Detroit Multi-pollutant Pilot Project: Hybrid Approach Modeling for Understanding Urban Air Quality

October 29, 2008

US-Canada Meeting

Detroit, MI

Detroit Multi-pollutant Pilot Project Team

Team Members (EPA/OAQPS)

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[1] Current on sabbatical to Johns Hopkins

[2] No longer at EPA

Why Detroit?

EPA implemented a project where the multi-pollutant & multi-resolution tools and methods could be implemented and tested.

- Multi-pollutant Issues
  - PM2.5
  - O3
  - Toxics
- Rich in technical data, research and analyses
  - Detroit Air Toxics Initiative (DATI)
  - Detroit Exposure and Aerosol Research Study (DEARS)
  - LADCO, Region V and Michigan DEQ
  - PM National Ambient Air Quality Standards RIA

Outline

While the Detroit Multi-pollutant Study includes multiple pollutants (HAPS&CAPS), we focus on evaluating a select group of HAPS for this presentation.

- Overview of Models/Method
  - CMAQ
  - AERMOD
  - Multiplicative Hybrid Approach
- Results
  - Modeled concentration
  - Model Performance evaluation
  - Risk Assessment (HEM-3)
- Spatial Fusion Application for Toxics
- Conclusions

Model Inputs

- Emissions Inventory
  - 2002 NEI: Integrated HAPs & CAPs
  - Local-scale EI improvements
    - Steel Mill Study Data, LADCO Nonroad Study, Solvent Study
  - Emissions Modeling Improvements
    - 1 km spacial surrogates and other improved land use based inventory data
  - Canadian EI Data
    - 2000
    - No HAP inventory
- Meteorological Data
  - 2002 MM5 data

Documentation of model inputs can be found in the "Technical Support Document for the Final Locomotive/Marine Rule: Air Quality Modeling Analyses"

http://www.epa.gov/scram001/reports/EPA-454-R-08-002.pdf

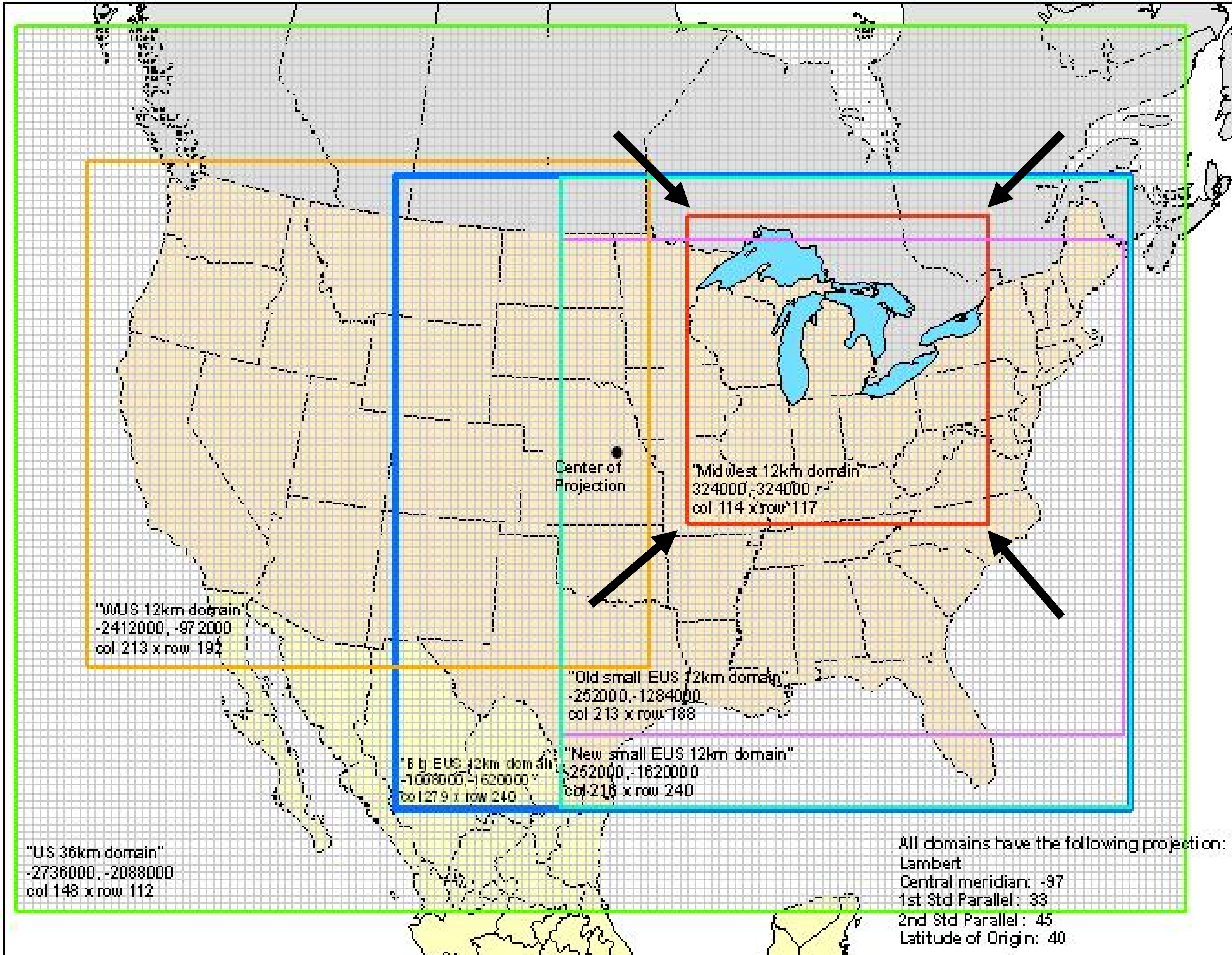
CMAQ v4.6.1

HAP	CAS#
Acrylonitrile	107-13-1
Carbon Tetrachloride	56-23-5
Propylene Dichloride	78-87-5
1,3-Dichloride Propene	542-75-6
1,1,2,2-Tetrachloride Ethane	79-34-5
Benzene	71-41-2
Chloroform	67-66-3
1,2-Dibromomethane	106-93-4
1,2-Dichloromethane	107-06-2
Ethylene Oxide	75-21-8
Methylene Chloride	75-09-2
Perchloroethylene	127-18-4
Trichloroethylene	79-01-6
Vinyl Chloride	7501-4
Naphthalene	91-20-3
Quinoline	91-22-5
Hydrazine	302-01-2
2,4-Toluene Diisocyanate	584-84-9
Hexamethylene 1,6-Diisocyanate	822-06-0
Maleic Anhydride	108-31-6
Triethylamine	121-44-8
1,4-Dichlorobenzene	106-46-7
Total Formaldehyde	50-00-0
Total Acetaldehyde	75-07-0
Total Acrolein	107-02-8
1, 3-Butadiene	106-99-0
Formaldehyde Emissions Tracer	50-00-0
Acetaldehyde Emissions Tracer	75-07-0
Acrolein Emissions Tracer	107-02-8

- CMAQ includes several new gas phase and aerosol phase HAPS
- Also includes Carbon Bond O5 (CBO5) chemical mechanism to allow for modeling of criteria and toxics
- http://www.cmaq-model.org/

HAP
Beryllium Compounds
Nickel Compounds
Chromium (III) Compounds
Chromium (VI) Compounds
Lead Compounds
Manganese Compounds
Cadmium Compounds
Diesel Emissions Tracer

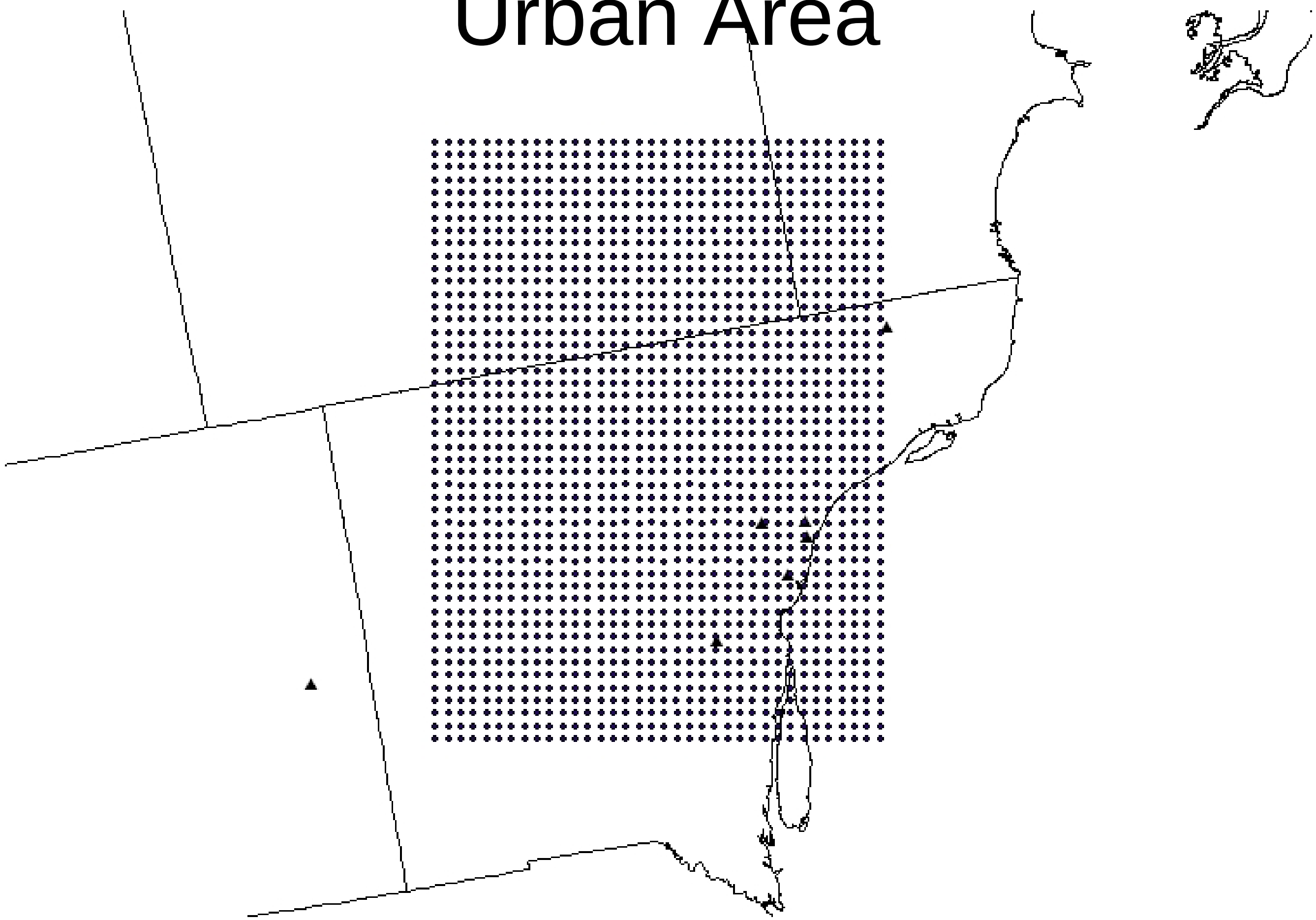
Source: Bill Hutzell, EPA/ORD


"Midwest 12km domain"
324000,-324000
col 114 x row 117
Center of Projection
"WUS 12km domain"
-2412000, -972000
col 213 x row 192
"Old small EUS 12km domain"
-252000,-1284000
col 213 x row 188
"New small EUS 12km domain"
-252000,-1620000
col 216 x row 240
"Big EUS 12km domain"
-1008000,-1620000
col 279 x row 240
"US 36km domain"
-2736000, -2088000
col 148 x row 112
All domains have the following projection:
Lambert
Central meridian: -97
1st Std Parallel: 33
2nd Std Parallel: 45
Latitude of Origin: 40

AERMOD

- EPA's preferred Dispersion Model: (http://www.epa.gov/scram001/dispersion_prefrec.htm)
- AERMOD 07026 used with small change to emissions temporal allocation options
- AERMOD Options Used
  - Deposition (Toxics Option)
  - Flat-terrain option
  - Downwash turned on for point sources
  - Urban Option used for sources in Detroit and Ann Arbor
- Meteorology: MM5 data supplied by MM5AERMOD Tool
  - 12 km grid which included the Detroit Metropolitan Airport
- Emissions: 2002 NEI v3 – Detroit specific
  - Emissions domain extends 36+ km around receptor domain
  - SMOKE and SAS code used to produce AERMOD emissions
- Pollutants modeled
  - PM2.5 components: NO3, SO4, EC, OC, Crustal
  - Benzene, 1,3-Butadiene,Naphthalene, Cadmium, Acetaldehyde, Nickel, Methylene chloride (Dichloromethane), Formaldehyde, Manganese, Diesel PM, and 1,4-Dichlorobenzene,p

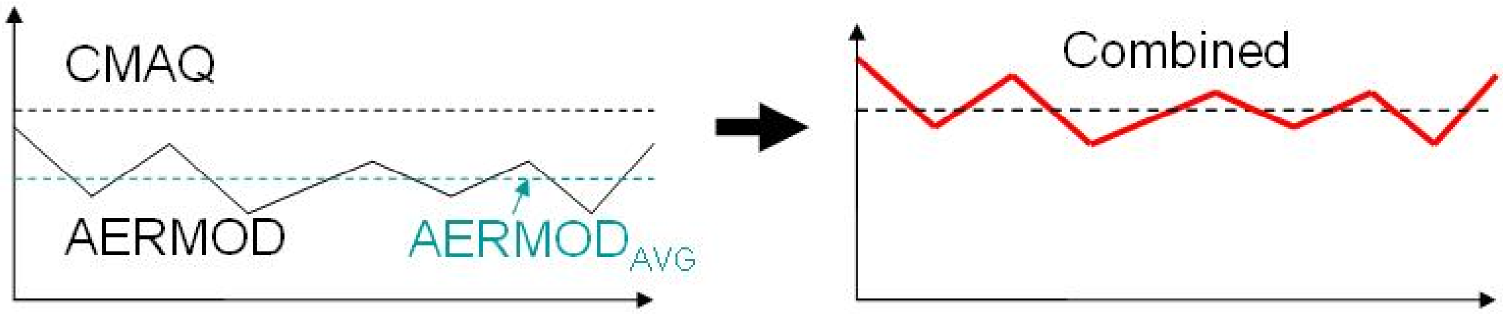
AERMOD Receptor Domain for Detroit Urban Area



AERMOD domain: 48x36km with receptors placed every 1km (1728 receptors)

Hybrid Approach

- Hybrid approach is a post-processing of CMAQ & AERMOD outputs to generate consistent AQ concentrations for the urban sub-grid and providing more resolved characterization for PM species & toxics



- Tested additive and multiplicative approaches and chose multiplicative

*CMAQ_primary * (AERMOD_rec/AERMOD_gridavg) + CMAQ_secondary*

Where:

CMAQ_primary and CMAQ_secondary are the primary and secondary CMAQ emissions of pollutant X within the relevant 12km

CMAQ grid cell (CMAQ = CMAQ_primary + CMAQ_secondary) AERMOD_rec = the concentration of pollutant X at an AERMOD receptor; and

AERMOD_gridavg = the average concentration of pollutant X at the AERMOD receptors located within the relevant 12km CMAQ grid cell (12km x 12km)

Human Exposure Model (HEM-3)

- Tool for estimating ambient concentrations, human exposures and health risks that may result from air pollution emissions.
- Accepts user-supplied gridded modeling results and uses a Voronoi Neighborhood Averaging (VNA) approach to interpolate pollutant concentrations at 1km receptor grids to Census block centroids.
- Estimates exposure/risk using the unit risk estimates and reference concentrations based on the latest values recommended by EPA for hazardous air pollutants (HAP) and other toxic air pollutants (http://www.epa.gov/ttn/atw/toxsource/table1.pdf).

Results: Model/Method Intercomparisons

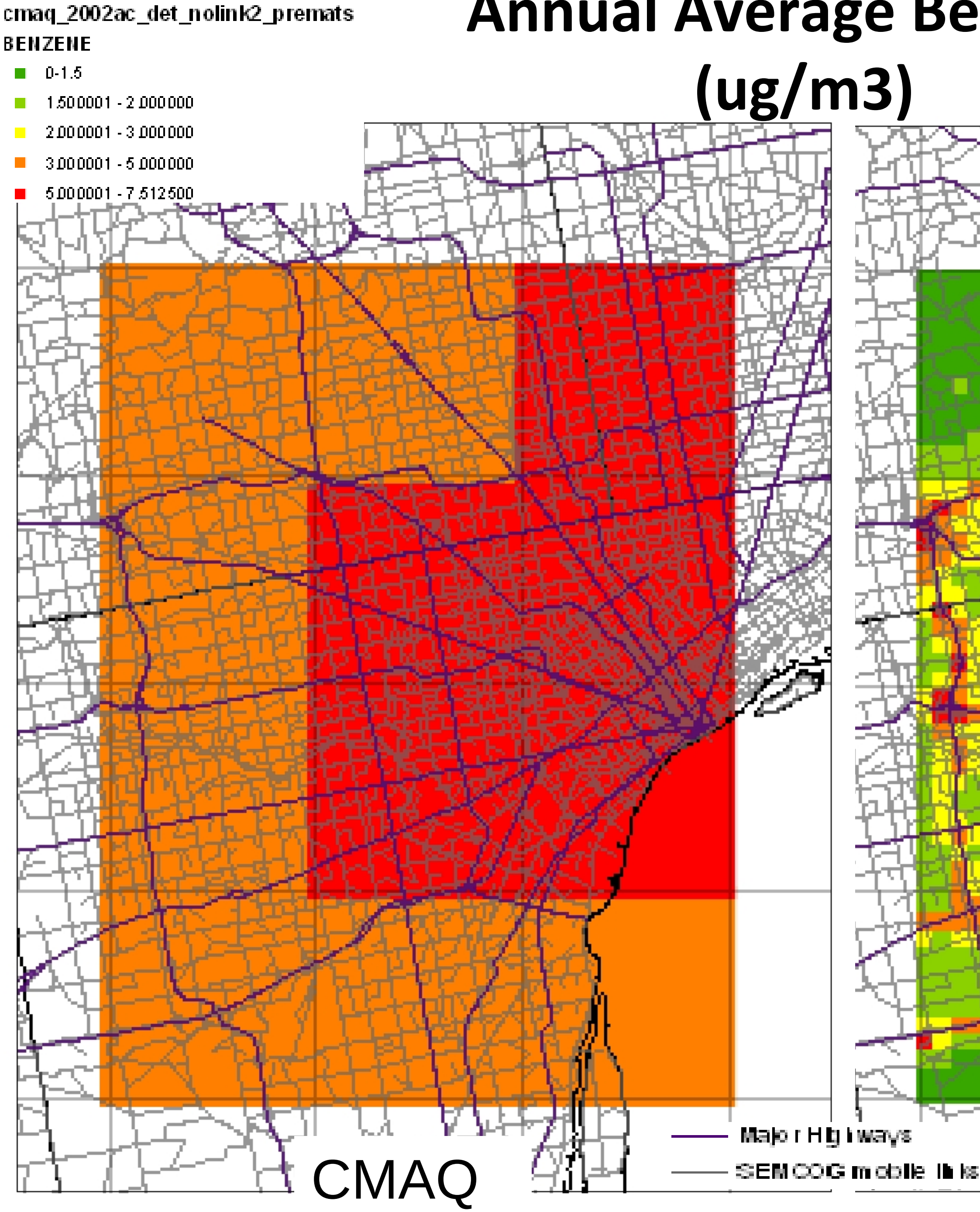
CMAQ vs. AERMOD vs. Hybrid:

- Benzene *(mostly primary)*
- Acetaldehyde *(mostly secondary)*

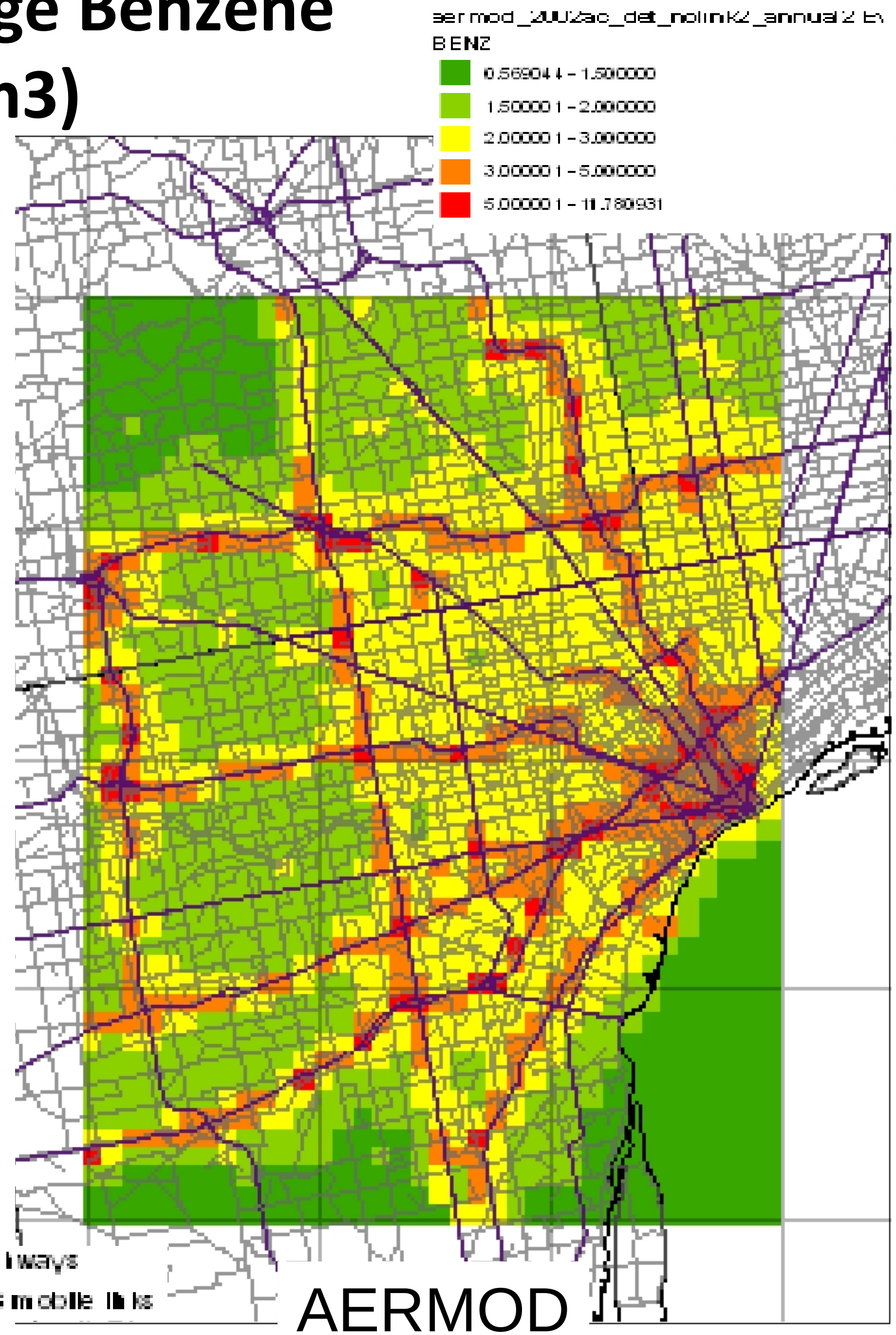
HEM-3

- Risk is calculated for: benzene, 1,3-butadiene, naphthalene, acetaldehyde, methylene chloride, formaldehyde, dichlorobenzene, cadmium, nickel & manganese using annual average modeled concentrations.

Annual Average Benzene (ug/m3)

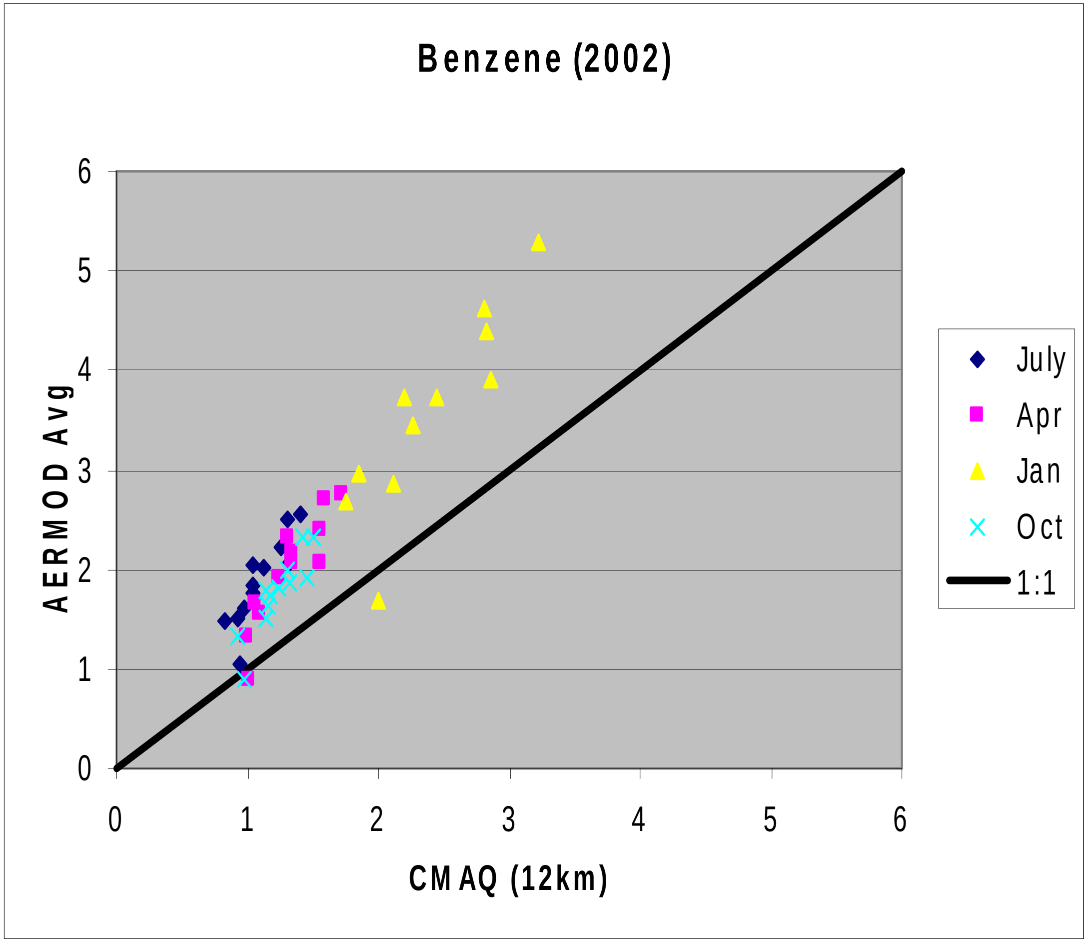


CMAQ



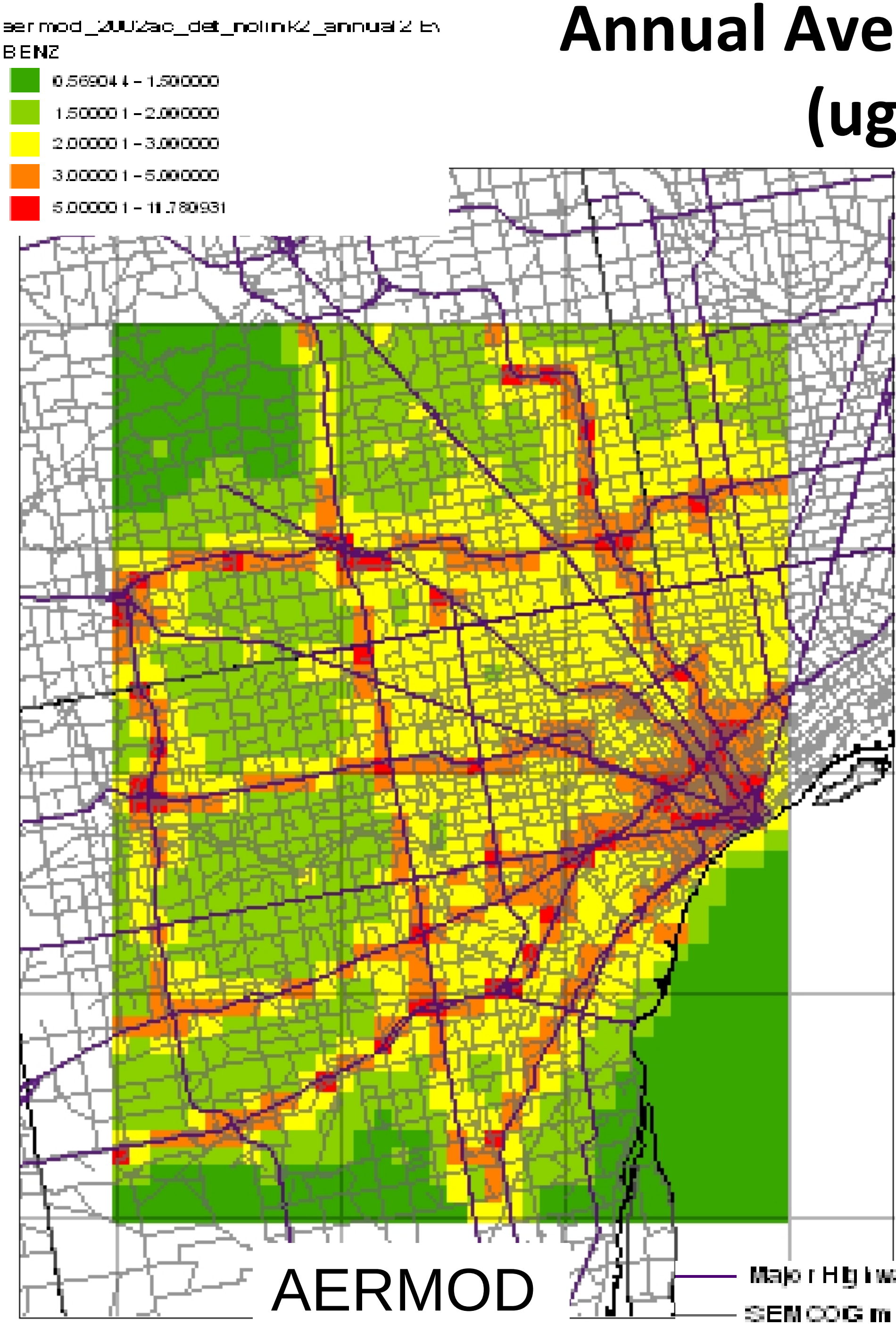
AERMOD

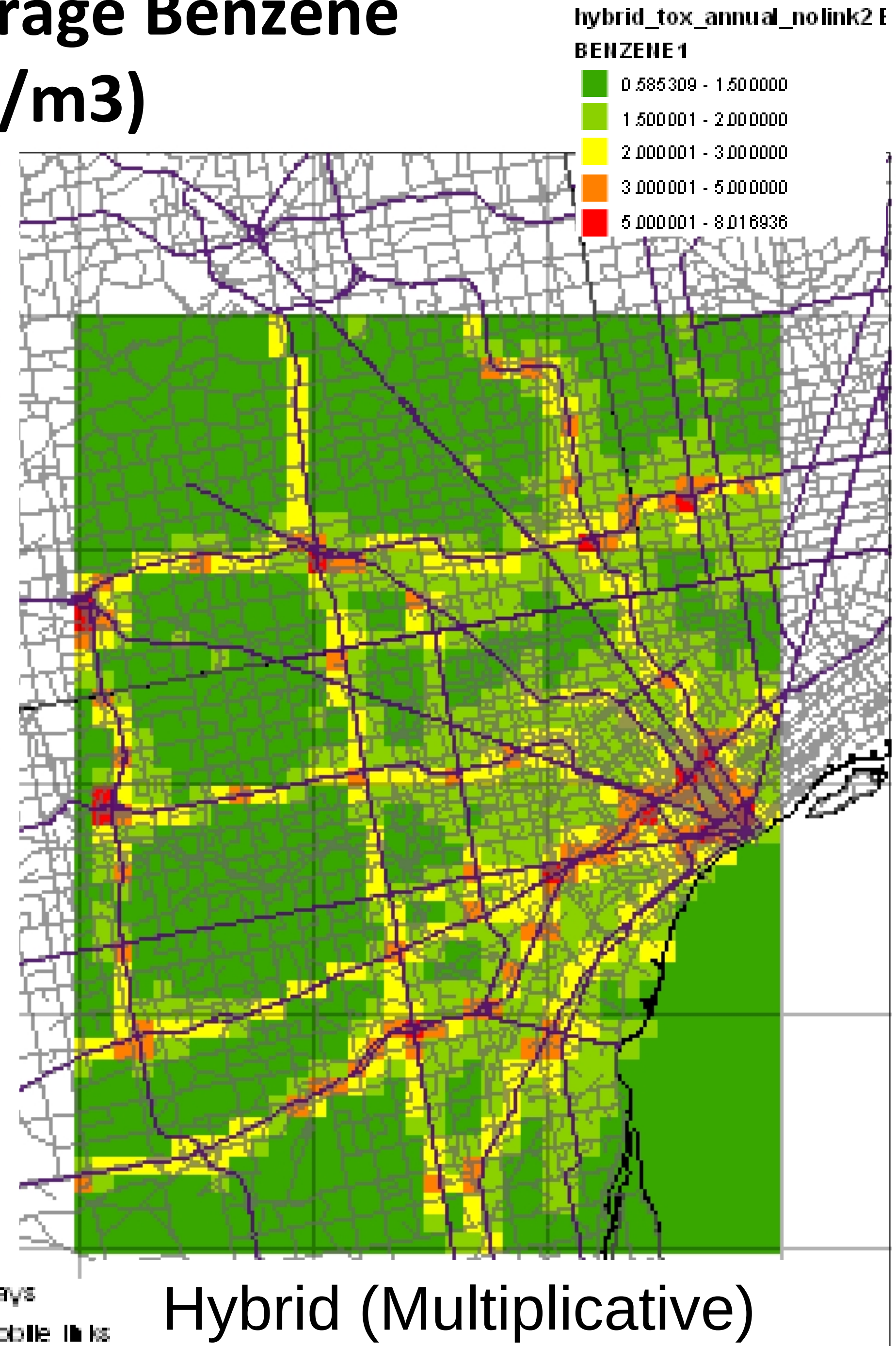
Average AERMOD values per 12km grid cell compared to CMAQ 12km



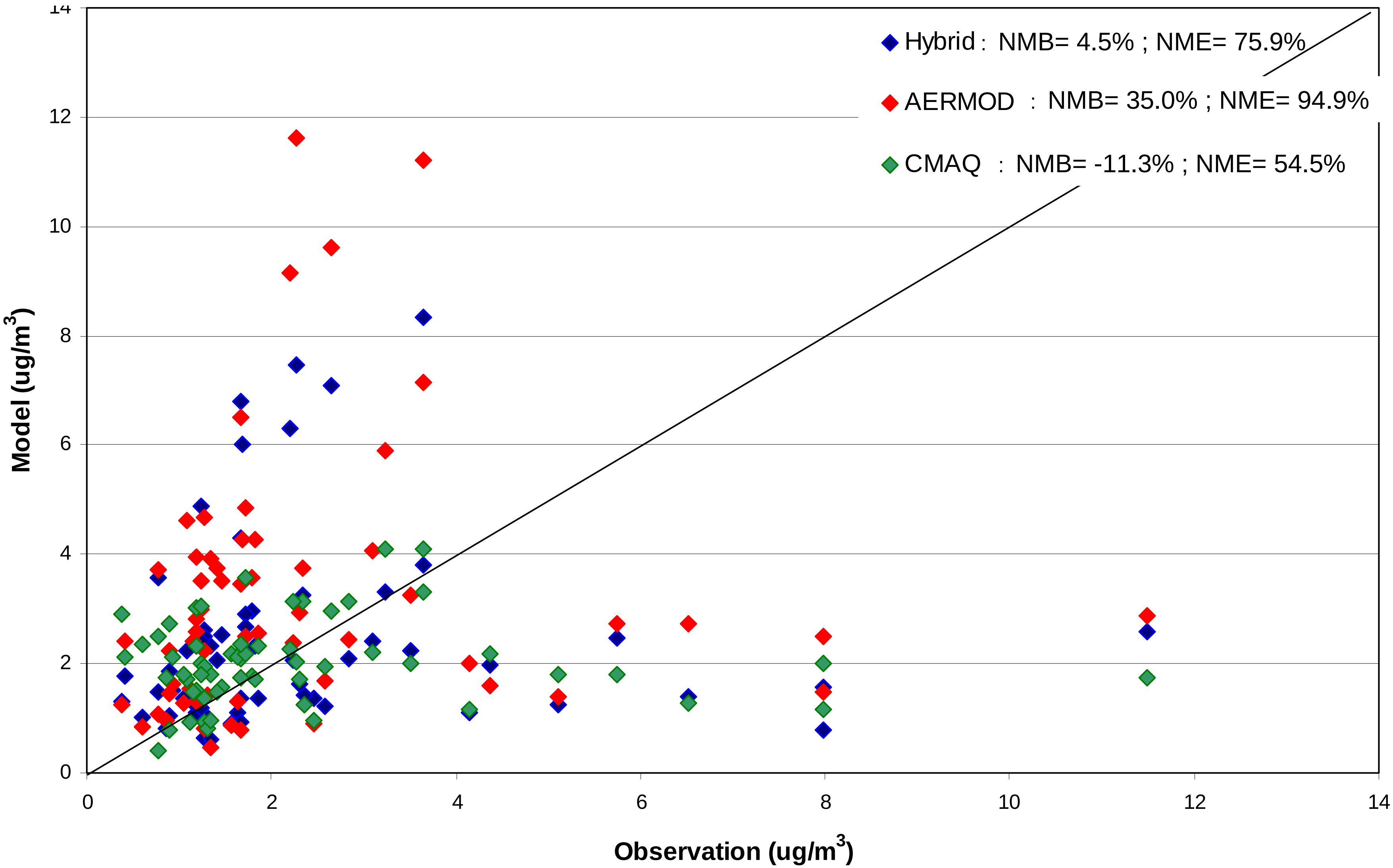
Summary: The average AERMOD concentrations per 12km grid cell agree well with the CMAQ values for all four seasons. Higher values from AERMOD could demonstrate the ability of AERMOD to pick up larger gradients (but not having an infinite number of receptors to cover the entire 12km domain), as well as CMAQ's inclusion of photochemical decay.

Annual Average Benzene (ug/m3)

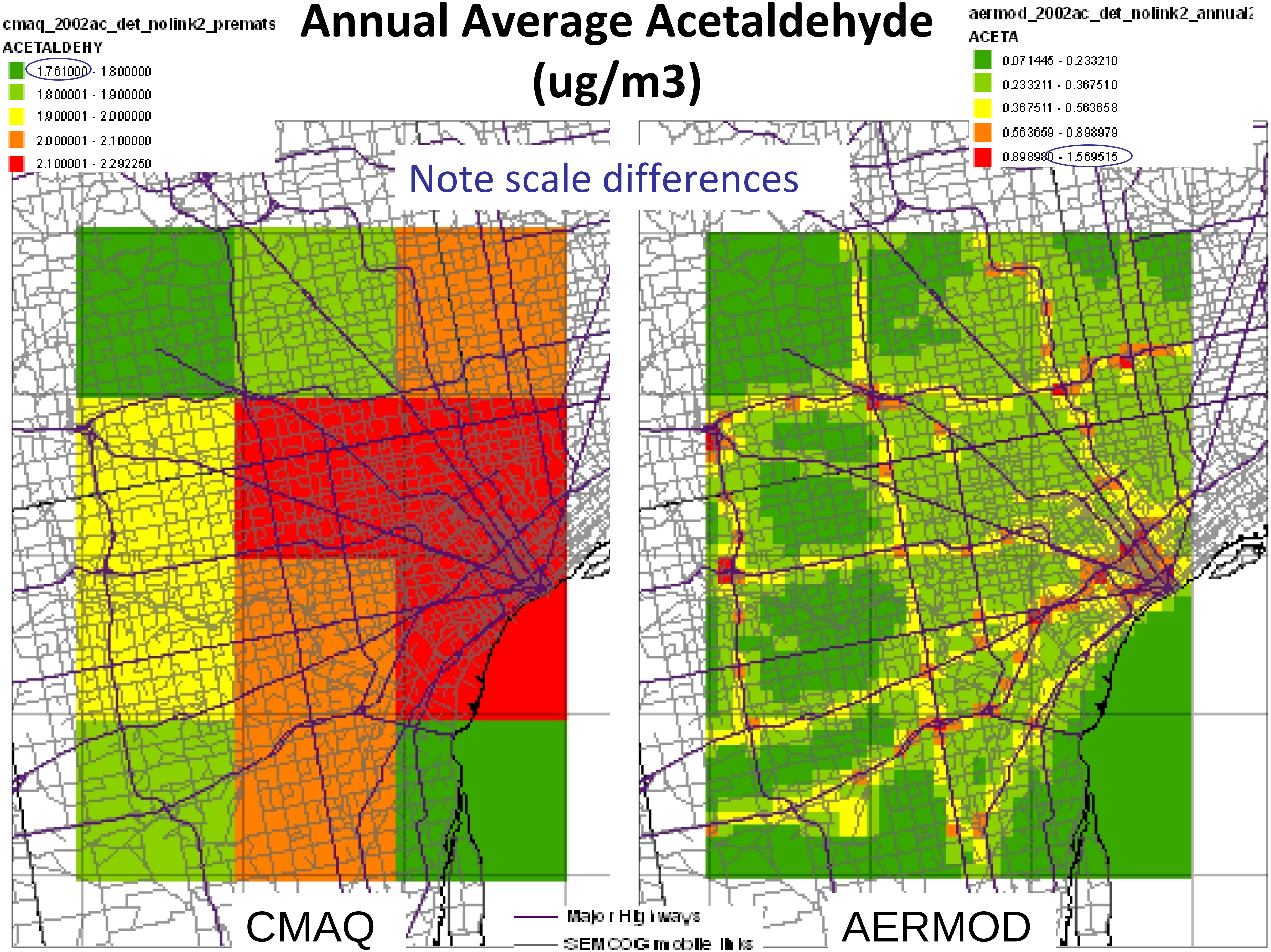




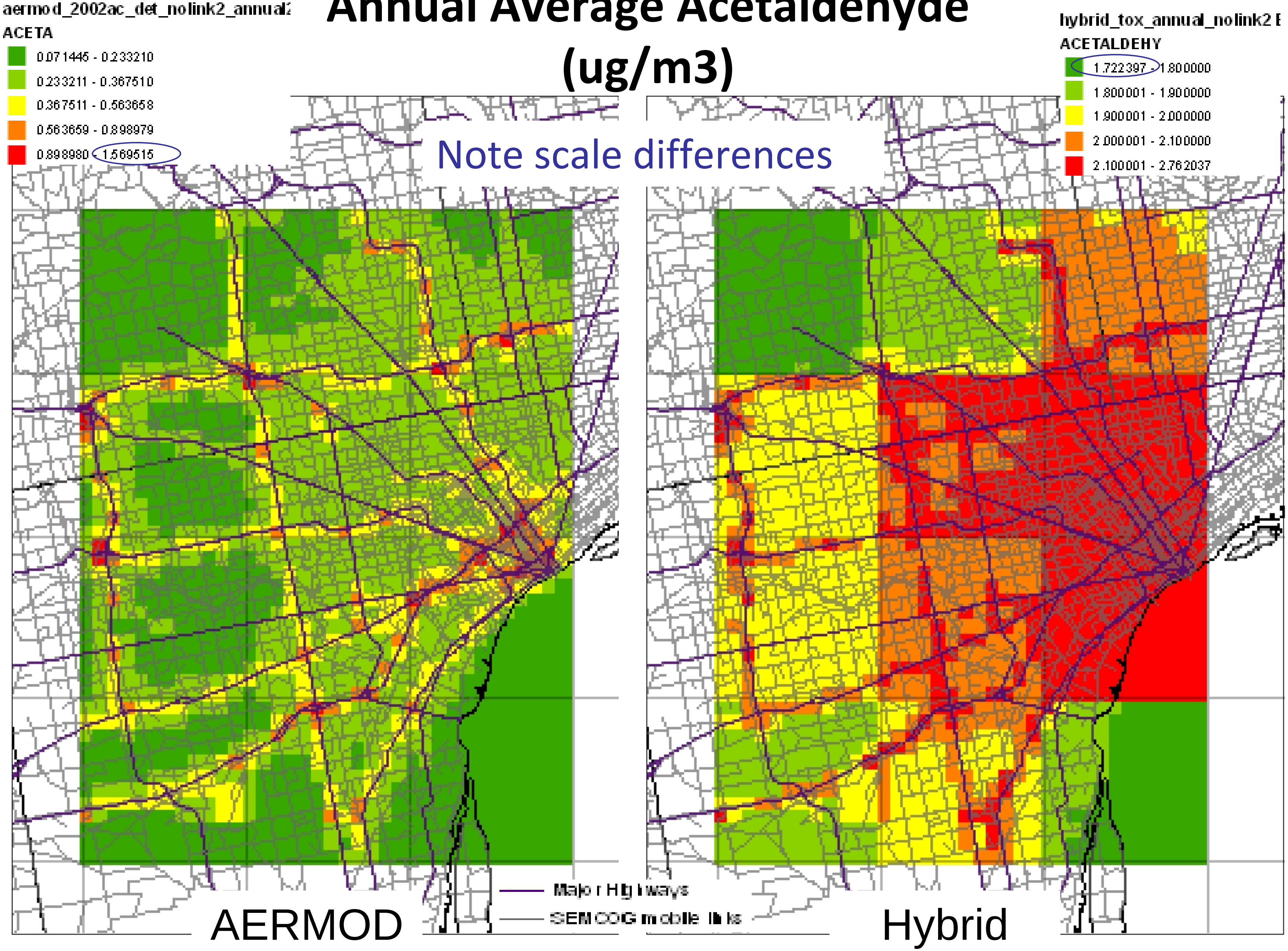
CMAQ, AERMOD & Hybrid Approach vs Measured Concentrations: Benzene (ug/m3)



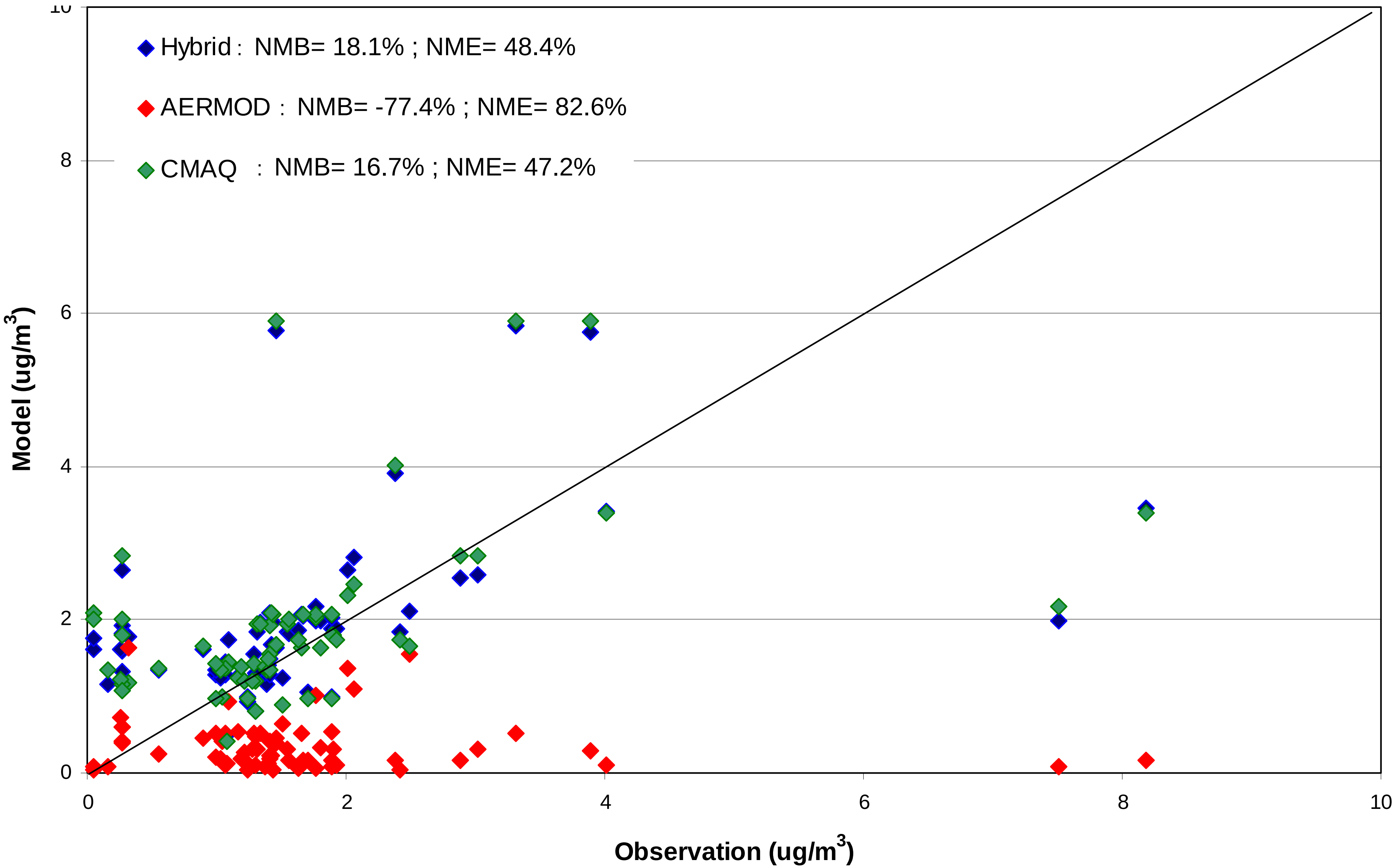
Annual Average Acetaldehyde (ug/m3)



Annual Average Acetaldehyde (ug/m3)



CMAQ, AERMOD & Hybrid Approach vs Measured Concentrations: Acetaldehyde (ug/m3)

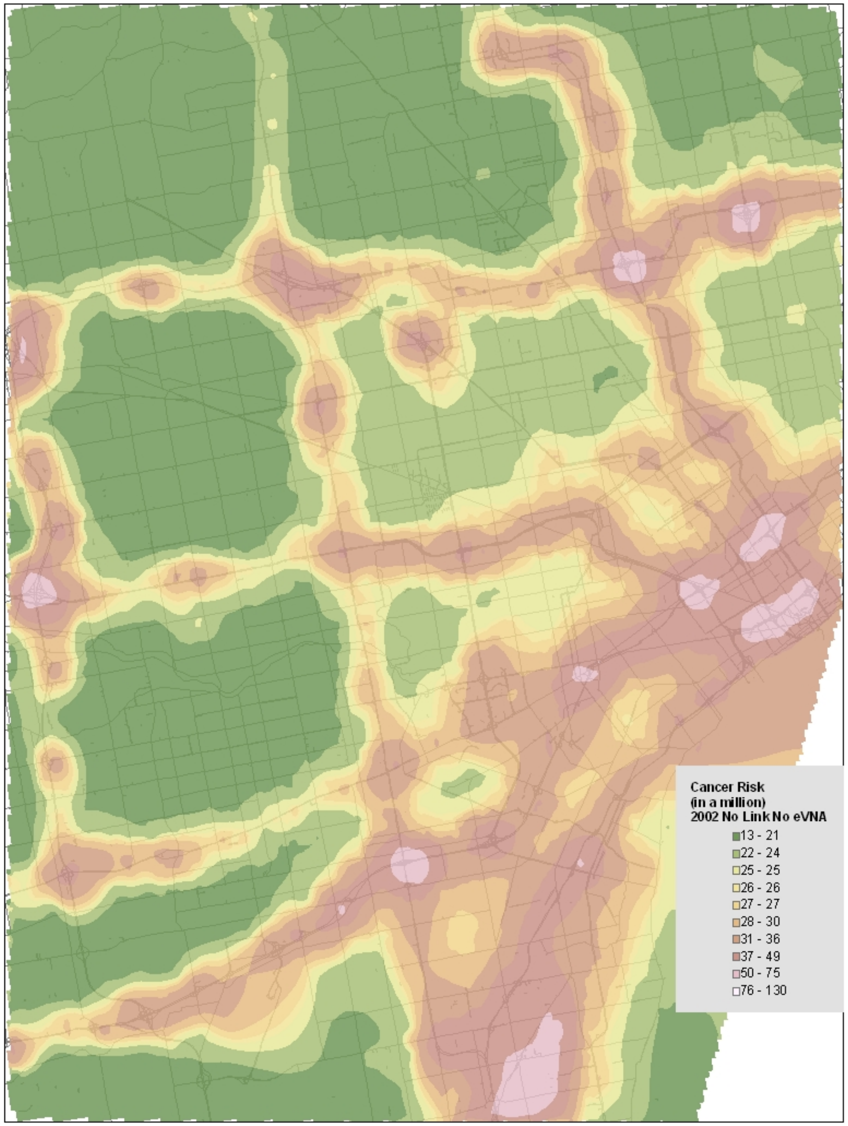


CMAQ vs. AERMOD vs. Hybrid Approach for Toxics

		Min	Max	Mean	Median
Benzene	Ambient	1.228	22.852	3.310	1.995
	CMAQ	1.213	3.230	2.132	1.744
	AERMOD	1.269	7.505	2.675	2.109
	Hybrid	1.009	5.547	2.001	1.590
Acetaldehyde	Ambient	0.779	3.446	1.697	1.610
	CMAQ	1.403	3.568	2.213	1.879
	AERMOD	0.180	0.987	0.379	0.301
	Hybrid	1.219	3.583	2.173	1.814
1,3-Butadiene	Ambient	0.028	0.178	0.087	0.063
	CMAQ	0.083	0.242	0.155	0.124
	AERMOD	0.131	0.742	0.242	0.179
	Hybrid	0.064	0.442	0.136	0.097
Formaldehyde	Ambient	1.248	16.982	3.713	2.765
	CMAQ	1.488	3.0562	2.206	2.113
	AERMOD	0.535	2.487	0.961	0.738
	Hybrid	1.028	4.412	1.931	1.622
Manganese (PM2.5)	Ambient	0.0030	0.0671	0.0164	0.0038
	CMAQ	0.0015	0.0281	0.0154	0.0210
	AERMOD	0.0003	0.0738	0.0101	0.0026
	Hybrid	0.0003	0.1033	0.0198	0.0105

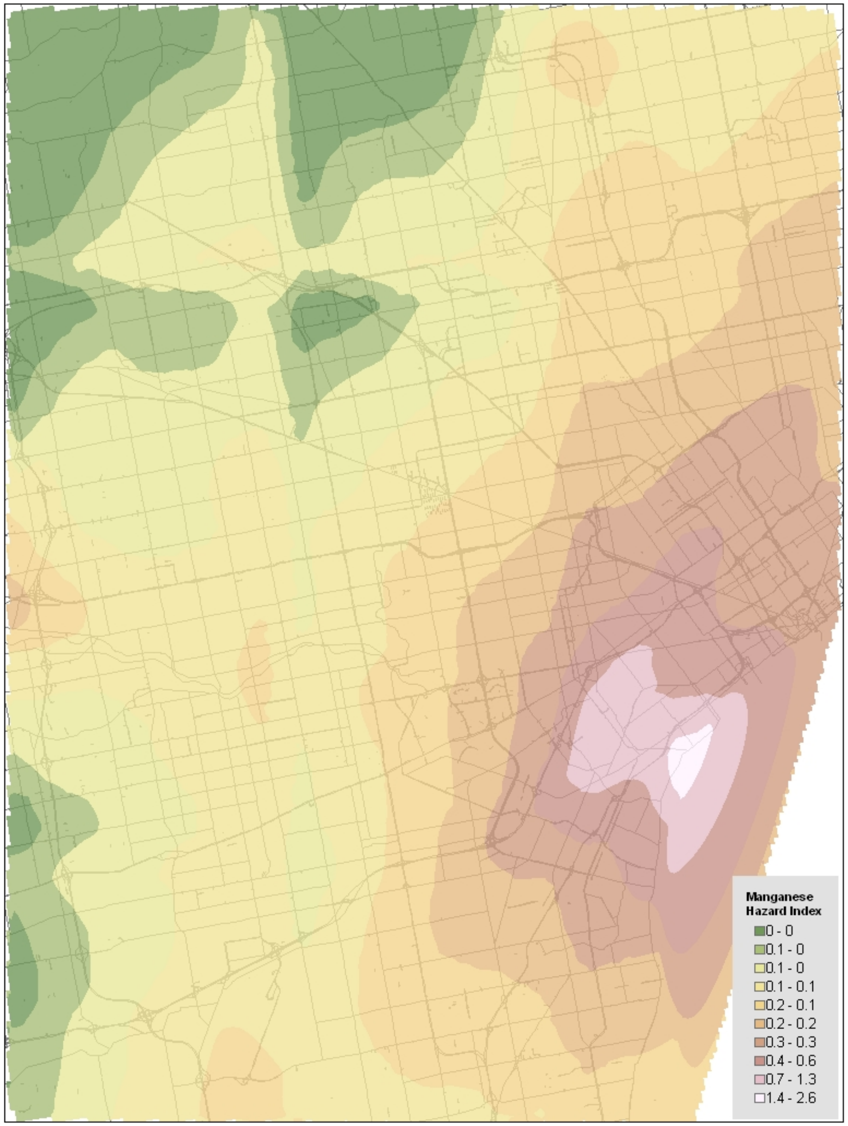
2002 Total Cancer Risk

(chronic)



Max Cancer Risk	7.4E-5
Max Cancer Risk Driver	Cadmium
Annual Incidence	0.8
Incidence Driver	Benzene
Population with Cancer Risk > 100 in a Million	0
Max Hazard Index	2.7
Max Hazard Index Driver	Manganese

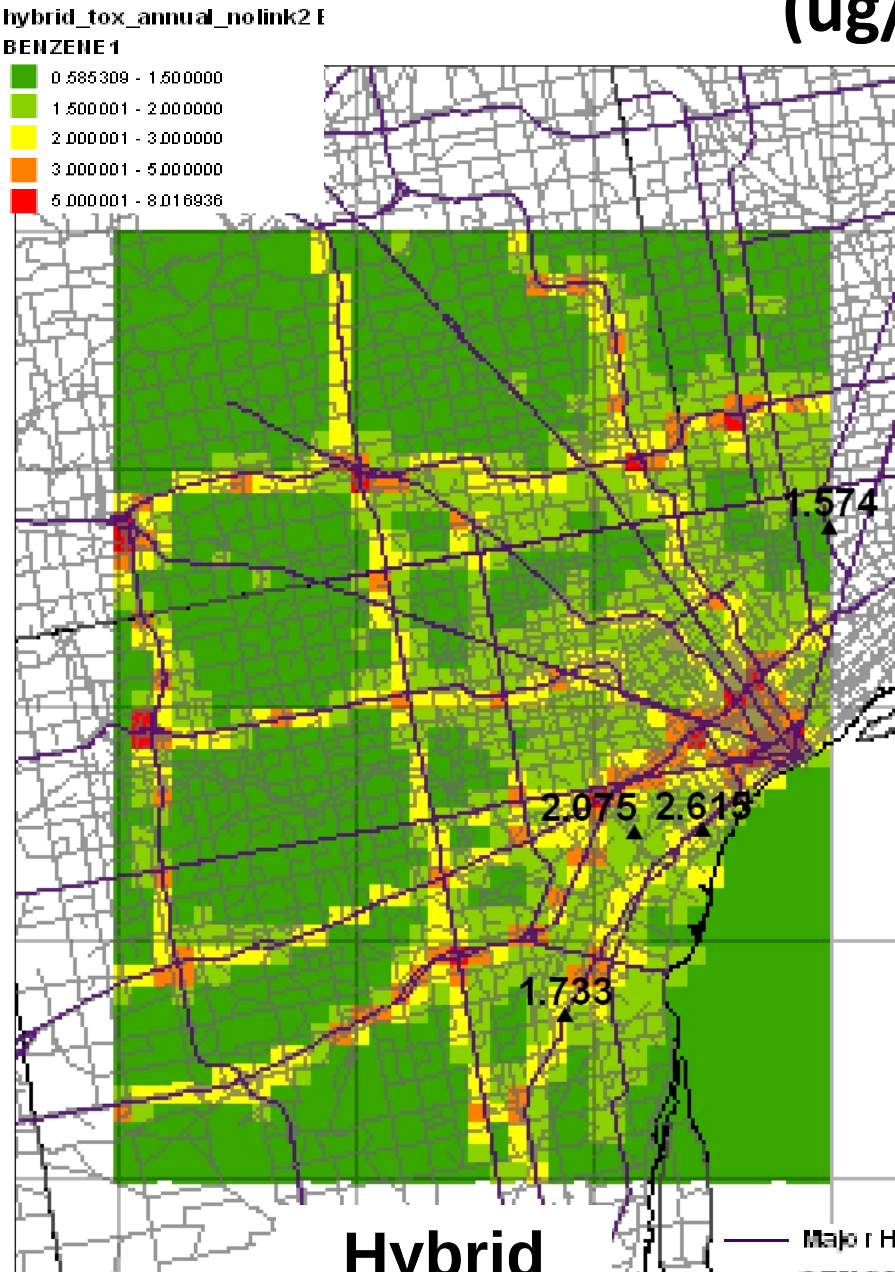
2002 Manganese Hazard Index



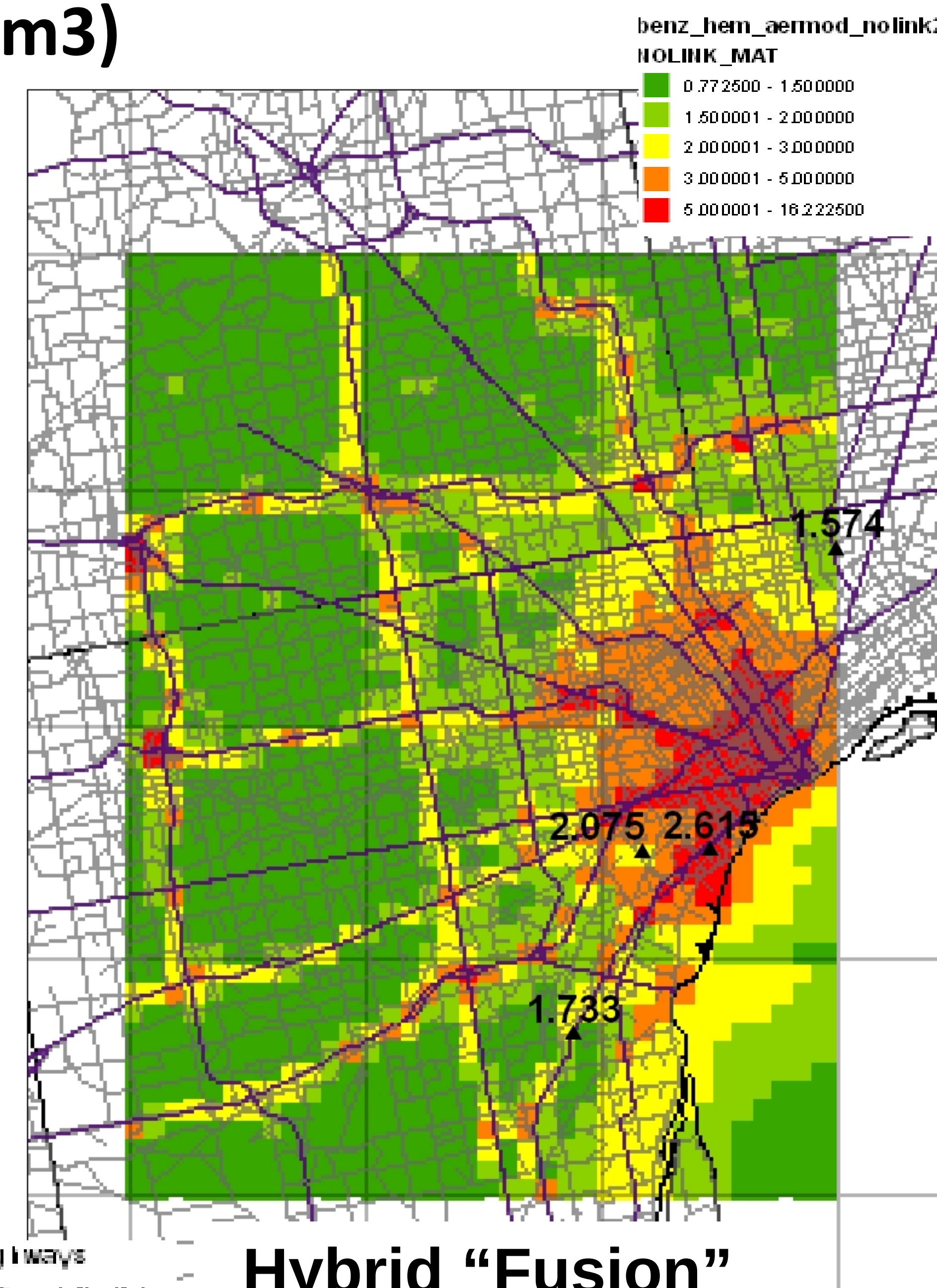
Can Spatial Fusion be used for toxics?

- The Modeled Attainment Test Software (MATS) tool is used to provide AQ input data to BenMAP
  - Creates a fusion of the ambient and modeled data across domain
  - Treats ambient data as “truth” and allows modeled data to provide gradient
  - Uses eVNA (enhanced Voronoi Neighborhood Averaging) approach
- In addition, MATS allows for a repeatable methodology that does not require “calibration” when different data sets are used.
- Readily available with the MATS software (http://www.epa.gov/scram001/modelingapps_mats.htm)
- Can we use it for toxics for HEM?
  - Tested as part of this project for several toxics (benzene, 1,3-butadiene, acetaldehyde, methylene chloride, formaldehyde & dichlorobenzene).
  - Input data are monthly averages from model & quarterly averages of monitored data to preserve seasonality.
  - Not done for all toxics (i.e. manganese, cadmium, nickel, naphthalene, & diesel PM) due to lack of sufficient monitoring data.

Annual Average Benzene (ug/m3)



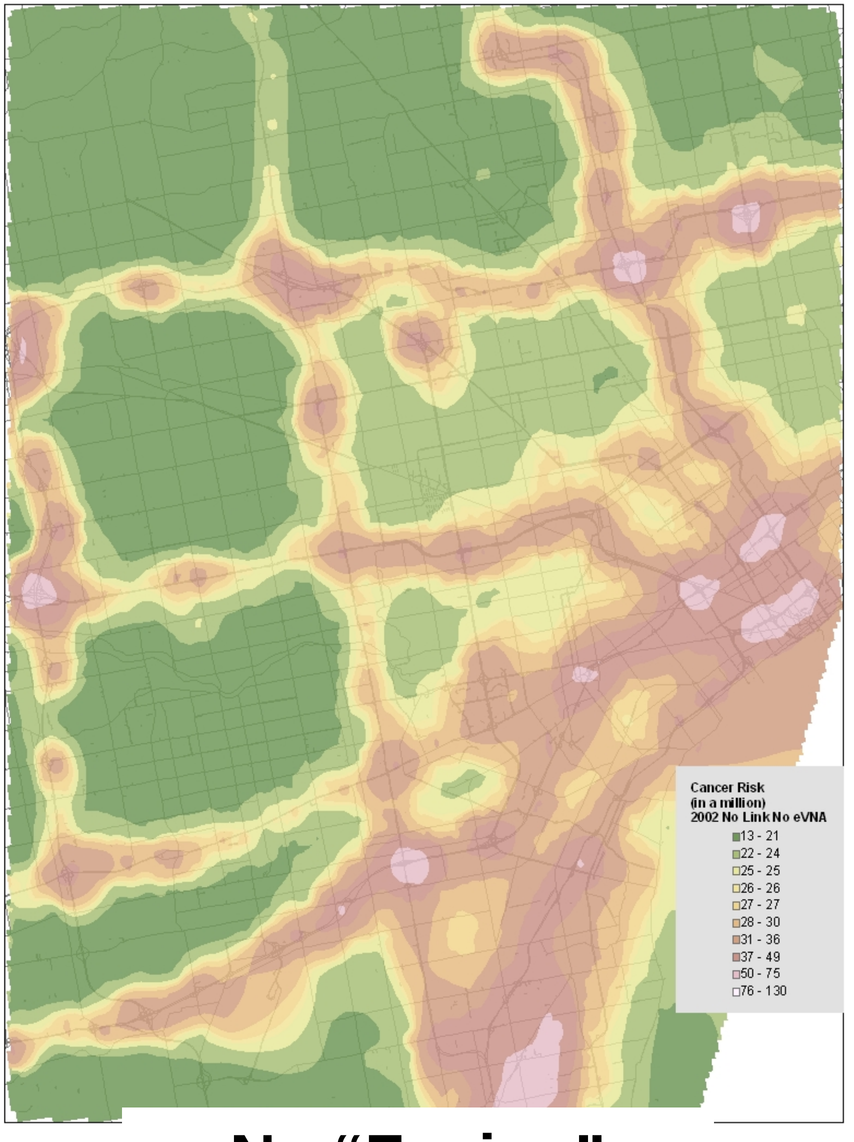
Hybrid



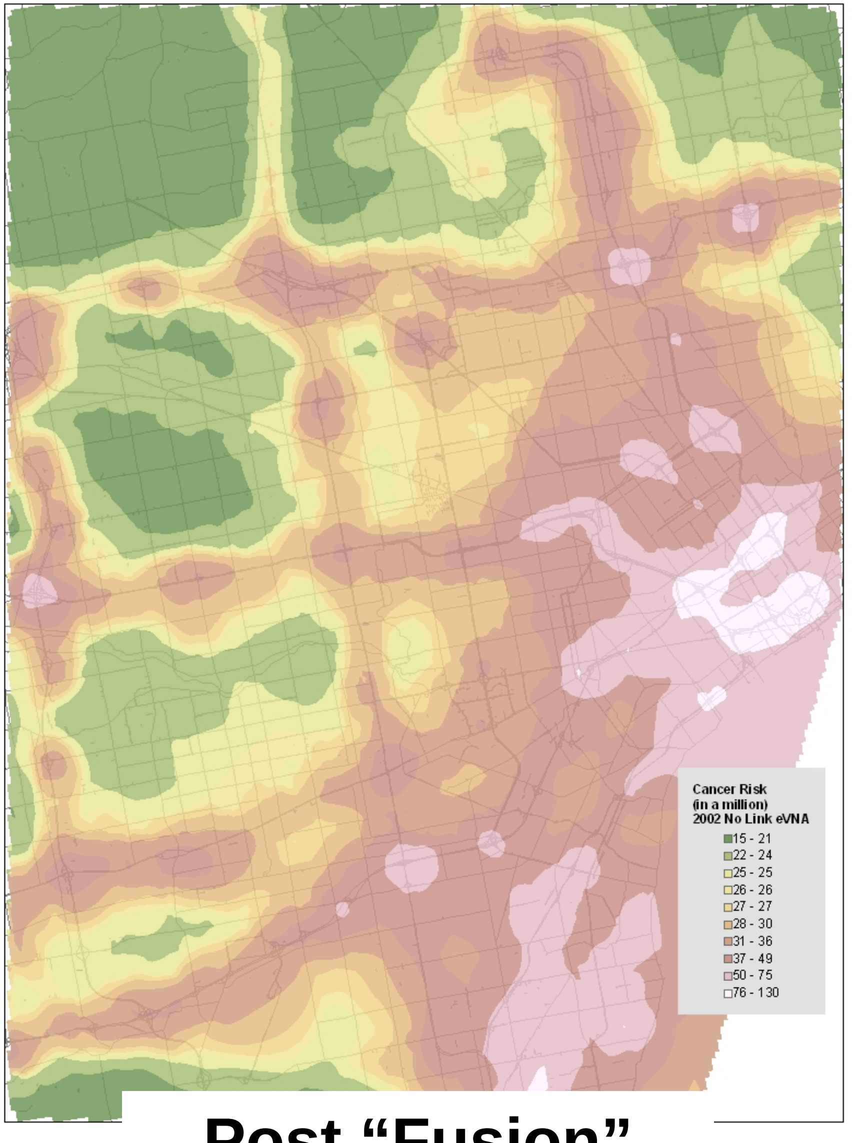
Hybrid “Fusion”

2002 Total Cancer Risk

(chronic; in a million)



No “Fusion”



Post “Fusion”

Results: 2002 Risk Estimates

Cancer

- Max risk 75% higher with “spatial fusion”
  - 130 in a million vs. 74 in a million
- Exposure/Incidence 33% higher with “spatial fusion”

- HAP driver changes from cadmium to benzene with “spatial fusion”

NonCancer

- Max hazard index (3, manganese) unaffected by “spatial fusion”

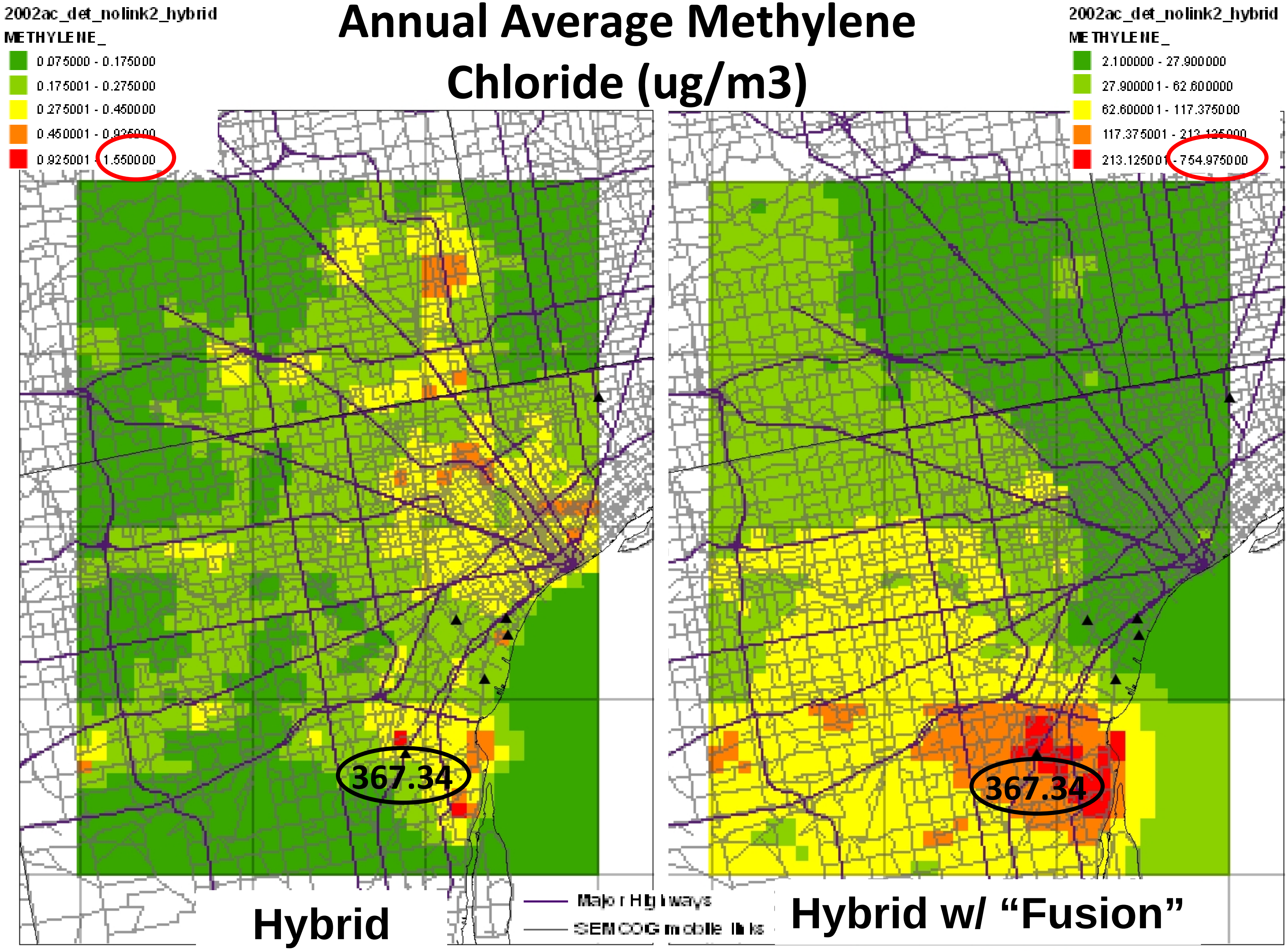
  - Manganese emissions not adjusted by “spatial fusion”

→Overall, using the “spatial fusion” approach via MATS tool is found to be an attractive method for improving air quality characterization by creating spatial surfaces for multiple pollutants that are consistent with monitored values.

“Lessons Learned”: Caveats for Toxics

- Since MATS tool uses monitoring data as “truth”, it is important to trust your monitoring data.
- For example, toxics monitoring data is more sparse and more susceptible to high measurements that are usually not included in the emissions inventory (“accidental release”)
- These very high measurements may bias your results. It becomes important to understand how these results will be used.
- Example for methylene chloride, where MDEQ could not explain exceptionally high values that did not occur at other monitors & source could not be identified. (This monitor was removed for this study.)

Annual Average Methylene Chloride (ug/m3)



Additional Caveats

- Important to also have confidence in your air quality modeling gradient, which influences the gradient adjustment done based on monitoring data as part of eVNA spatial fusion.
  - Model performance will depend on:
    - Model science (e.g. dispersion)
    - Meteorological data (e.g. wind direction)
    - Emissions inventory accuracy at local scale

Conclusions

- AERMOD and CMAQ seem to compare well for many primary species. AERMOD alone has difficulty when the pollutant has large component due to secondary formation (e.g. acetaldehyde, nitrate), as expected given AERMOD's lack of chemistry.
- Demonstrated the existence of local gradients & importance of local-scale air quality information.
- Multiplicative Hybrid Approach is one way to get air quality concentrations at a local scale.
  - However, resources required to run AERMOD for an urban area for many pollutants have us looking into fine-scale photochemical modeling.
- "Spatial fusion" via eVNA is an attractive technique for blending modeled and monitored data. It allows the model to be used in a relative sense (i.e. to generate spatial gradient), while the monitored values represent the "truth." However, it illustrates the importance:
  - Local scale emissions inventory data for AQ modeling
  - This technique also illustrates the importance of having high quality measurements for the pollutant(s) of interest.