Predicting Fate and Transport of Toxic Air Pollutants using CMAQ

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Outline

- How this work contributes to EPA’s mission and fits in with other work that has been presented here
- Specifics of the CMAQ-TX model applications
- Some preliminary results
- Finer “community scale” modeling and applications in urban areas
- What we are planning to do in the future

Three current activities involve Toxic Air Pollutant modeling with CMAQ

- Mercury Modeling
  - Supports analyses of Clear Skies Initiative controls and international assessments
  - Multimedia linkages
- HAPs modeling at large scales (36 km)
  - Supports the National Air Toxics Assessment (NATA)
  - Characterizes peak and background concentrations of HAPs and their sources
  - Provides boundary conditions for finer-scale modeling
- Urban and community-scale modeling (1-12 km)
  - Develops tools for local risk assessments and control strategy development, provides input for Human Exposure Models
  - Simulates airborne releases of hazardous agents at fine scales in urban environments (Homeland Security applications)
  - Gives us a better capability for assessing subgrid variability from within-grid sources and photochemistry, and to introduce this information into exposure models

Why currently-used methods aren't sufficient

- Monitoring
  - Can't get the spatial distribution
  - Not always available at all times and places for all species
- Routine dispersion modeling (ISC, etc.)
  - Doesn't account for wind shear
  - Can't track plumes beyond 50 km
  - Can't handle chemistry correctly
  - Doesn't include biogenic sources

First application of air toxics modeling (large-scale) is the National Air Toxics Assessment (NATA)

Every 3 years, EPA conducts a national-scale assessment of the pollutants of greatest concern. This assessment includes:

1. Compiling emissions inventories of toxic air pollutants from outdoor sources
2. Estimating concentrations over the U.S. using ASPEN
3. Estimating population exposures using HAPEM
4. Characterizing potential public health risk due to inhalation of air toxics for both cancer and non-cancer effects.
5. Comparing concentration fields from CMAQ with ASPEN and revising health risk calculations to account for significant differences

Toxic air pollutants studied under the NATA

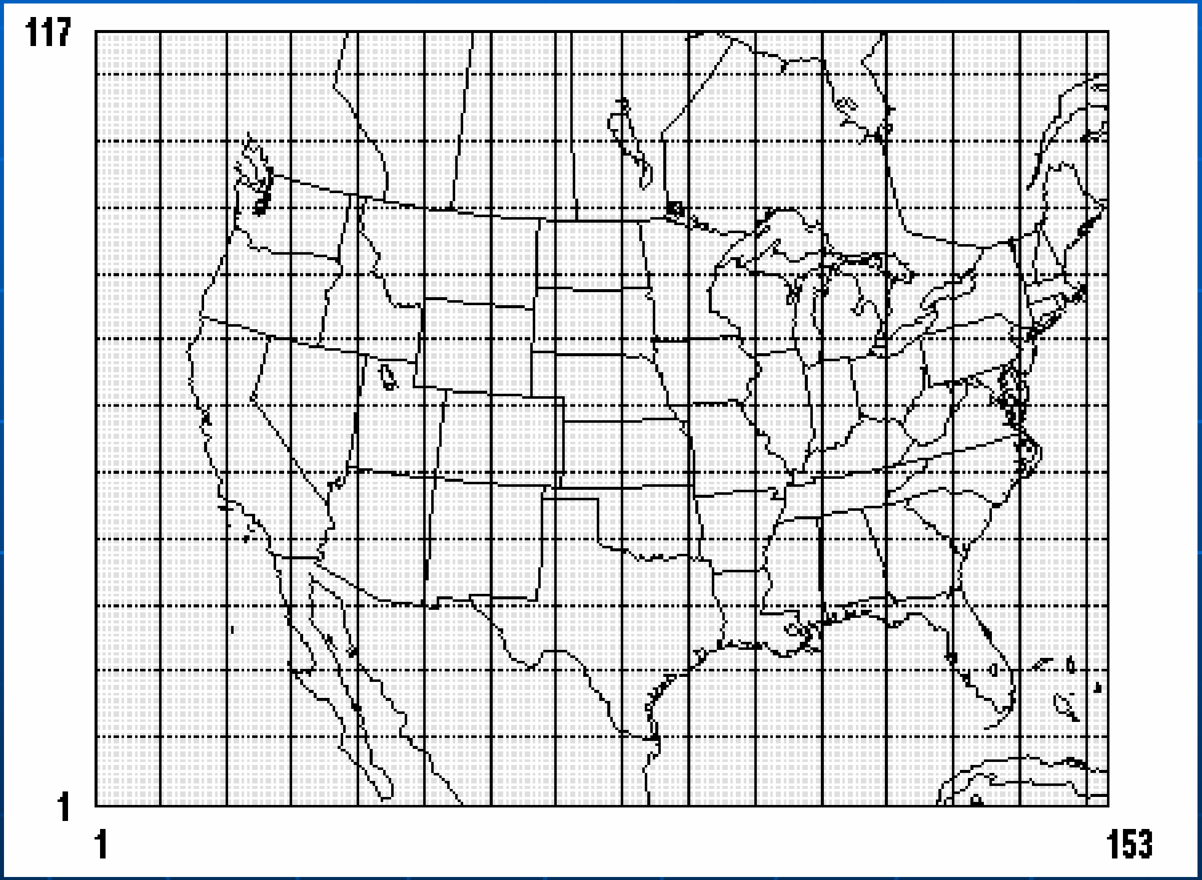
acetaldehyde	chloroform	hexachlorobenzene	tetrachloroethane
acrolein	1,3-dichloropropene	hydrazine	trichloroethylene
acrylonitrile	ethylene dibromide	methylene chloride	vinyl chloride
1,3-butadiene	ethylene dichloride	perchloroethylene	napthalene*
benzene	ethylene oxide	propylene dichloride	
carbon tetrachloride	formaldehyde	quinoline	
arsenic	chromium	lead	nickel
beryllium	coke oven emissions	manganese	polychlorinated biphenyls (PCBs)
cadmium	diesel particulate matter	mercury	polycyclic organic matter (POM)

NATA Model domain
36-km grids across the continental U.S.

Grid:
15 vertical layers
153 columns by
117 rows

Simulation period:
Jan 1 –Dec 31, 2001
10-day spin-up

Platform:
IBM SP2



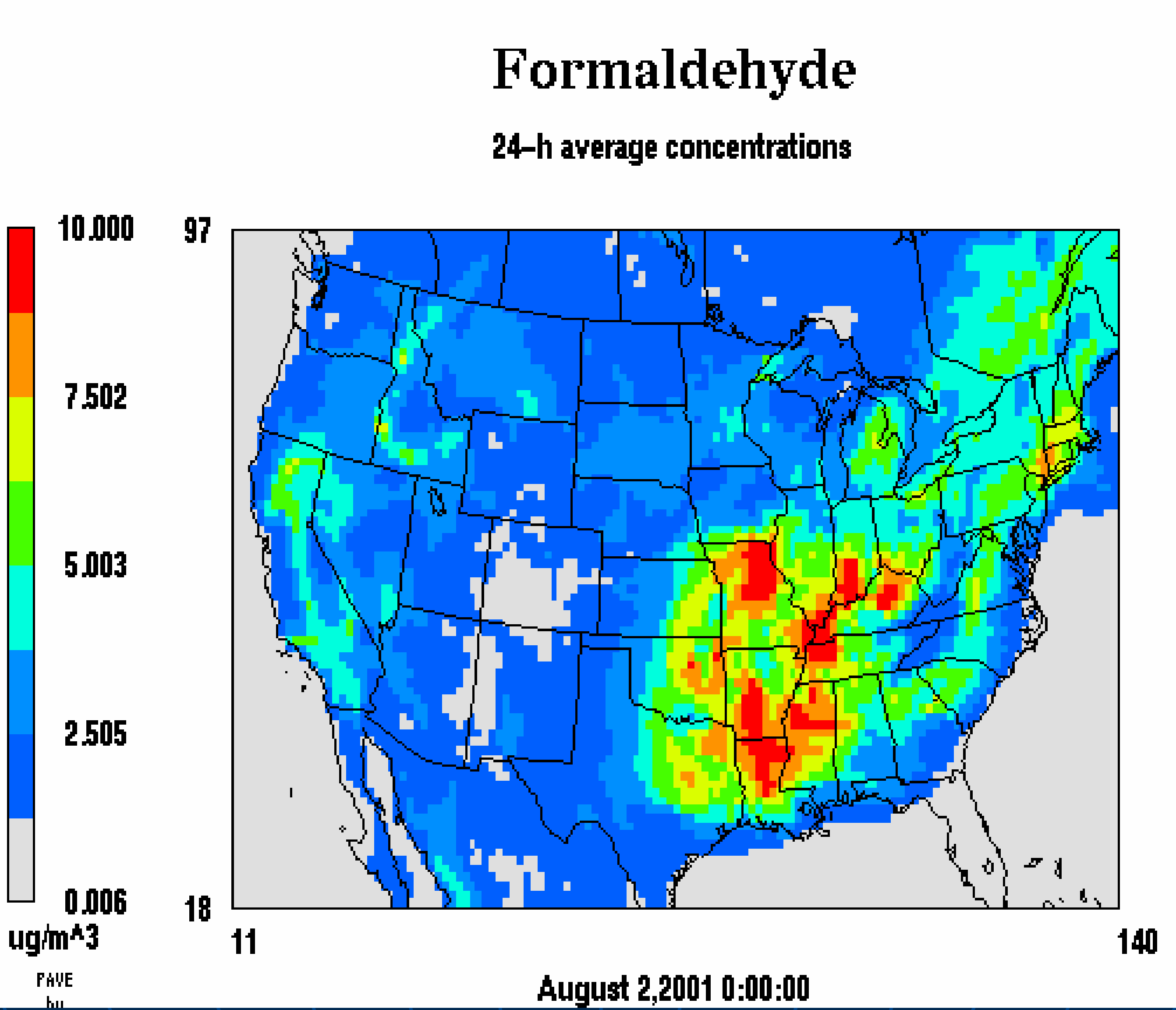
CCTM, Meteorology and Emissions

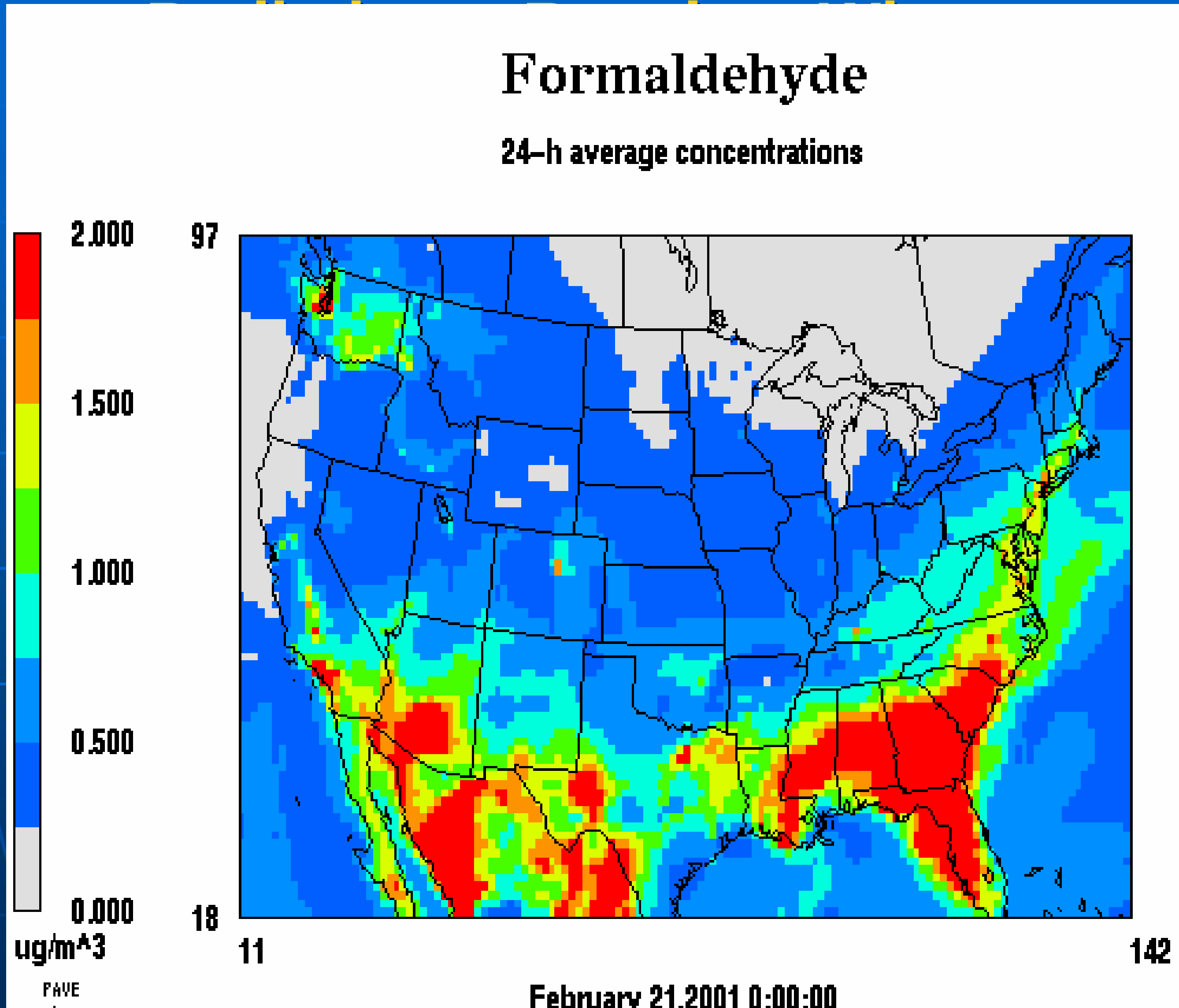
- CMAQ v4.3, September 2003
- Includes aqueous chemistry but no aerosols (future simulations to include aerosols)
- EBI solver
- Meteorology from MM5v3.6, 34 vertical layers
- MM5 files processed with MCIP v.2.2
- Emissions of criteria pollutants using NEI v.2
- Emissions of toxic pollutants from NEI v.3
- Biogenic emissions from BEIS v3.11
- Processed with SMOKE v.2.0 with new plume rise calculations

Chemical Mechanisms

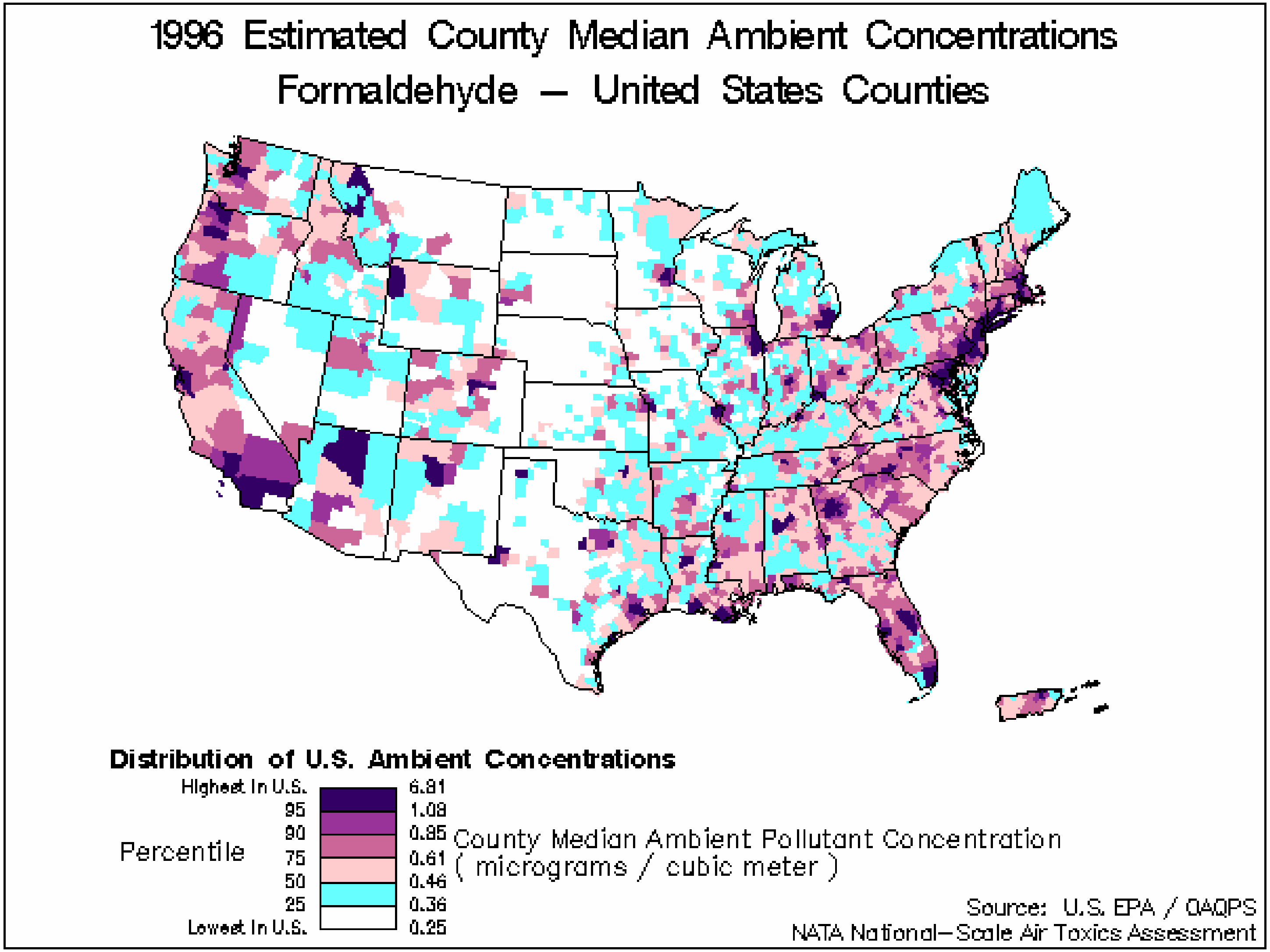
- First Simulation uses CB4TX1
  - Release version of CB4 with modifications to include explicit HAPs
  - Formaldehyde and acetaldehyde are explicit
  - VOC HAPs only in first simulation
  - Tracking of concentrations due to primary emissions for:
    - Formaldehyde
    - Acetaldehyde
    - Acrolein from 1,3-butadiene
  - Other HAPs only have degradation offline
- Sensitivity studies with SAPRC99TX2

Preliminary Results - Summer

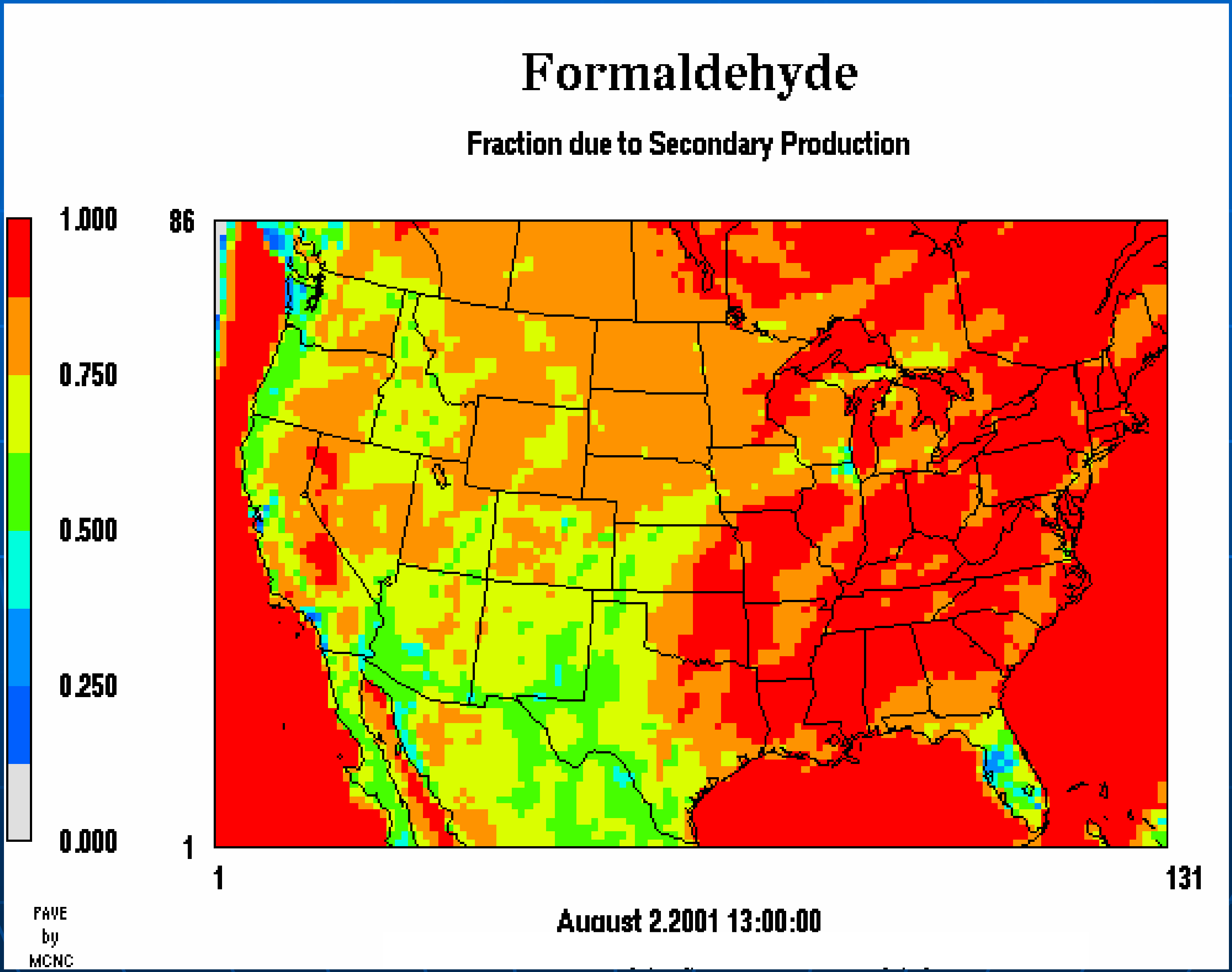



Formaldehyde
24-h average concentrations
2.000
1.500
1.000
0.500
0.000
ug/m^3
97
18
11
142
February 21,2001 0:00:00
PAVE

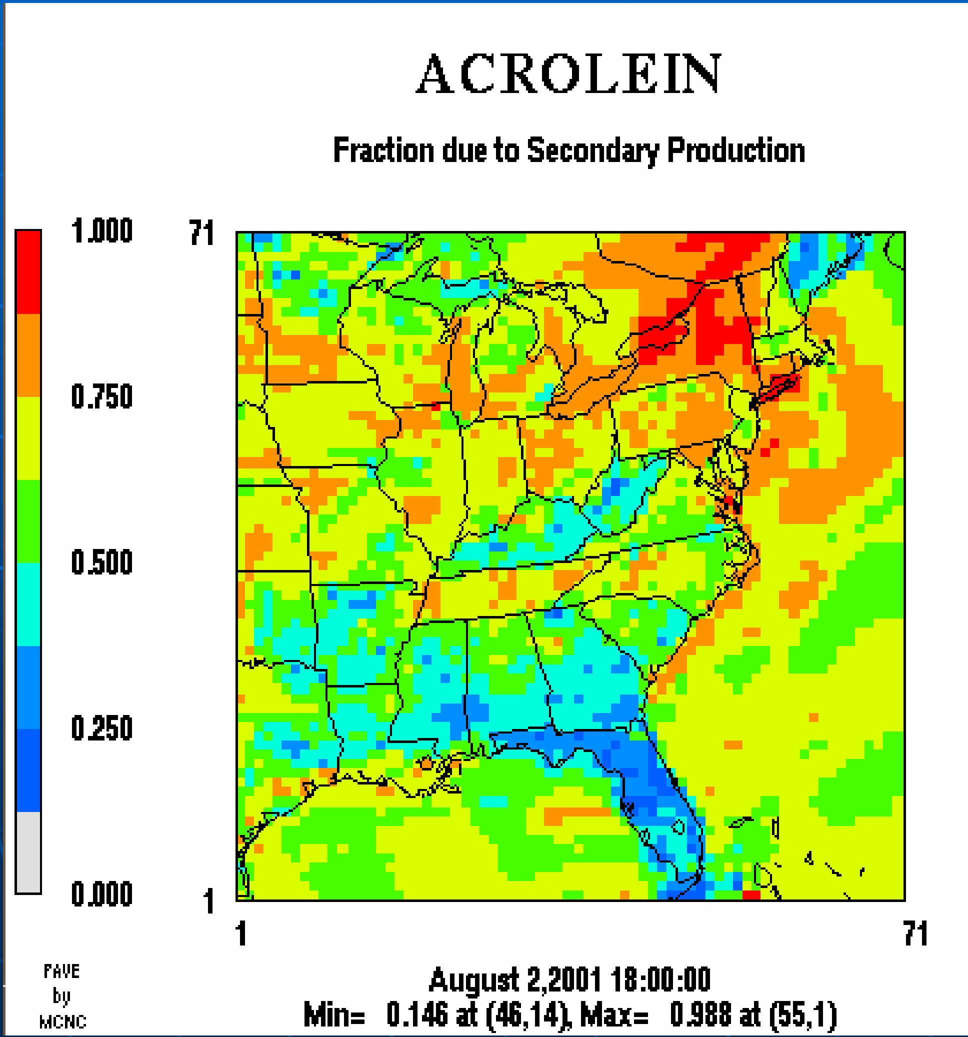
We expect that CMAQ predictions will differ, both in magnitude and spatial distribution from previous NATA-ASPEN concentrations



Secondary Production from other VOCs is the dominant source of atmospheric formaldehyde



Other chemicals can also have significant, but variable secondary production



Some questions that we are trying to answer with this information

- What are the largest sources of toxic aldehydes? How important are biogenic sources in determining concentrations of toxics?
- What conditions tend to maximize concentrations of HAPs? When/where is deposition the greatest?
- Are seasonal and diurnal variations significant enough to affect calculated exposures?
- How do we account for both hot spots and secondary production? (How fine does the grid resolution have to be?)

Extension of Air Toxics Modeling to Urban and Community Scales

- Exposure assessments are primarily for urban population centers.
- Urban meteorological fields, dispersion parameters are strongly influenced by urban features such as buildings and their distribution, street canyons, vegetative canopy, etc.
- To account for the effects of urban morphology, we are incorporating Urban Canopy Parameterizations (UCPs) in CMAQ’s meteorological processor, MM5.

First application of air toxics modeling at urban scales is the Philadelphia risk assessment

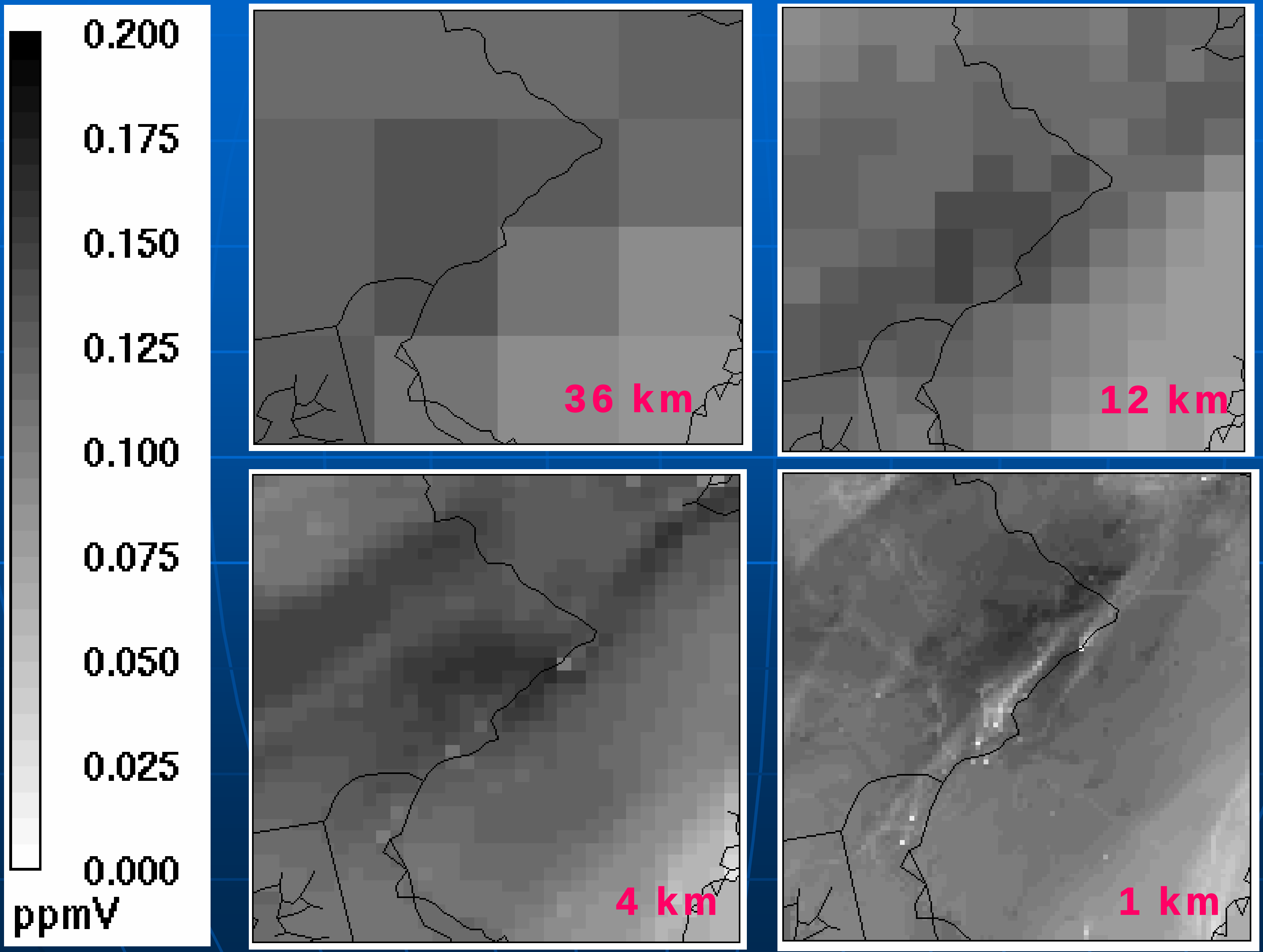
ORD/NERL/AMD is collaborating with Region 3 and the State of Delaware to conduct a joint pilot risk assessment of toxic air pollutants within the Philadelphia and state of Delaware, involving:

1. Determining concentrations from annual CMAQ simulations at 12, 4 and 1 km
2. Compiling a highly-resolved inventory of sources of HAPs
3. Estimating subgrid concentrations distribution (using ISC)
4. Estimating population exposures using HAPEM modified to handle SGV distributions
5. Characterizing potential public health risk due to inhalation of air toxics for both cancer and non-cancer effects.

CCTM, Meteorology and Emissions

- Nested grid domains of 12, 4, and 1 km centered over Philadelphia and Delaware
- CMAQ model, chemical mechanism, solver, and emissions files are same as used in NATA simulation
- Boundary and initial conditions extracted from NATA simulation
- MM5 to be run in a one-way nested configuration: 108, 36, 12, 4 (and 1 km horizontal grid spacing) .
  - UCPs to be used only for the 1 km domain.
  - Turbulent scheme model: Gayno-Seaman PBL with turbulent length scale of Bougeault and Lacarrere (1989).
- Computational platform: Linux, 8 nodes, 16 processors

More structure is apparent when "nesting" down from regional to fine scale



Ozone, July 14, 1995, 6PM local time

Questions that we are trying to answer

- Can we model SGVs with parameterizations?
- Can we develop accurate meteorological fields for CMAQ urban applications at fine scales?
- What degree of within-grid concentration variability do we find in CMAQ simulations? How does this vary for different grid resolutions?
- Can we improve risk assessments by conducting AQ modeling at fine scales and including within grid (SGV) variability?

Status of Urban Toxics Modeling

(Paradigm: Drive risk-based exposure models with both resolved (CMAQ) and SGV (PDFs) concentration distributions)

- Currently applying prototype for applications in Philadelphia and Houston
- Developing, testing and refining the prototype urban canopy parameterizations (UCP) in MM5 (Houston)
- Developing PDFs of sub-grid variability for different parent grid resolutions
  - Within grid photochemistry using LESChem
  - Primary sources: Developing parameterizations from physical, CFD and dispersion modeling
- Using Philadelphia application to evaluate the methodology, including comparison with comprehensive ISC results

Follow up Work: near-term (1-2 y) to mid-term (3-5 y)

Large-Scale

- Work with OAQPS to explore the use of CMAQ results to improve the NATA
- Expand the list of pollutants simulated to include species such as particle-bound toxics such as metals, PAHs
- Apply improvements to next NATA

Urban Scale

- Initial demonstration of linkage of CMAQ and SGV concentration distributions to human exposure models.
- Improve, apply urbanized MM5 to CMAQ.
- Improved modeling of subgrid scale processes in another urban area (Houston)
- Refine, apply, evaluate nested CMAQ and PDFs in another city (TBD).

Summary

- The CMAQ model is being applied for air toxics applications
  - Initial simulations are being performed over the continental US, for high priority gas-phase toxics
  - Simulations of Mercury concentrations and deposition are being performed and compared with other models
  - The continental simulations are being used to provide boundary conditions for finer-scale simulations, nesting down over urban areas
- CMAQ simulations will improve the way that EPA predicts concentrations of HAPs
  - For species with significant secondary production
  - When diurnal variations of concentrations can change the exposure significantly
  - When concentrations are transported large distances
- Fine-scale modeling with CMAQ and corresponding SGV is being developed to improve population exposure estimates