An initial linkage of the CMAQ modeling system at neighborhood scales with a human exposure model

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AMD Research
Community-scale modeling for air toxics and homeland security

Objective: Develop numerical modeling tools for simulating ambient concentrations of airborne substances in urban settings at spatial scales ranging from <1-10 km for assessing human exposures.

Motivation: Tools are needed to assess the small-scale variability in ground-level concentrations that occurs from the release of toxic air pollutants in an urban setting. These tools can benefit the National Assessment of Air Toxics (NATA) program and other human exposure modeling programs.

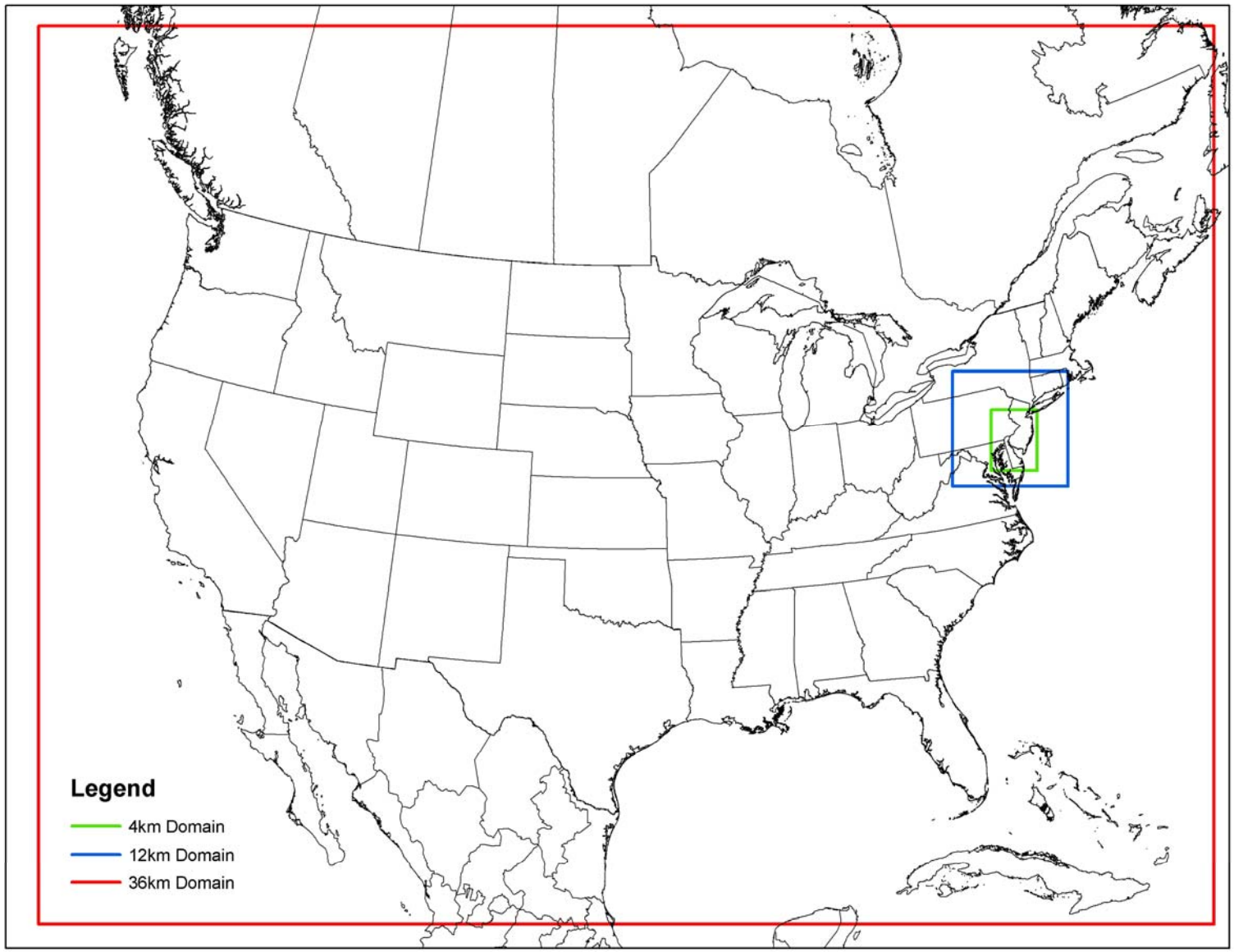
Science Question

Can a chemical transport model (such as CMAQ) successfully augment traditional Gaussian plume modeling approaches for estimating annual ambient concentration estimates of air toxics for human exposure assessments in urban settings?

Study Approach
Development of an initial prototype to support human exposure models

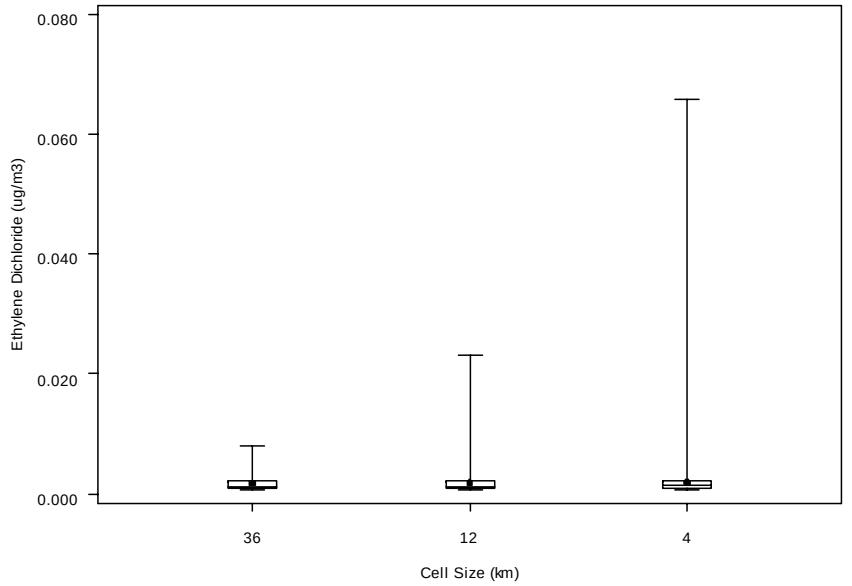
- Establish collaborations with Delaware, Region 3, and OAQPS
- Use the 36 km CMAQ simulations for boundary conditions
- Apply CMAQ at 12 & 4 km to Philadelphia for 2001
- Compare CMAQ with available air toxic observations
- Link annual CMAQ results to HAPEM5
- Assess practicality of using CMAQ

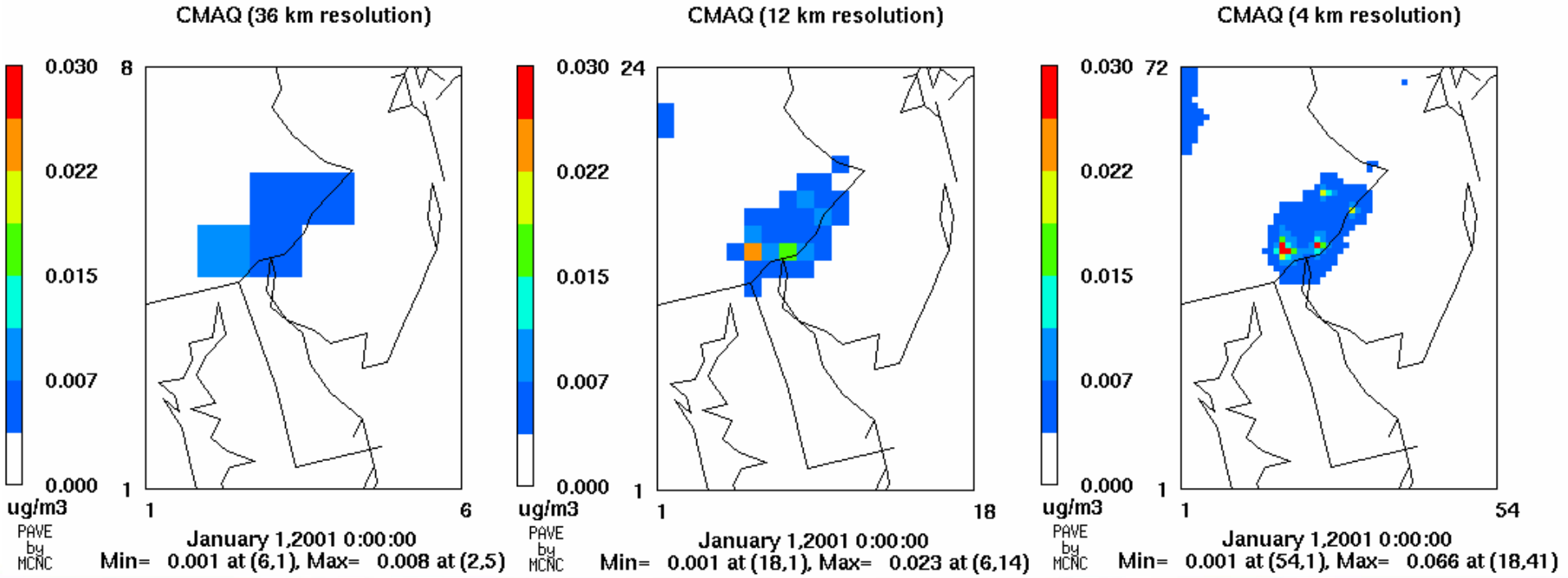
CMAQ modeling domains (36, 12, 4 km)



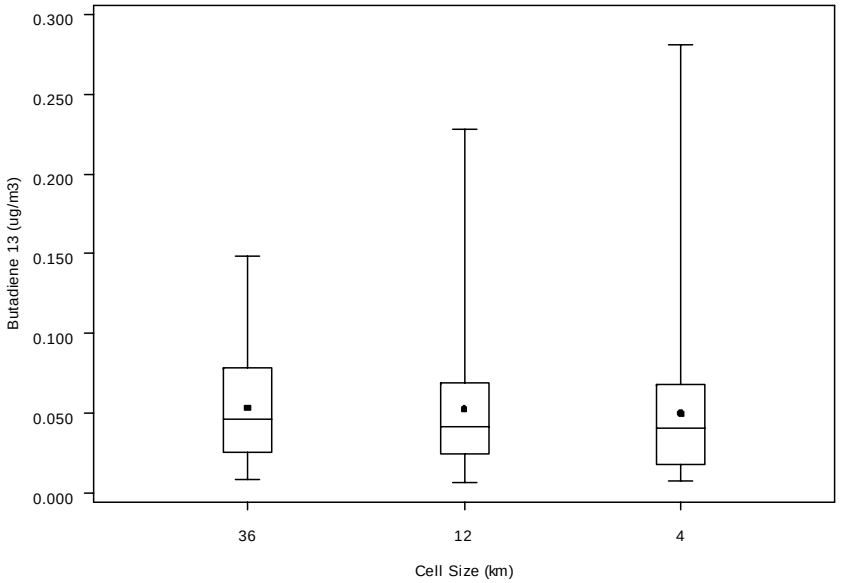
Ethylene Dichloride Annual average (2001) CMAQ

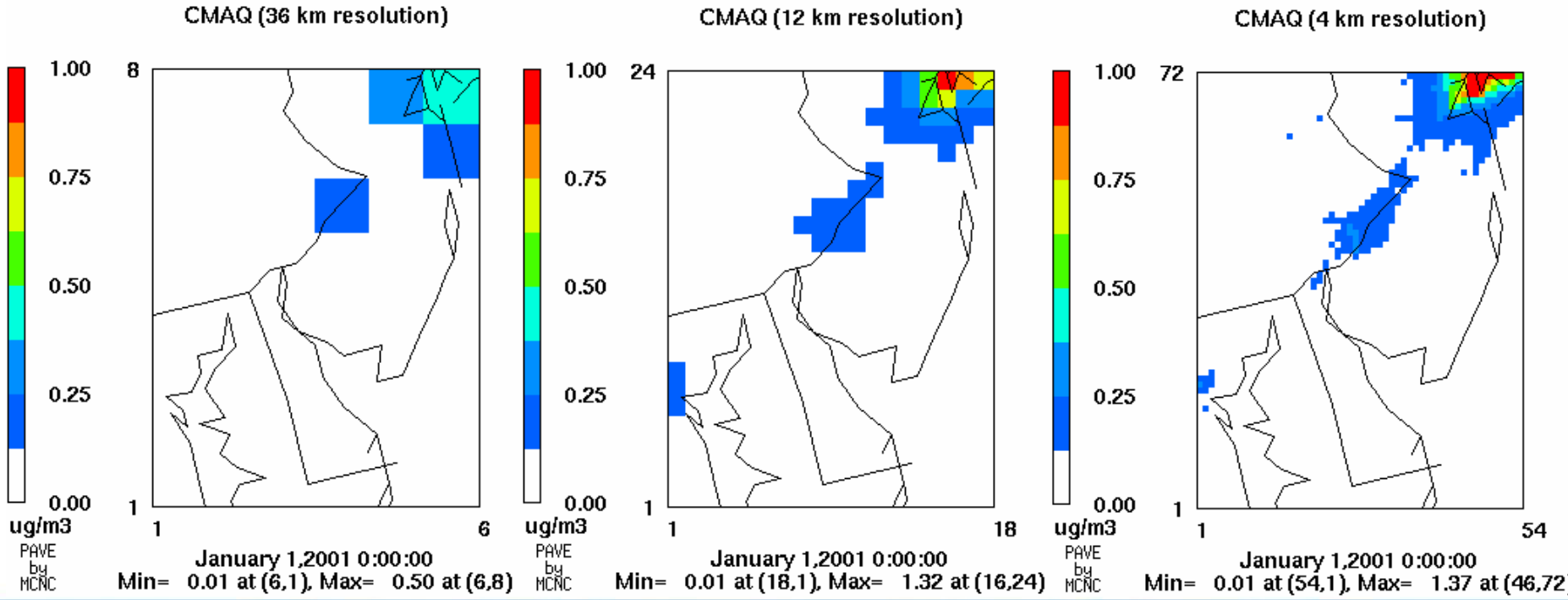
… impact of grid size on modeling air toxics in the Philadelphia area



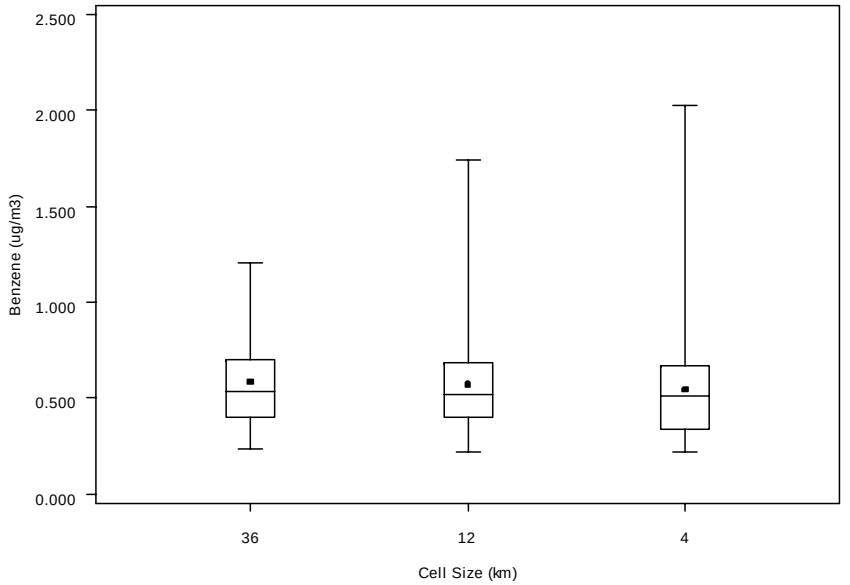


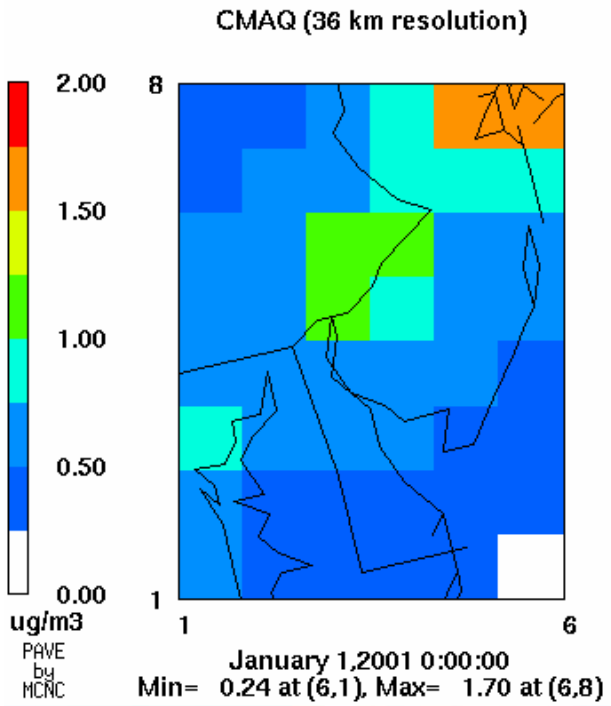
1,3-Butadiene
Annual average (2001)
CMAQ

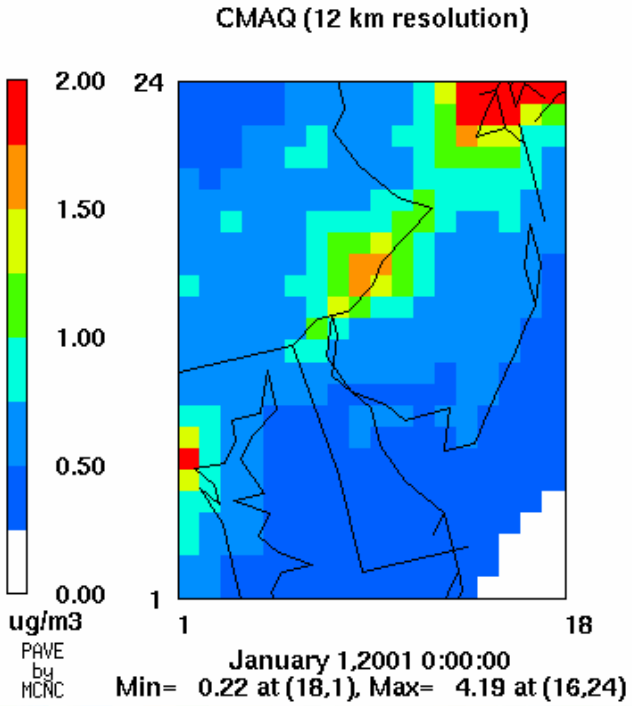


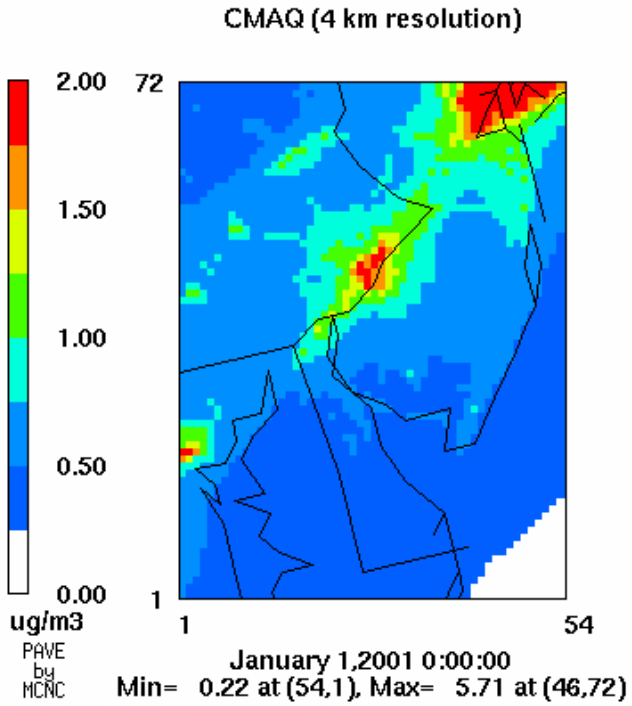


Benzene
Annual average (2001)
CMAQ

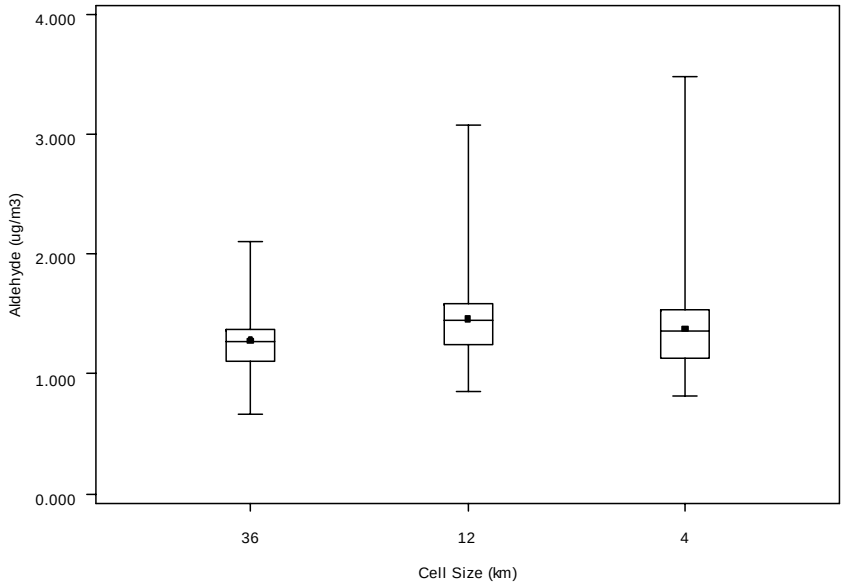


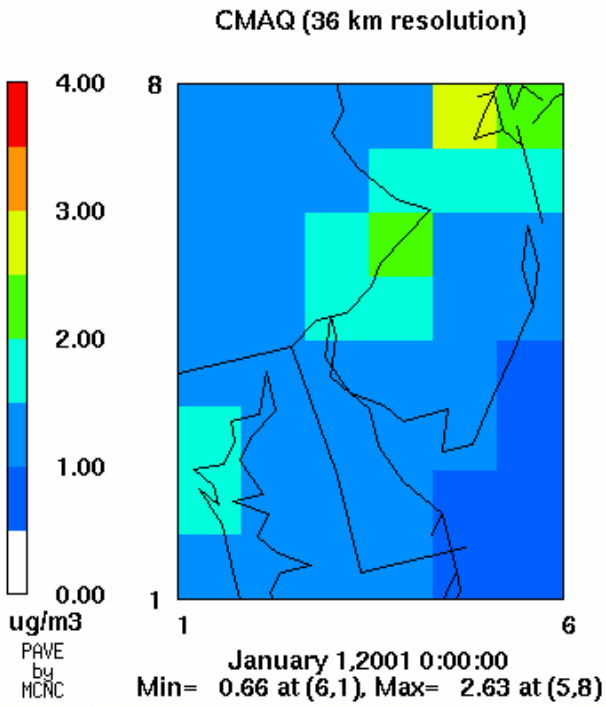


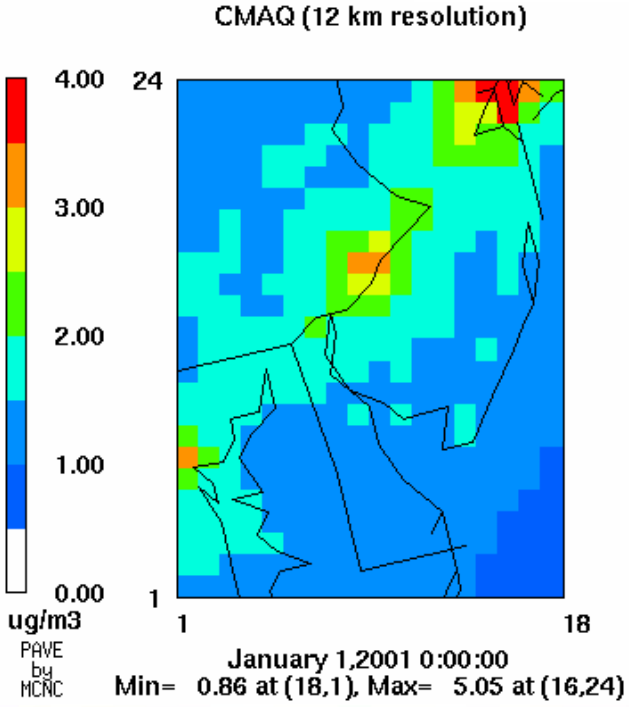


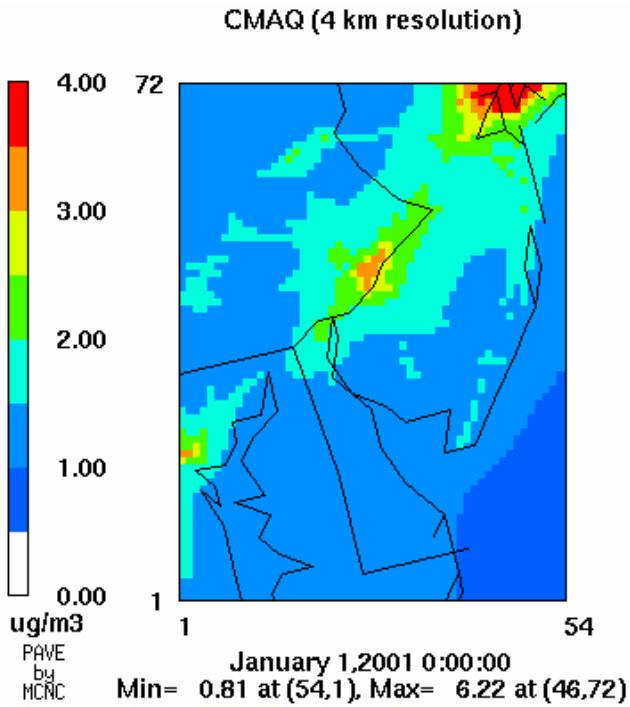


Acetaldehyde
Annual average (2001)
CMAQ



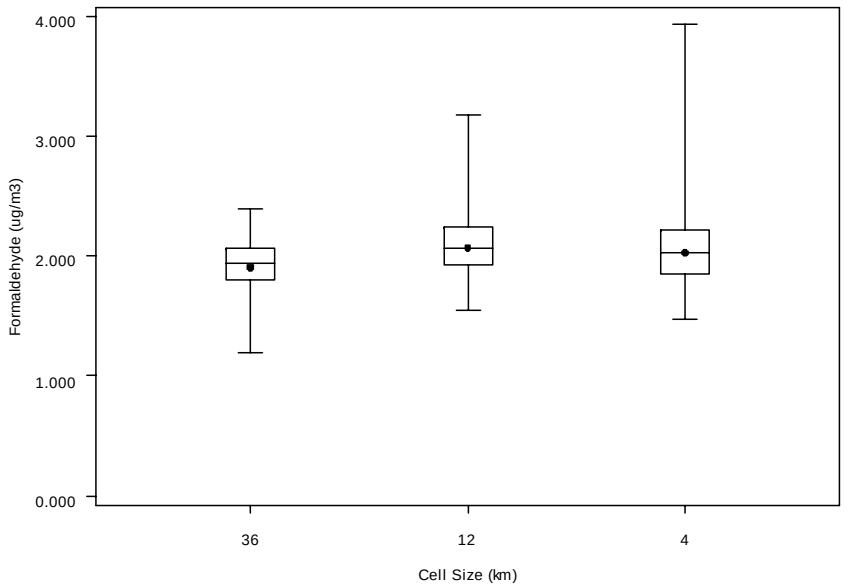


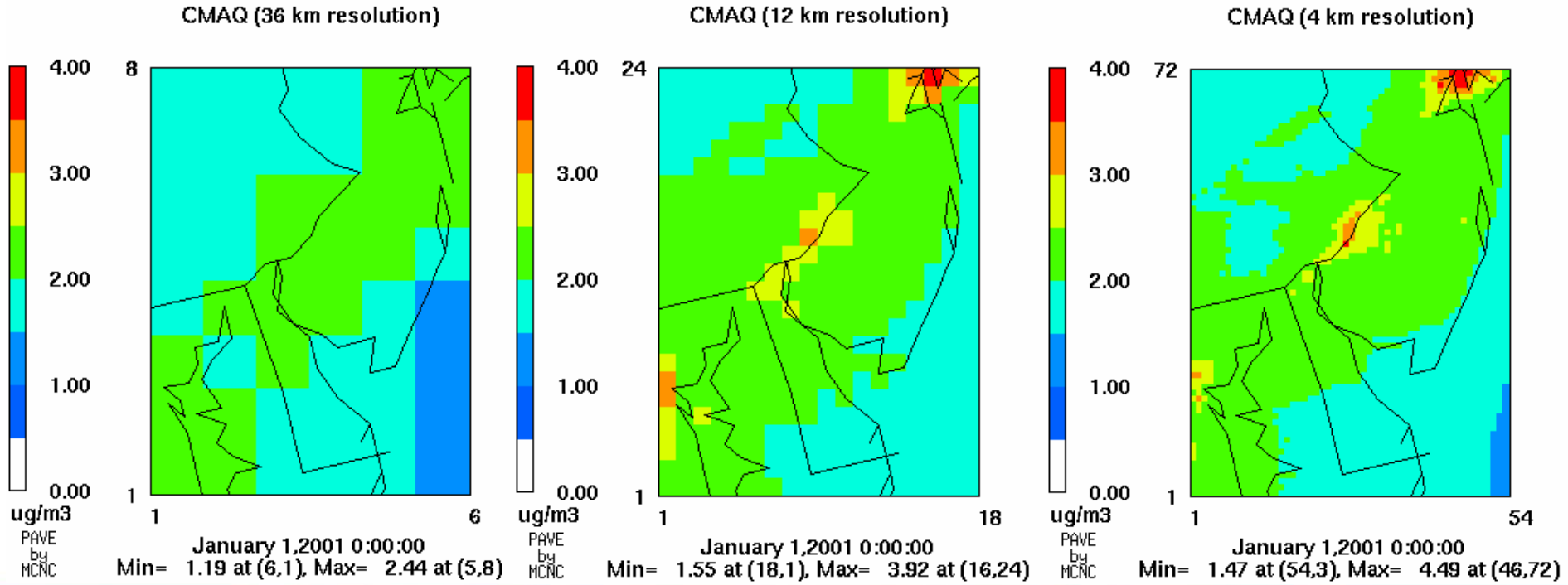




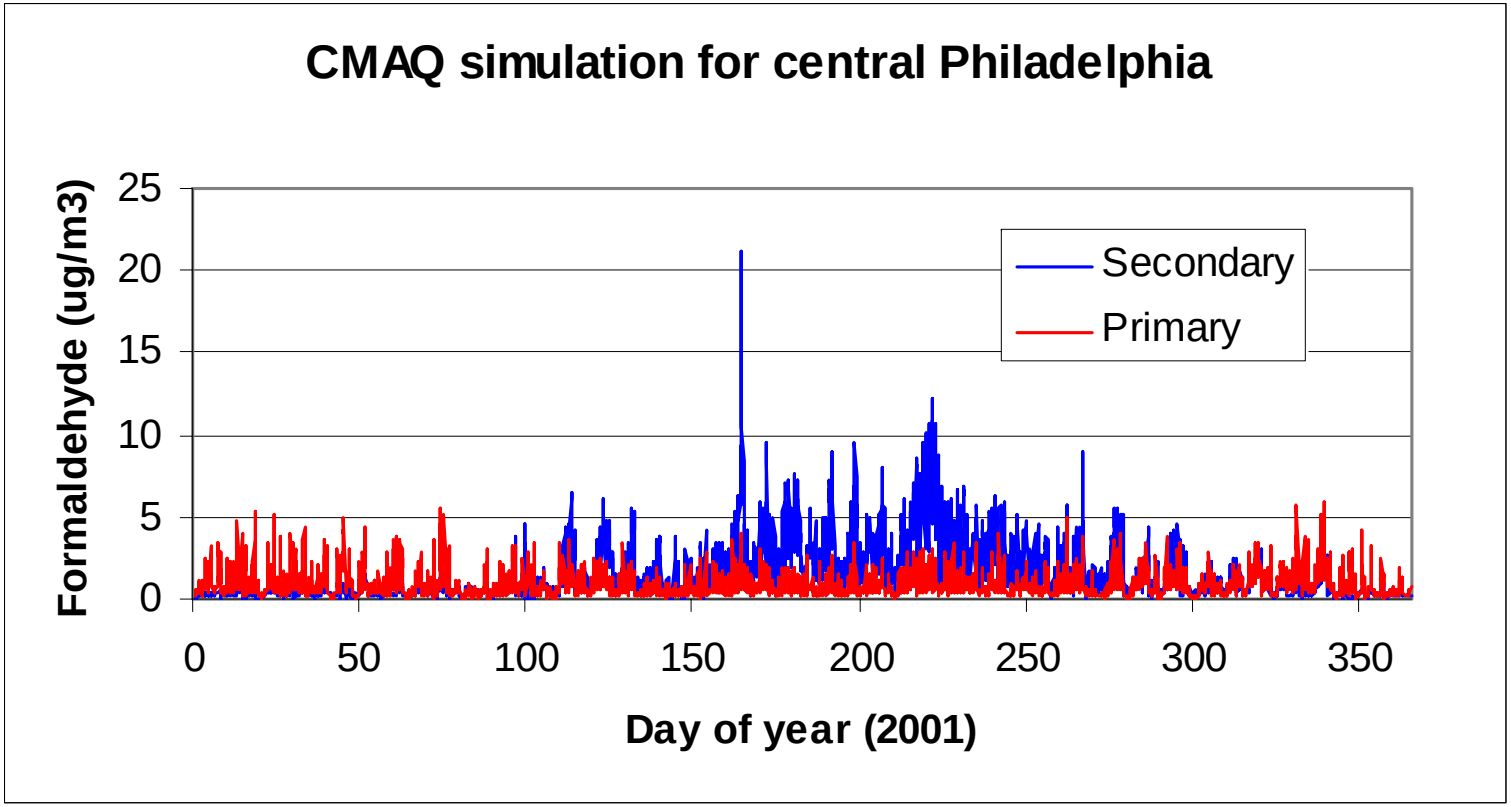
Formaldehyde
Annual average (2001)
CMAQ

...while the means are comparable, the 4 km grids provide more spatial variability than the 12/36 km grids





CMAQ can differentiate primary and secondary formaldehyde in an urban area. The time series shows a 4 km grid cell (26,47) over central Philadelphia. Data are grouped into three-hour averages.



Comparison of air toxic concentrations measured at the Camden, NJ, site to CMAQ (layer 1). All samples, except benzene, are 24-hour averages; benzene is a 1-hour average.

		Mean (ug/m^3)			Std. deviation (ug/m^3)		
Compound	n	Obs	4 km	36 km	Obs	4 km	36 km
1,3-Butadiene	28	0.33	0.18	0.12	0.34	0.12	0.08
Formaldehyde	44	3.68	2.91	2.25	3.21	2.13	1.52
Acetaldehyde	44	2.09	2.49	1.92	1.42	1.20	0.78
Benzene	1328	1.11	1.02	0.77	1.06	0.71	0.40

...based on this limited comparison, CMAQ compares favorably to observations

Linkage of annual CMAQ results to HAPEM5

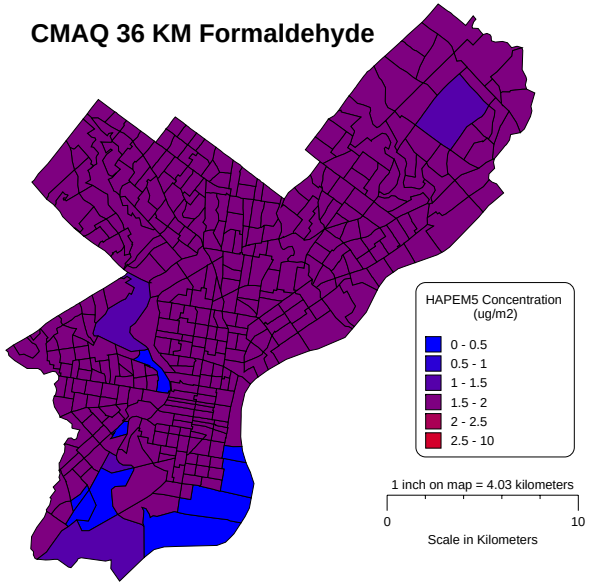
- Hazardous Air Pollutant Exposure Model (HAPEM5)
  - › Screening-level exposure model
  - › Predicts “apparent” inhalation for general population in a census tract
  - › Attempts to account for behavior of demographic groups for indoor and outdoor microenvironments
  - › Uses annual 3-hr average ambient concentrations assumed at the centroid of each census tract
  - › Ingests statistical distribution info (median, mean, and 90th-percentile)

- CMAQ results
  - › Aggregated into annual 3-hr time bins
  - › Concentration distribution from the grid cell overlaying a centroid was used in HAPEM5

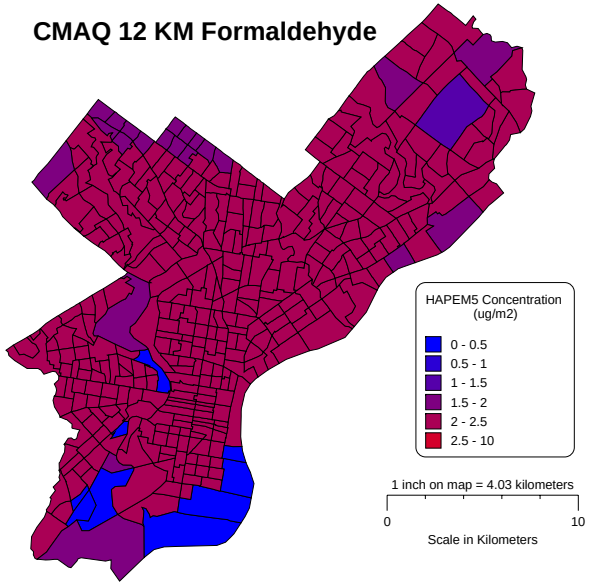
HAPEM5 results for Philadelphia based on CMAQ annual (2001) simulations

Formaldehyde (mean)

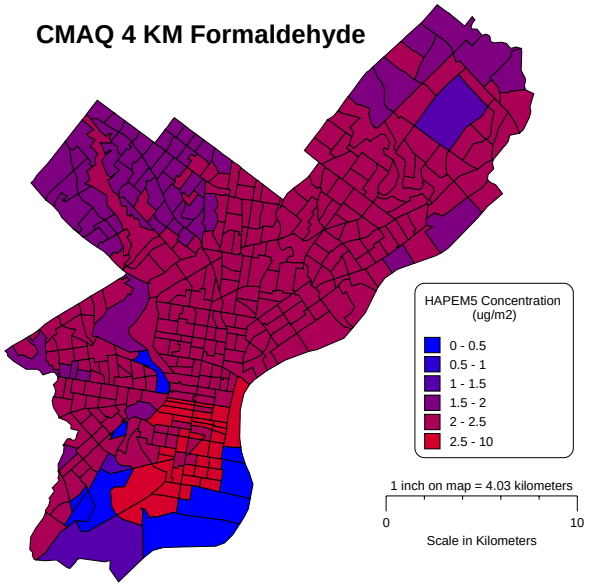
CMAQ 36 KM Formaldehyde



CMAQ 12 KM Formaldehyde



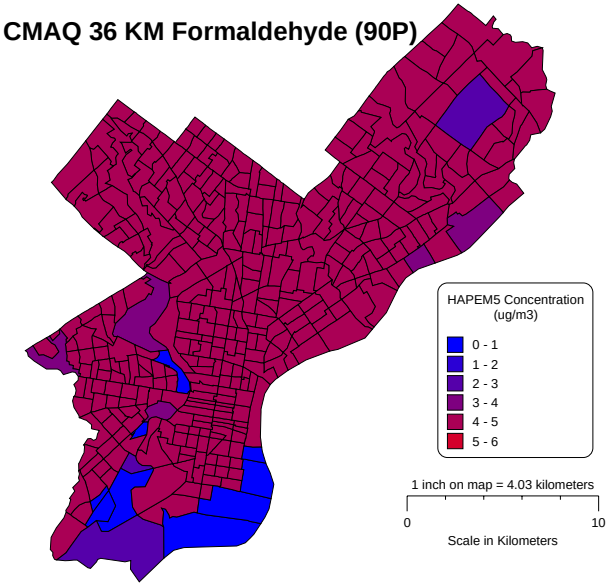
CMAQ 4 KM Formaldehyde



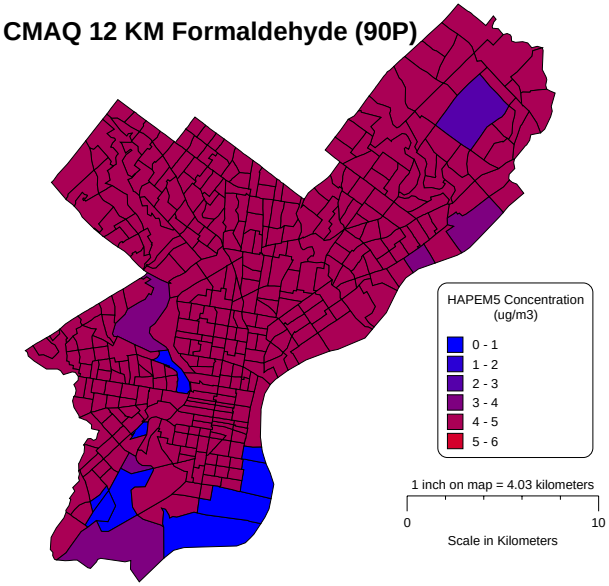
HAPEM5 results for Philadelphia based on CMAQ annual (2001) simulations

Formaldehyde (90th-percentile)

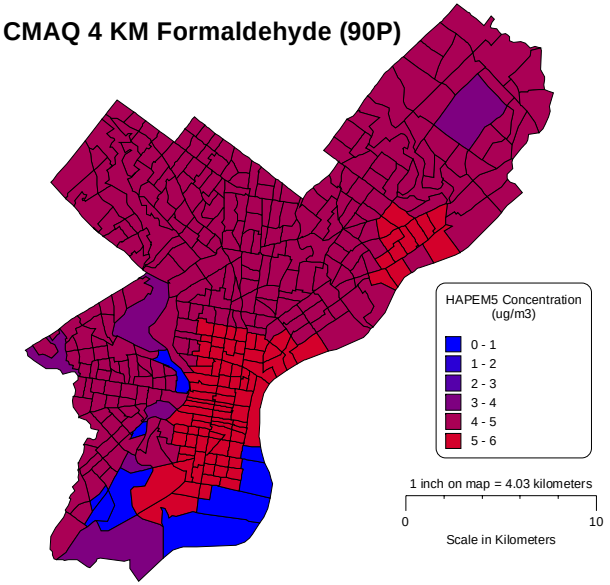
CMAQ 36 KM Formaldehyde (90P)



CMAQ 12 KM Formaldehyde (90P)



CMAQ 4 KM Formaldehyde (90P)



Average Philadelphia exposure levels (ug/m3) computed with HAPEM5

	CMAQ 4 km			NATA
Compound	Median DD	Mean DD	90% DD	Mean DD
Benzene	0.96	1.26	2.63	2.23
Formaldehyde	1.63	2.15	4.60	2.57

*DD = Diurnal Distribution

... CMAQ can be used to provide statistical distributions to human exposure models.

Is it practical to apply CMAQ to model air toxics in urban areas?

- Annual simulation on EPA's IBM eServer Cluster 1600 (w/ 8 CPUs):
  - 12 km (45 x 45 grid cells): 55 hours
  - 4 km (54 x 72 grid cells): 146 hours
- Simulation times on a Linux cluster are comparable
- With modern computer resources, annual urban simulations are quite manageable

Future opportunities for linking CMAQ to human exposure models at urban scales

- Integrate approach with ISCST or AERMOD
- Extend capability to a finer grid resolution (~1 km)
- Perform more extensive model evaluation
- Link with the SHEDS human exposure model
- Explore application to other regions for other toxics

An initial linkage of the CMAQ modeling system at neighborhood scales with a human exposure model

Disclaimer: Although this work was reviewed by EPA and approved for publication, it may not necessarily reflect official Agency policy.

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