

# Resolving Community Scale in Air Toxics Modeling Applications

Vlad Isakov

Air-Surface Processes Modeling Branch  
Atmospheric Modeling Division  
National Exposure Research Laboratory  
EPA Office of Research and Development

EPA Regional/State/Local Modelers Workshop  
New Orleans, LA

May 16-18, 2005



RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*

**Objective:** Develop and evaluate modeling tools for simulating ambient pollutant concentrations in urban settings at spatial scales <1-10 km for assessing human exposures.

**Motivation:**

- Tools are needed to assess the small-scale variability in ground-level concentrations of air toxics in an urban setting.
- These tools will benefit the NATA program and human exposure modeling clients within EPA.

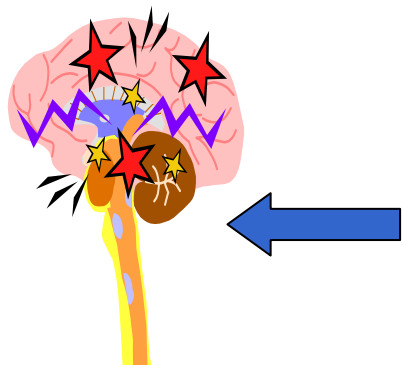
**Problems in modeling air toxics:**

- A large number of HAPs with widely varying properties
- Need concentrations over a range of spatial scales
- Sparse or no measurements for most compounds

**HAPs are** chemicals which can cause cancer, neurological or reproductive damage or other adverse health effects to humans and ecosystems. 189 are defined, including benzene, xylene, mercury, PAHs, chloroform, etc.



# Assessments Can Be Done At Different Scales: National, Urban, and Neighborhood Level



# Why focus on community level?

- many sources have local impact



RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*

# Why focus on community level?

- people live near major freeways

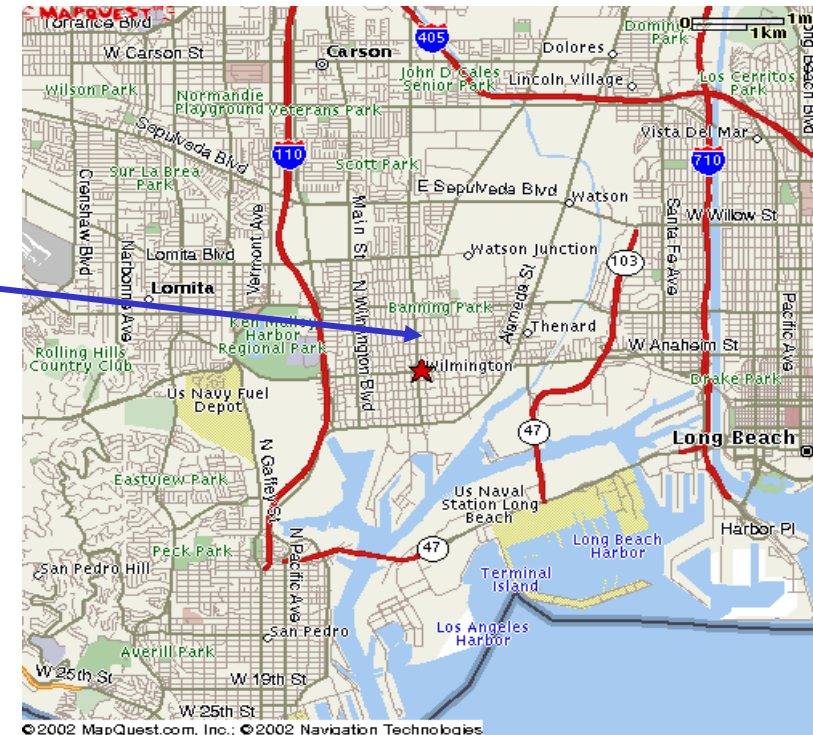


RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*

# Why focus on community level?

- people live near industrial activities



## Example – Wilmington, California



RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*



# Resolving Community Scale – Three Modeling Approaches

- DETERMINISTIC:

  - **Regional Modeling + Local Dispersion**

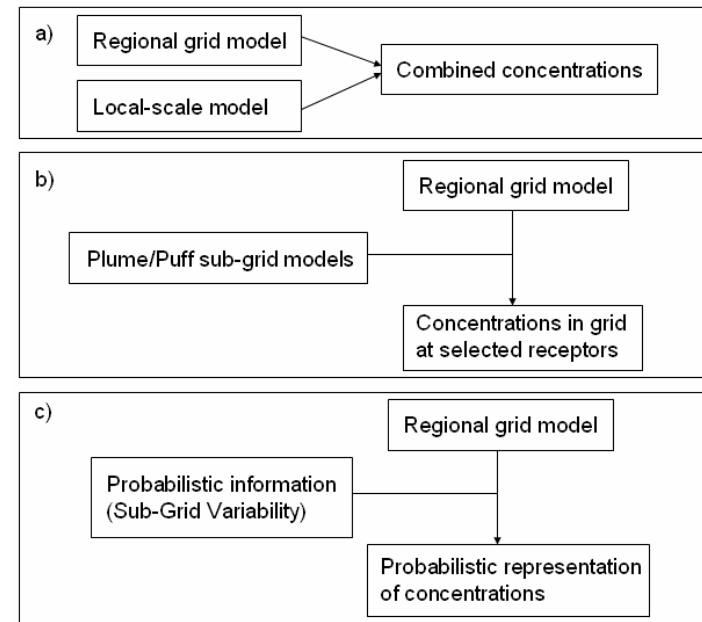
    - CMAQ model provides regional background concentrations
    - Local plume dispersion model provides fine-scale details

*Current limitation: Procedure needed to ensure no double-counting of emissions between regional and local scale model*

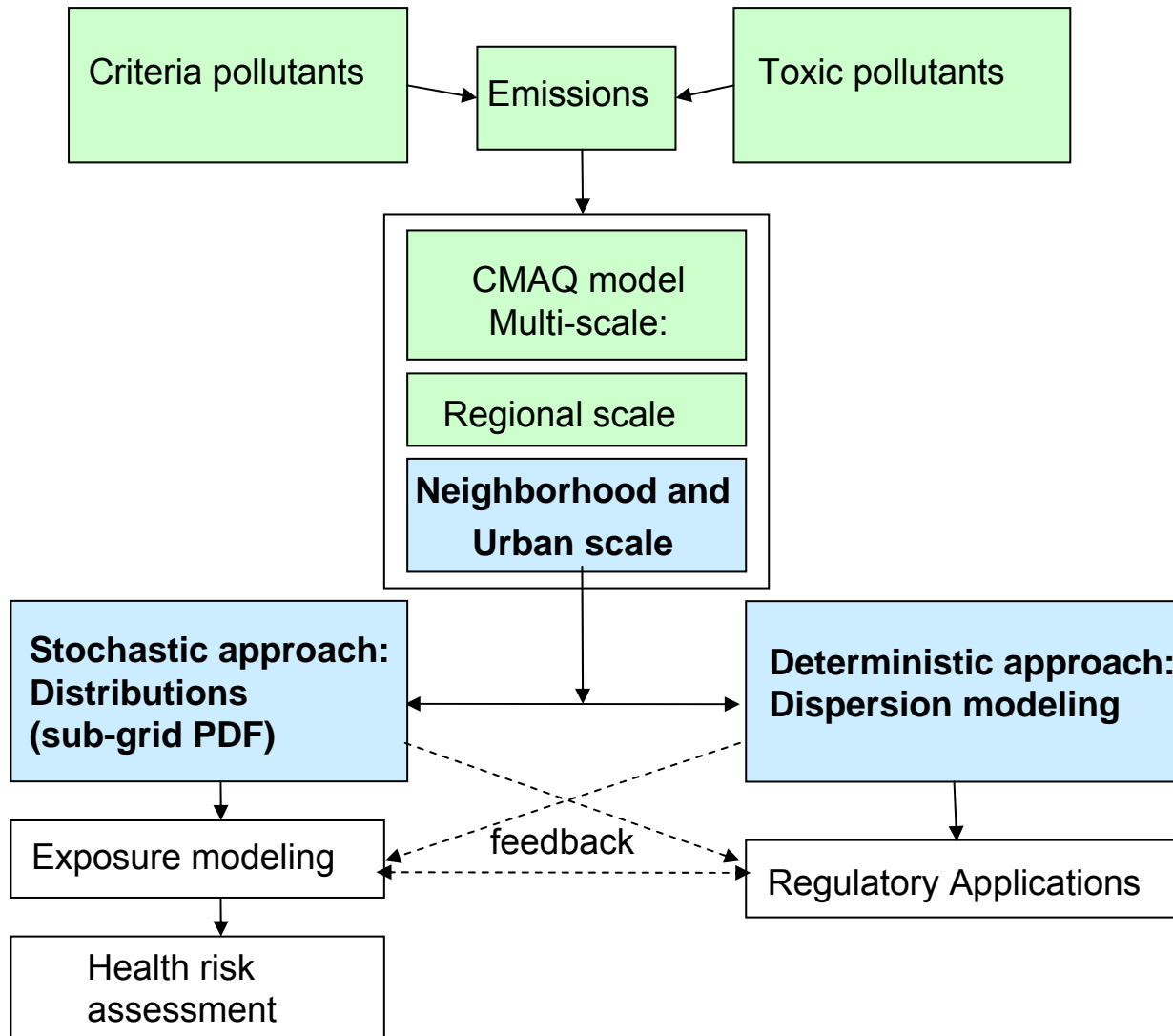
- HYBRID APPROACH: **Plume/Puff Sub-grid Modeling** within Regional Grid Model.

*Current limitation: High computational burden, prevents application to large number of sources, not available at this time*

- PROBABILISTIC: **Regional Modeling + SGV**  
(next presentation by Jason Ching)



# AMD's Conceptual Approach



# AMD's Air Toxics Modeling Capabilities

## National-scale to Hot-spots

### Introduction of CMAQ for Air Toxic Assessments

- Traditionally, CMAQ was used for criteria pollutants, regional applications, using deterministic approach, to support regulations

### Current Implementations

- 1999 NATA assessment using CMAQ at 36 km
- Nested CMAQ annual runs at 12 and 4 km for the Philadelphia modeling domain
- Provide local details from dispersion models (AERMOD, ISCST3 or ASPEN)

### Addressing the research question

- Can CMAQ successfully replace and/or augment traditional Gaussian plume modeling approaches for air toxics exposure assessments in urban settings?

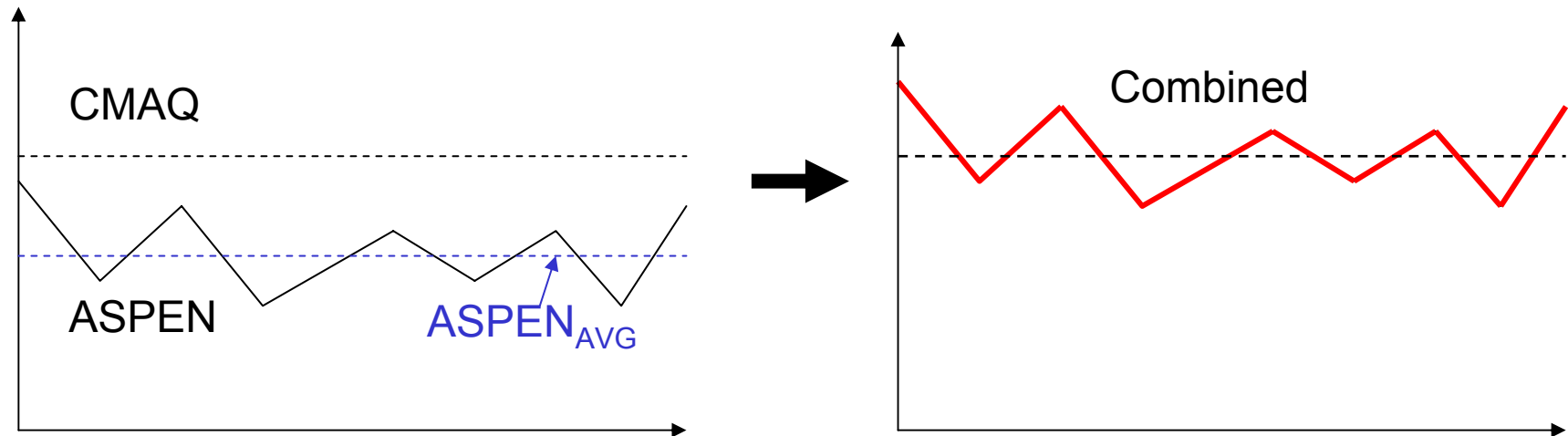


# An Approach to Provide Local Details from Dispersion Model to CMAQ: ASPEN and CMAQ combination

Procedure:  **$(ASPEN - ASPEN_{AVG}) + CMAQ$**

- 1) Calculate ASPEN average for each CMAQ grid cell ( $ASPEN_{AVG}$ )
- 2) Calculate ASPEN differences at each receptor:  $(ASPEN - ASPEN_{AVG})$
- 3) Add ASPEN differences and CMAQ values for each cell

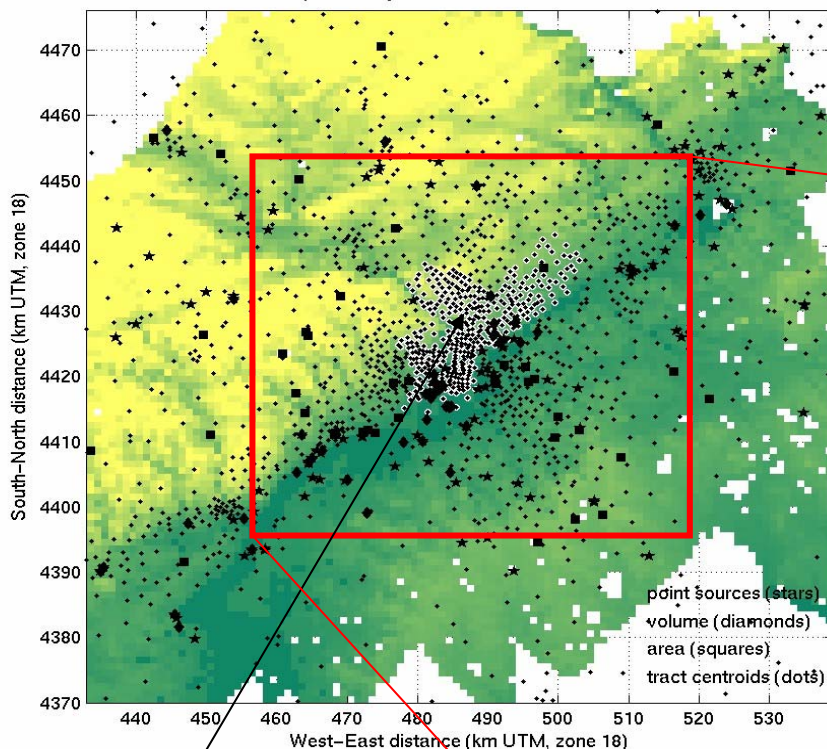
Note: If negative  $((ASPEN - ASPEN_{AVG}) + CMAQ < 0) \rightarrow$  check inventory



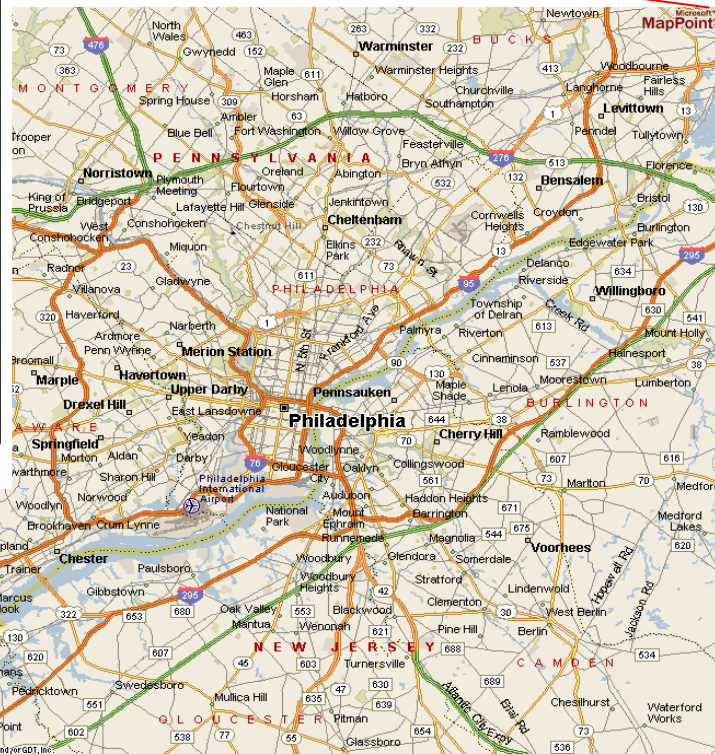
# Application: Philadelphia Air Toxics Study

## CMAQ combined with local details from ASPEN

Philadelphia Study – Locations of Emission Sources



## Modeling Domain



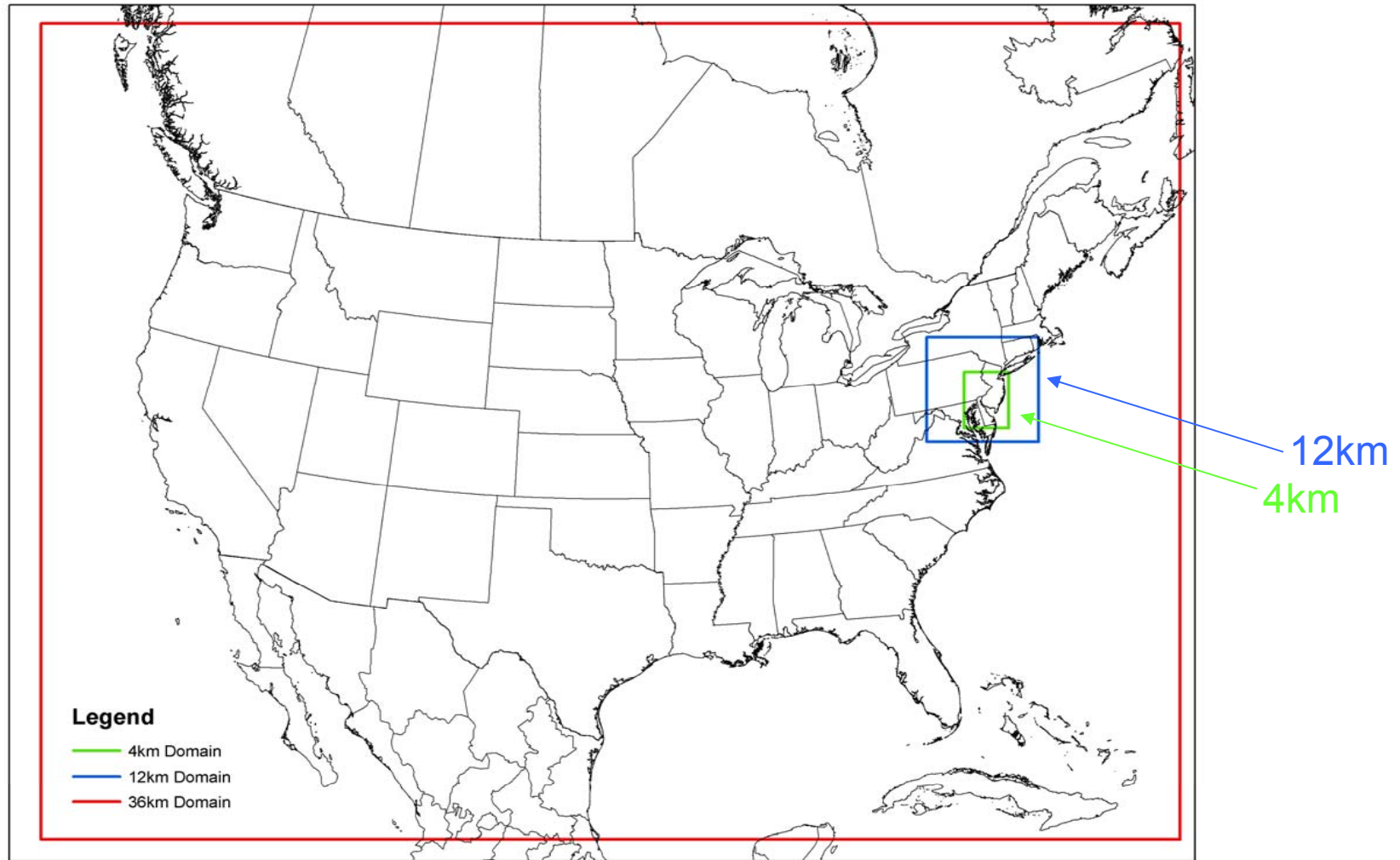
## Census Tract Centroids (Philadelphia County)

RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*

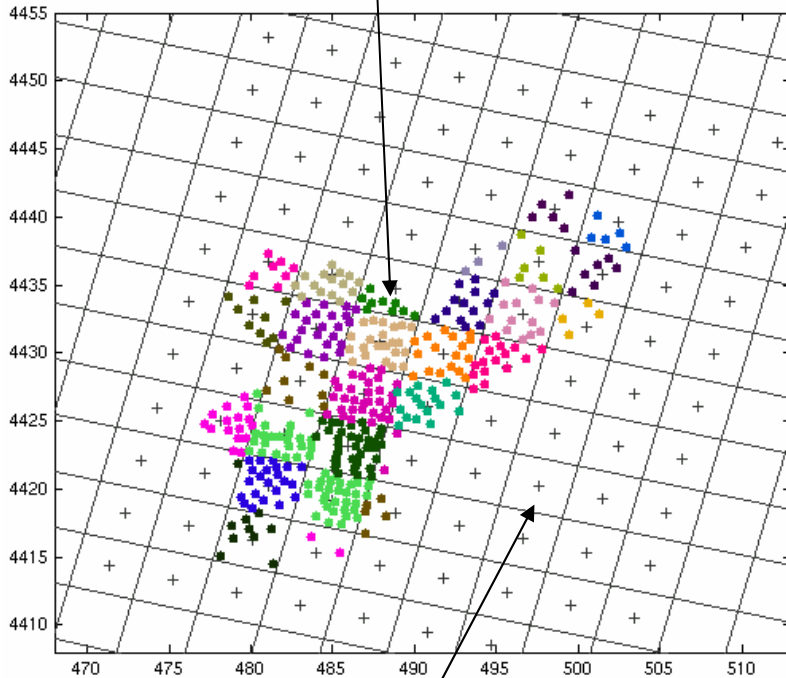


# CMAQ modeling applications for air toxics in Philadelphia



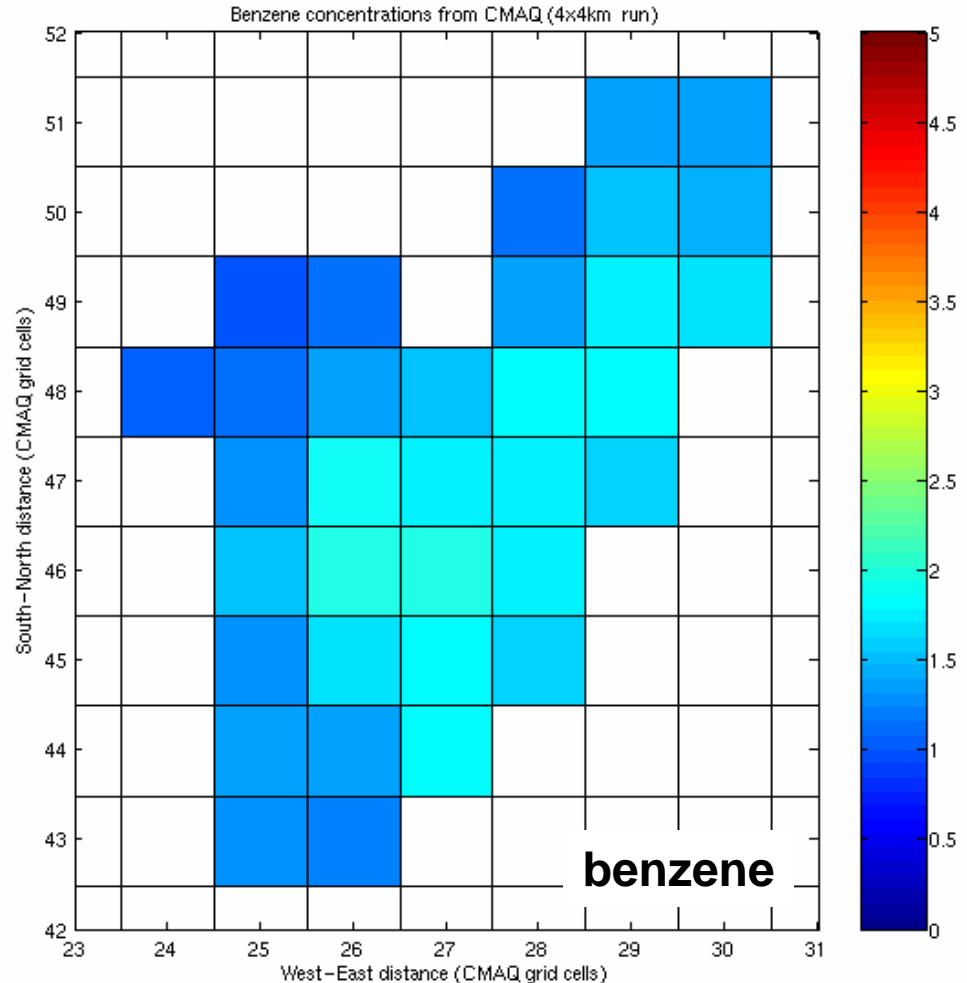
# CMAQ results (4km x 4km grid)

Census tract centroids in Philadelphia county  
(tracts in different 4x4km grid cells are shown  
in different colors)



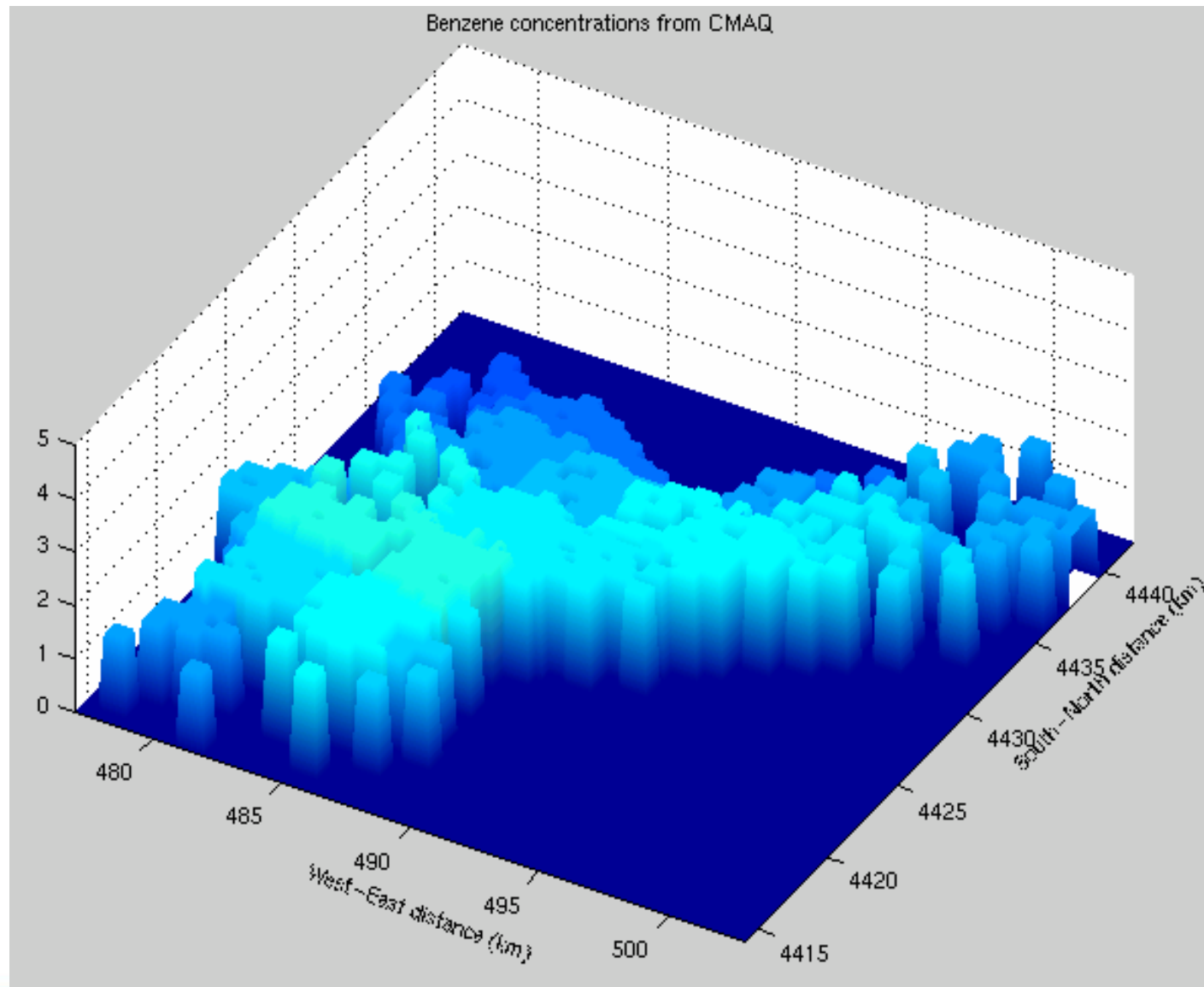
CMAQ 4x4km grid cells

Gridded benzene concentrations  
in Philadelphia county



# Philadelphia Case Study – CMAQ combined with local details from ASPEN

## 3-D view, benzene concentrations from CMAQ



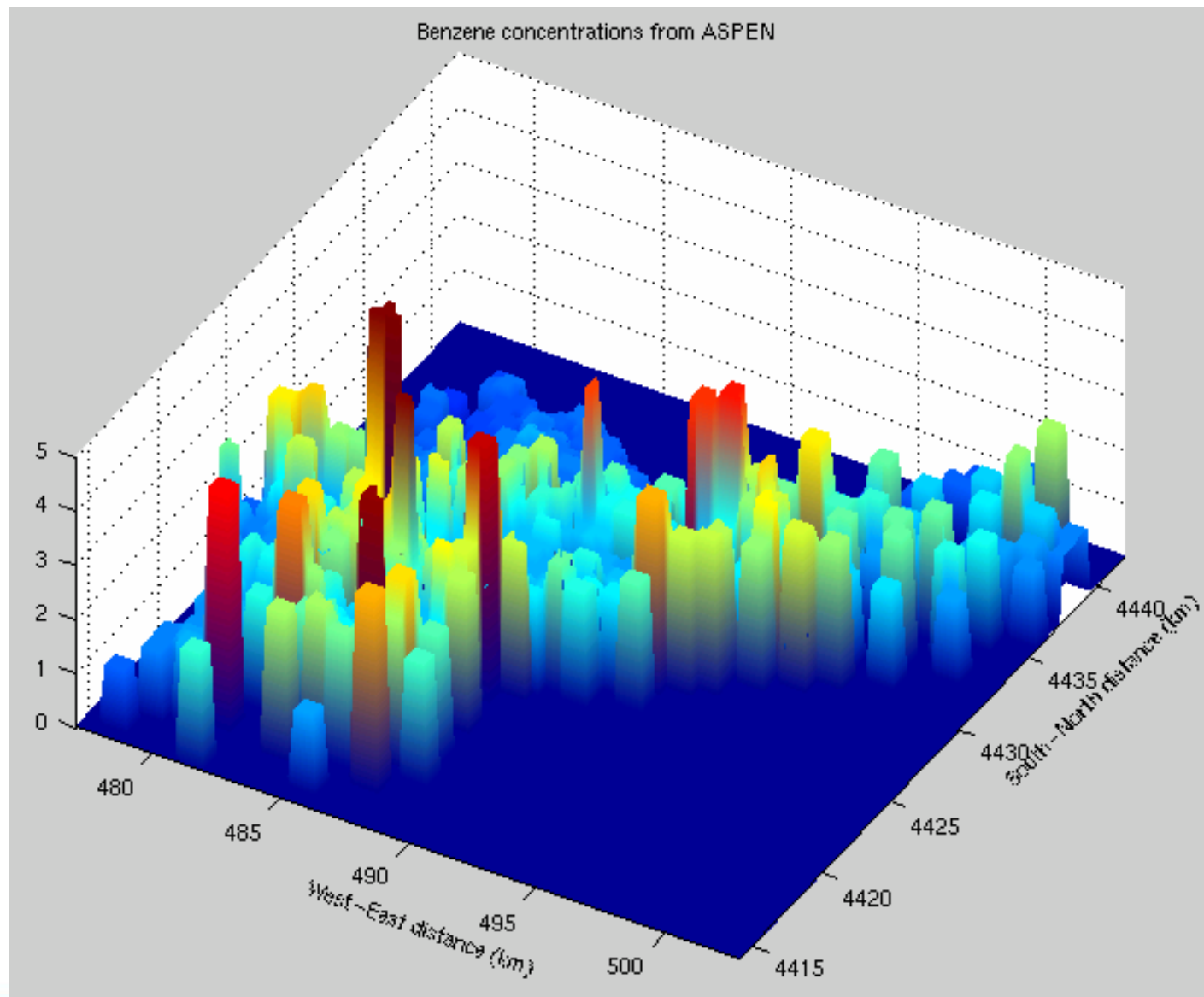
RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*



# Philadelphia Case Study – CMAQ combined with local details from ASPEN

## 3-D view, benzene concentrations from ASPEN



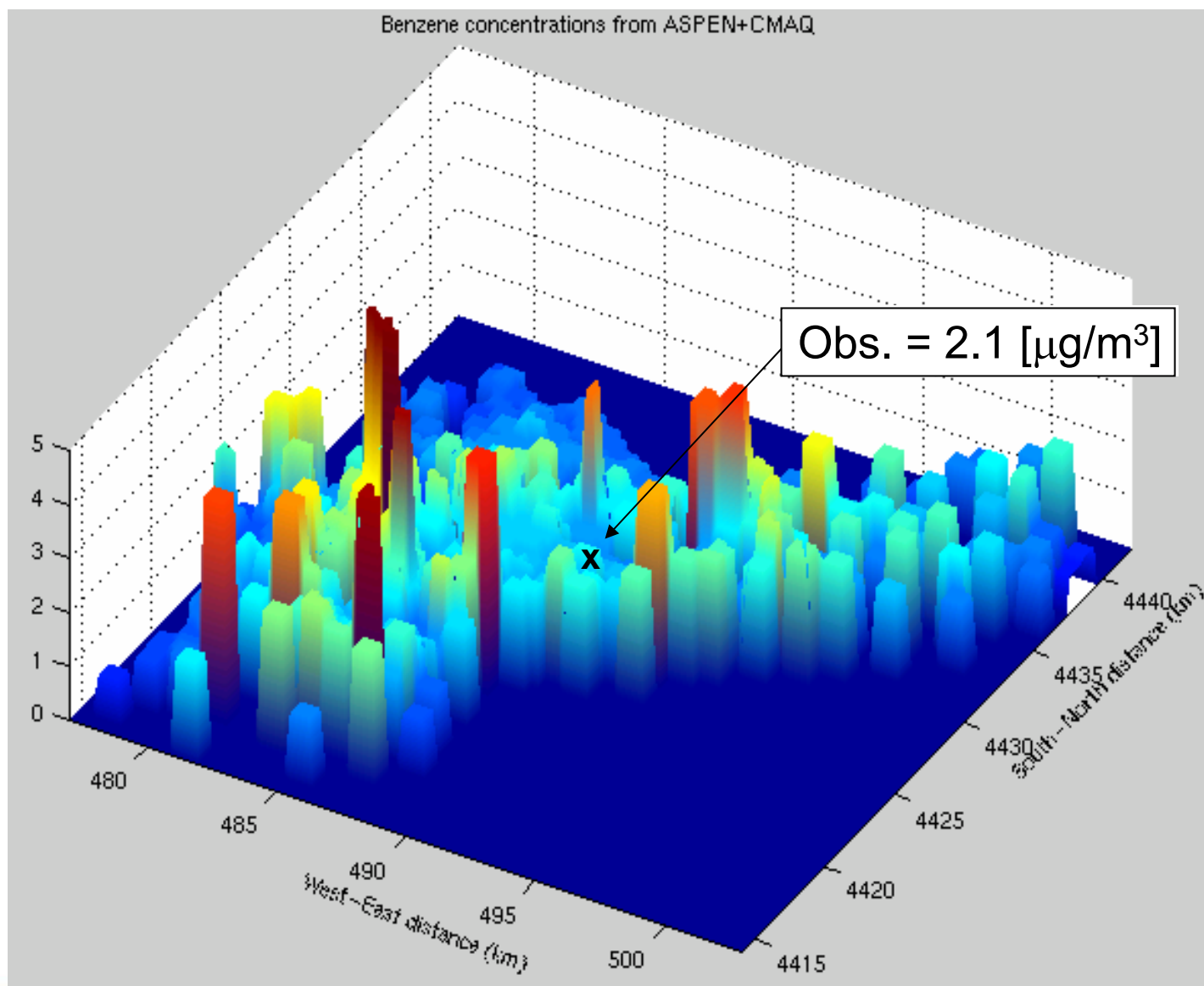
RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*



# Philadelphia Case Study – CMAQ combined with local details from ASPEN

3-D view, combined benzene concentrations: ASPEN + CMAQ

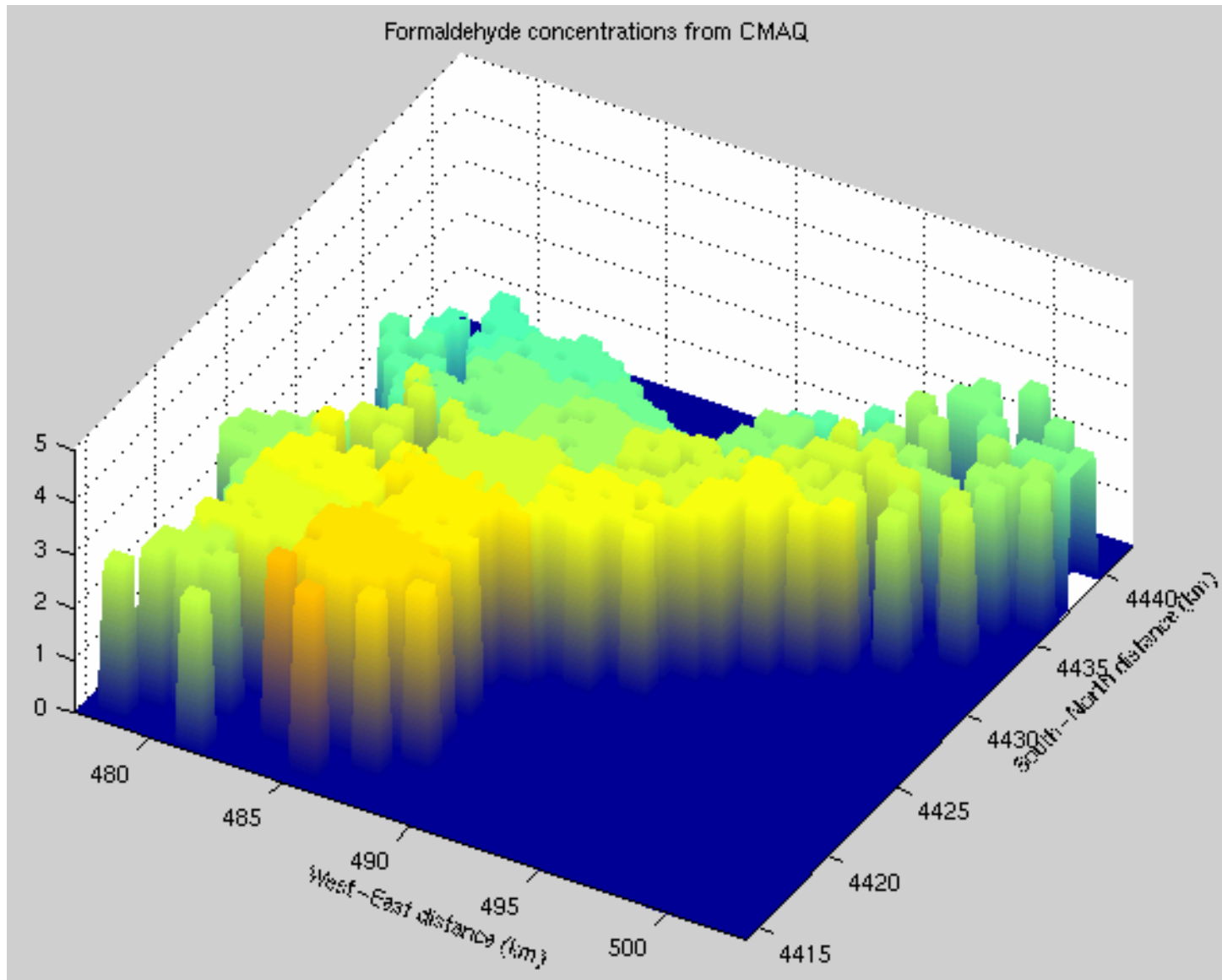


RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*

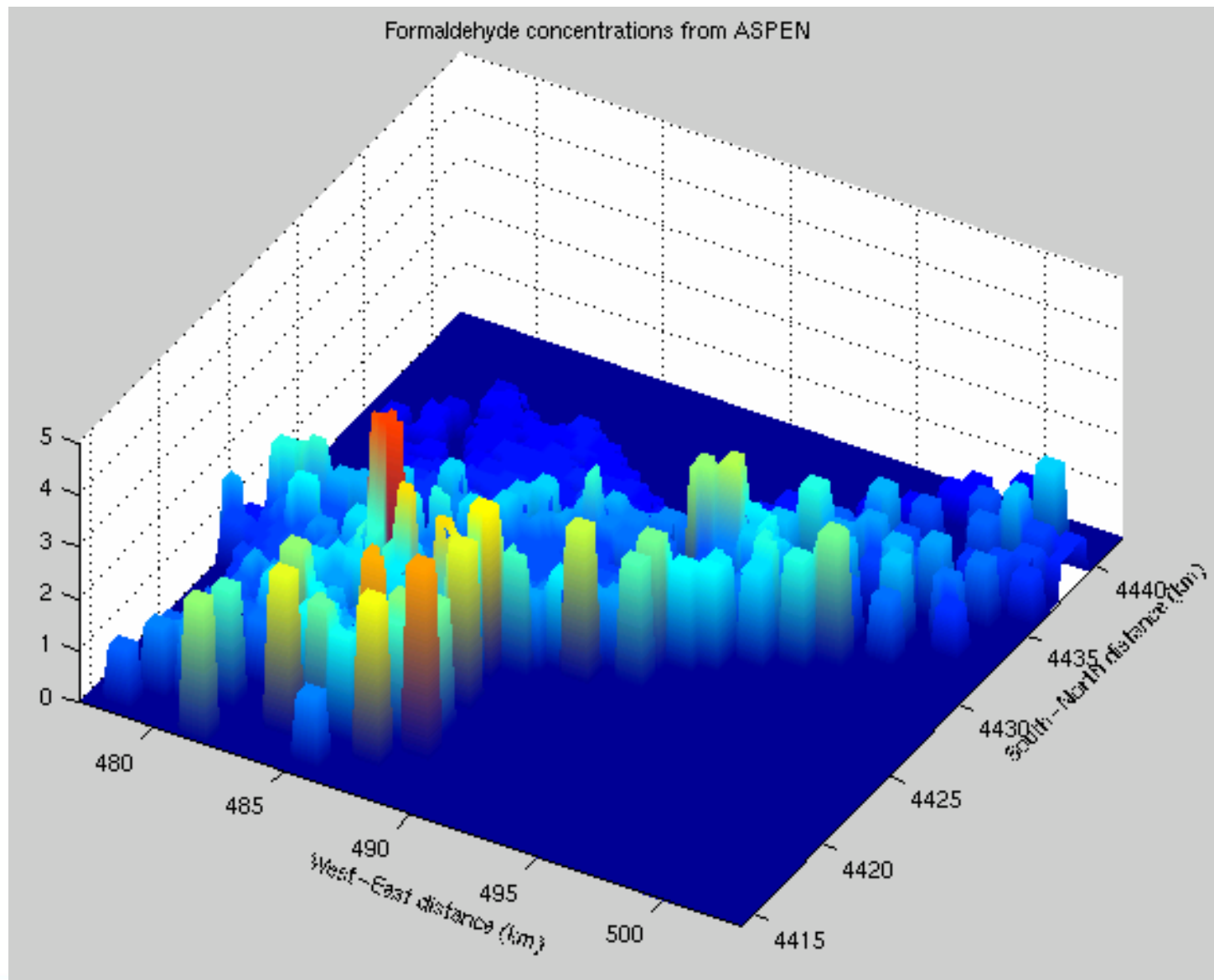
# Philadelphia Case Study – CMAQ combined with local details from ASPEN

## 3-D view, formaldehyde concentrations from CMAQ



# Philadelphia Case Study – CMAQ combined with local details from ASPEN

## 3-D view, formaldehyde concentrations from ASPEN



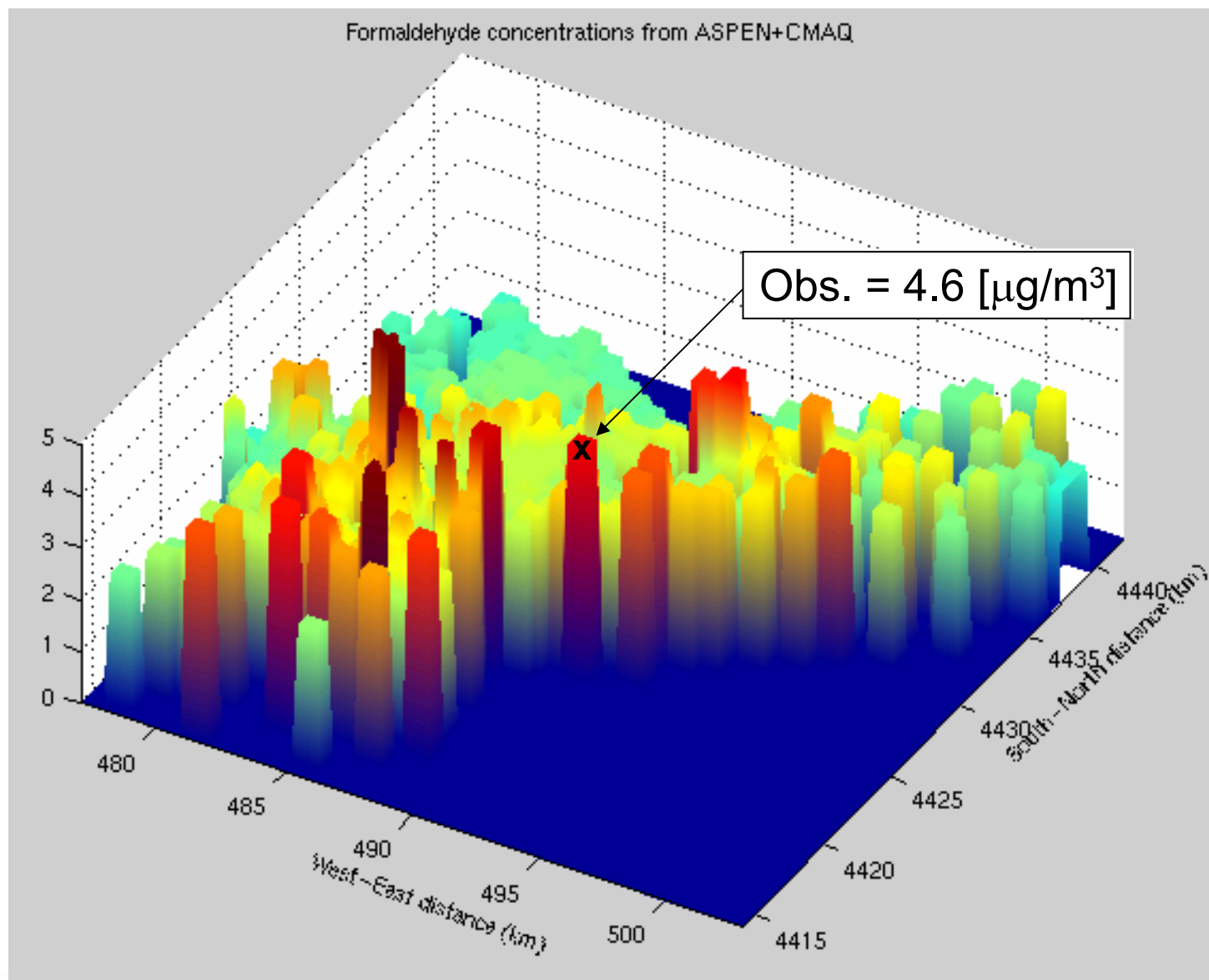
RESEARCH & DEVELOPMENT

*Building a scientific foundation for sound environmental decisions*



# Philadelphia Case Study – CMAQ combined with local details from ASPEN

3-D view, combined formaldehyde concentrations: ASPEN + CMAQ

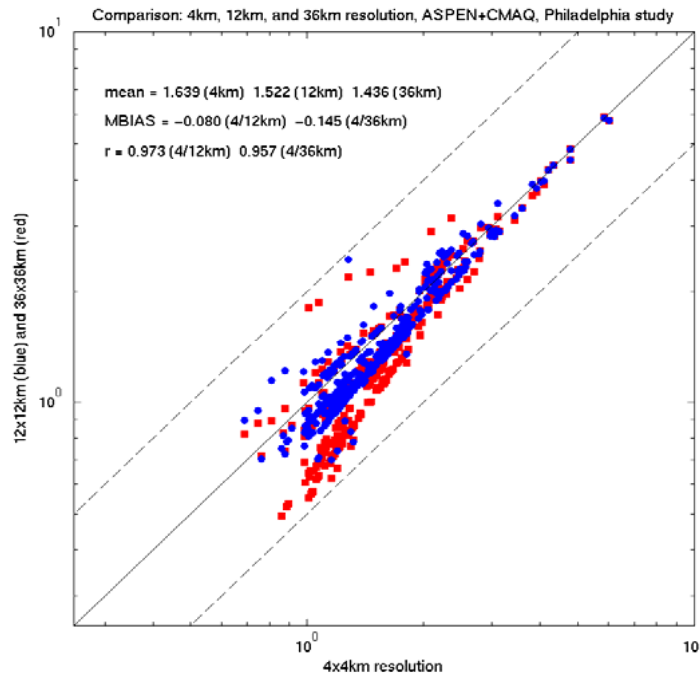


RESEARCH & DEVELOPMENT

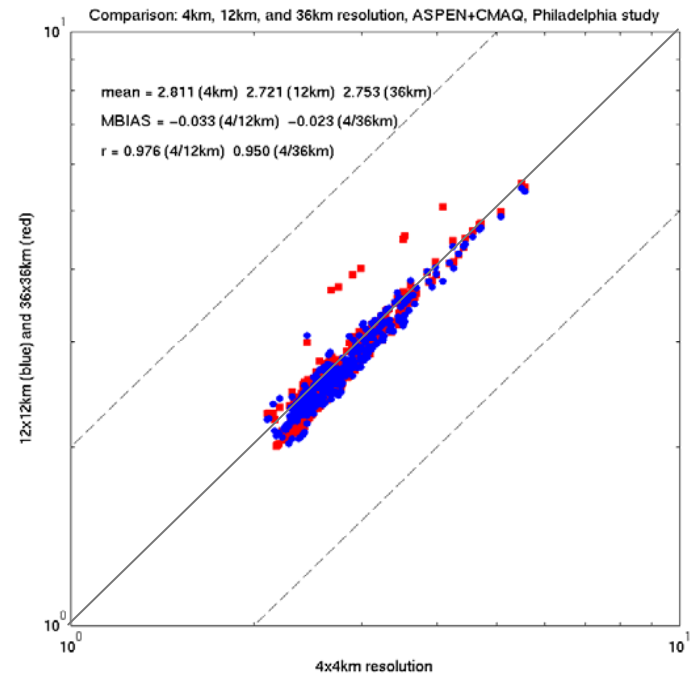
*Building a scientific foundation for sound environmental decisions*

# Various CMAQ resolution: 4km, 12km, and 36km – Is it important for estimating exposures?

benzene



formaldehyde



Conclusion: 12km resolution seems appropriate when CMAQ is combined with local details from ASPEN



## **The approach has been applied to Philadelphia**

- CMAQ provides regional background and contribution from chemically reactive pollutants
- Local details in pollutants concentrations are provided by ASPEN dispersion model



# Linkage: Air Quality into Exposure Model

## CMAQ Multi-scale (4,12,36) Applications for Human Exposure Modeling Assessments

### **Hazardous Air Pollutant Exposure Model (HAPEM-5)**

- Screening-level exposure model
- Predicts “apparent” inhalation for population in census tract
- Accounts for behavior of demographic groups for indoor and outdoor micro-environments
- Uses annually averaged diurnal distribution (3-hr blocks) of ambient concentrations at each census tract centroid
- HAPEM-5 provides statistical distribution information (median, mean, and 90<sup>th</sup>-percentile)

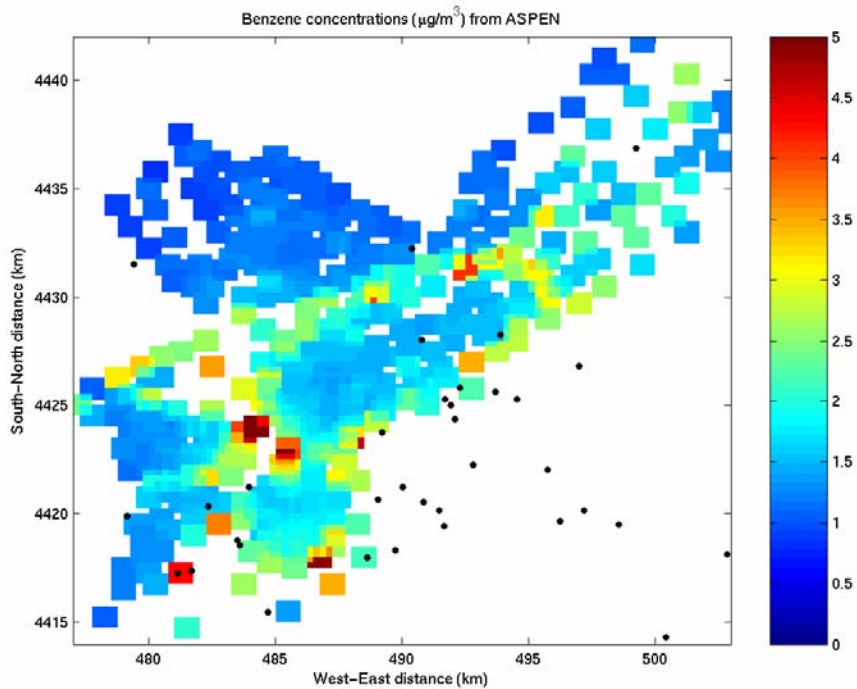
### **Inputs into HAPEM-5**

- Aggregated into annual 3-hr time bins for each grid cell
- Concentrations from the CMAQ grid cell overlaying a centroid
- CMAQ enhanced by local details from ASPEN dispersion model

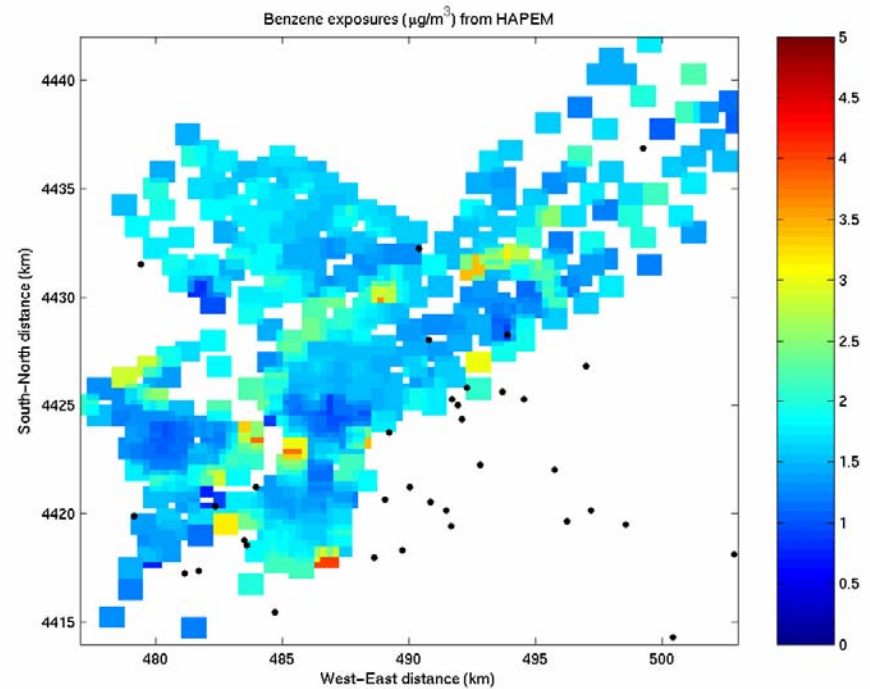


# Model results – Benzene, Philadelphia County

Concentrations from CMAQ+ASPEN



Exposures from HAPEM



# Conclusions

- Providing spatially resolved data is essential for exposure modeling (local details are provided by dispersion models: ASPEN, ISCST or AERMOD)
- Regional background and contribution from chemically reactive pollutants can be obtained from CMAQ simulations
- 12km resolution seems appropriate when CMAQ is combined with local details from dispersion models
- Temporal variations in pollutant concentrations are important for estimating exposures



# The End

Thank you for your attention

Collaborations:

Jason Ching, Al Cimorelli, Bill Hutzell, Deborah Luecken, Ted Palma, Tom Pierce, Joe Touma

**Disclaimer:** *The research presented here was performed under the Memorandum of Understanding between the U.S. Environmental Protection Agency (EPA) and the U.S. Department of Commerce's National Oceanic and Atmospheric Administration (NOAA) and under agreement number DW13921548. This work constitutes a contribution to the NOAA Air Quality Program.*

