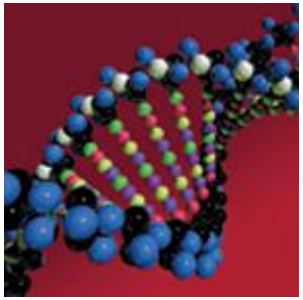
Fine-scale Modeling of Urban Toxics, PM and Ozone for Detroit using the CAMx and CMAQ Photochemical Grid Models


Greg Yarwood, Ou Nopmongcol, Tan Sakulyanontvittaya ENVIRON
Karen Wesson, US EPA

August 4, 2010

ENVIRON

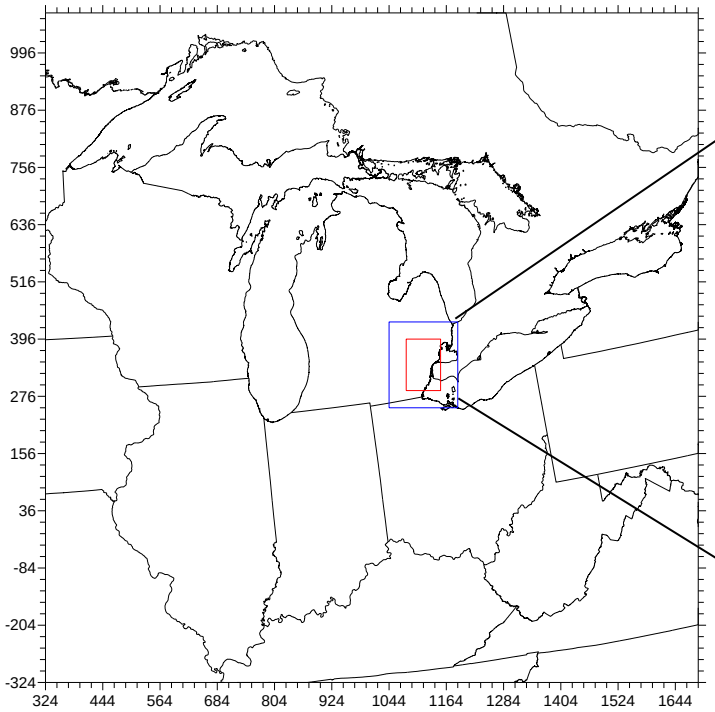
Detroit Fine-Scale Modeling

- Demonstrate and evaluate two grid models
  - CMAQ and CAMx
  - Grid resolutions as fine as 1 km
  - Plume-in-grid (PiG) with CAMx for ~500 point sources
  - Model January and July, 2002
  - EPA also has CMAQ/AERMOD hybrid model results
- Emissions and meteorology developed by EPA
  - SMOKE and MM5
- Photochemical modeling performed by ENVIRON
  - Special Toxics version of CMAQ
  - CAMx toxics modeled using RTRAC (reactive tracer) option
- EPA performing the model evaluation

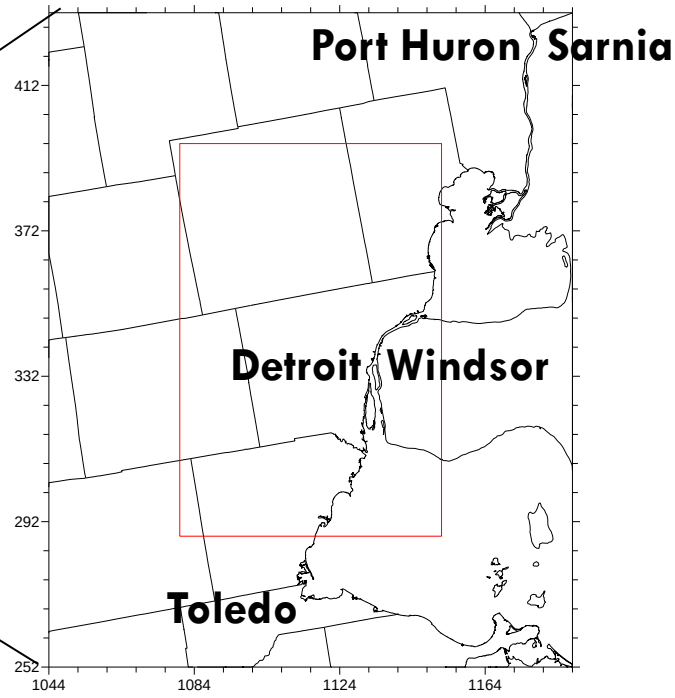
Pollutants Modeled with CMAQ and CAMx

- Ozone
- PM (primary and secondary components)
- Toxic gasses (38 species)
  - Formaldehyde (primary vs. secondary)
  - Acetaldehyde (primary vs. secondary)
  - Butadiene and acrolein
  - Aromatics
  - Chlorinated organics
  - Others
- Toxic particulates (17 species)
  - Diesel PM
  - Metals: Cr(III), Cr(VI), Mn, Pb, Ni, Hg, Cd, Be
  - Metals resolved to coarse and fine fractions of PM

Detroit Multi-Pollutant Modeling Grids



12 km Regional Grid



4 km and 1 km nested grids

- Nested grid modeling domains for both CMAQ and CAMx
  - Regional 12 km grid with boundary conditions from continental 36 km grid
  - Local 4 km and 1 km grids

Modeling Tools

CMAQ

- Special model version (4.6.1i) with toxic species added
  - Pre-select toxics hard coded into the model
- 1-way grid nesting
- No plume in grid

CAMx

- Standard model version (4.52) with toxics modeled using the RTRAC Probing Tool
  - Toxics selected at run time via input file (RTRAC chemistry parameter file)
- 2-way grid nesting
- Plume in grid

CAMx RTRAC Chemistry Parameter File

```
CAMx Version        |VERSION4.5
Description         |Toxics for Detroit project with CB05
No of gas tracers   |38
No of aero tracers  |17
No photolysis rxns  |7
No thermal rxns     |54
Gas Tracers
No.  Name       P/S   SNAM   lower bnd H-law     T-fact    Diffrat   Reactvty  Rscale
   1 FORM_P     PRIM         1.00E-12      3200     -6800      1.29  0.0       1.0
   2 BUTA       PRIM         1.00E-12     0.014         0      1.73  0.0       1.0
   3 NAPHTH     PRIM         1.00E-12         2     -3600      2.67  0.0       1.0
   4 ACR_P      PRIM         1.00E-12       8.2         0      1.76  0.0       1.0
   5 ACET_P     PRIM         1.00E-12        14     -5600      1.56  0.0       1.0
```

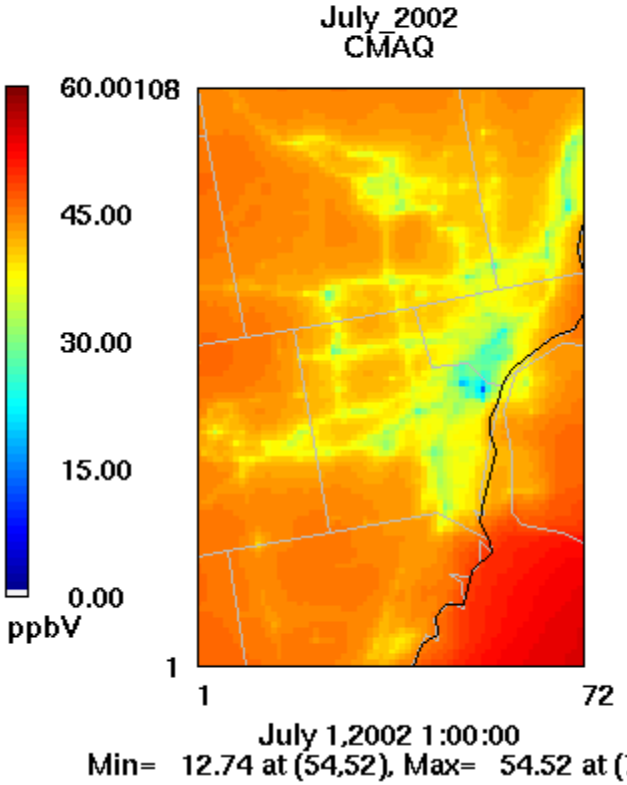
```
Aero Tracers
No.  Name       lower bnd  Density   Low cut   Upper cut
  1  BERYLLIU_F  1.00E-09       3.0      0.04        2.50
  2  BERYLLIU_C  1.00E-09       3.0      4.30       10.00
  3  CADMIUM_F   1.00E-09       3.0      0.04        2.50
  4  CADMIUM_C   1.00E-09       3.0      4.30       10.00
```

```
Photolysis reactions
Toxic            Rxn #    Factor
FORM_P         75           2.749
SFORM          75           2.749
ACET_P         87            1.0
```

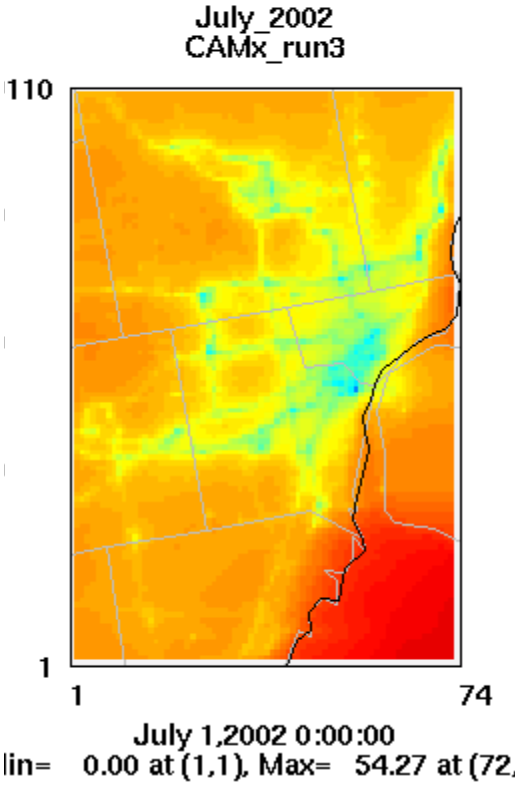
```
Thermal reactions and rates
Toxic     React    A(ppm-1min-1)  Ea (K)     B         Tref
ACRYNITRL OH      7.0464E+03       0.0       0.0        1.0
BENZENE   OH      3.6260E+03     207.0       0.0        1.0
ETHDIBROM OH      1.5120E-02     422.0       2.0        1.0
```

July Mean Ozone (ppb)

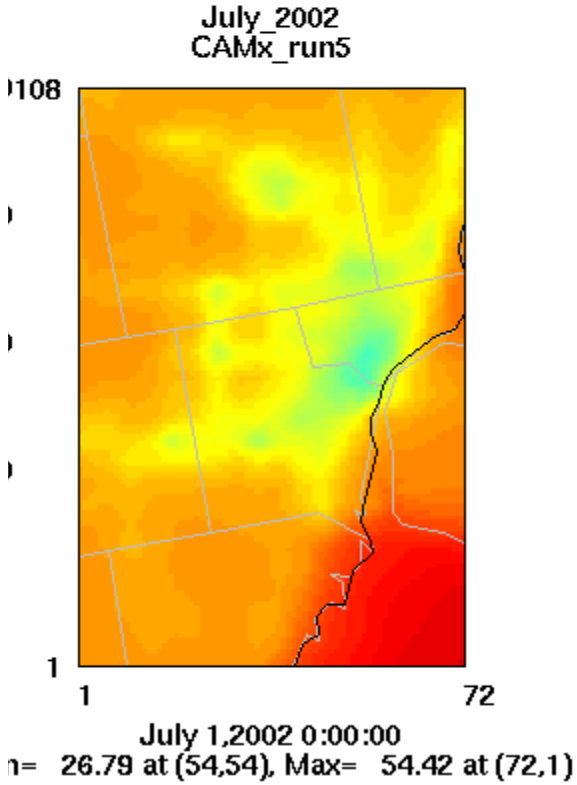
CMAQ 1 km grid



CAMx 1 km grid

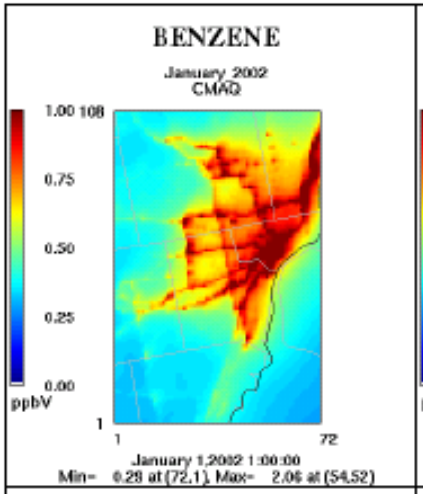
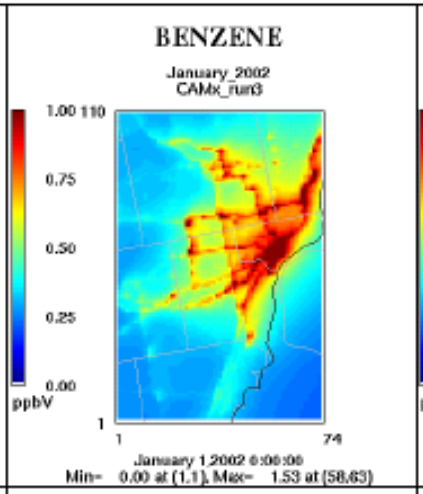
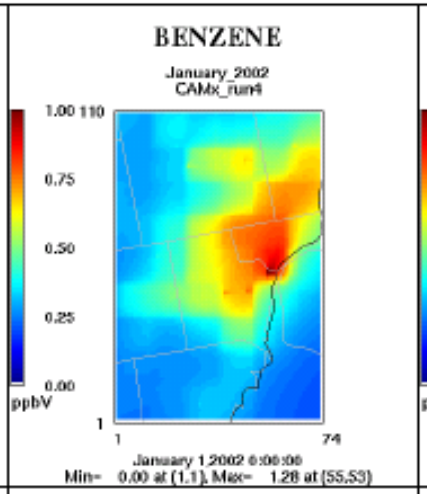
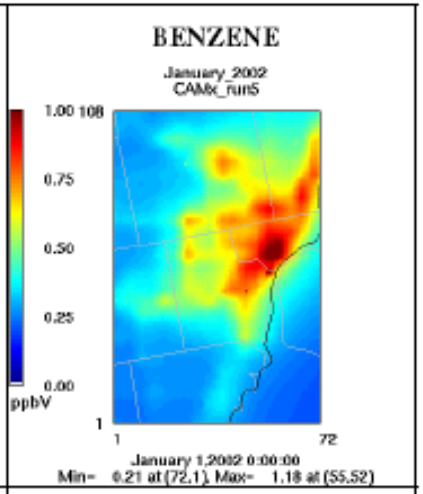
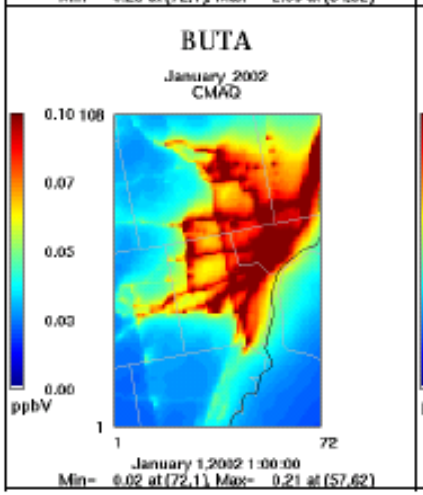
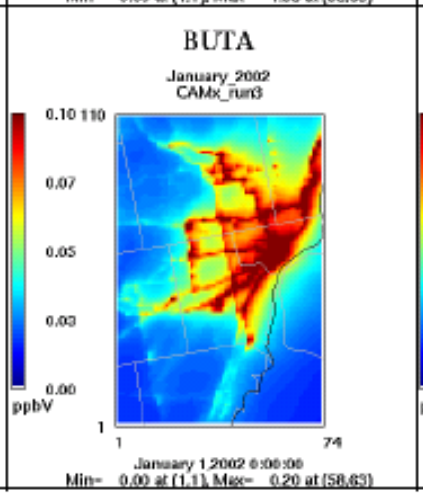
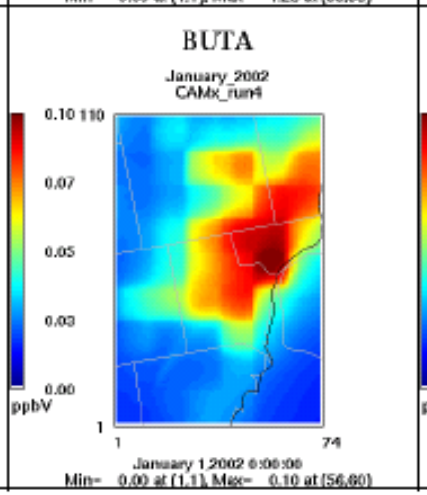
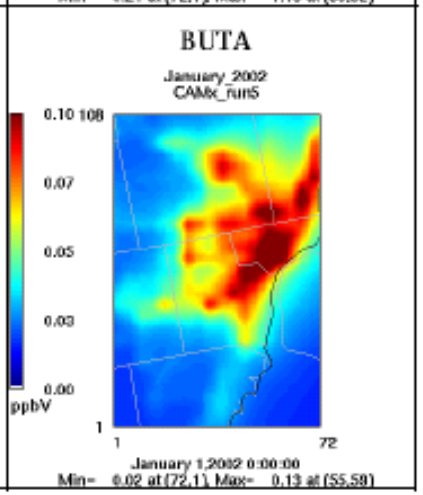


CAMx 4 km grid + PiG

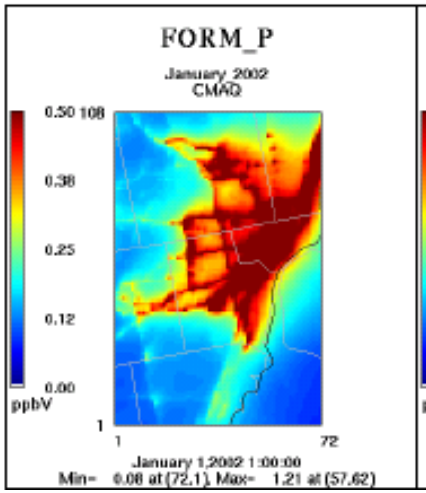
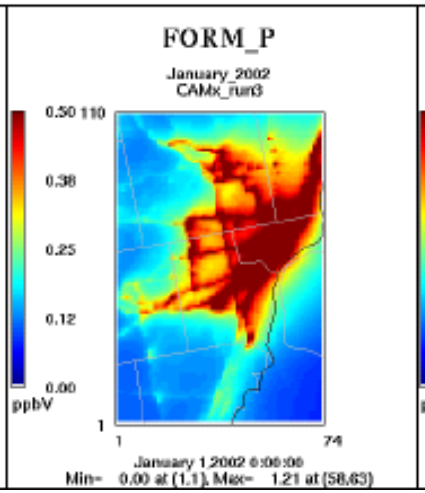
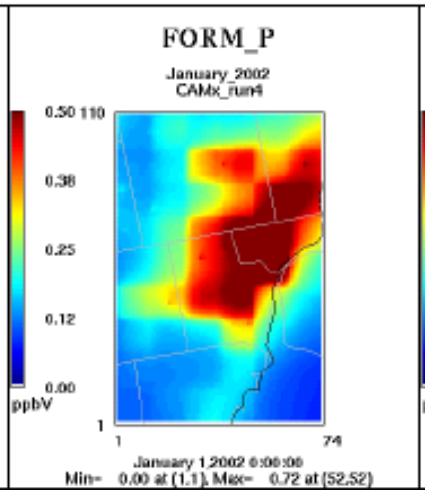
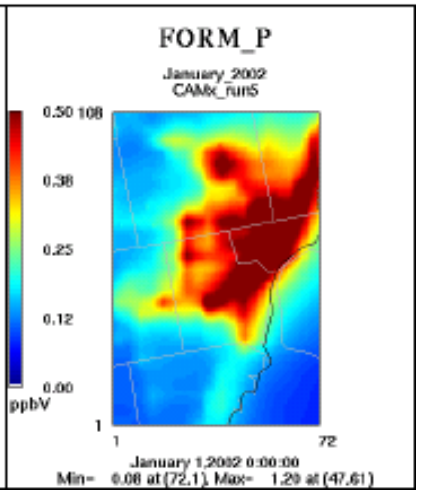
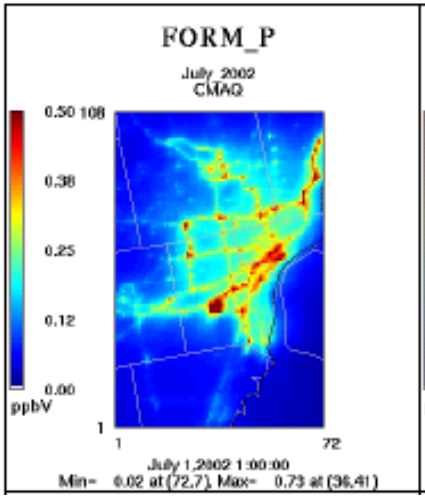
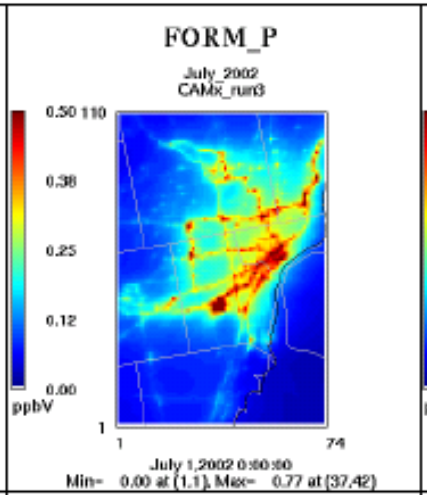
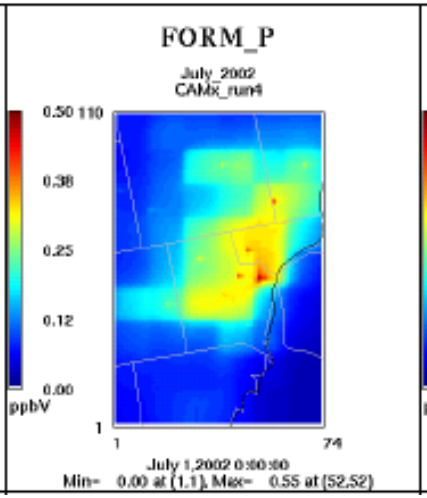
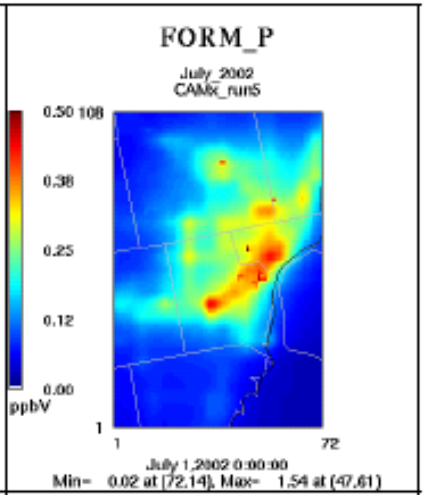


- Ozone is a regional pollutant
- Mean ozone shows titration by NOx along roadways and in urban areas
- Ozone higher over Lake Erie – more production, less destruction

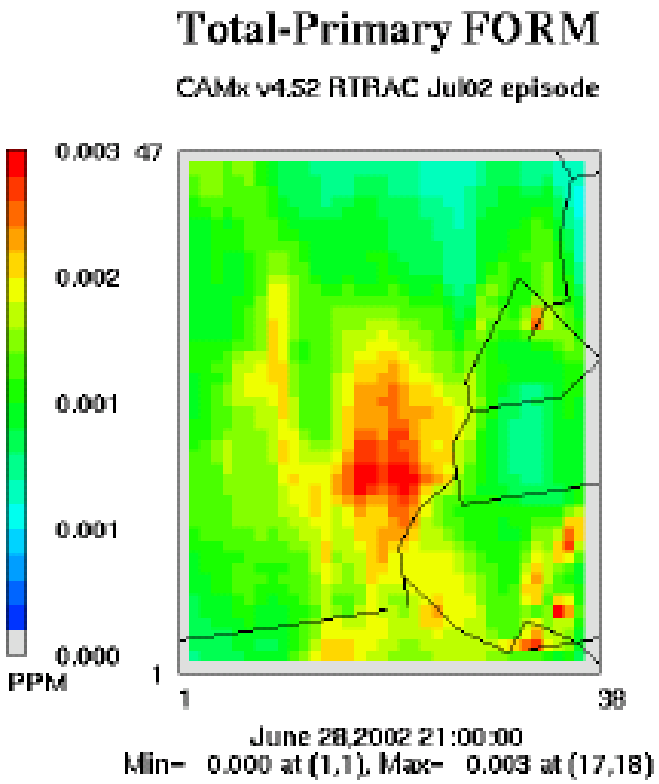
Jan 2002 Benzene and 1,3-Butadiene (ppb)

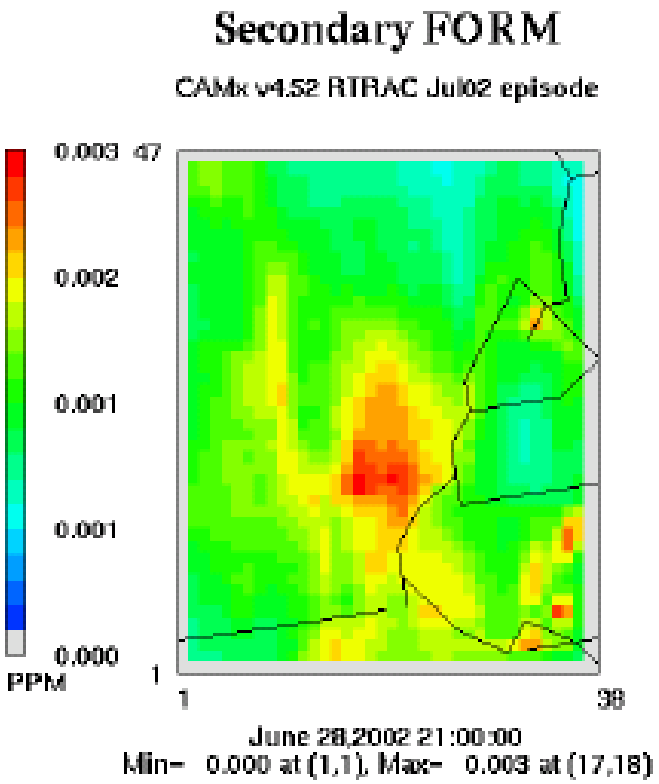
CMAQ 1 km	CAMx 1 km	CAMx 1 km with 12 km emissions	CAMx 4 km + PiG
			
			

Primary Formaldehyde (ppb)

	CMAQ 1 km	CAMx 1 km	CAMx 1 km with 12 km emissions	CAMx 4 km + PiG
Jan 2002				
July 2002				

RTRAC Method for Secondary Formaldehyde





- CMAQ calculates secondary formaldehyde from difference between total and primary formaldehyde tracer – CAMx can do the same (shown on left)
- RTRAC can directly track secondary formaldehyde formed in gas-phase chemistry (shown on right) which is simpler and theoretically more accurate
- Results are very similar

Computational Performance

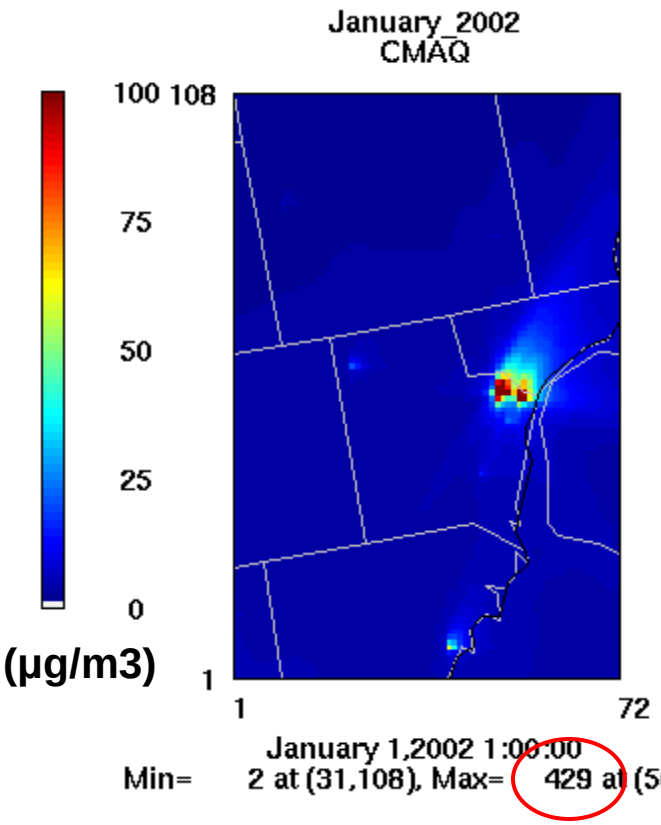
Table 4-1. Computer usage for CMAQ and CAMx configurations for a summer episode using 2 CPU cores at 2.83 GHz.

Model	Configuration	Disk Usage	Execution Time
CMAQ	1 Grid 12-km domain* (114 x 117 cells)	3832 MB	1 hr 50 min
CMAQ	1 Grid 4-km domain (36 x 45 cells)	455 MB	15 min
CMAQ	1 Grid 1-km domain (72 x 108 cells)	2286 MB	2 hrs 40 min
CMAQ total for 3 Grids 12/4/1-km		6573 MB	4 hrs 45 min
CAMx	Configurations 2 3 Grids 12/4/1-km	781 MB	2 hrs 50 min
CAMx	Configurations 3 3 Grids 12/4/1-km with Flexi-nesting	781 MB	2 hrs 50 min
CAMx	Configurations 4 2 Grids 12/4-km with ~400 PiG sources/1-km sampling grid	622 MB	1 hr 50 min

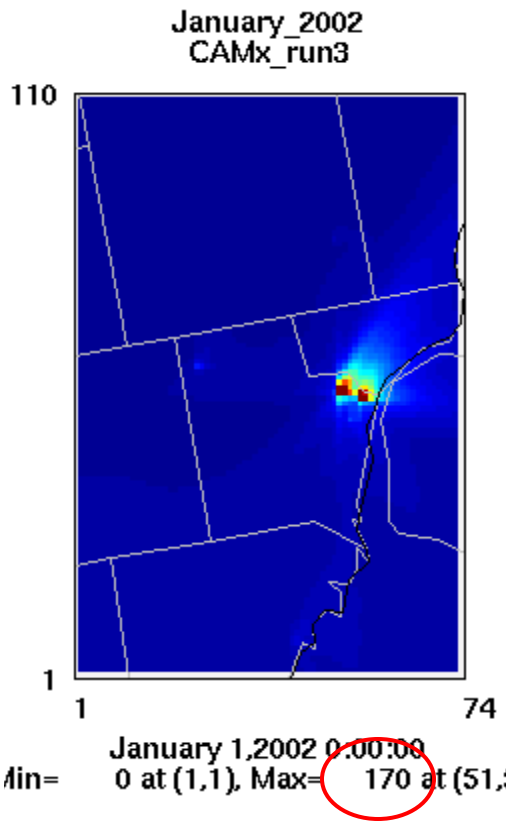
- CAMx used less CPU time than CMAQ (1:50 vs 4:45)
- CAMx used less disk space (781 MB vs 6573 MB)
- Both used far less CPU time than AERMOD

January Mean Manganese (µg/m^3)

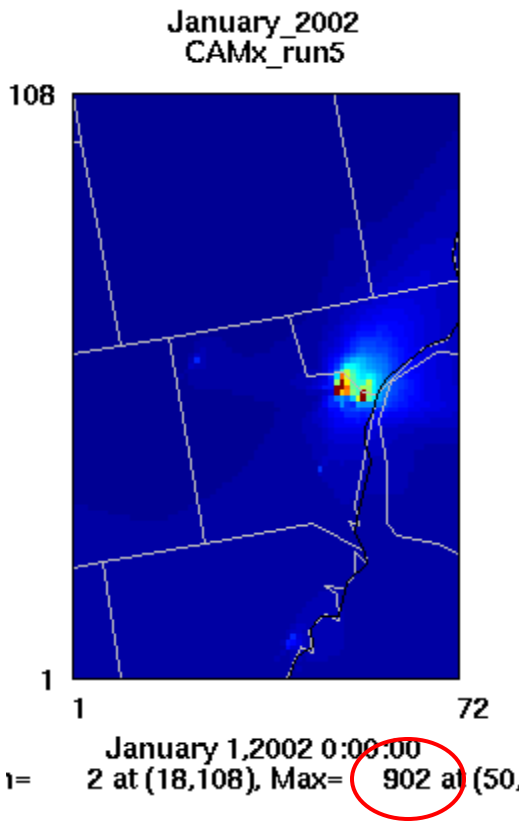
CMAQ 1 km grid



CAMx 1 km grid



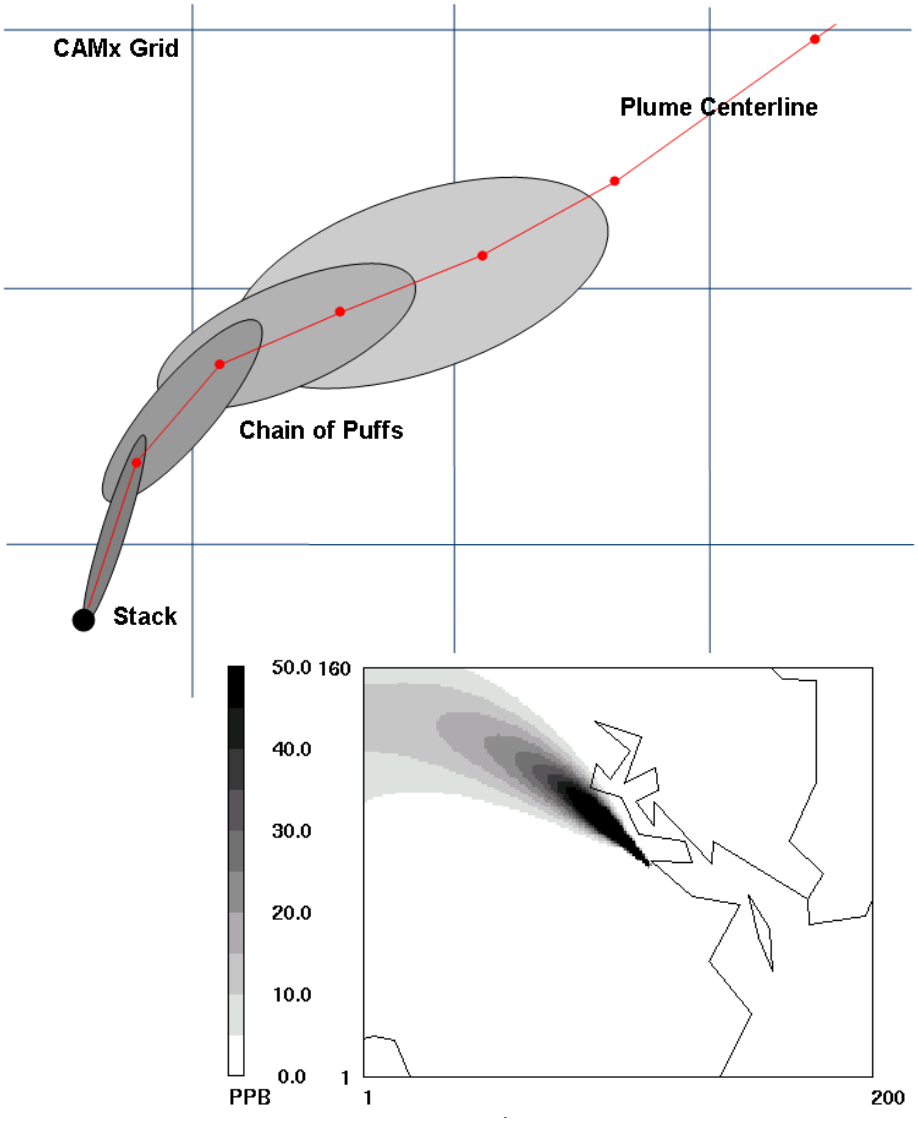
CAMx 4 km grid + PiG



- **Manganese a local issue near specific point sources**
- **Peak concentrations depend upon model and configuration**
- **Plume-in-grid predicts the highest concentration near (at) the source**

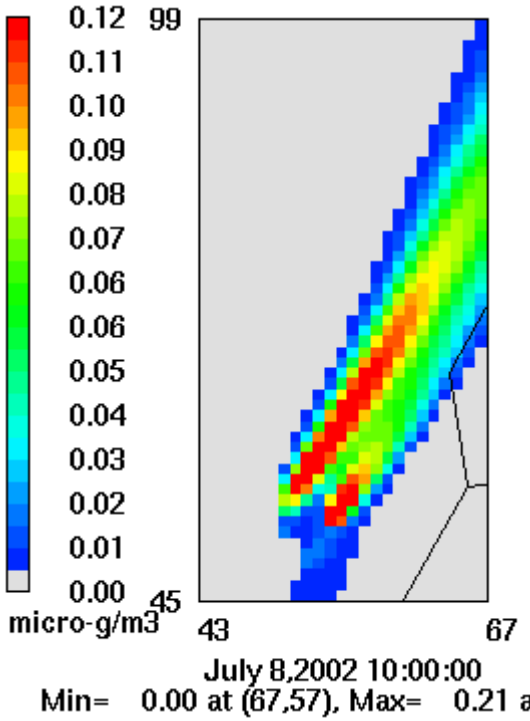
CAMx Plume-in-Grid

- Hybrid grid/puff model
  - Puff model embedded within a grid model
- Selected point source emissions released into the puff model
  - Puff model handles near source dispersion and chemistry
  - Can use a "sampling grid" to combine the puff with grid concentrations
- Emissions transferred to the CAMx grid when puffs grow sufficiently large
  - Grid model handles regional chemistry, transport

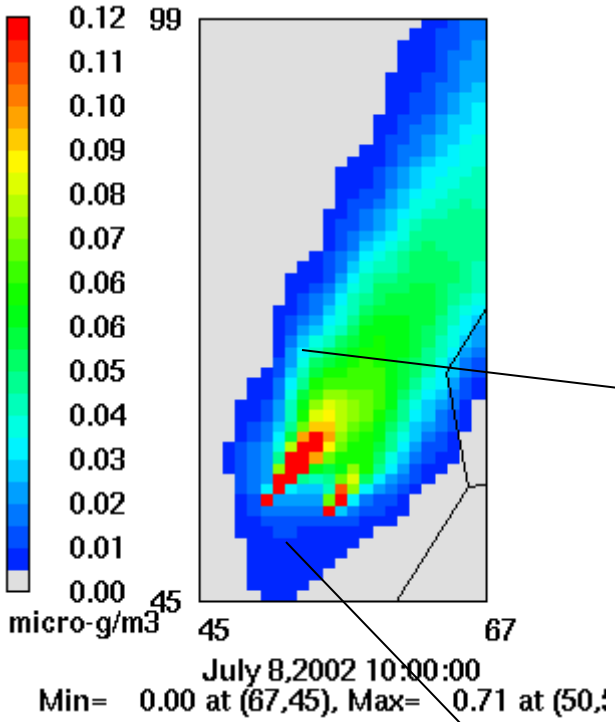


Closer Look at Mn with1 km grid vs. 4 km grid + PiG

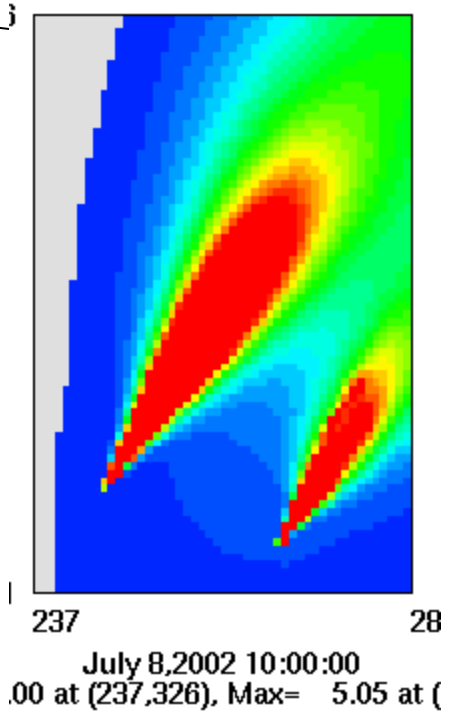
CAMx 1 km grid



CAMx 4 km grid + PiG with 1 km sampling grid



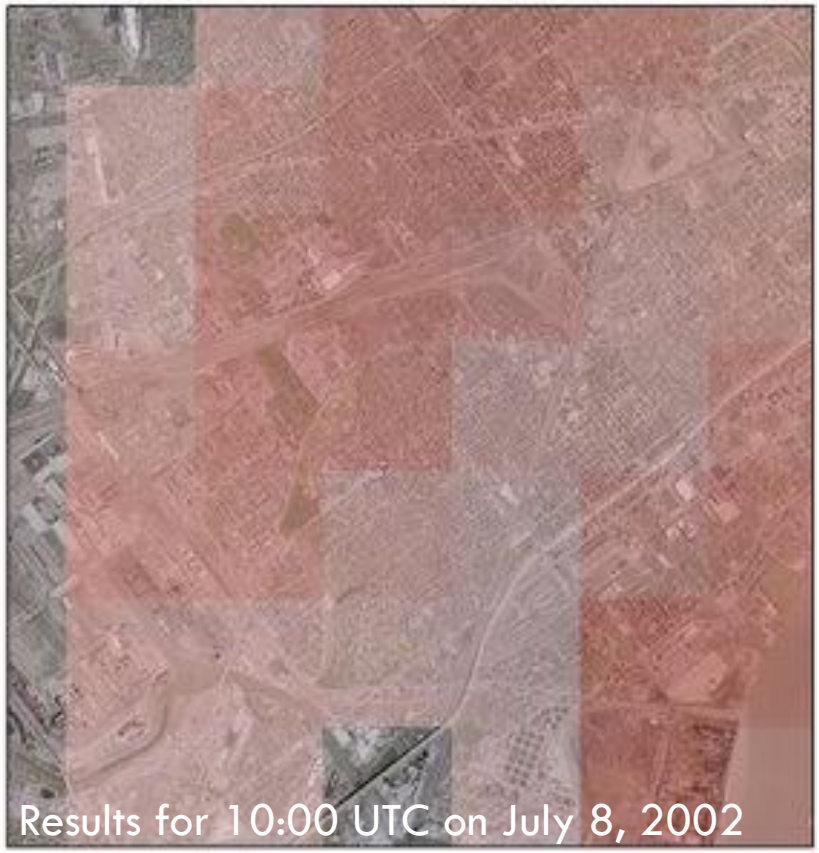
Zoom in by using a finer sampling grid at 200 m rather than 1000 m



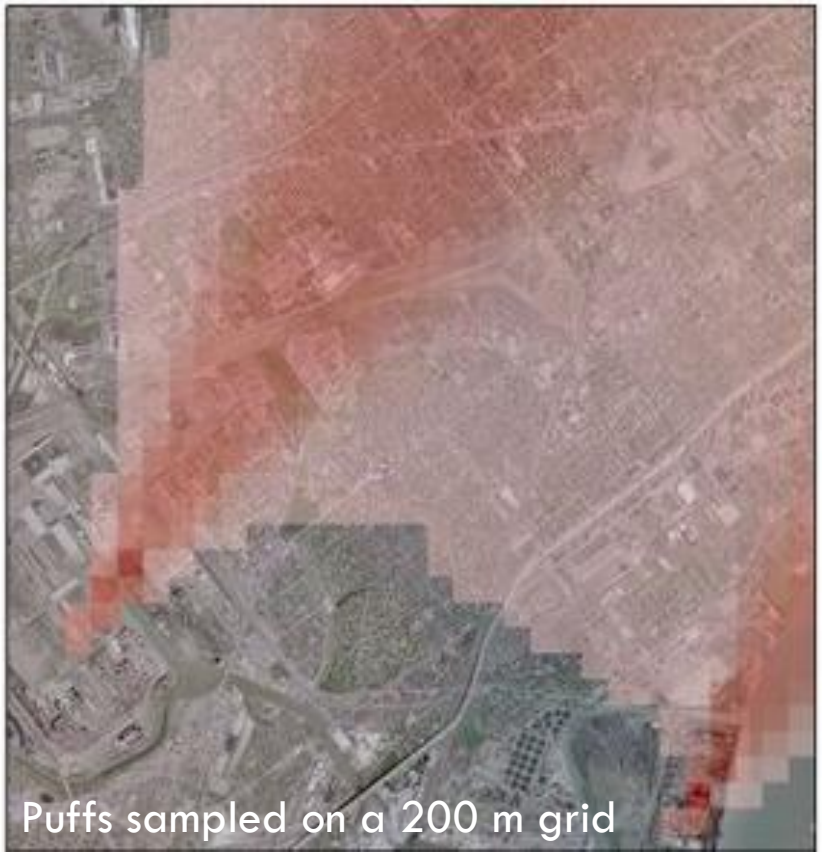
- **Focus on an hour with consistent winds**
- **Differences near source are better plume resolution by PiG**
- **Differences further downwind due to 4 km vs. 1 km grid**

Close Look at Manganese Point Sources

CAMx 1 km grid



CAMx 4 km grid + PiG



- **Plume-in-grid (PiG) better resolves near source impacts**
- **Maximum impacts with PiG occur inside these facility fence lines**

End of Slides