (chemistry, wet and dry deposition);
  - and on the complexity of the approach.
- The choice of model depends on a combination of the available data and the needs of the researcher

# Choice of Models

- U.S. EPA's detailed recommendations  
[http://www.epa.gov/scram001/guidance/guide/appw\\_03.pdf](http://www.epa.gov/scram001/guidance/guide/appw_03.pdf)
- Many of the models are available for direct download at the U.S. EPA Support Center for Regulatory Air Models (SCRAM)  
<http://www.epa.gov/scram001/>
- On-line course offered by the Air Pollution Training Institute  
[http://yosemite.epa.gov/oaqps/EOGtrain.nsf/DisplayView/SI\\_410\\_0-5?OpenDocument](http://yosemite.epa.gov/oaqps/EOGtrain.nsf/DisplayView/SI_410_0-5?OpenDocument)
- Advanced courses on air quality modeling  
<http://www.wessex.ac.uk/courses/air-quality/page-3.html> (PZ)  
<http://www.shodor.org/os411/>  
<http://www.weblakes.com/training/index.html>  
<http://trinityconsultants.com/Training/>
- My 1990 APM book online:  
<http://www.envirocomp.com/pops/airpollution.html>
- Comprehensive AQM book series:  
<http://envirocomp.org/books/aqm.html>



# Modeling of Emergencies

- Emergency preparedness
  - Modeling of pre-defined possible events
  - Preparation of “what if” scenarios
  - Training
- Emergency response
  - Semi-automatic computer systems to guide decision-makers during accidental releases
  - Fast response is essential
- Accident Reconstruction
  - Assessment of responsibility
  - Litigation

# Plume/Puff Modeling

- EPA models vs. other models
- Simple models (e.g., a steady state Gaussian Plume model) vs. complex models (e.g., a dynamic puff model)
- Example of application of [MONTECARLO](#) (20 y ago)
- Today's animation capabilities – [M case](#)

# Examples...

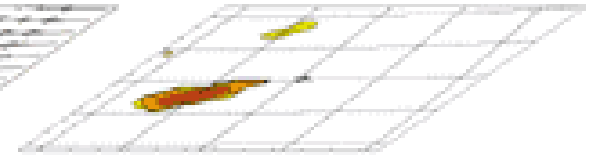


Tire Fire in Tracy, CA (August 1998) – emergency forecast

# Examples...



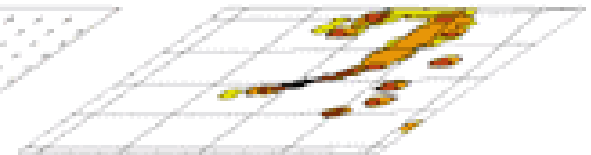
35,000 feet



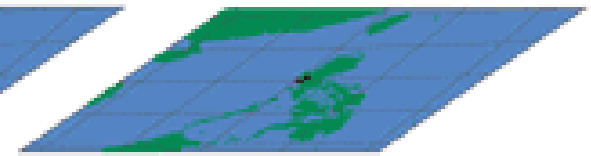
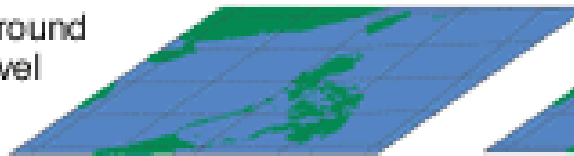
15,000 feet



2,500 feet



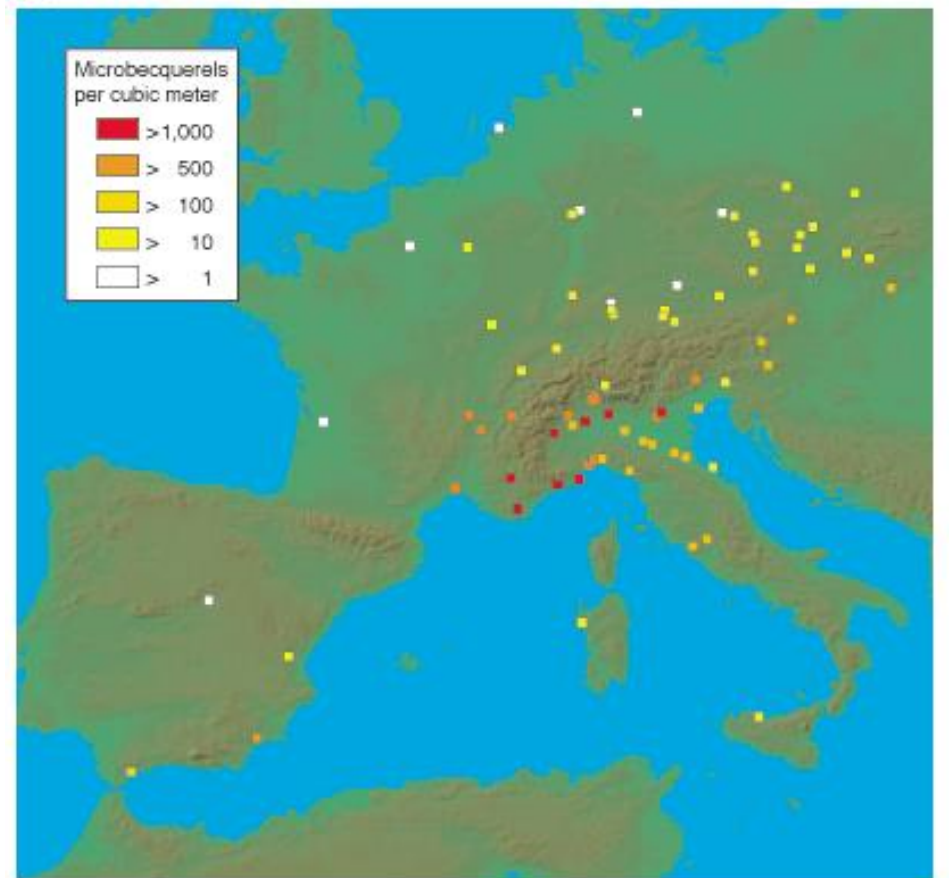
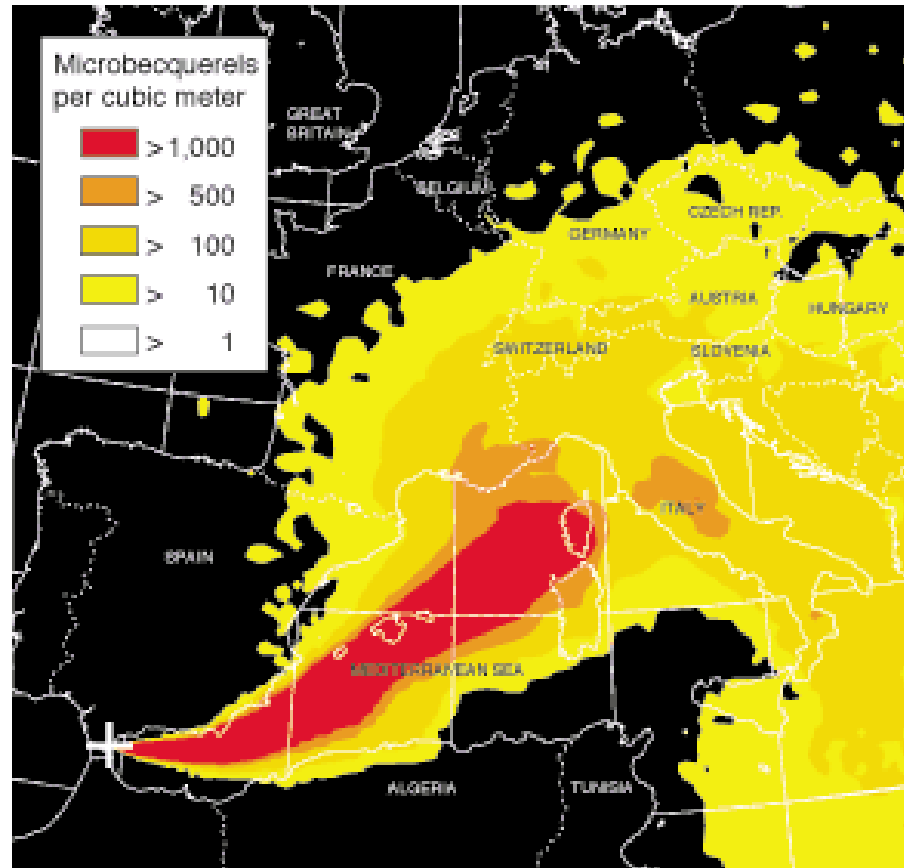
Ground level



Wind field forecast  
to determine where  
volcanic ash would travel

Dispersion model  
calculation of relative  
ash-cloud density

## Examples...

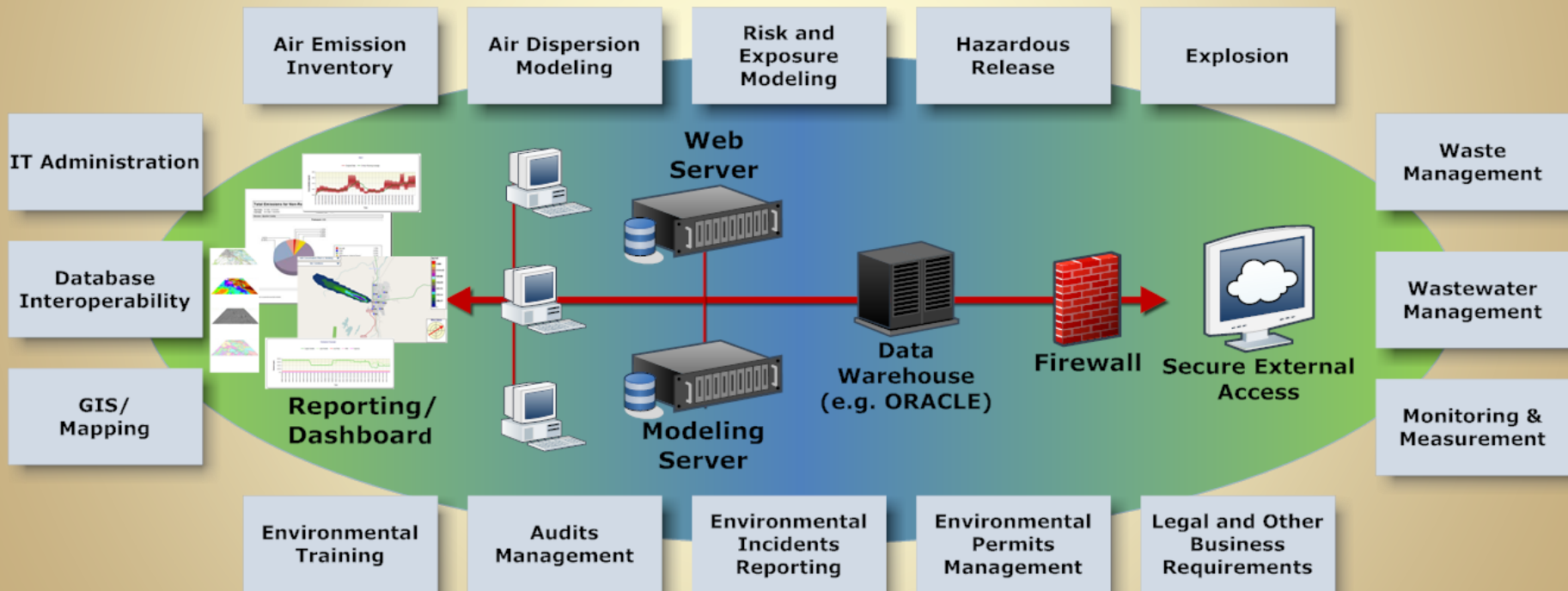


Radioactive Release: Cesium-137  
from Algeciras, Spain  
(last week of May 1998)

# In the Future...

- Fully computerized emergency response systems
- Automatic computer modeling and forecast
- Warning and decision support
- ... even Artificial Intelligence features

# CONCEPTUAL OVERVIEW – (Courtesy of Lakes Environmental Software)



# Animations

The hyperlinks below activate two animations:

1. [Real time](#) plume animation of a fictitious accidental release
2. Animation of the [plume forecast](#) in the following hours for a fictitious accidental release



# Thanks!

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# Wisdom!

1. The serenity to accept the things I cannot change;
2. The courage to change the things I can;  
and most importantly:
3. The wisdom to know the difference