OBSERVED AND HIGH RESOLUTION MODELED POLLUTANT FIELDS USING FINE-SCALE AND HYBRID MODELING APPROACHES FOR WILMINGTON, DELAWARE

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Outline

- Sub Grid Variability (SGV) – an inherent property of all grid models
- Methods for incorporating SGV
- Quantification of SGV from a number of studies
  - Fine-scale CMAQ simulations
    - Philadelphia 12,4,1.33 km: 1999 & 2001
    - Delaware 1 km: 1999 & July 2001
  - Local-scale modeling
    - Delaware
    - Philadelphia
  - Mobile van measurements in Wilmington

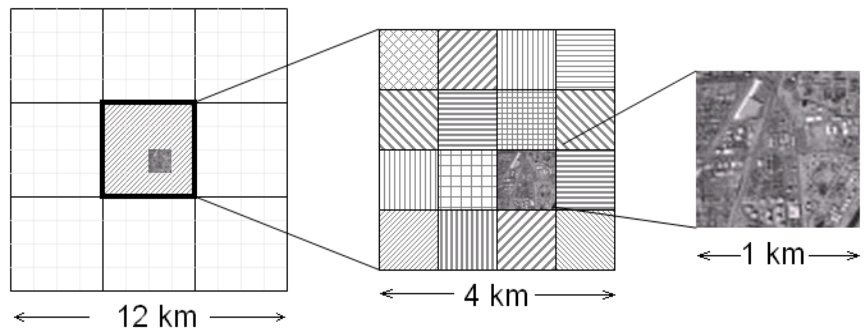
BACKGROUND & Rationale

- Characterization of air toxic hot spots is necessary but it is difficult
  - With monitoring network
  - With coarse-scale grid modeling
- Grid modeling (e.g., w/CMAQ) provides
  - Volume average concentrations
  - But not variability within the grid
- Human exposure assessment requirements
  - From multiple pollutants
  - Over various time scales and activity patterns
  - Most pronounced in vicinity of hot spots

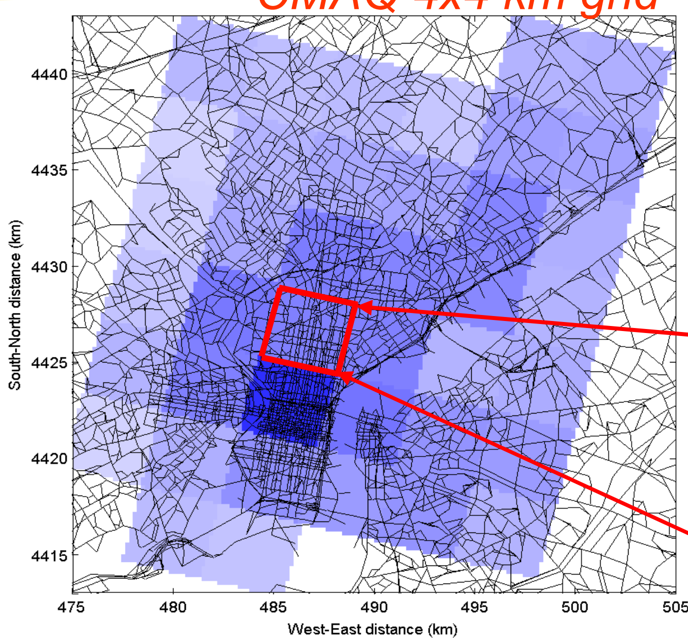
The problem:

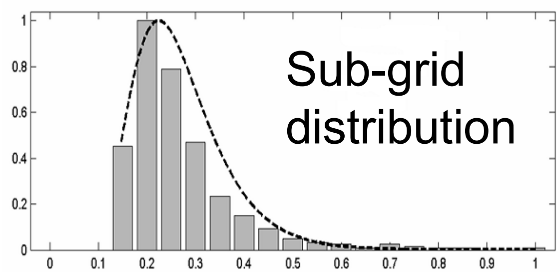
For every grid resolution, there are unresolved sub-grid features.

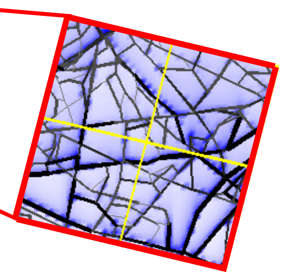
For many air quality model applications, while desirable, current models are typically unable to resolve both regional and local scale features.



CMAQ 4x4 km grid







Local details within a grid cell

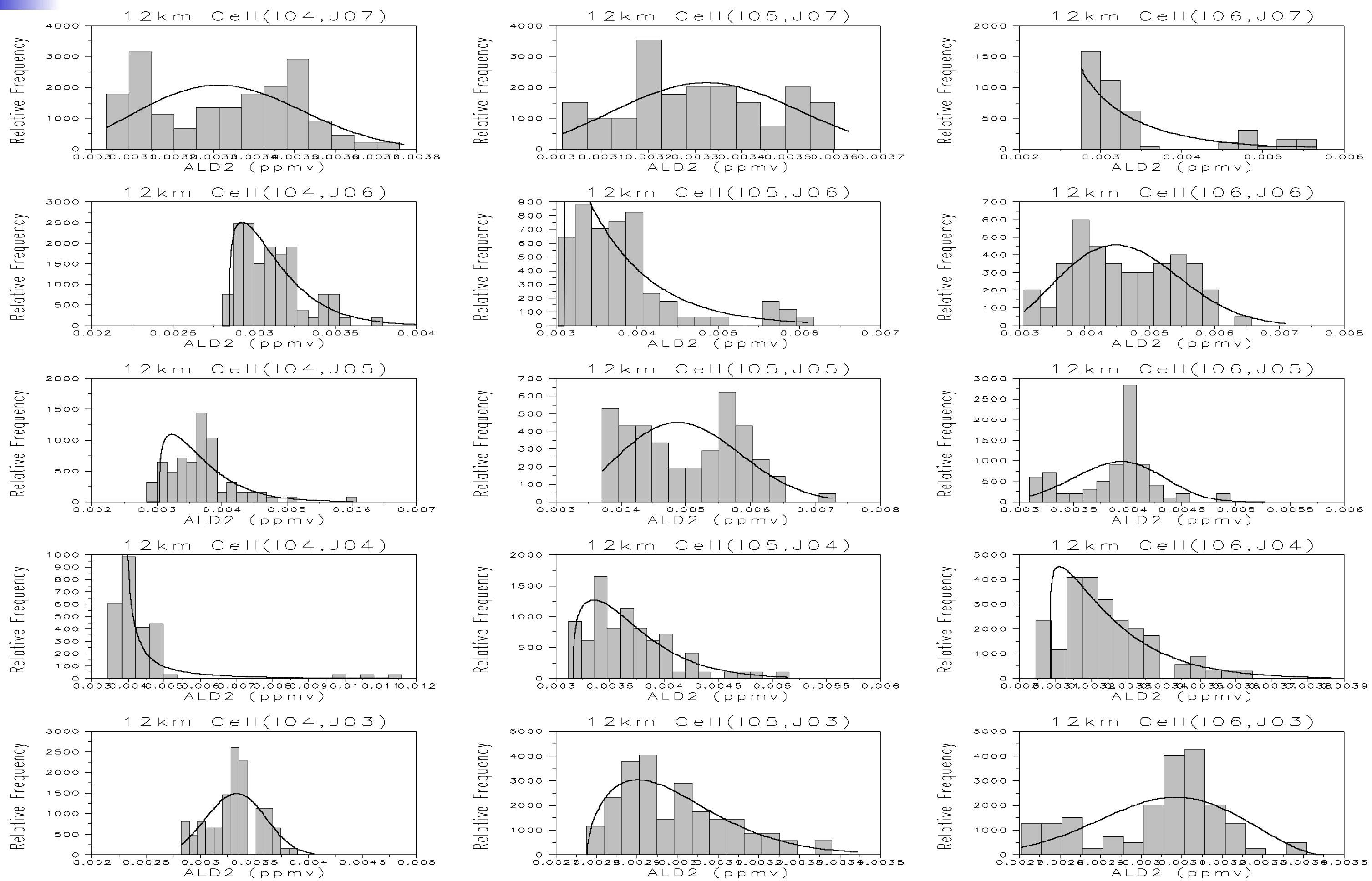
Detailed fine-scale measurements are needed for model evaluation

SGV & Neighborhood Scale (N-S) Modeling Features

- CMAQ provides multi-scale, grid resolved concentrations
- Modeling at N-S
  - Valuable when significant variability is present at that scale
  - Still underestimates variability.
- SGV can be derived from
  - Fine-scale CMAQ
  - Local-scale modeling
  - Photochemistry in turbulent flows
  - Measurements
- SGV
  - Essential for improved human exposure assessments
  - Treated as concentration PDFs

Acetaldehyde relative histograms with **Weibull probability density function** fits **(heavy lines)** for 12 km grid cells derived from blocks of 81 1.33 km grid values at 15:00 LST from the CMAQ simulation of Philadelphia

14 July 1995. Central cell is Central Philadelphia



Adjusting CMAQ Concentrations
For SGV

$$SAC = C_g * f_1 (C_{SGV})* f_2 * \lambda \qquad (1)$$

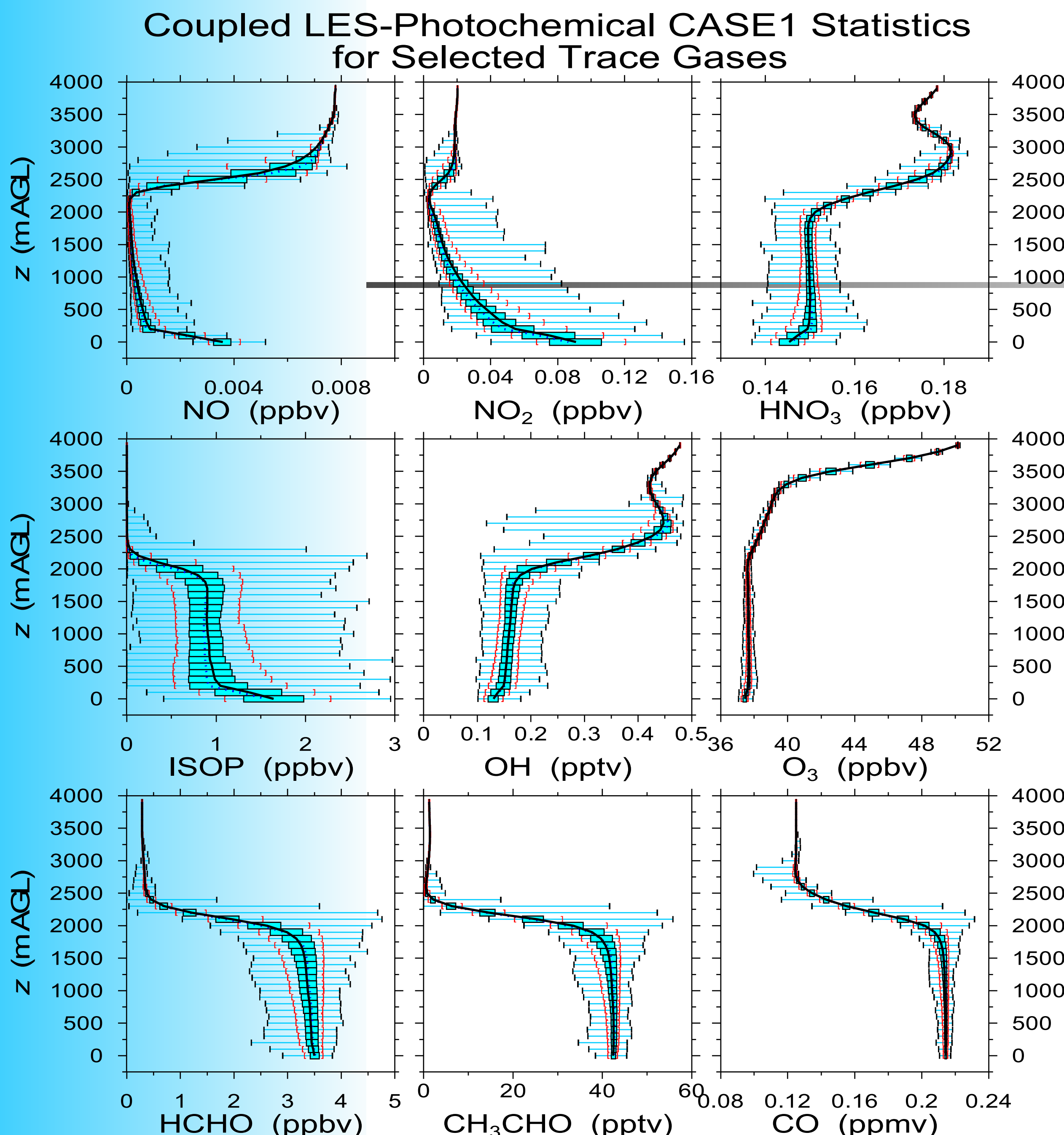
f_1 Factor based on modeled/monitored SGV
f_2 Factor for photochemical-dynamical contributions
λ Coefficient or weighting factor for variability
& spatially variable

f_1 is the focus of current investigations, e.g.,

$$f_1(C_{SGV}) = 1 + C_{SGV} / C_g = 1 + COV \qquad (2a)$$

Other suggested C_{SGV} options include but not limited to:

- 95th or other percentile of the distribution (2b)
- Peak (or range)/cell mean. (2c)



Courtesy: Jerold A. Herwehe

Vertical Profiles of Trace Gas Statistic

Minimum, Maximum

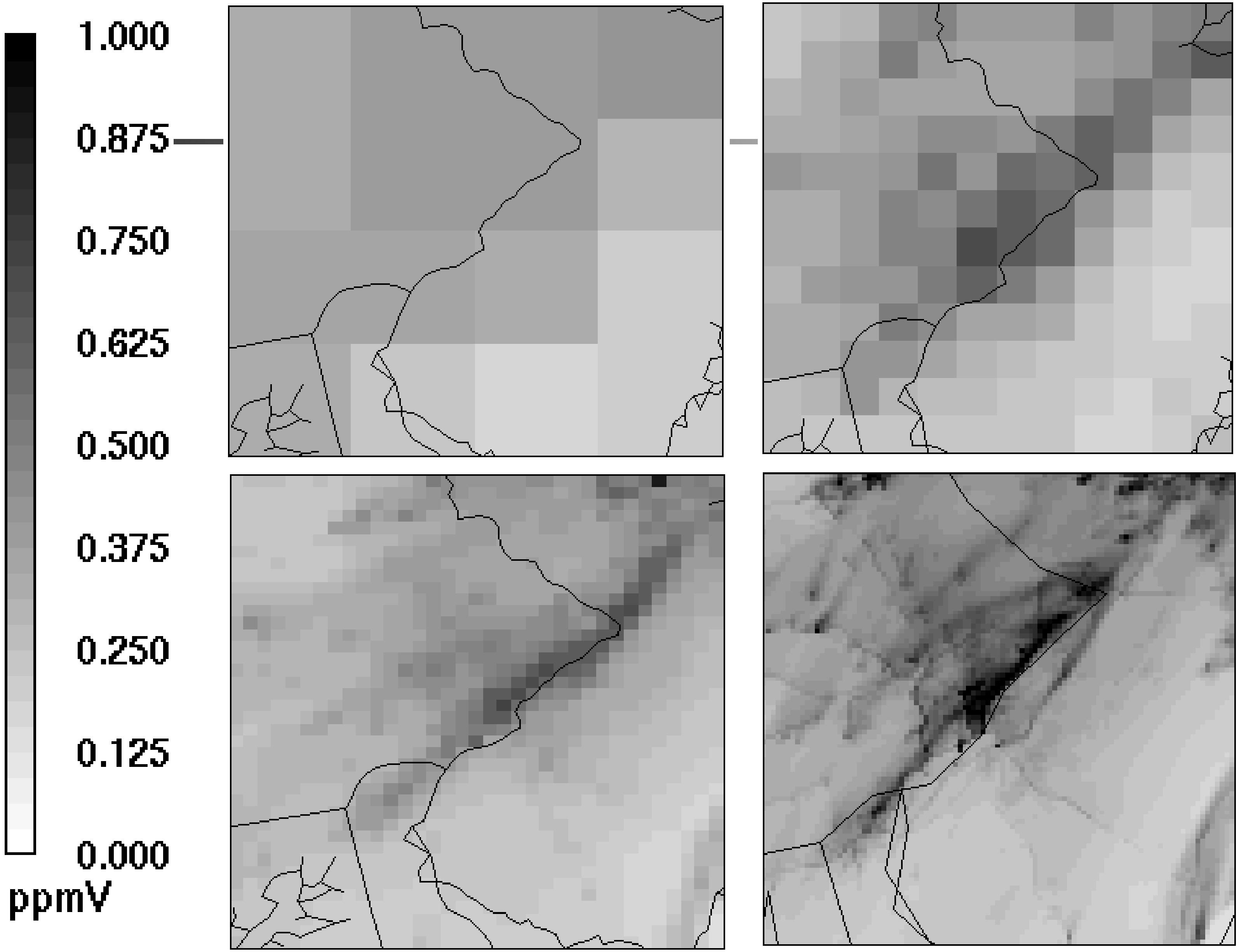
10th and 90th percentiles (red brackets),

1st and 3rd quartiles (cyan box)

Median (blue dashed line)

Mean (black line)

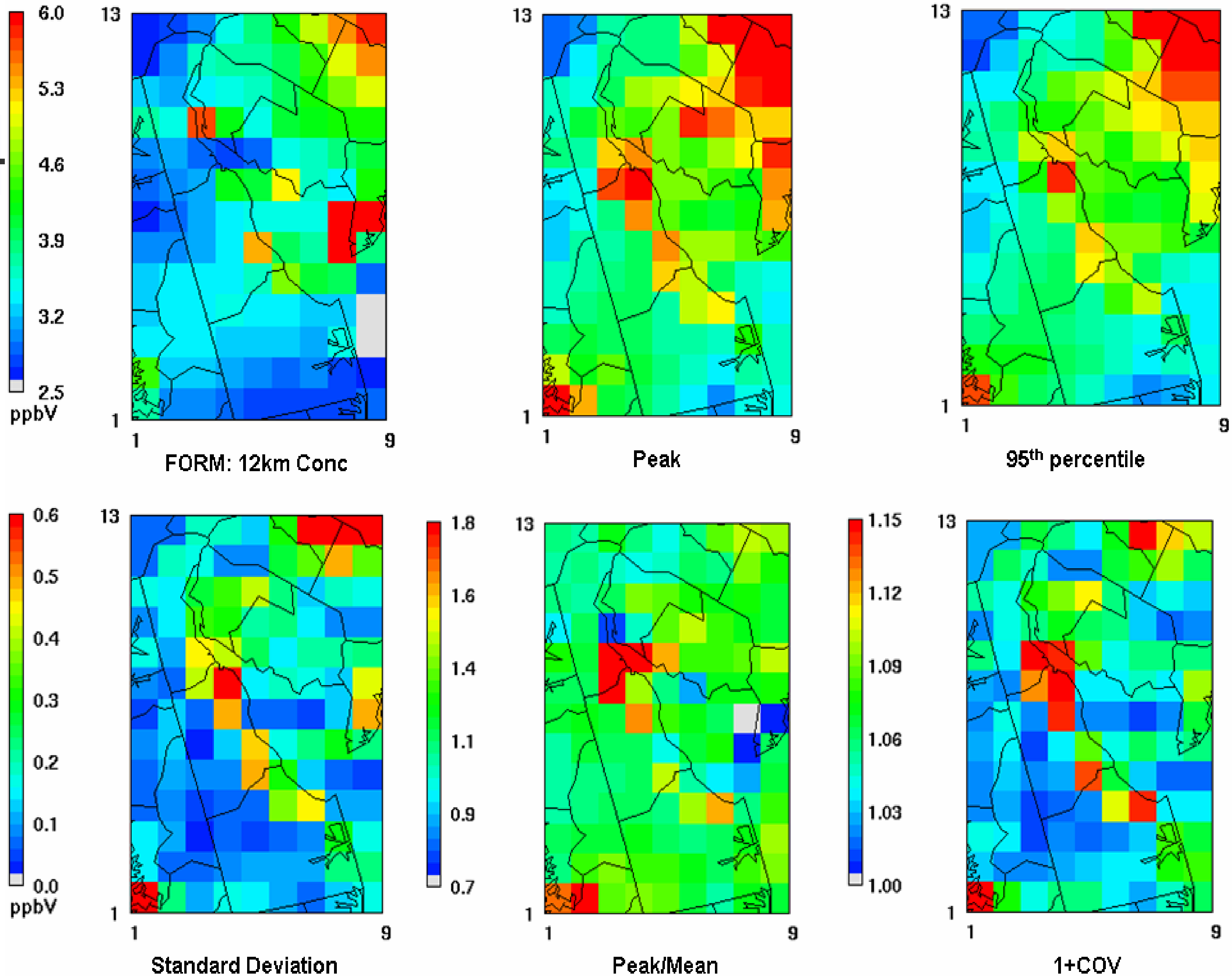
CO Jul 14, 95, 6pm (local)



SGV based on Fine-Scale Modeling

- Modeling from regional to fine scale (Delaware domain) at 1-km grid resolution by 1-way nesting – MM5 & CMAQ
- Modified CB-IV treats 20 gas-phase air toxics & provides primary and secondary components of carbonyl compounds
- 1999 NEI Emissions processed w/SMOKE

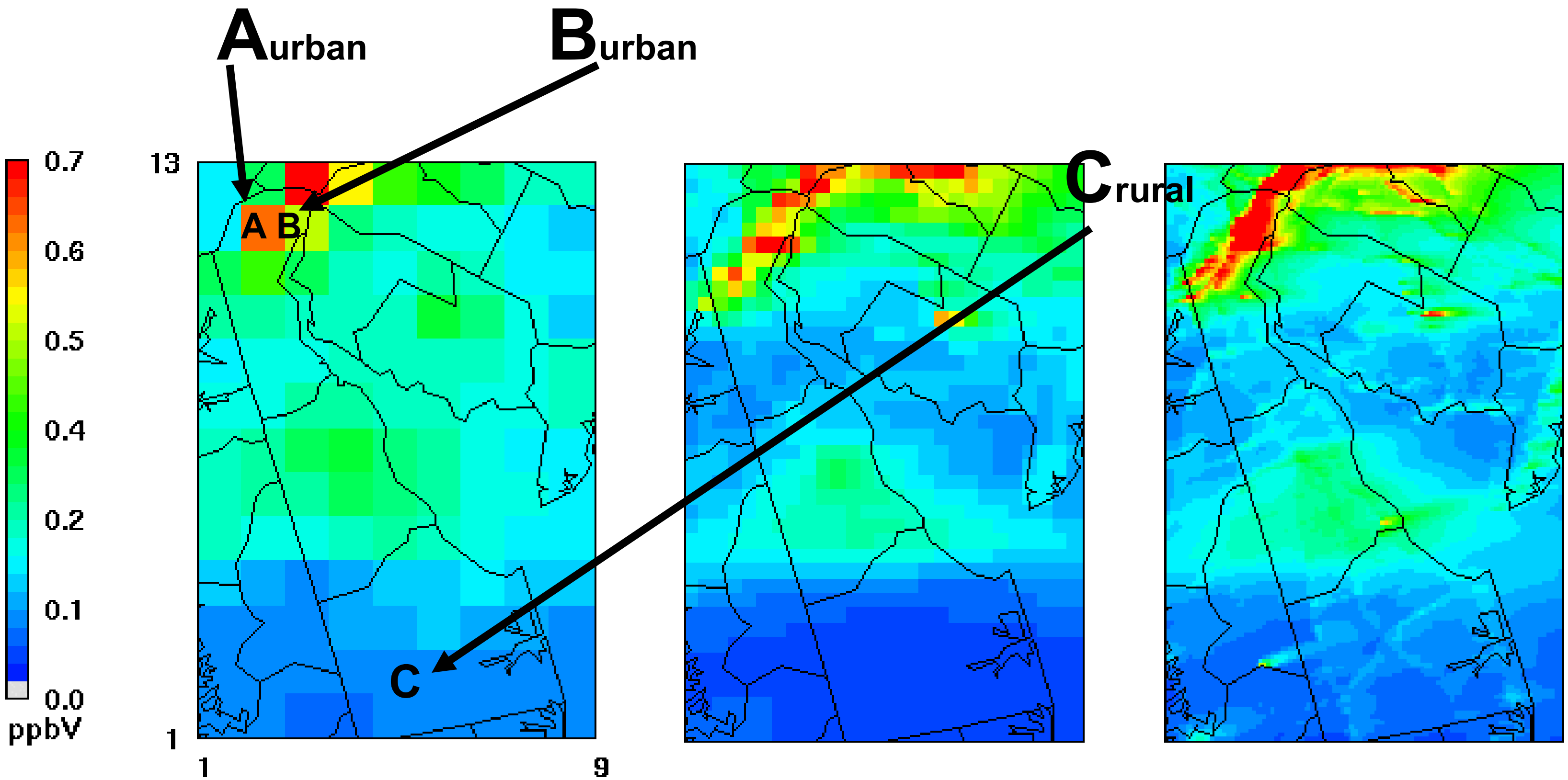
12 km HCHO SGV and SAC results



Delaware Episodic Modeling Study

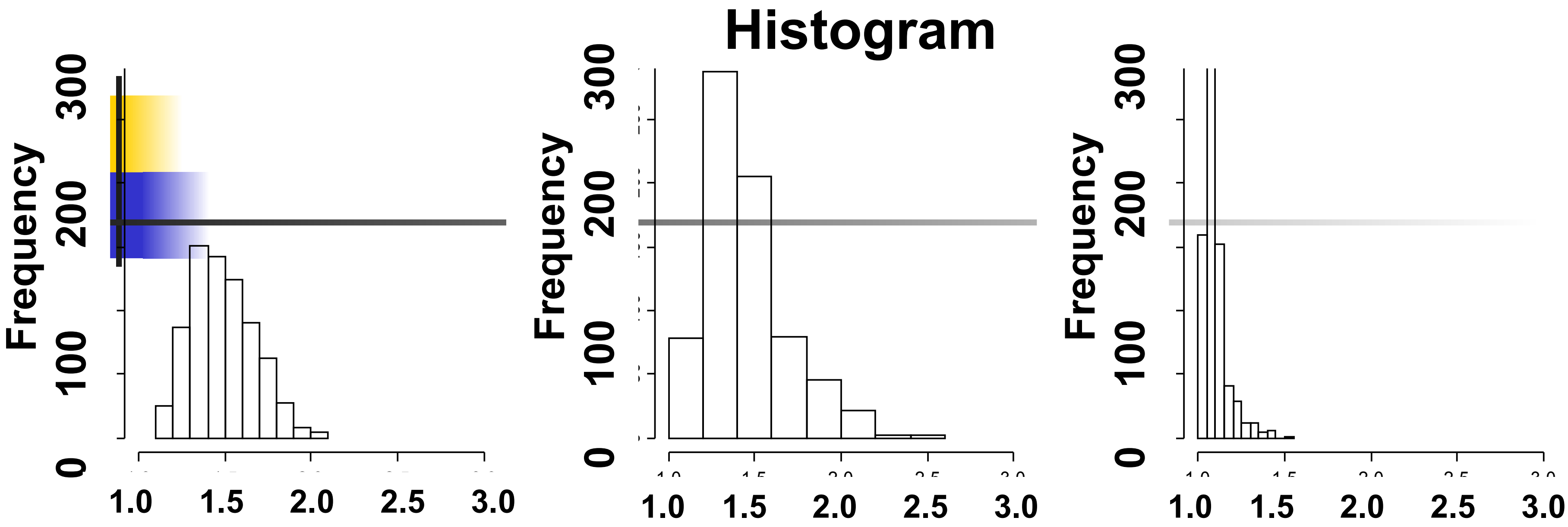
Benzene

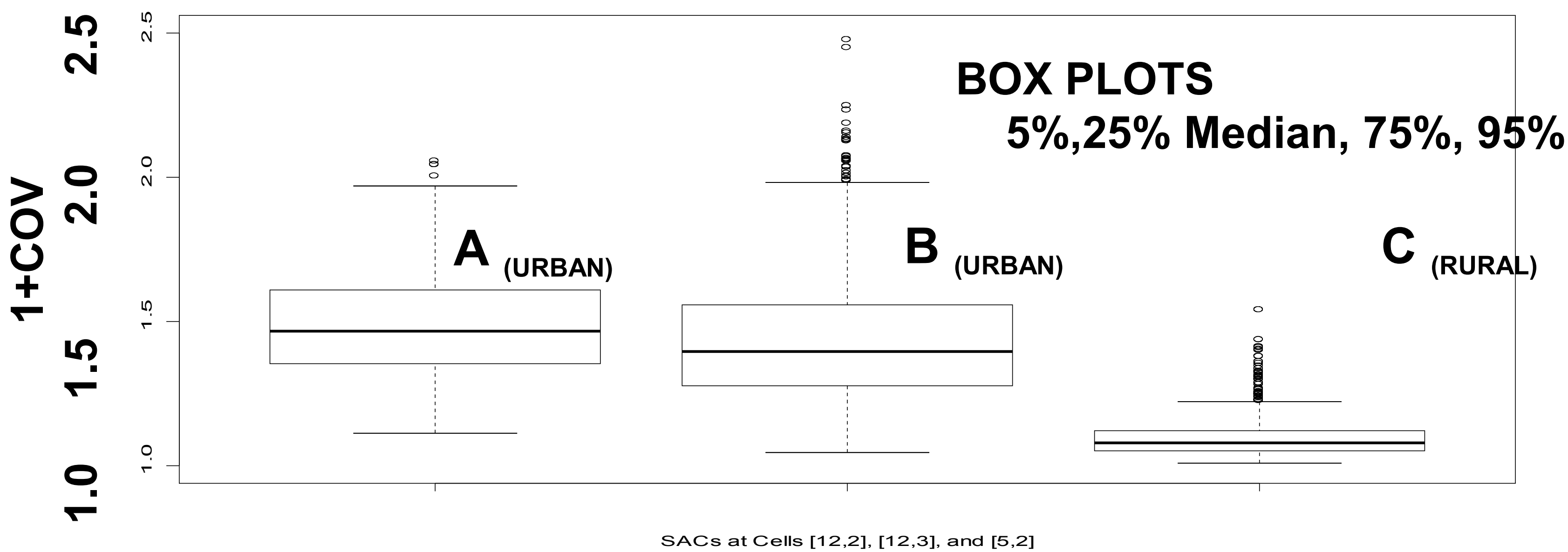
16th July 2001 at 11:00 UTZ



(A) 12 km **(B) 4 km** **(C) 1 km**

Benzene (July 2001) 1+COV

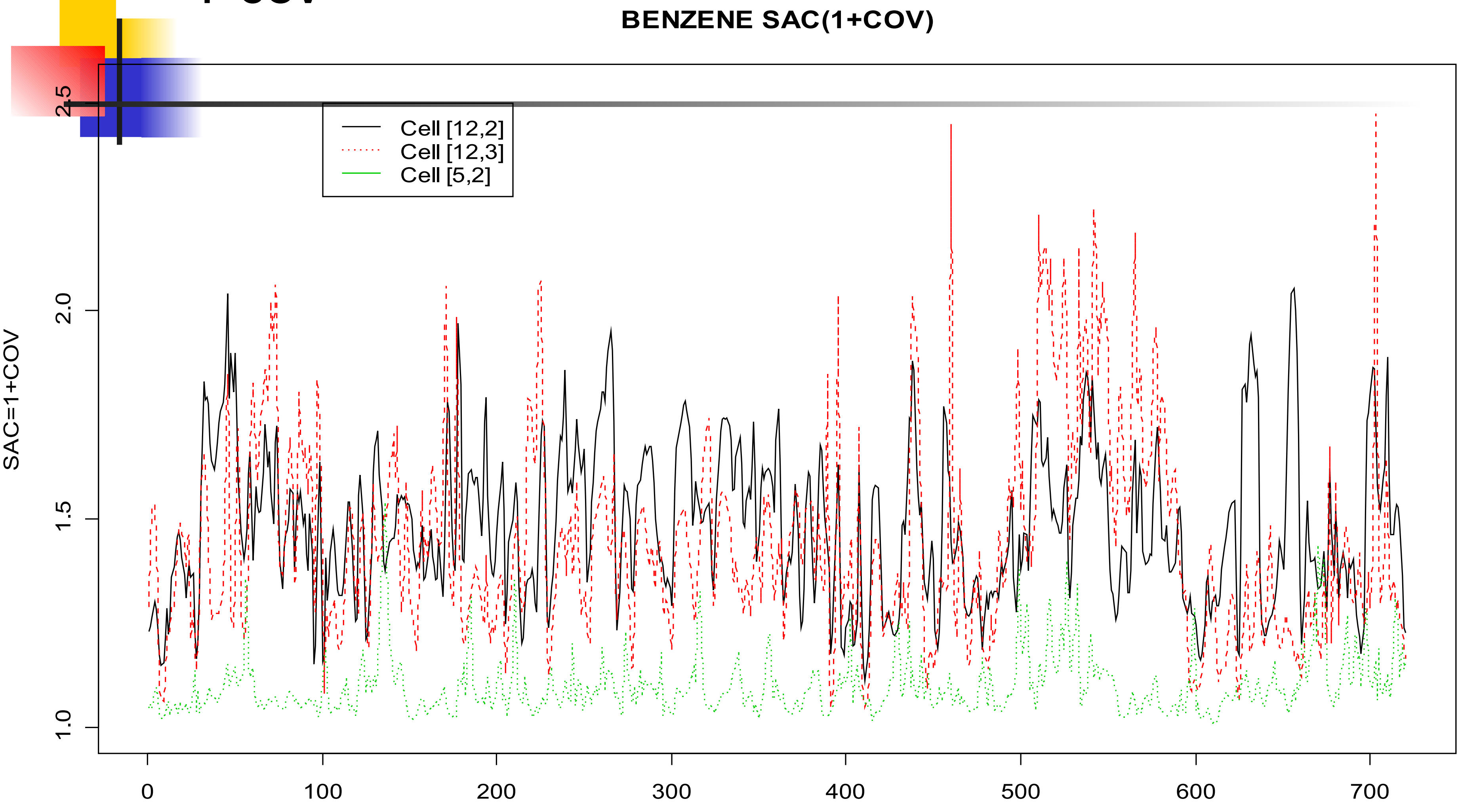




Benzene (ppb) (July 2001) Wilmington,DE

Black(A) **A** Red(B) **B** Green (C) **C**

1+COV

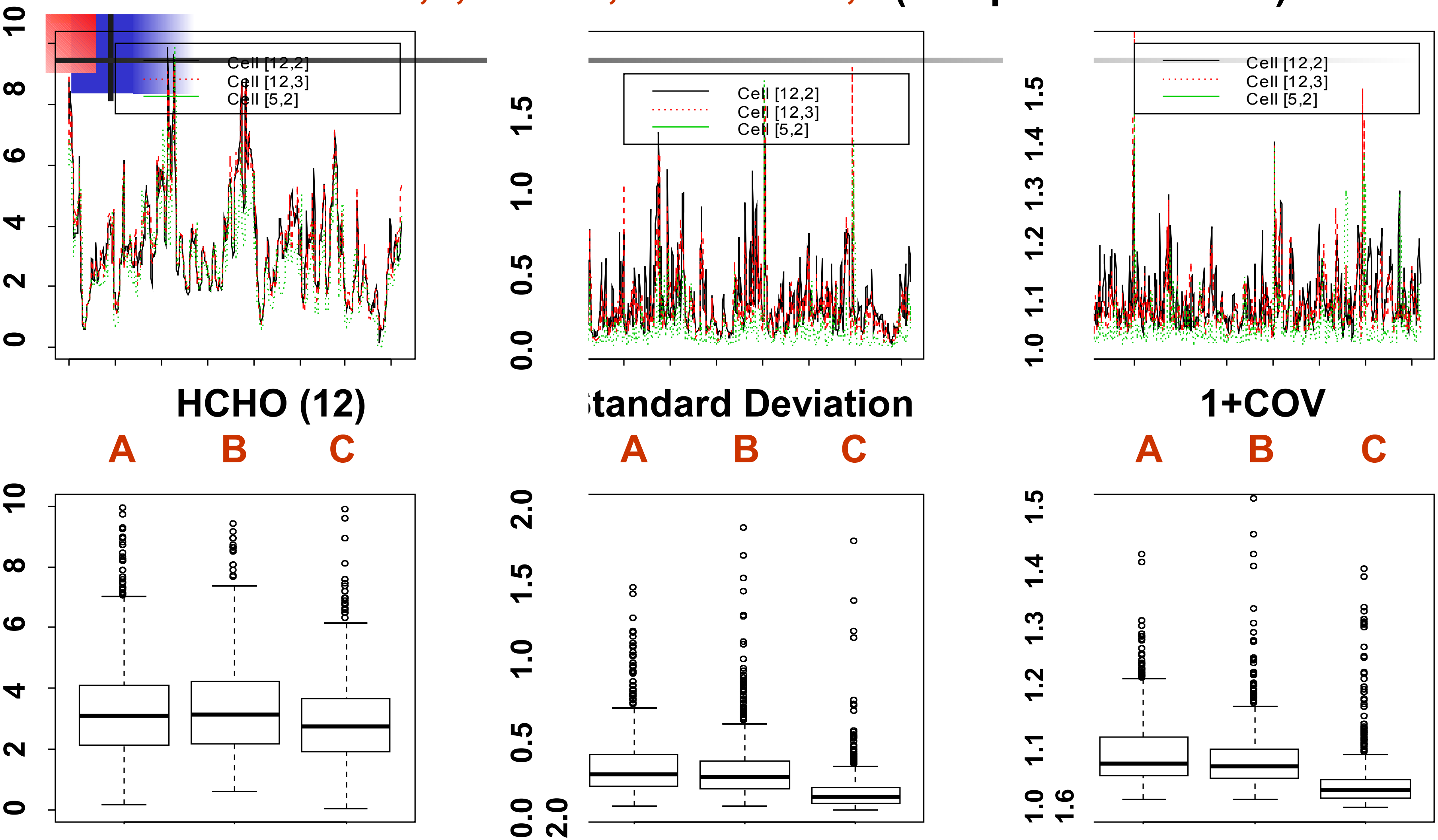


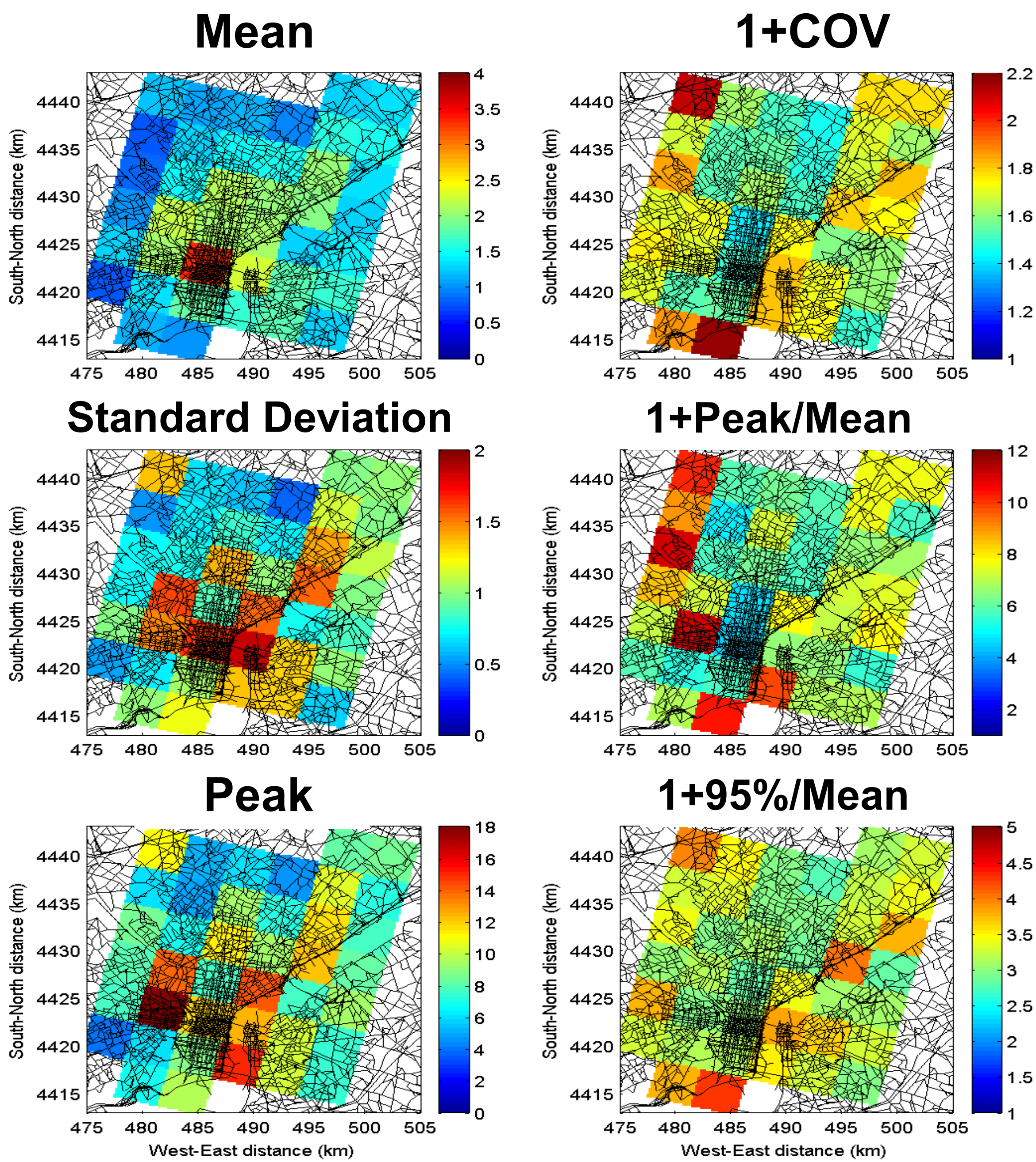
Jul 1 4 8 12 16 20 24 28 Aug 1

Time series & Box plots for HCHO

CMAQ(12), Std Dev, SAC factor (COV)

Grids A: 12,2; B: 12,3 and C: 5,2 (see previous slide)





PHILADELPHIA COUNTY

CMAQ Annual (2001) simulation of Benzene (ug/m3) using 4 km grids

SGVs & SAC factors are derived from ISCST3 model. Road links are shown as background.

COMMENTS:

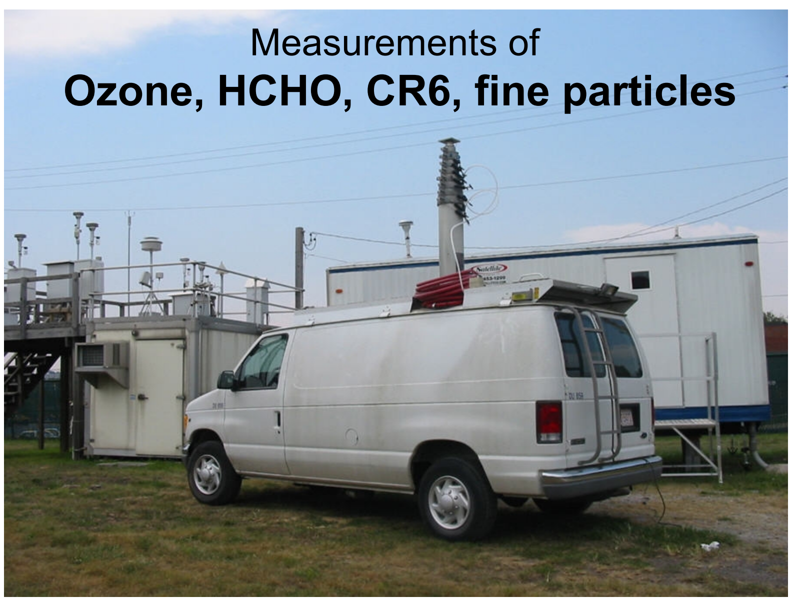
CMAQ: Range of variability from 0-4 ug/m3

SAC factor:

(1) Not necessarily spatially correlated with gridded CMAQ results
(2) COV > 2X gridded values
(3) Peak/Mean > 10 X Mean
(4) 95th percentile ~5X Mean

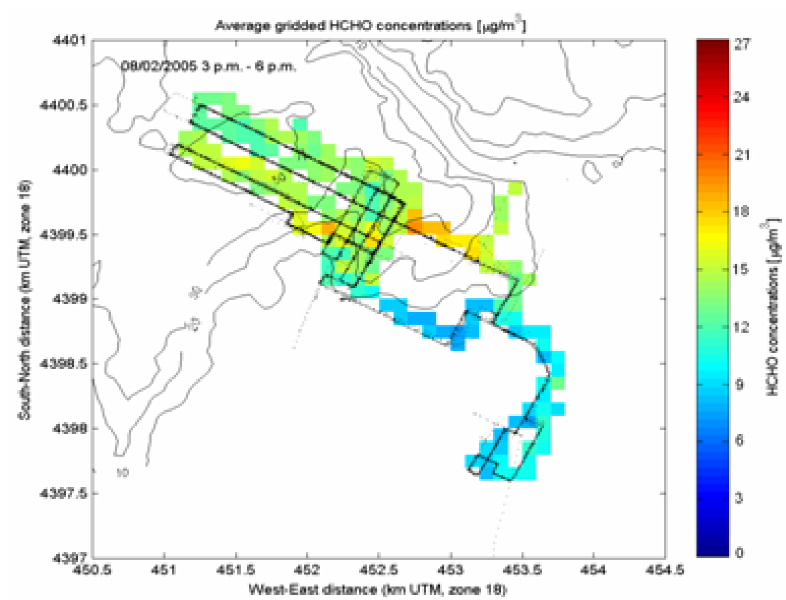
A rich database of air toxics measurements to provide:

(2) Better understanding of the micro-level air quality impacts of emission sources.
(2) Enhanced spatial resolution of the ambient toxics dataset through city and variability at spatial scales of order 100m by *mobile* measurements
(3) Means to evaluate our hybrid approach

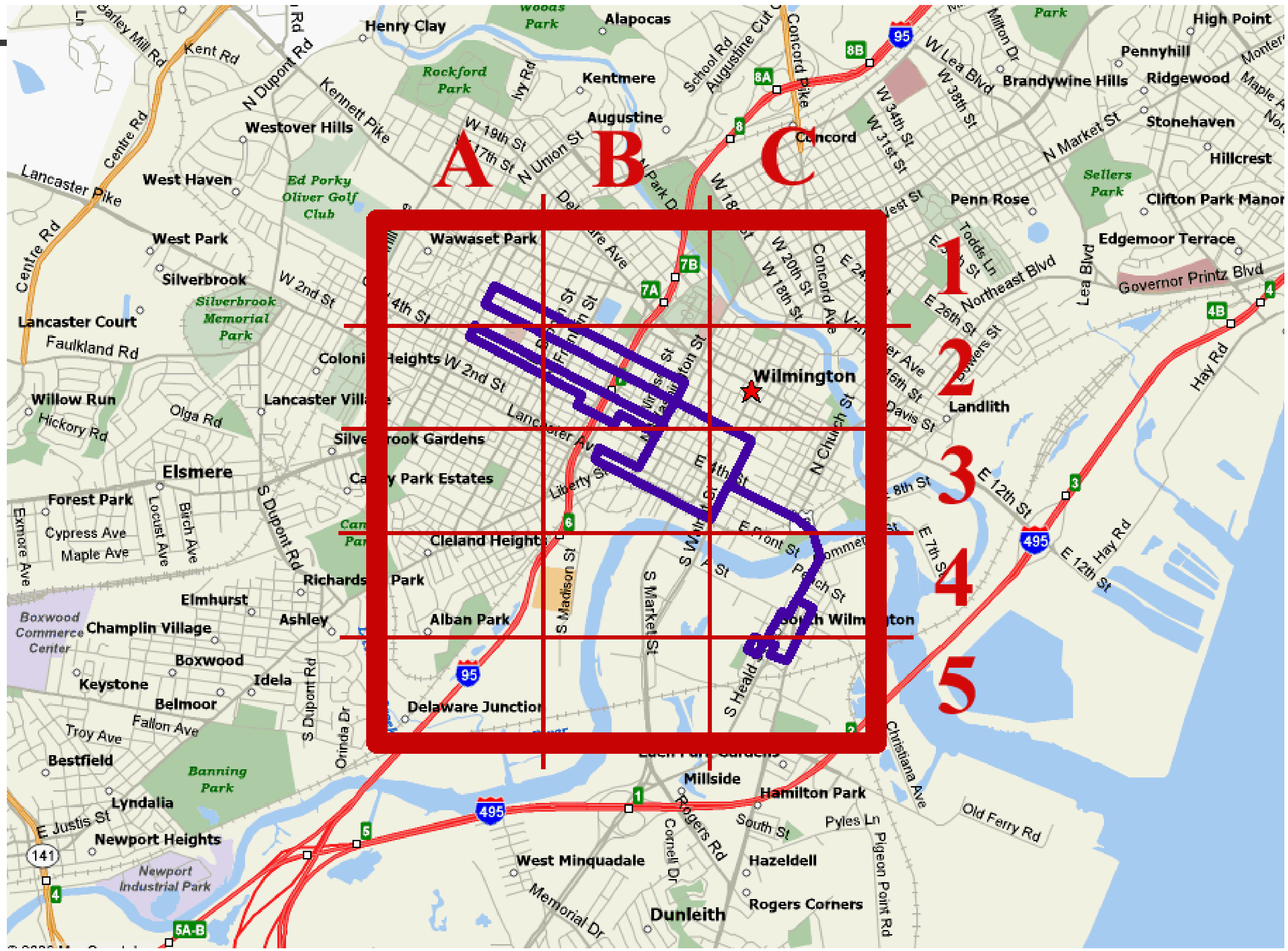


Spatial distribution of HCHO:

4 km Domain (Afternoon of August 2, 2005.)

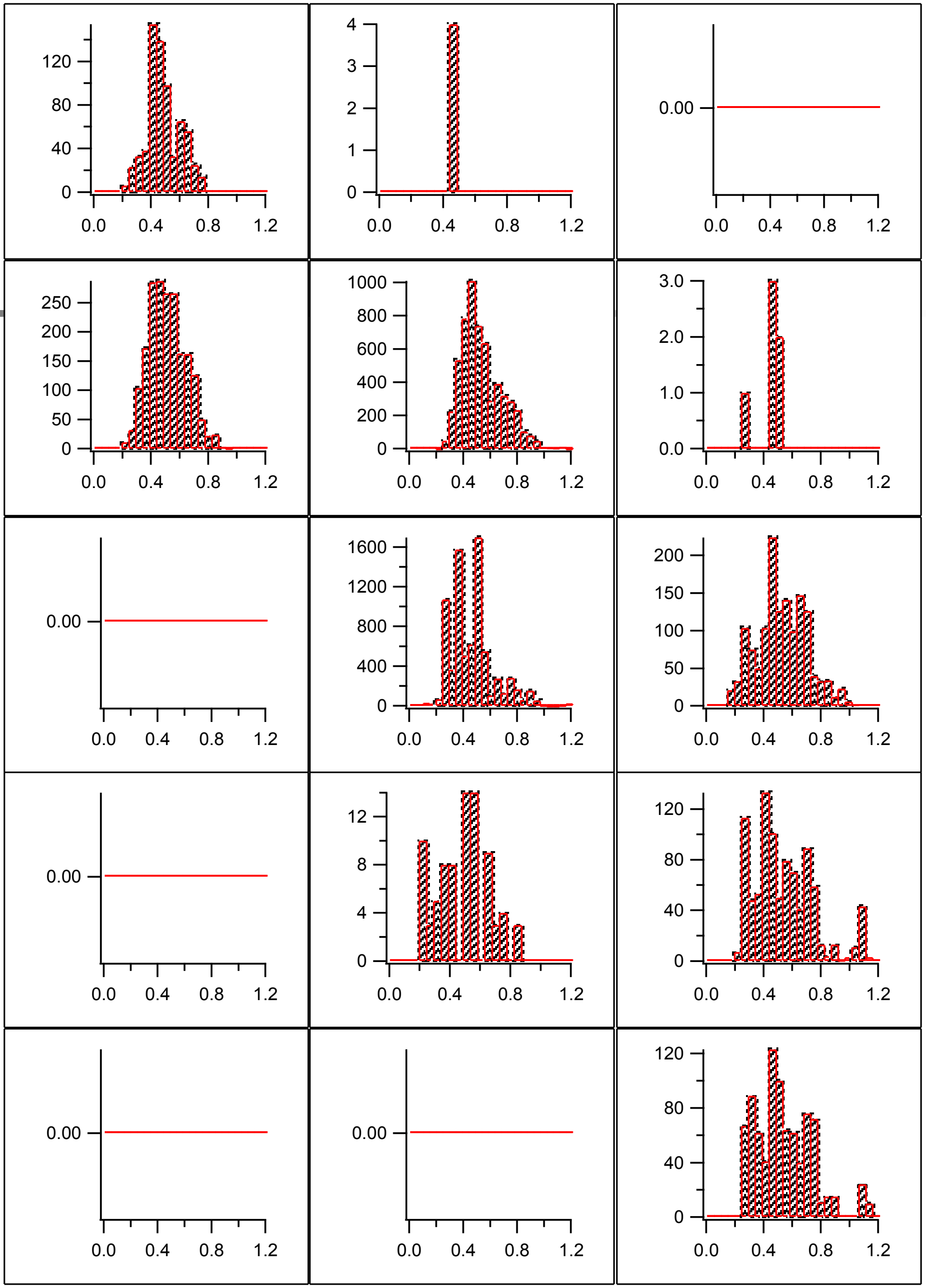


Grids for concentration distribution at neighborhood scales

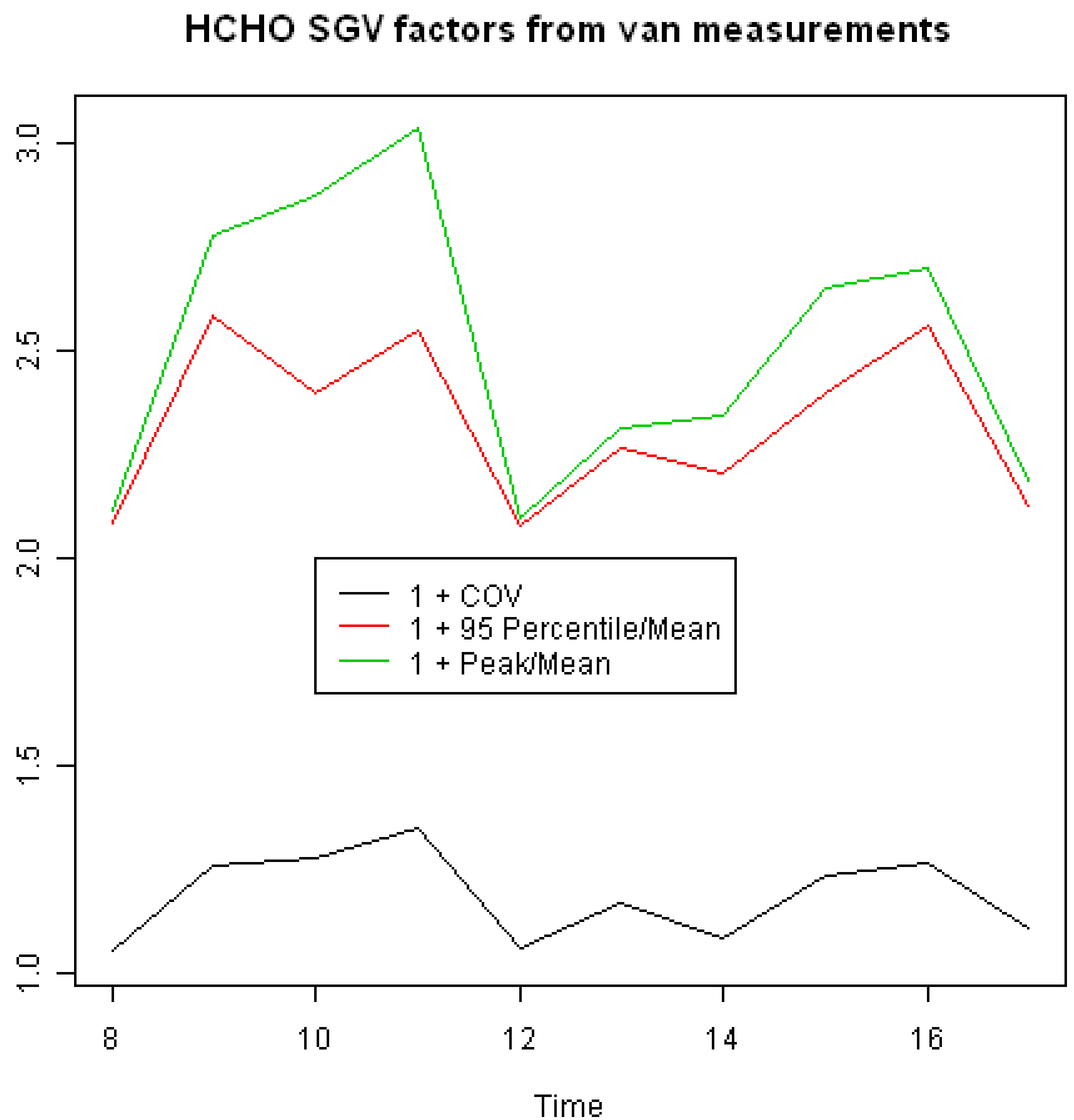


Neighborhood scale variability of formaldehyde (summer 2005)

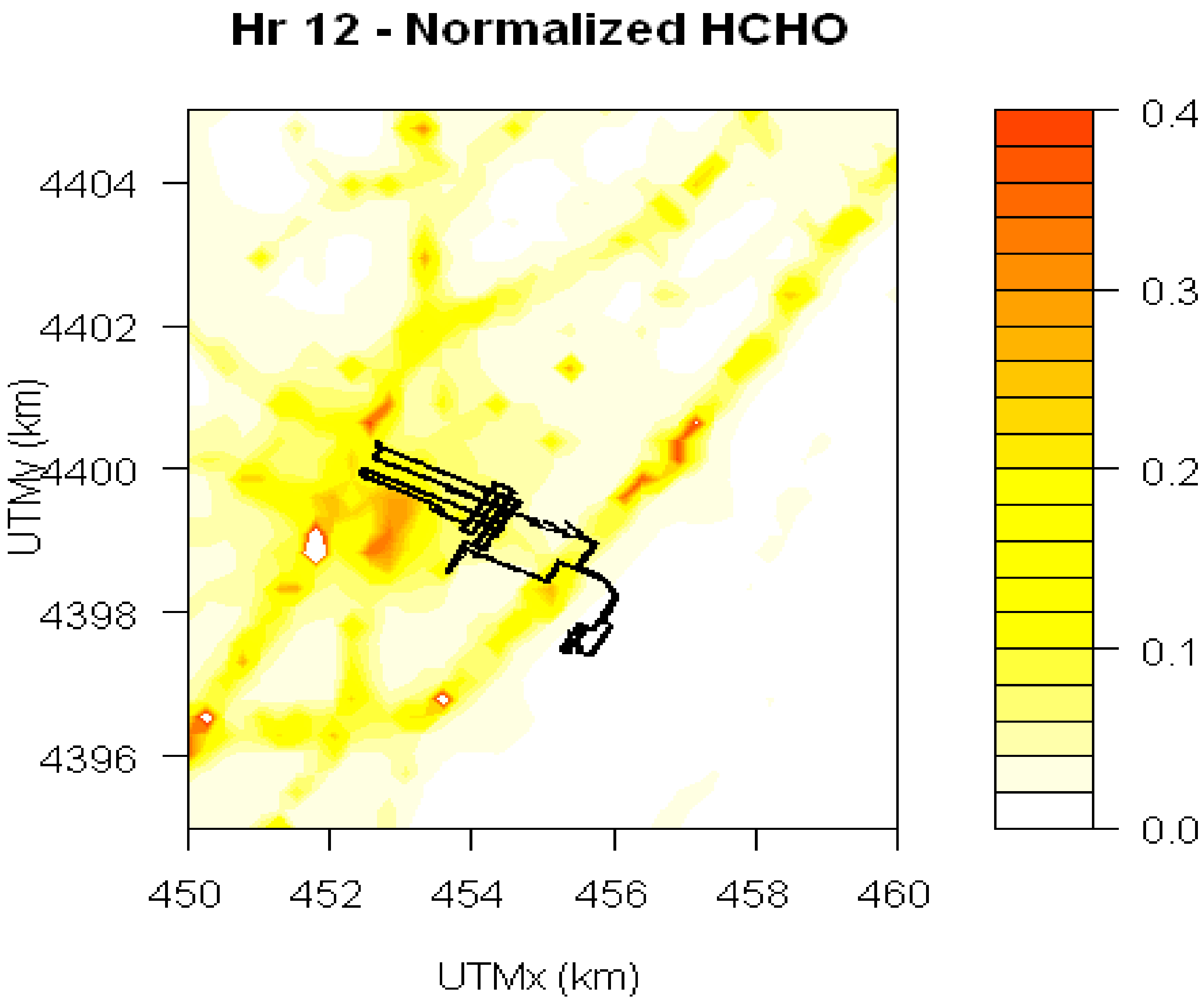
- The X-axis shows the concentration of HCHO in $\mu mol/m^3$
- The Y-axis shows the number of observations.



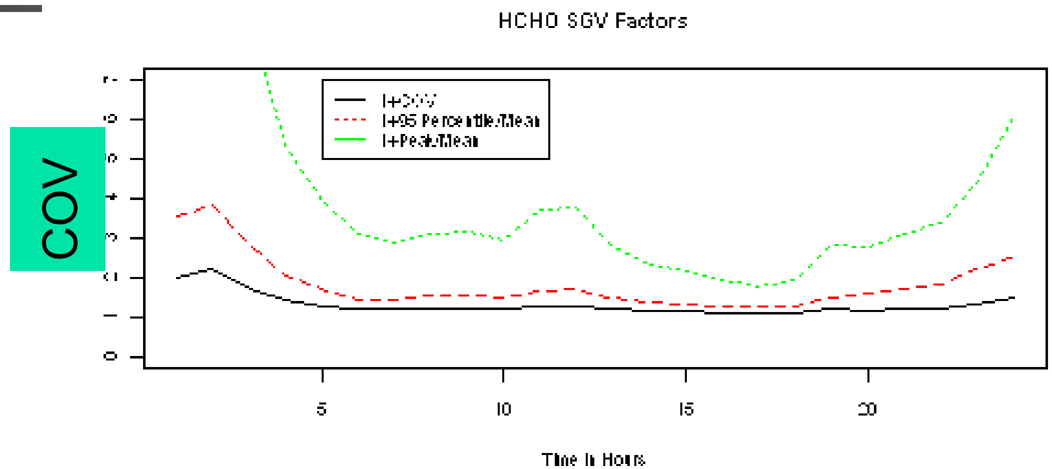
Factor f_1 based on van measurements for summer 2005 campaign

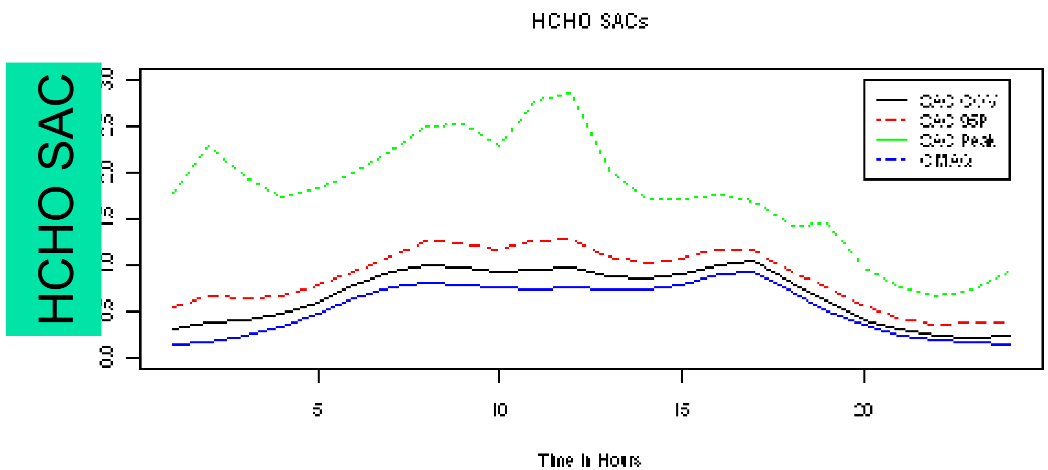


Example of local contributions of HCHO using AERMOD for the hybrid approach



Factor f_1 based on AERMOD modeling for a 4x4 km cell over Wilmington, DE





SUMMARY

- **SGV**
  - **an inherent property of all grid models**
  - **Varies with grid size**
- **SAC**
  - **A method to incorporate SGV results with CMAQ.**
  - **SGV factors f_1 can be based on fine-scale CMAQ, local-scale modeling, or from measurements.**
  - **Characteristics SAC factors varied for different:**
    - **pollutant species**
    - **emission densities and mixtures**
    - **grid sizes**
    - **averaging periods**
    - **Lambda – application dependent**