CMAS Workshop, September 20, 2005

Session 5: Urban/Regional Model Applications and Evaluation

Incorporating Sub-Grid Variability Concentration Distributions with CMAQ

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Synopsis of Presentation

- **Given: SGV is an inherent property of all grid models.**
- **Discuss Method to Introduce Sub grid Variability (SGV) into CMAQ simulations for use in Exposure Assessments and other Applications**
- **Sample Illustrative Results**
  - **Philadelphia 4 km: 2001 annual study**
  - **Delaware 12 km: Episodic (July 2001)**
  - **Houston 4 km study: Episodic (Texas 2000)**

METHODOLOGY

Definitions:

C_g	CMAQ grid cell simulation
C_{SGV}	SGV for each CMAQ grid
SAC	SGV adjustment to C_g
$f(C_{SGV})$	Weighting function or SAC Factor

Apply a SGV weighting function to C_g to produce:

"SGV Adjusted Concentration" defined as:

$$SAC = C_g * f(C_{SGV}) \quad (1)$$

For this study, we propose a SAC factor such that

$$f(C_{SGV}) = 1 + (C_{SGV}) / C_g \quad (2)$$

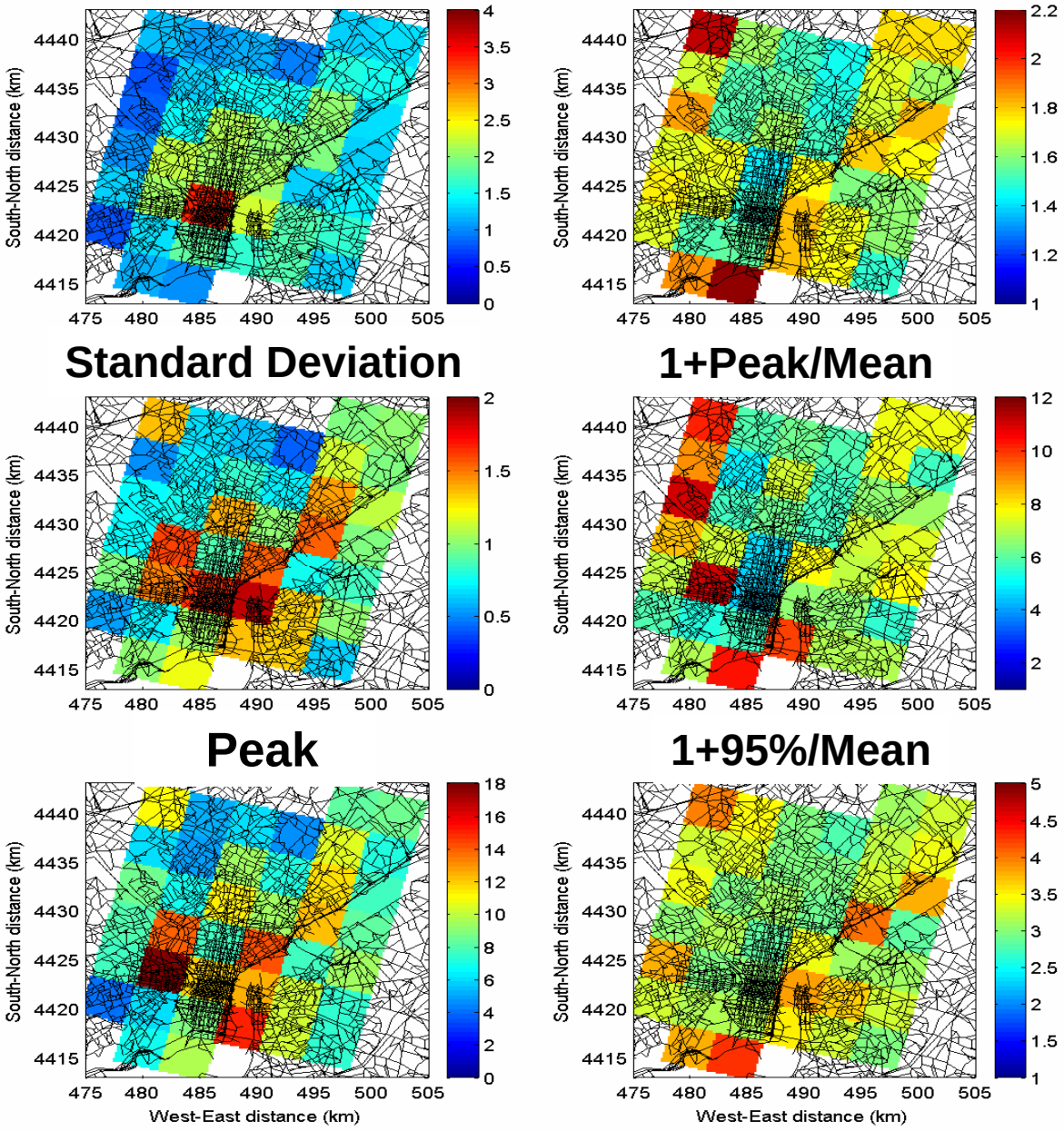
Suggested C_{SGV} options include but not limited to:

- Standard Deviation
- 95th Percentile of the distribution (or other percentile values)
- Peak (or range)/cell mean.

Examples: Preliminary Results

- **Annual simulations of CMAQ-AT**
  - **For Exposure Assessment exercise**
  - Philadelphia Study (2001) CMAQ-AT simulation (w/ CBIV)
  - 36 km, 12 km, and 4 km one-way nested runs
  - **4 km gridded SGVs & SAC factors based upon local scale modeling**

- **Episodic simulations**
  - **Delaware** Study (July 2001) CMAQ-AT
    - 36-12-4-1 km one-way nested simulations
    - **12 km gridded SGVs, SAC factors from 1 km CMAQ simulations**
  - **Houston** (Texas 2000): 8/22-9/2, 2000) CMAQ-AT
    - 36-12-4-1 km one way nested simulations
    - **4 km gridded SGVs, SAC factors from 1 km CMAQ simulations**



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

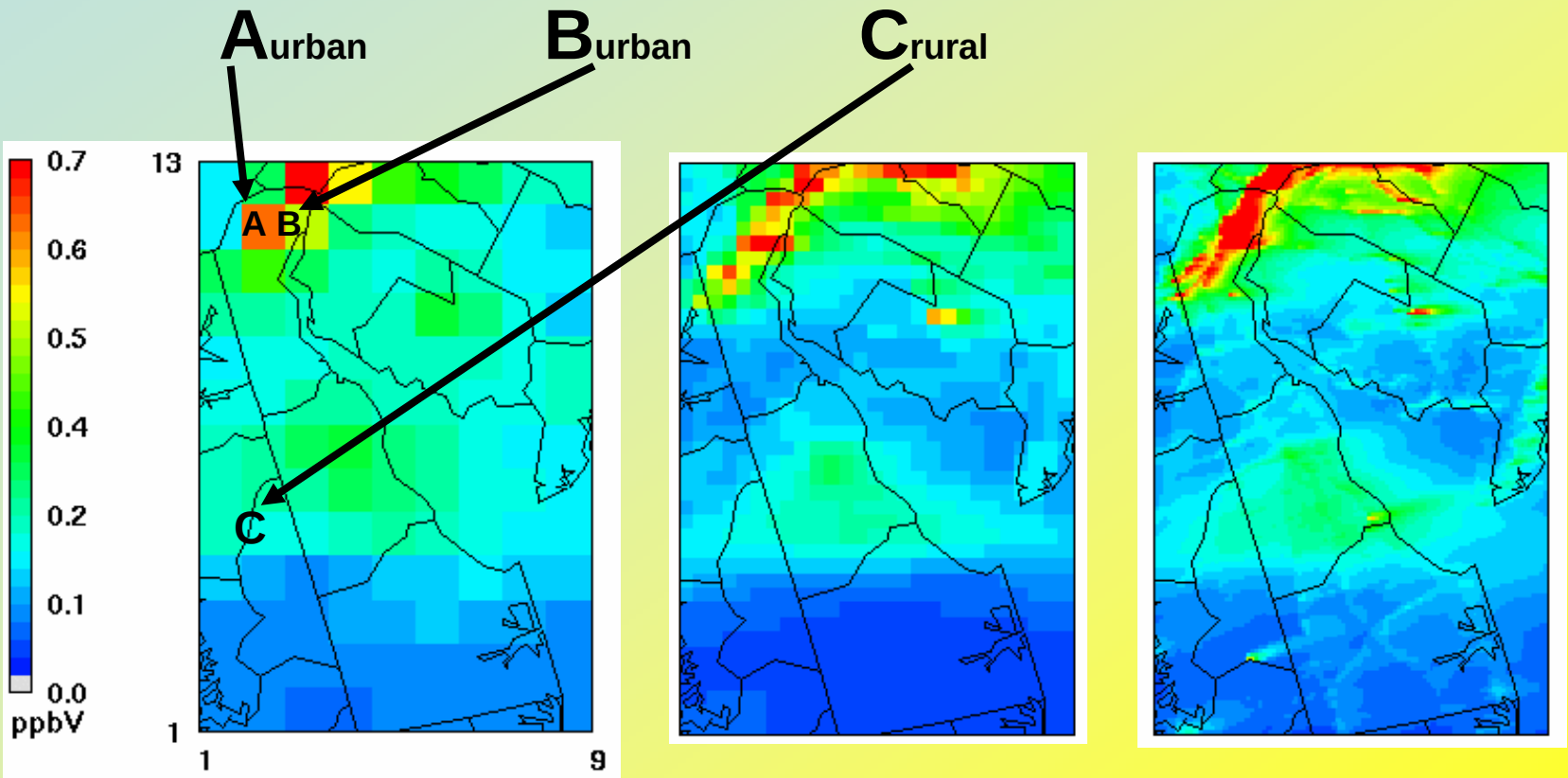
SAC factor:

(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

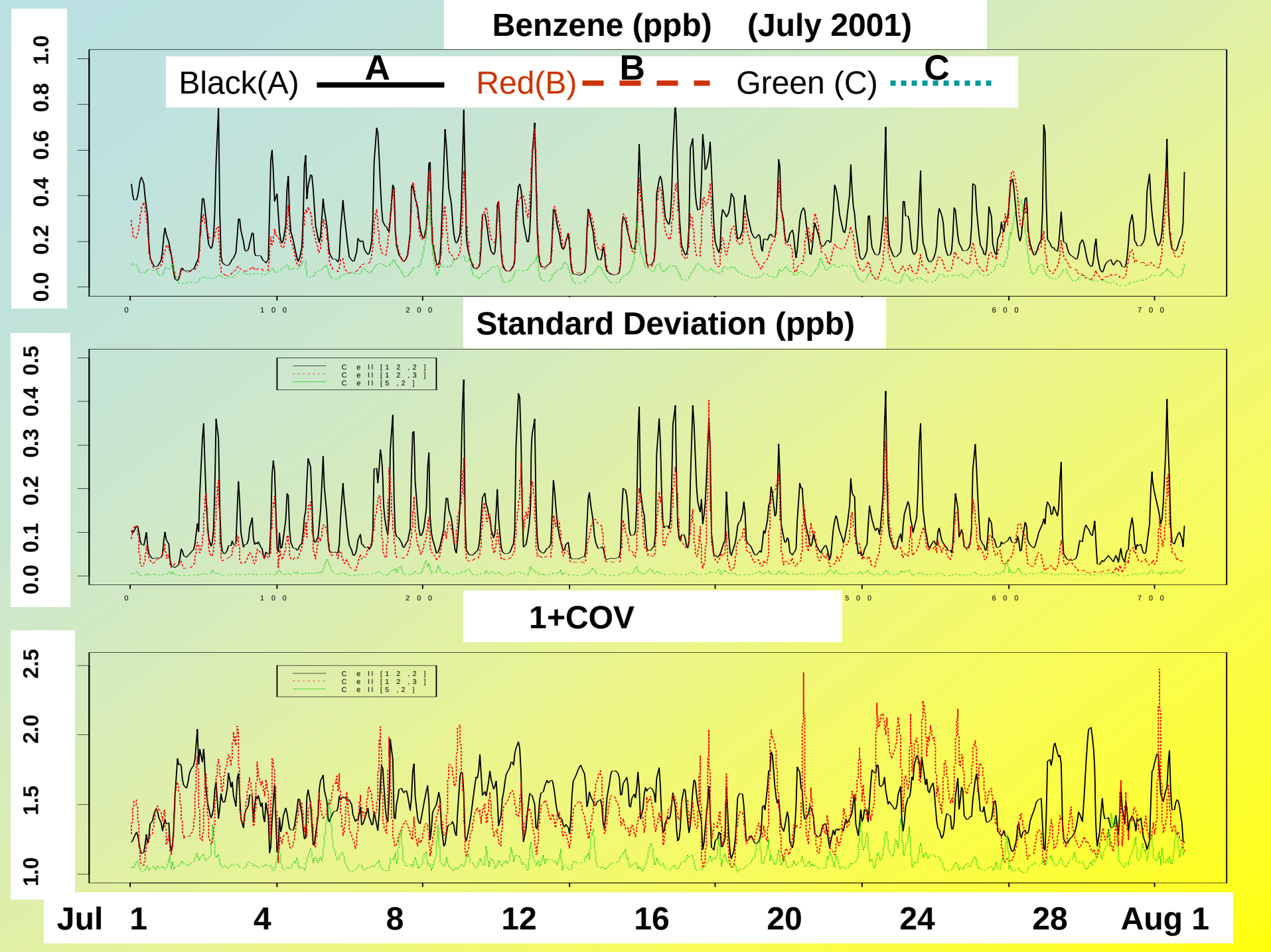
Delaware Episodic Modeling Study

Benzene

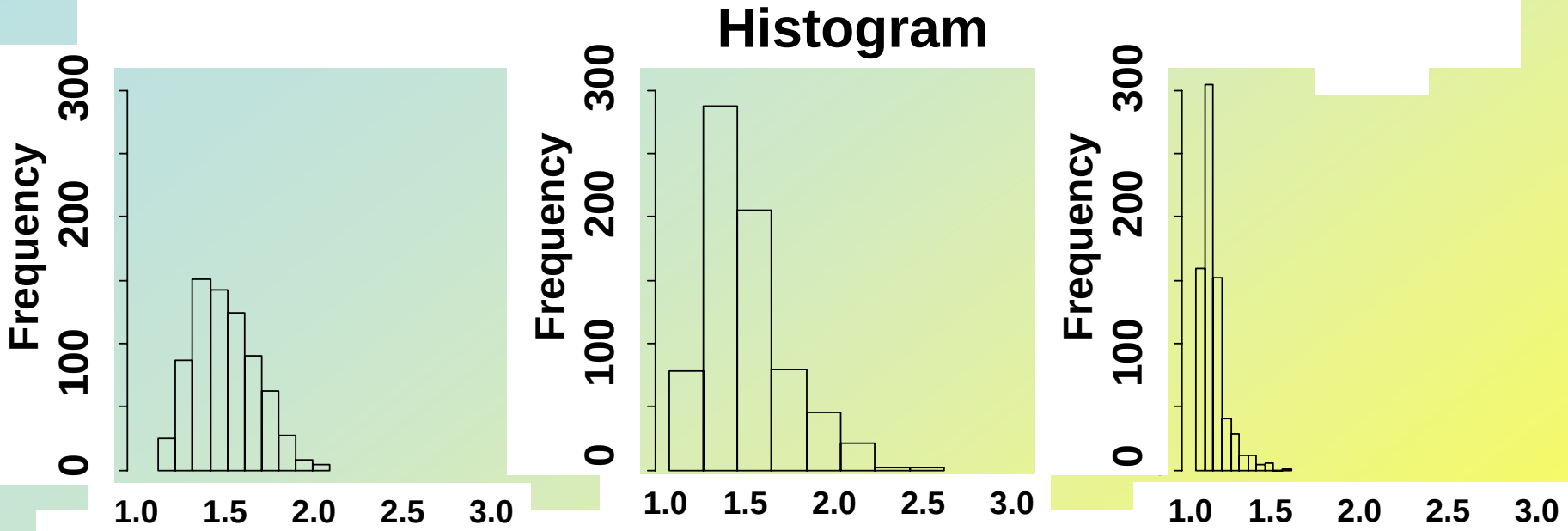
16th July 2001 at 11:00 UTZ

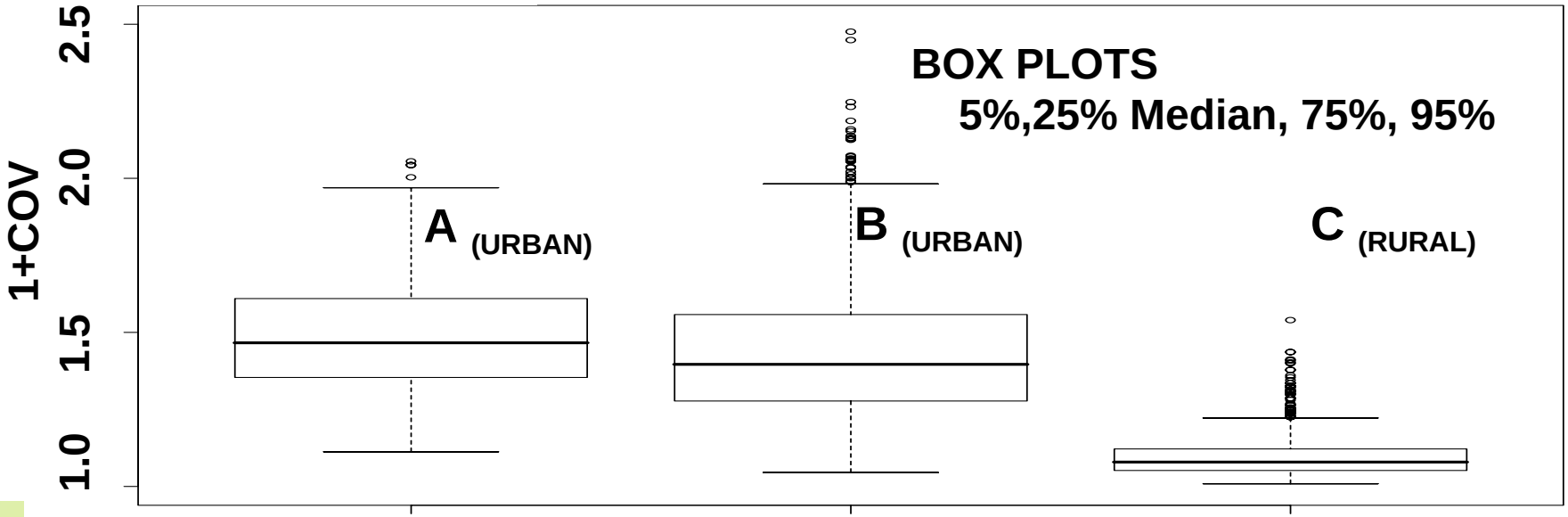


(A) 12 km **(B) 4 km** **(C) 1 km**


Benzene (ppb) (July 2001)
Black(A) A
Red(B) B
Green (C) C
0.0 0.2 0.4 0.6 0.8 1.0
0 100 200 600 700
Standard Deviation (ppb)
0.0 0.1 0.2 0.3 0.4 0.5
0 100 200 500 600 700
1+COV
1.0 1.5 2.0 2.5
Jul 1 4 8 12 16 20 24 28 Aug 1

Benzene (July 2001) 1+COV

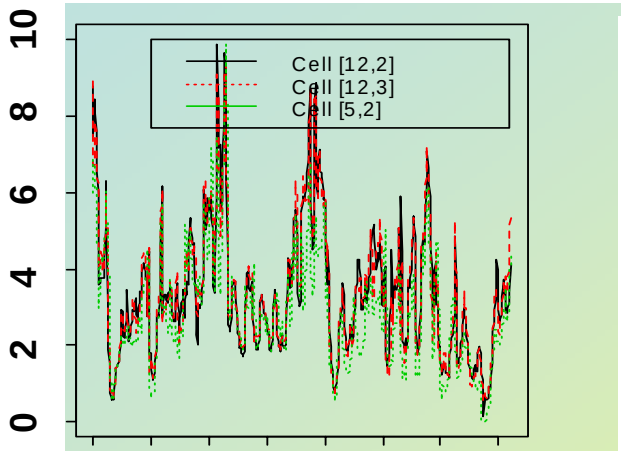




Time series & Box plots for HCHO

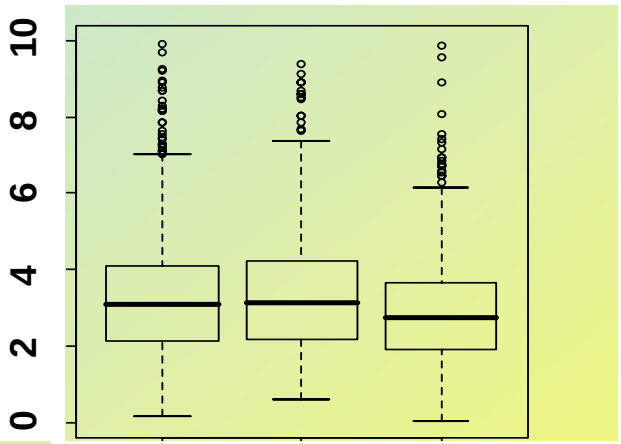
CMAQ(12), Std Dev, SAC factor (COV)

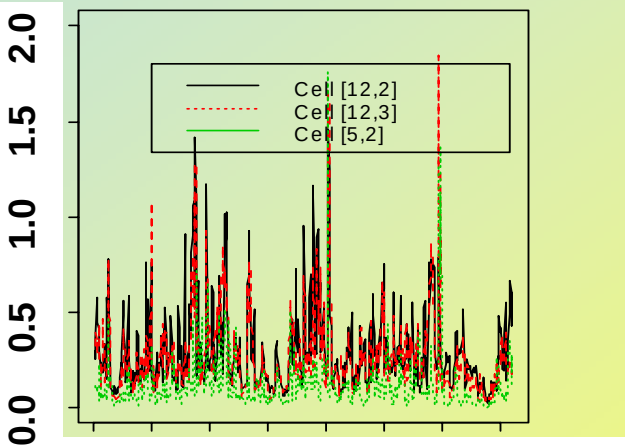
Grids A: 12,2; B: 12,3 and C: 5,2 (see previous slide)



HCHO (12)

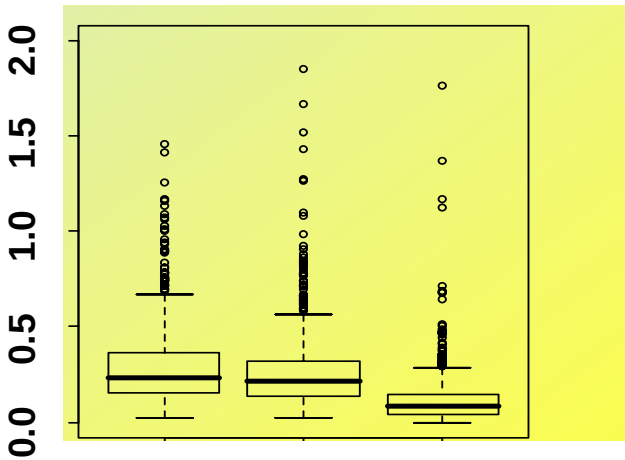
A B C

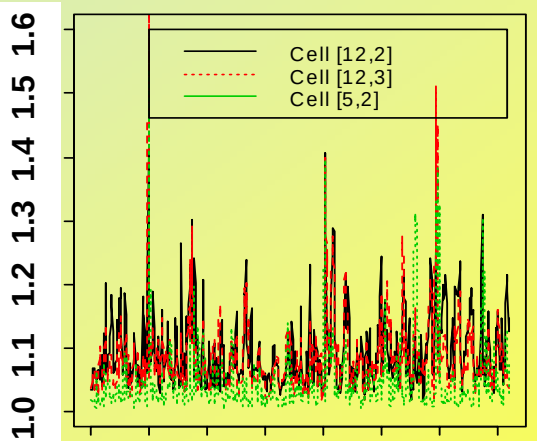




Standard Deviation

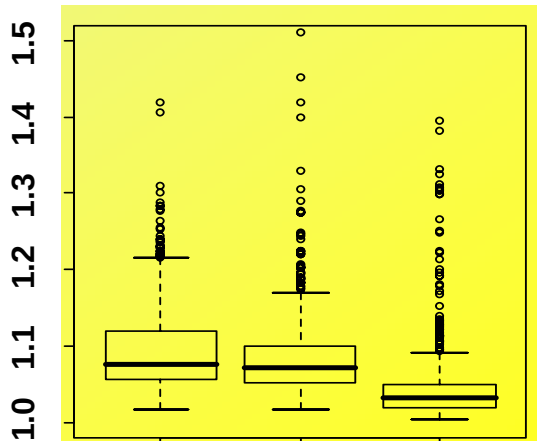
A B C





1+COV

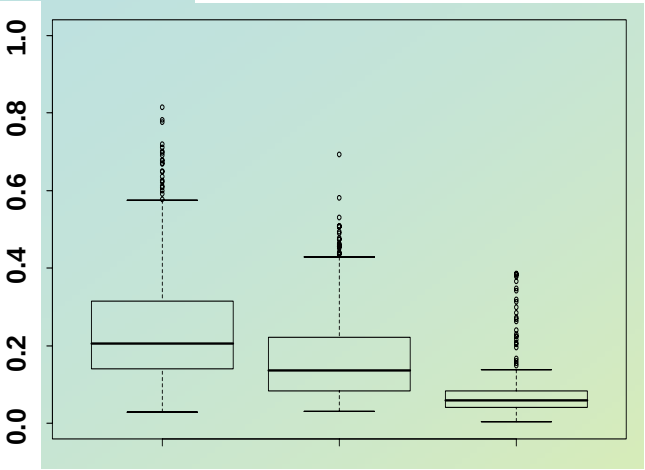
A B C



Box Plots for Benzene and Ozone

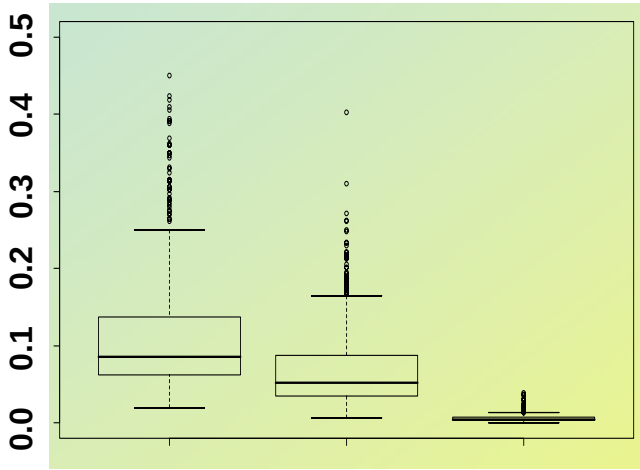
CMAQ (12), Std Dev, SAC factor (COV)

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



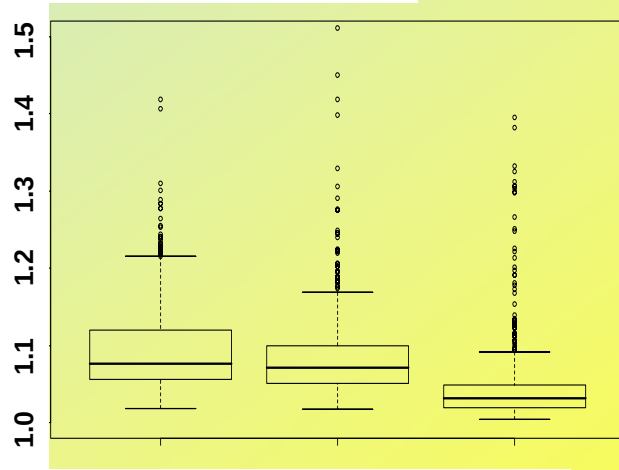
Benzene (12)

A B C



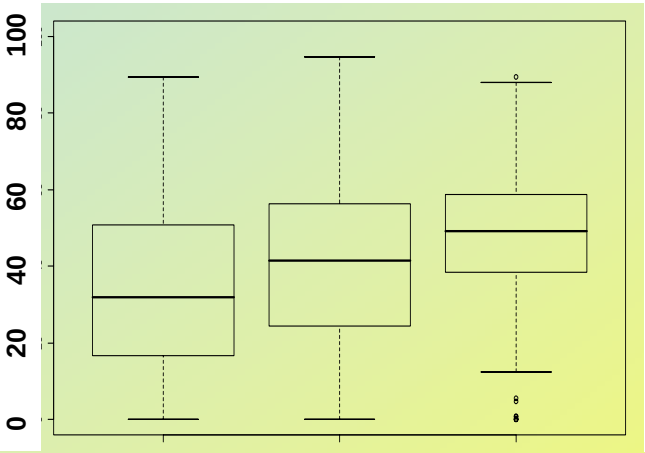
Standard Dev

A B C

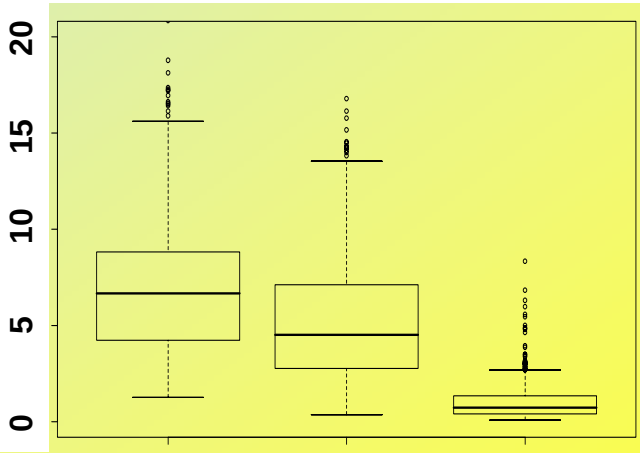


1+COV

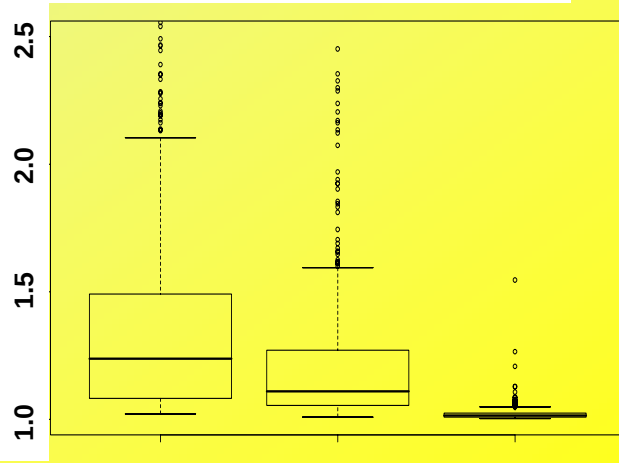
A B C



Ozone (12)



Standard Dev



1+COV

Points of Delaware Study

- Introduced SGV factor as 1+COV

- Characteristics of SAC Factors
  - Urban typically greater than rural
  - SAC factors for pollutant species
    - HCHO 1+COV
    - Median < 10%
    - 95th %tile < 20%
  - Benzene
    - Median < 10%
    - 95th %tile < 20%
  - Ozone
    - Median < 20%
    - 95th %tile < 100%

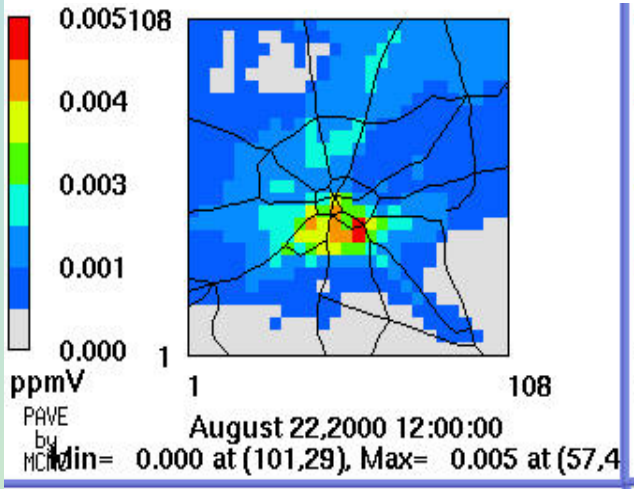
  - Distribution above 95th %tile varied
    - By pollutant species
    - By grid location

Preliminary Results: Houston, TX

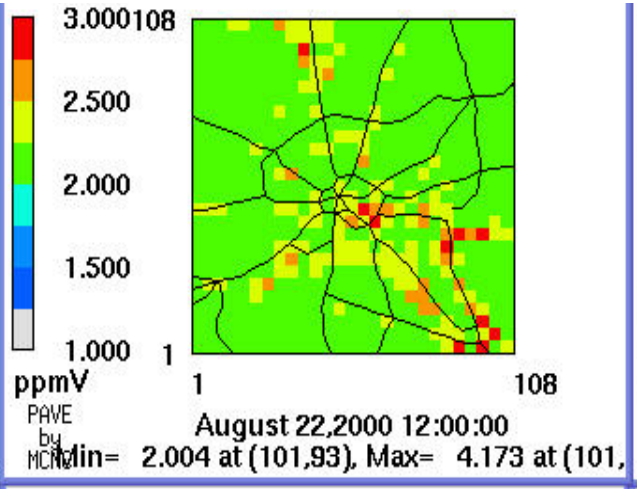
- Episodic CMAQ-AT simulations (w/SAPRC-99 with 23 toxics species)
- 36 km, 12 km, 4km and 1 km one-way nested MM5 and CMAQ simulations; Day specific diurnal SST in MM5, including Galveston Bay
- 4 km gridded SGVs & SACs based on 1 km CMAQ outputs
- Presentation of CMAQ and SACs for the species:
  - CO: Primarily inert mobile source toxic
  - Formaldehyde: Photochemically active air toxic
  - Ozone: Photochemical oxidant
  - Also: Benzene, Acetaldehyde and 1-3 Butadiene

Houston: 4 km Results HCHO (8/22, 2000@ 12Z)

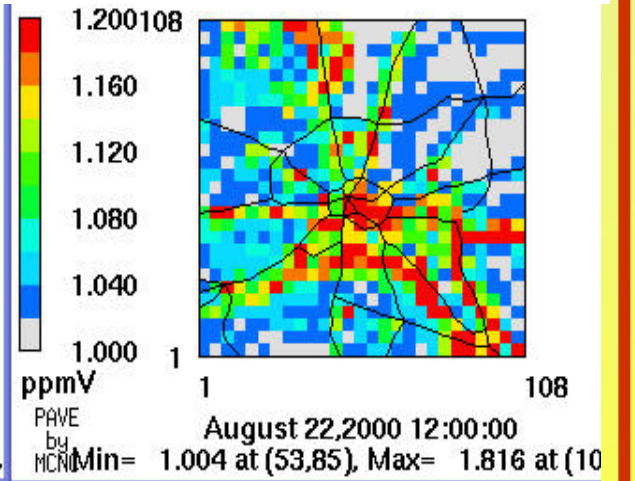
HCHO



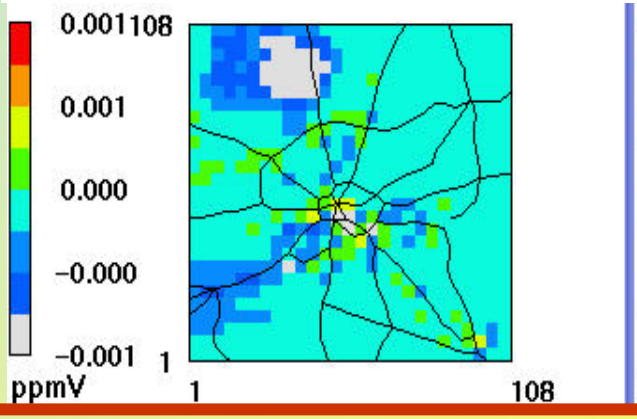
1+Peak/Mean



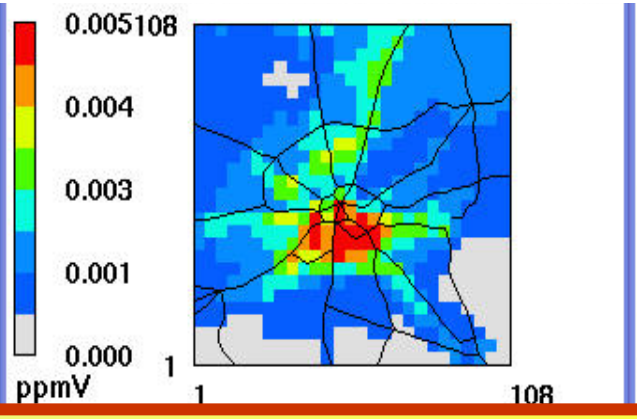
1+COV



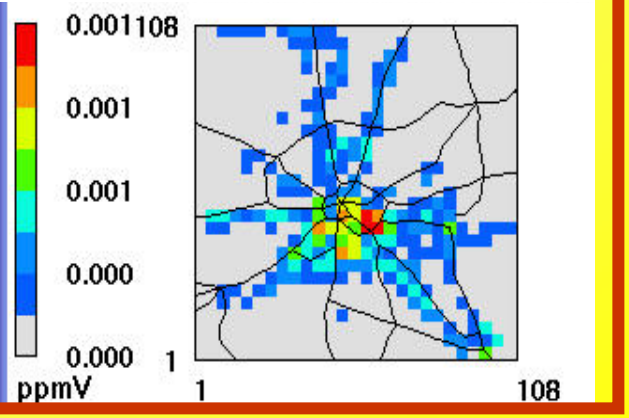
Mean-4 km Parent



Peak



Standard Dev

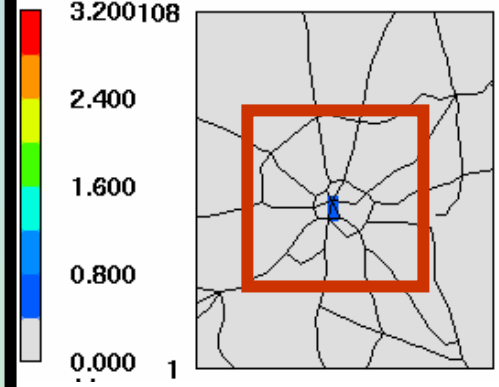


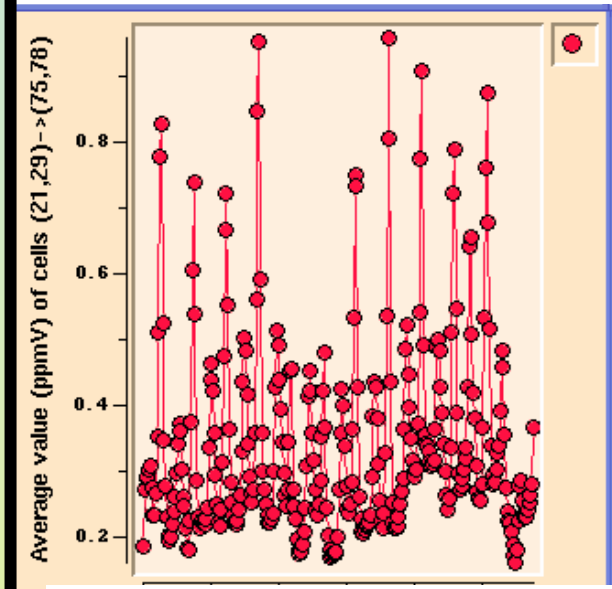
NOTES ABOUT HCHO

- Regional contributions can be significant
- SACs are under predicted.
  - Since much of the variability is from primary sources, needs local scale modeling to obtain more representative SACs
- Comparative:
  - Highest values of Concentration, Peak, Std Dev in urban area
  - Highest values of SACs are distributed throughout domain
- SACs Domain results
  - COV of order 10%
  - Peak/Mean of order 20%
- SACs cell by cell results
  - COV of order >20%
  - Peak/Mean of order > factor of 2

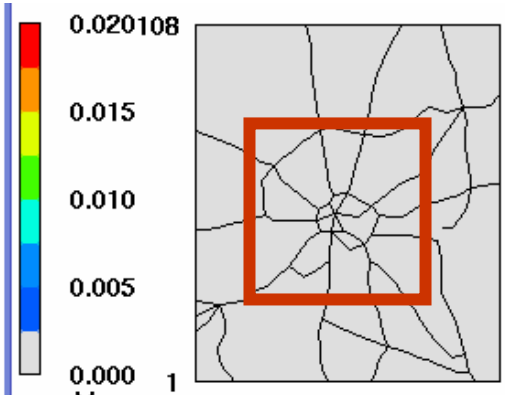
CMAQ (4km parent) for Small Domain (Central Houston)

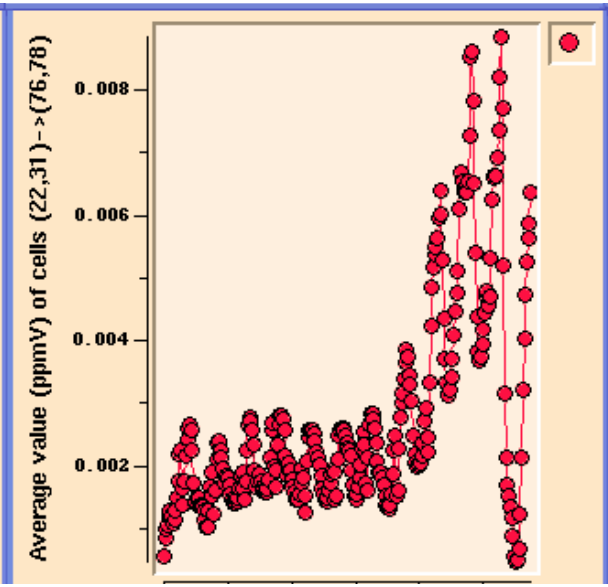
CO



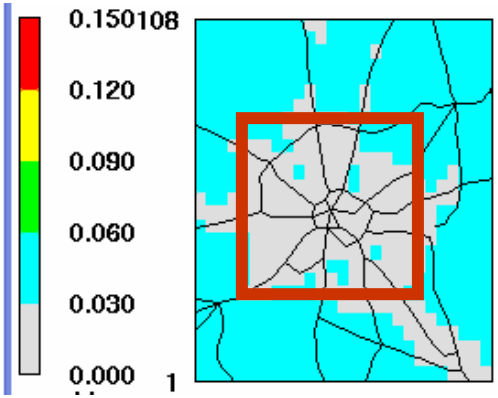


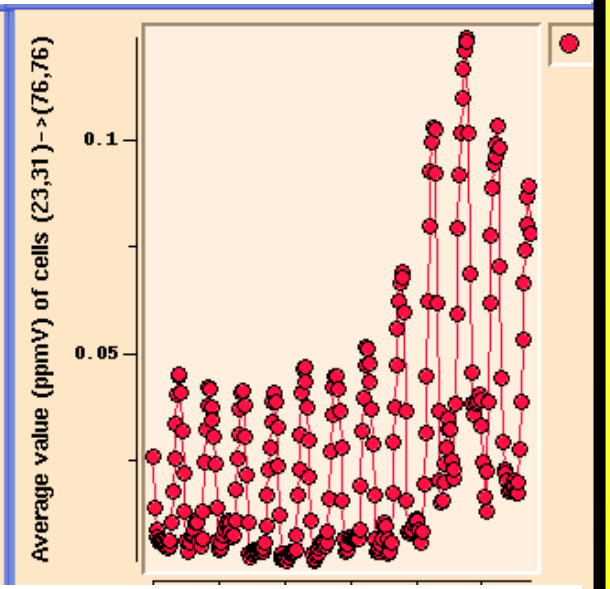
HCHO





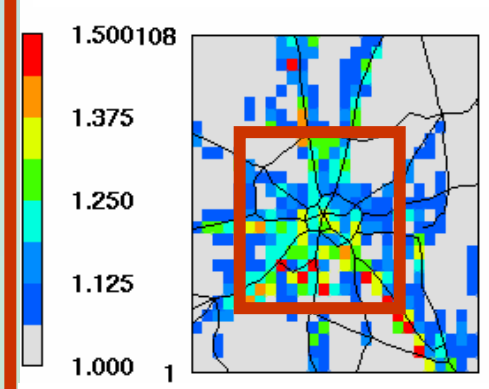
Ozone

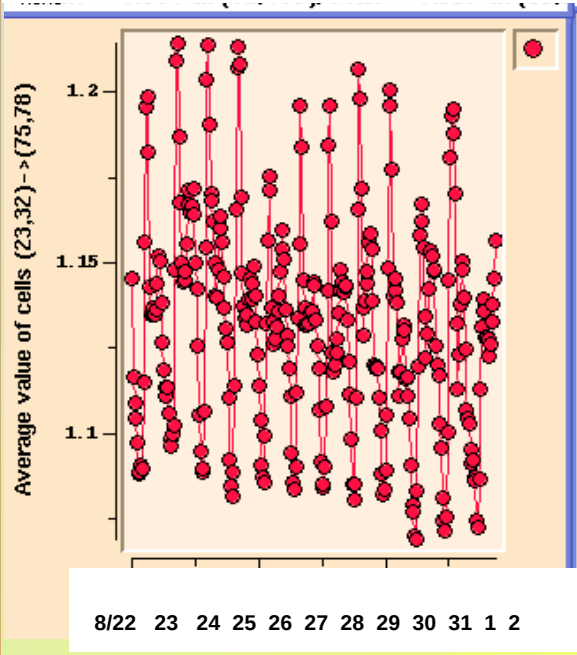




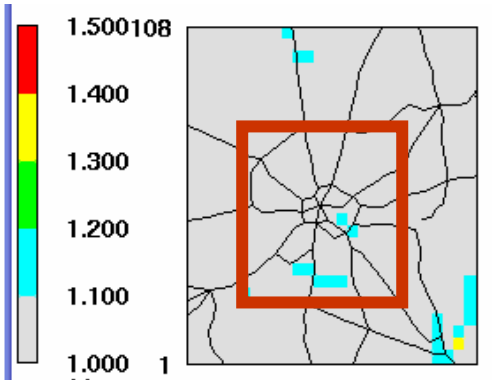
(1+COV) for Small Domain (Central Houston)

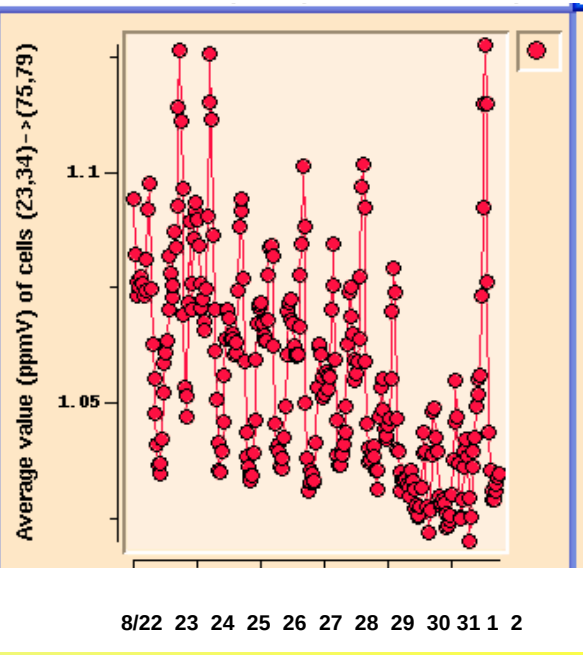
CO



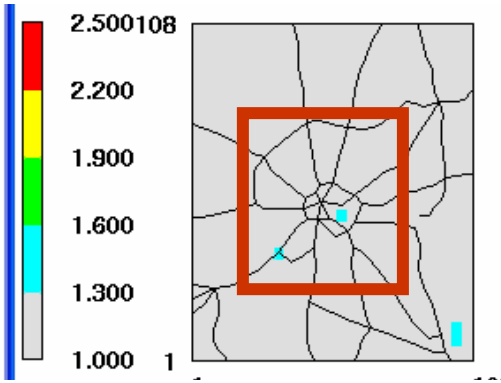


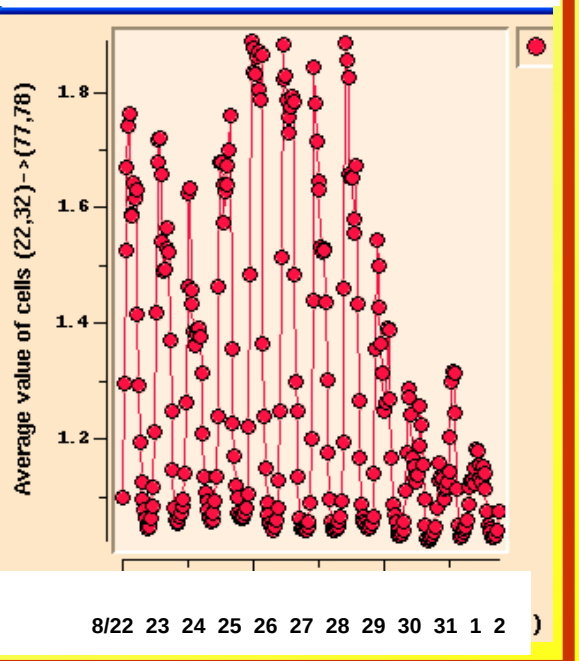
HCHO





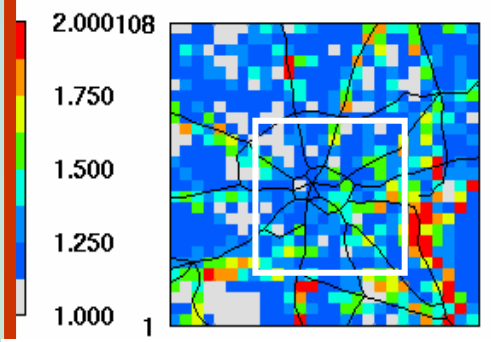
Ozone

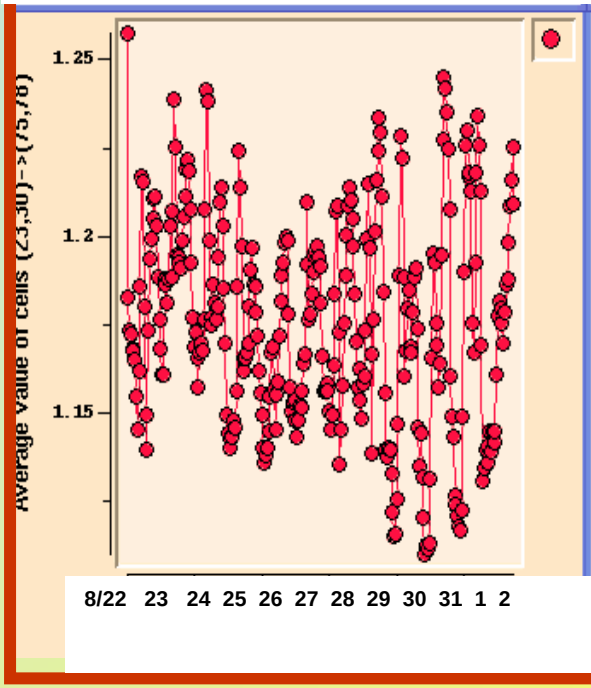




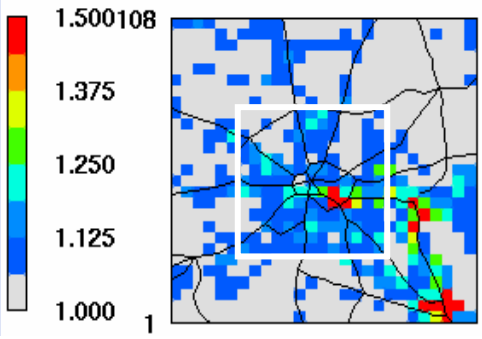
1+COV for small domain (Central Houston)

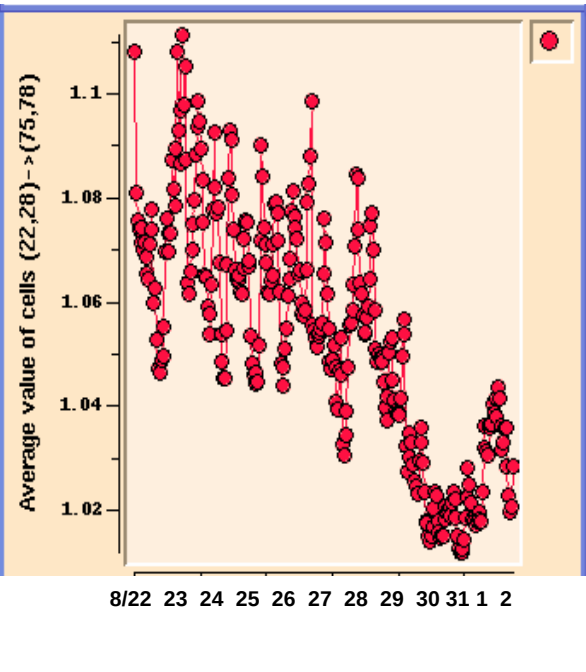
Benzene



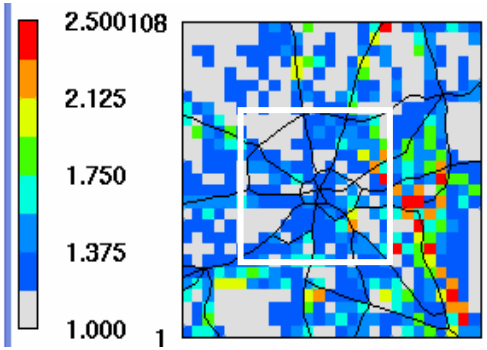


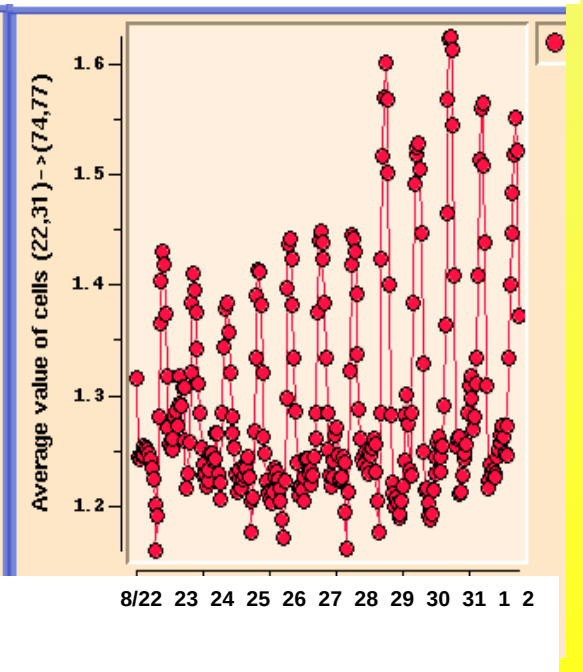
Acetaldehyde





1-3 Butadiene





NOTES: 12 Day (small domain) sequence

- **CO**
  - Diurnal variability significant
  - Temporal trend weak
  - COV small domain order 15%
  - COV cell by cell order 50%

- **HCHO**
  - Diurnal variability varies over period
  - Temporal trend apparent- decrease over period
  - COV small domain 2% to 10%
  - COV cell by cell 10% to 50%

- **Ozone**
  - Diurnal variability dominant, amplitude decrease at end of period
  - Temporal trend weak
  - COV small domain order 10% with diurnal peaks >80%
  - COV cell by cell Night of order 150%; daytime 10-20%

SUMMARY

- **SGV is an inherent property of all grid models. Its properties vary with grid size. We seek effective ways to utilize SGVs for applications.**
- **SAC, an ad hoc suggestion/method to incorporate SGV results with CMAQ.**
- **Results of SAC and SAC factors are based on SGVs from local scale and fine scale CMAQ model simulations for episodic and annual simulations.**
- **Characteristics SAC factors varied for different:**
  - **pollutant species,**
  - **emission densities and mixtures,**
  - **grid sizes**
  - **averaging periods.**

Discussion and Implications

- **SAC factors can be significant; their characteristics and magnitudes differ for different pollutants**

- **Investigations needed to determine optimal and appropriate SAC factors for applications (not all SACs are equal) including:**
  - **Exposure, health risk assessments**
  - **Model evaluation**
  - **Weight of Evidence –RRF/DV(C&F) analyses for SIPS**

- **Improved SGVs are needed for more robust SACs to reveal more fully, the SGV contents at very fine scales (sub km grid resolutions)**
  - **Use of LESchem for SGVS due to fine scale photochemical-dynamics**
  - **Use of local scale modeling for primary, relatively inert species**
  - **Improved spatial resolution of emission inventories**
  - **Appraise and conduct evaluation studies**

- **Operations research needs: Develop operational parameterizations of SAC factors by space, by pollutant species, by grid size, by monitoring site, by hot spot areas, etc**
  - **Use of CDFware (Herwehe) for parameterizations**
  - **Histograms are time and space dependent; What is appropriate averaging times?**

Emerging opportunities for development and utilization of SACs
- **Highway Initiatives**
- **Exposure Studies**
- **Saturation monitoring projects**

Invitation to CMAS: Your interest and participation towards furthering developments on SAC methodology and to the propagating of their operational implementations and advanced applications.

Go SAC it to 'em

Thank you

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. Although it has been reviewed by EPA and NOAA and approved for publication, it does not necessarily reflect their policies or views.***