Data analysis for multipollutant planning

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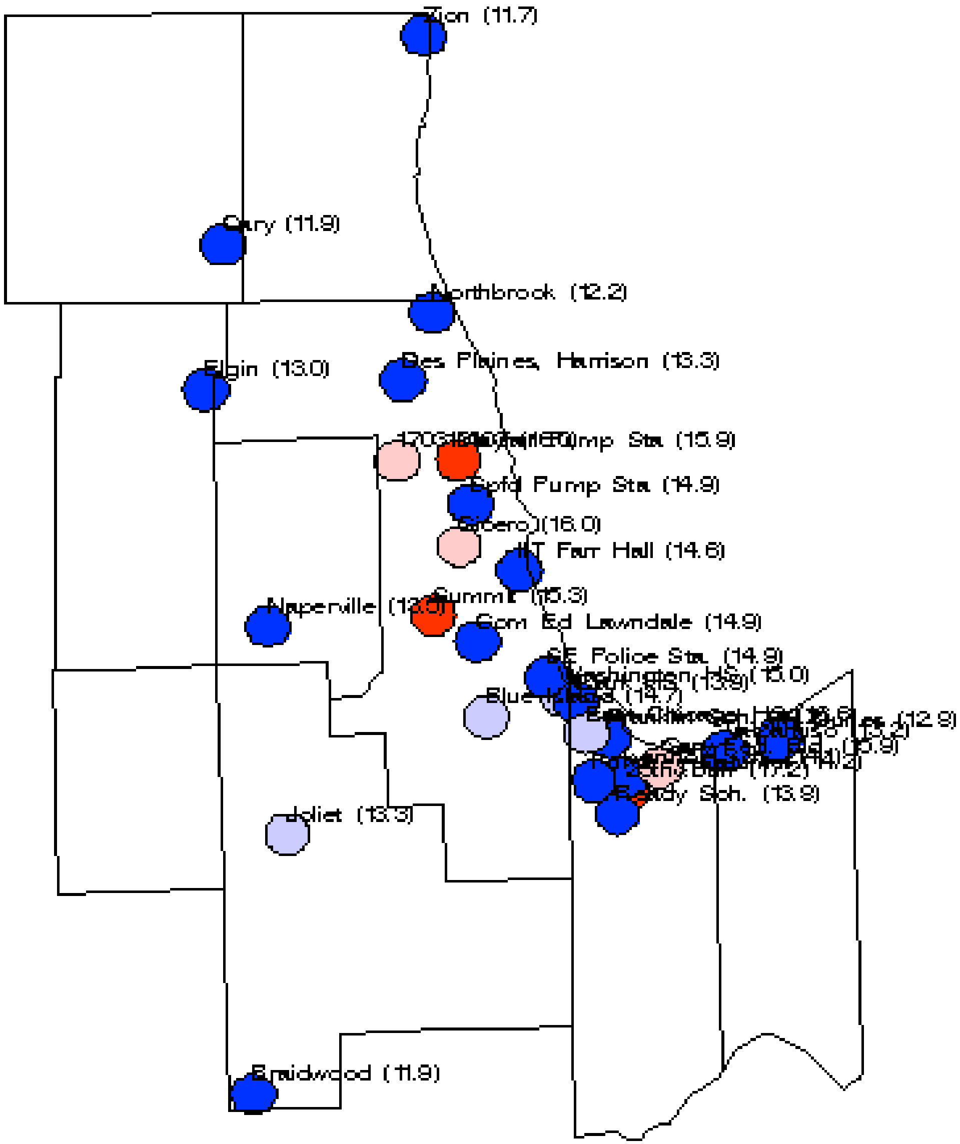
Donna Kenski

LADCO/MRPO

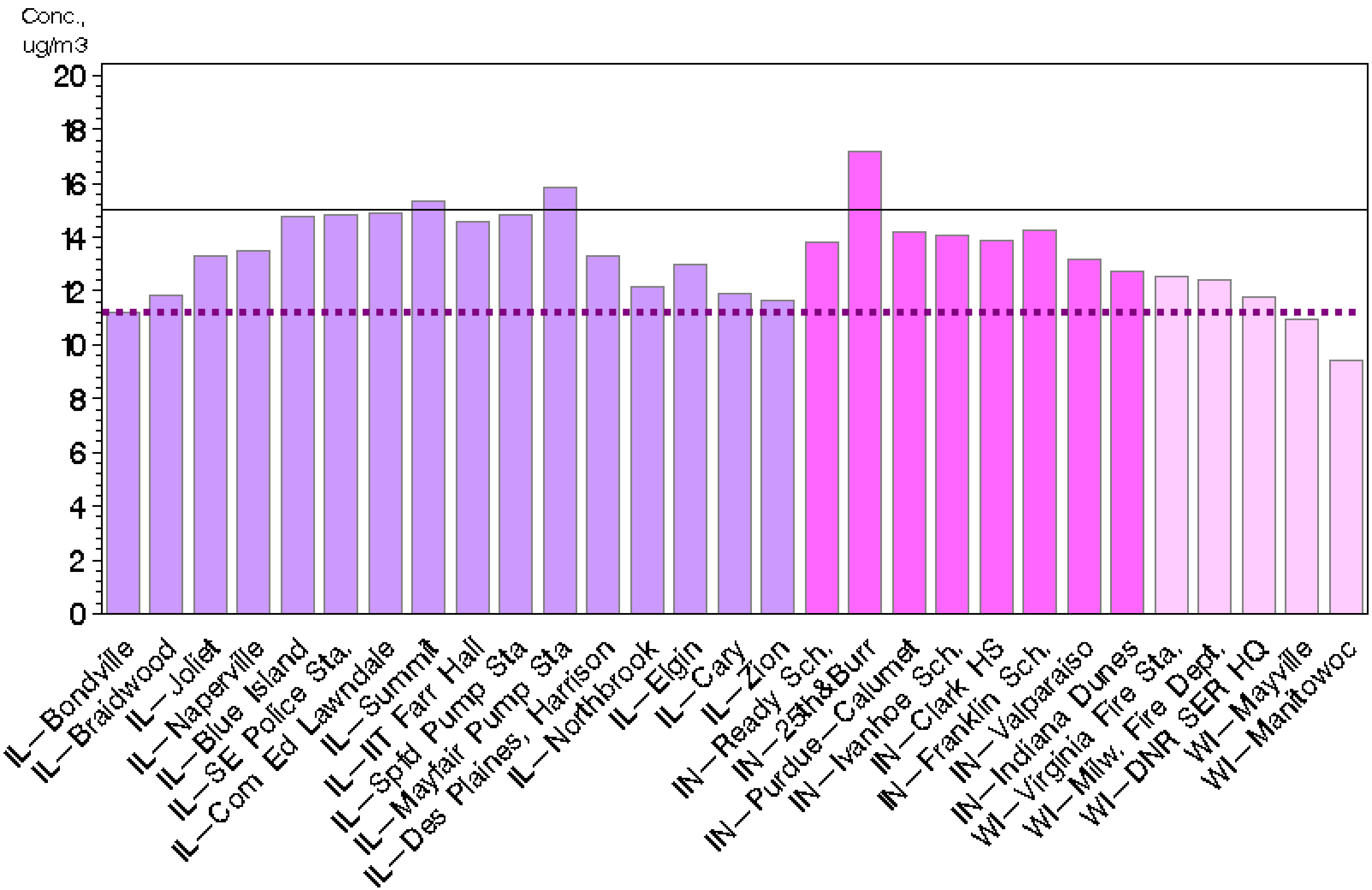
What can ambient data tell us about sources of PM2.5, toxics, and other pollutants?

- How do we quantify local primary source contributions to urban PM2.5 nonattainment, as distinguished from regional or widespread urban sources? What roles do precursor gases play?
- Data available:
  - FRM mass
  - continuous mass
  - speciation (24-hr and some near-continuous)
  - meteorology
  - special studies—OC speciation, continuous metals, mass spec, criteria gases, ammonia
- Tools and techniques available:
  - Descriptive/exploratory/visualization
  - Receptor models (includes CMB, PMF, factor analysis, UNMIX)
  - Thermodynamic models
  - Trajectory analyses, CPF

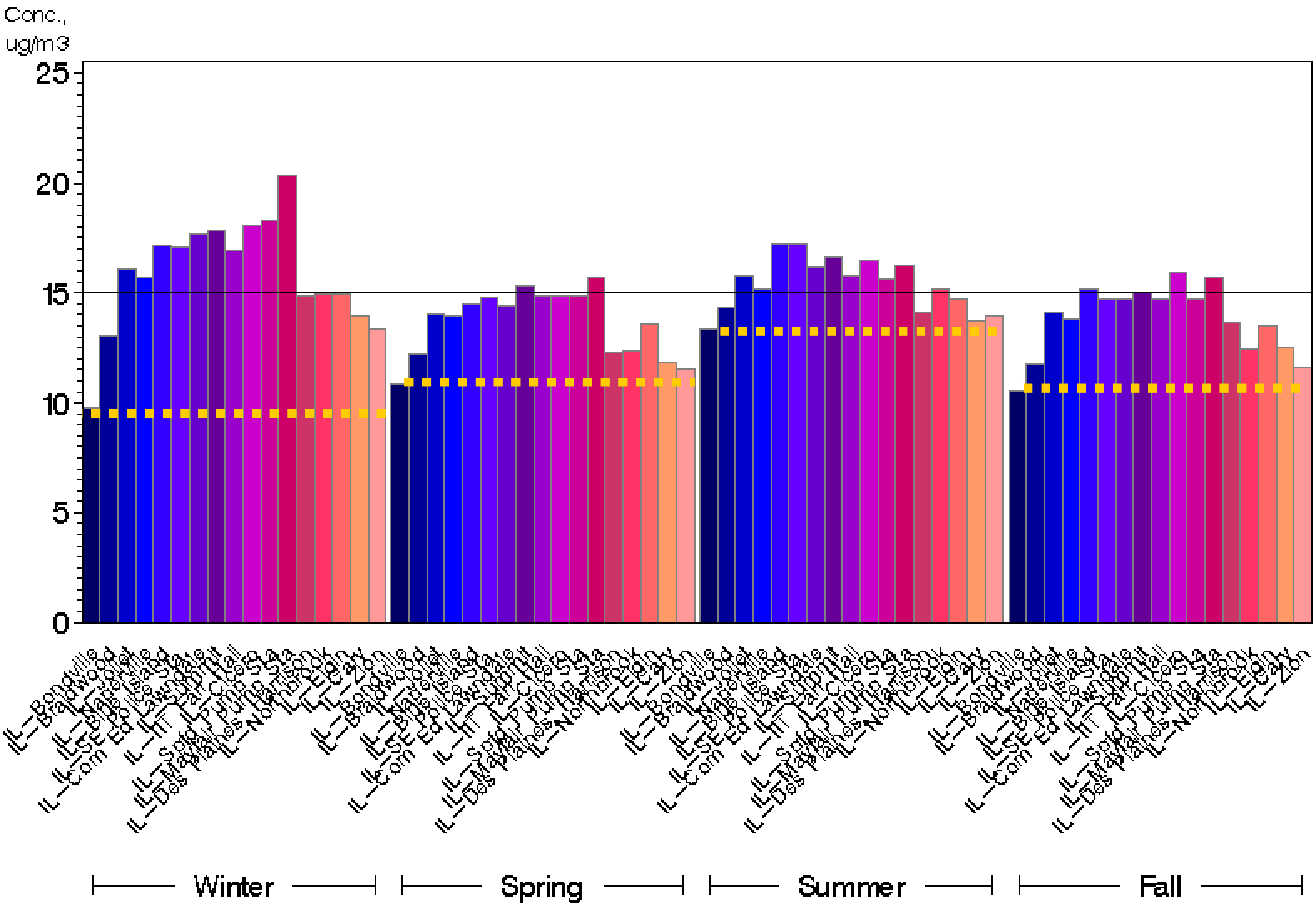


Chicago/Gary

Three-Year Average PM2.5, 2002-2004

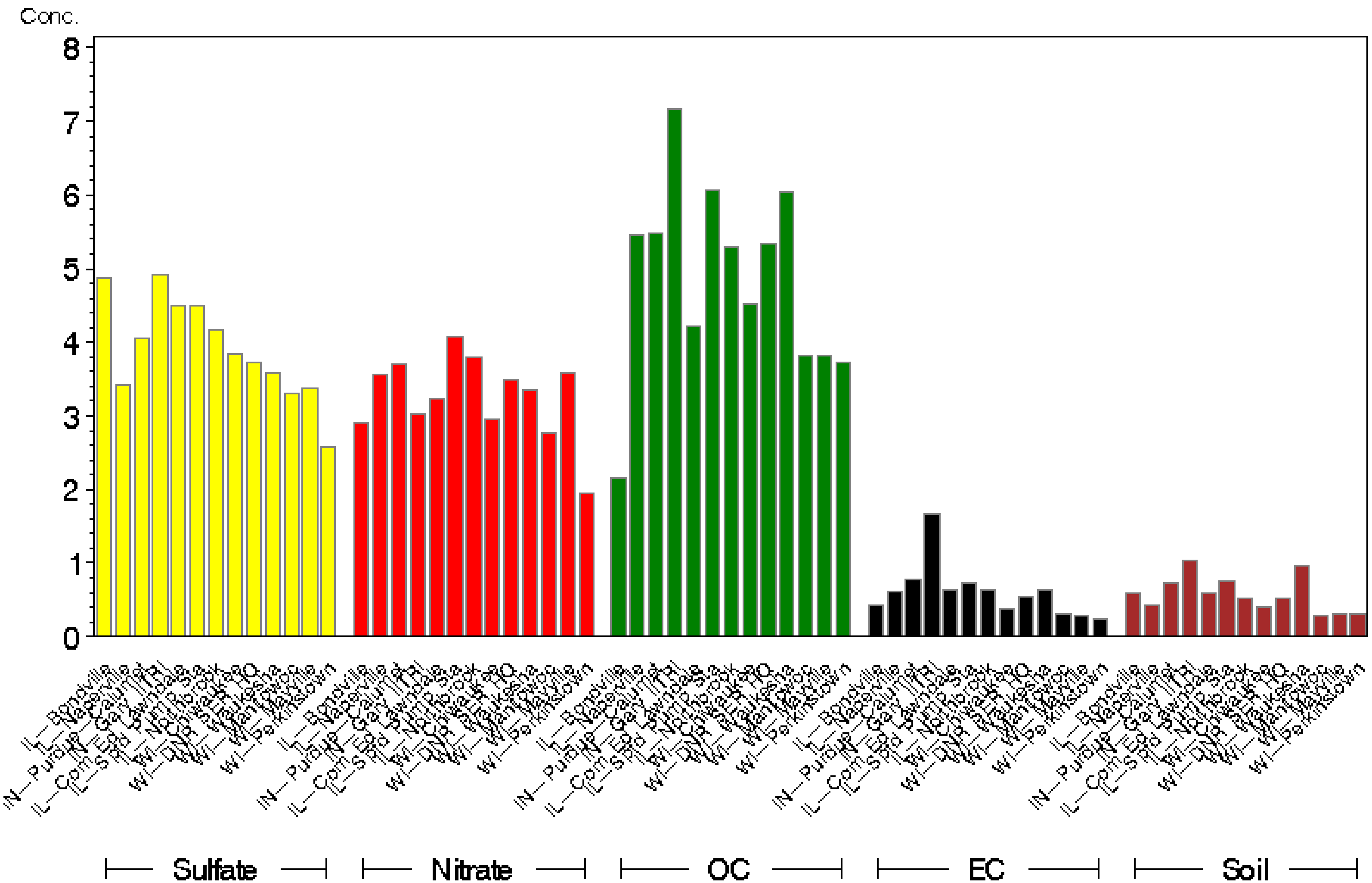


FRM Average Concentration by Season, Chicago, 1999–2005



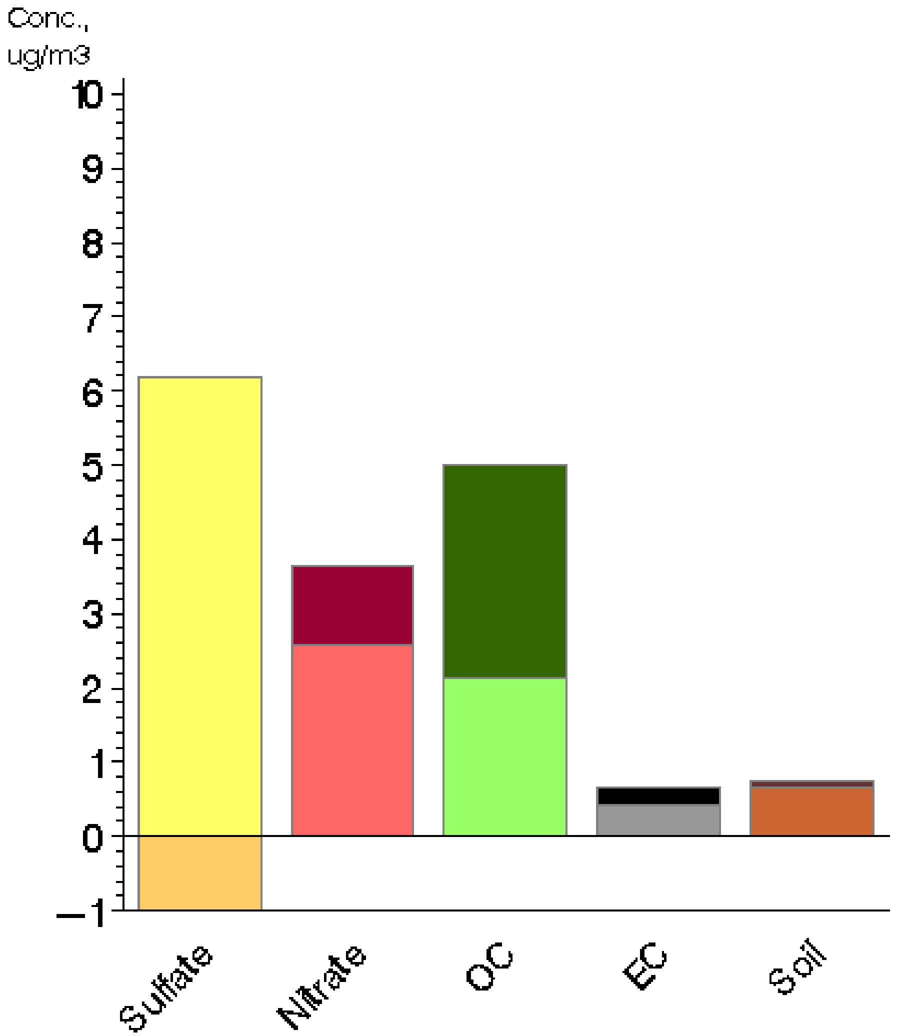
PM2.5 Components -- Average, 2002-2004

Reconstructed Mass



Chicago Urban Excess, Annual, by Species

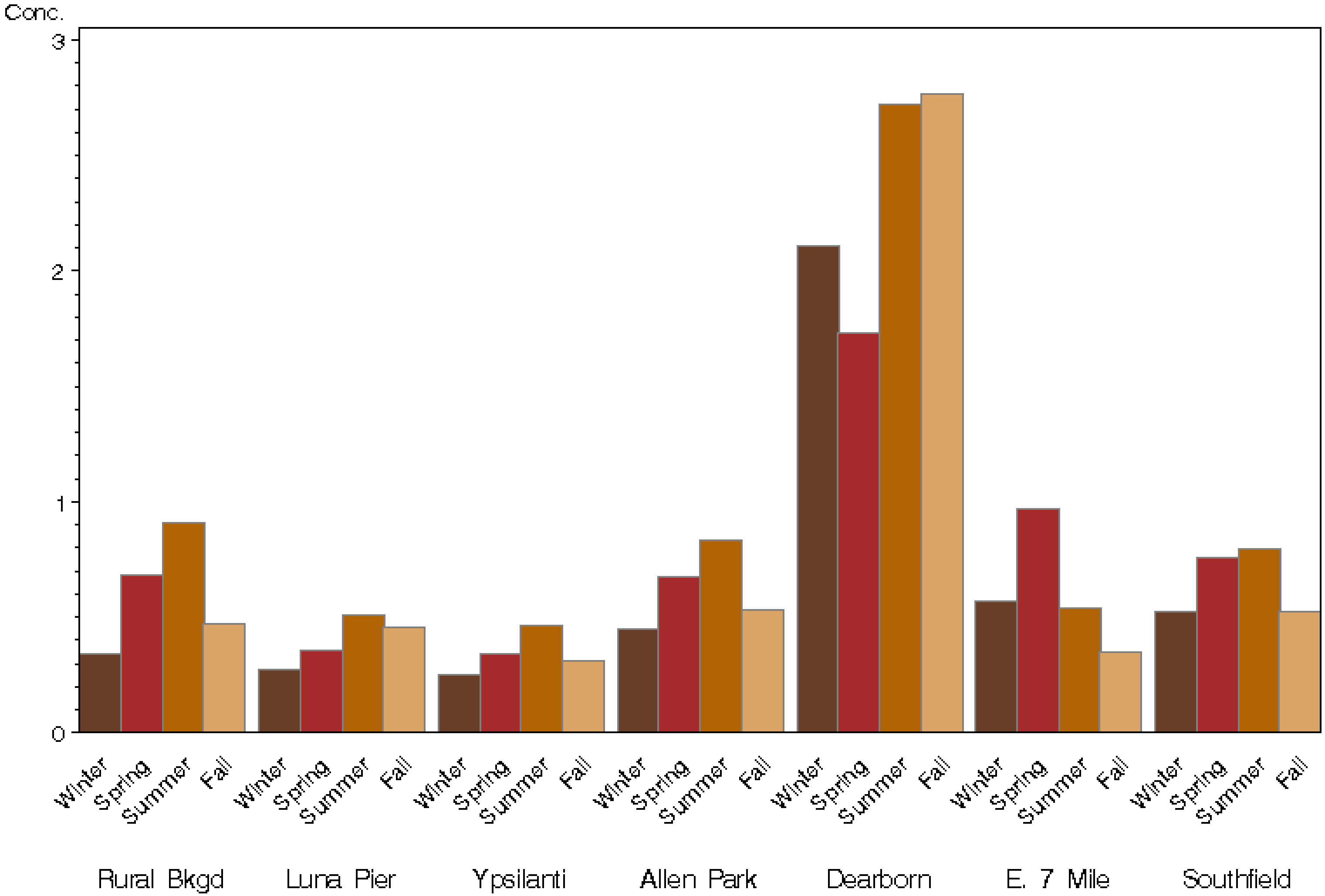
Bondville–Livonia Annual Average Used for Regional Background Estimation

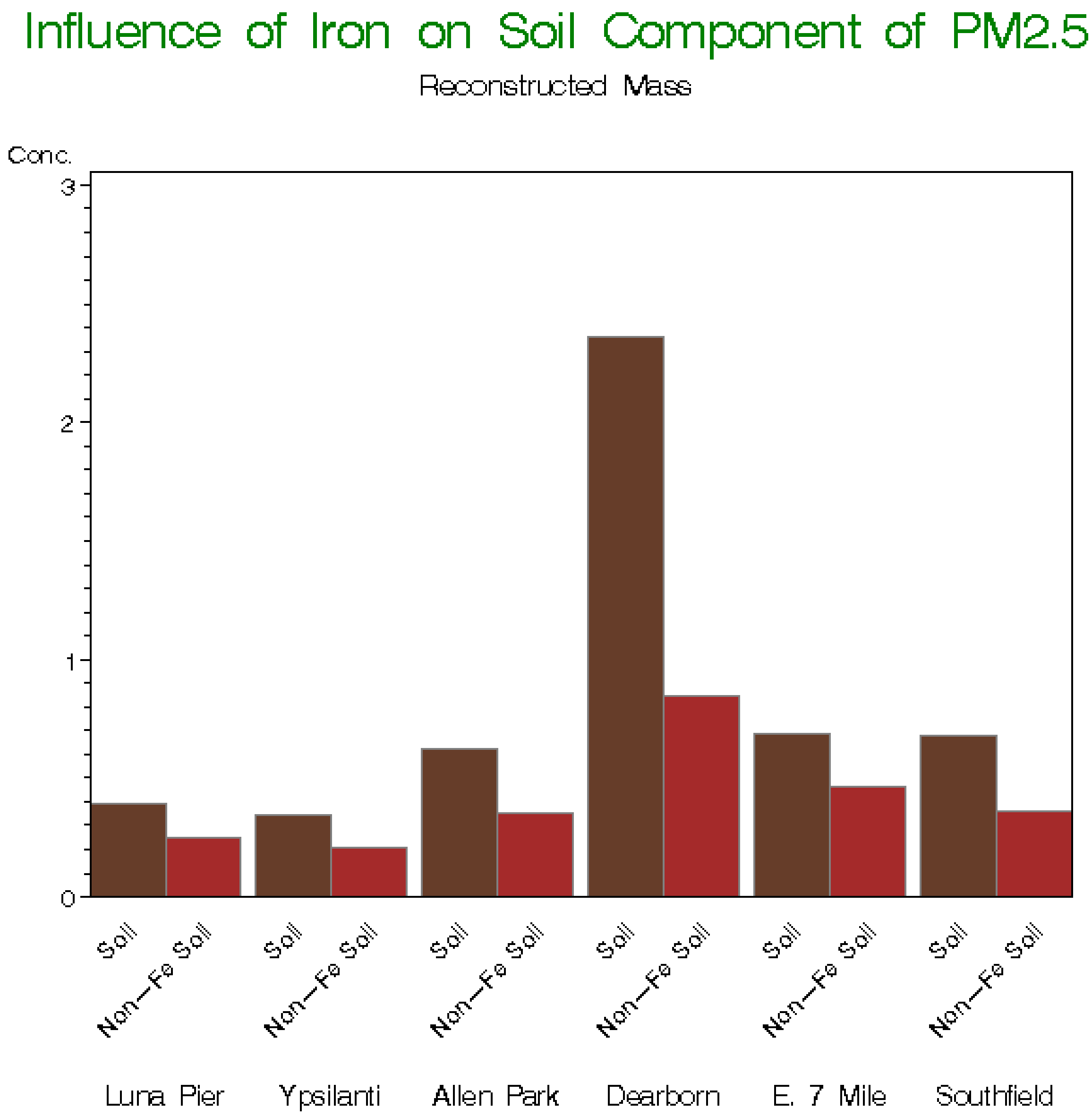


Light color bars are regional background; darker bars are urban excess

Seasonal and Spatial Variability in Soil

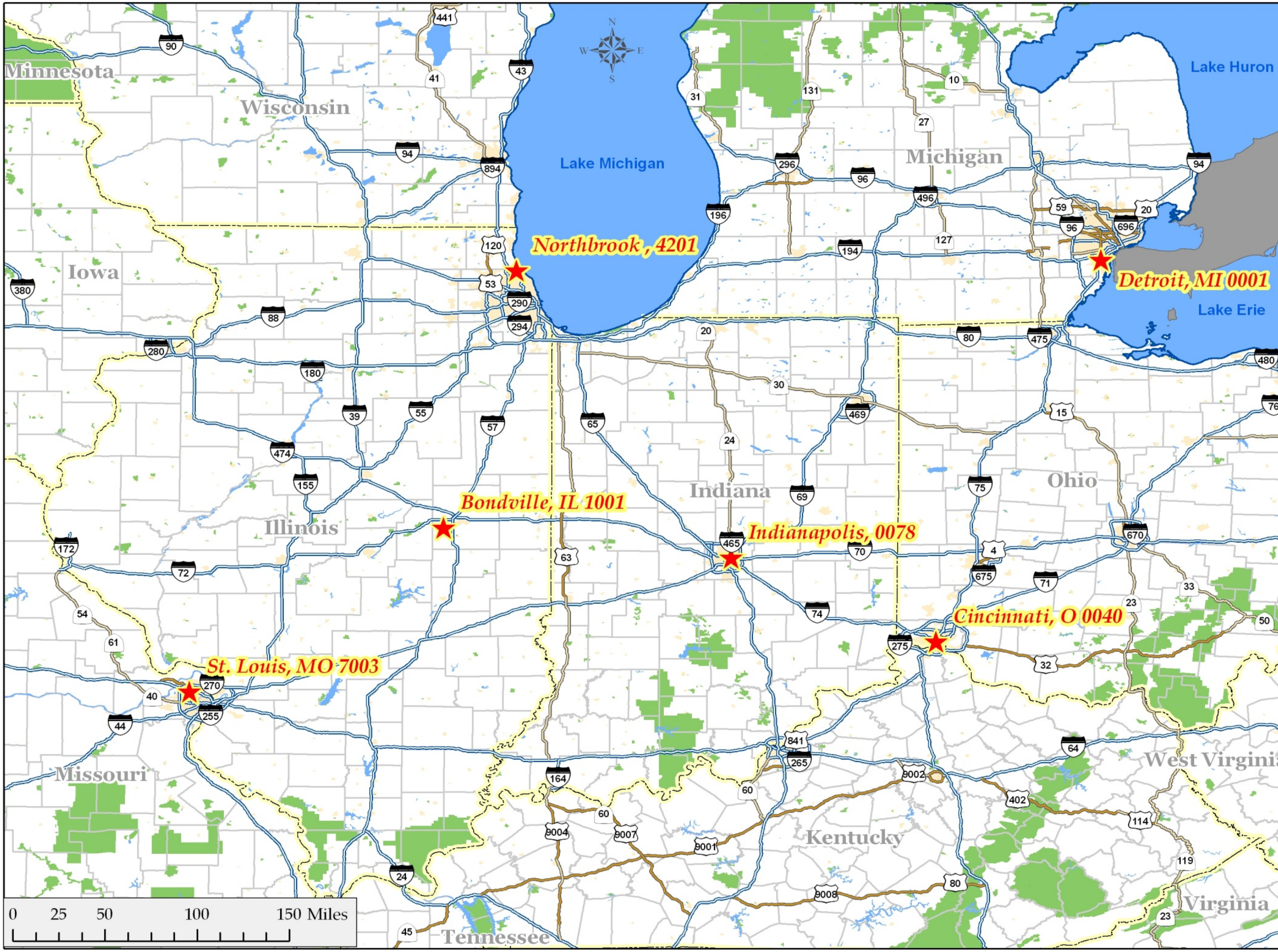
Reconstructed Mass



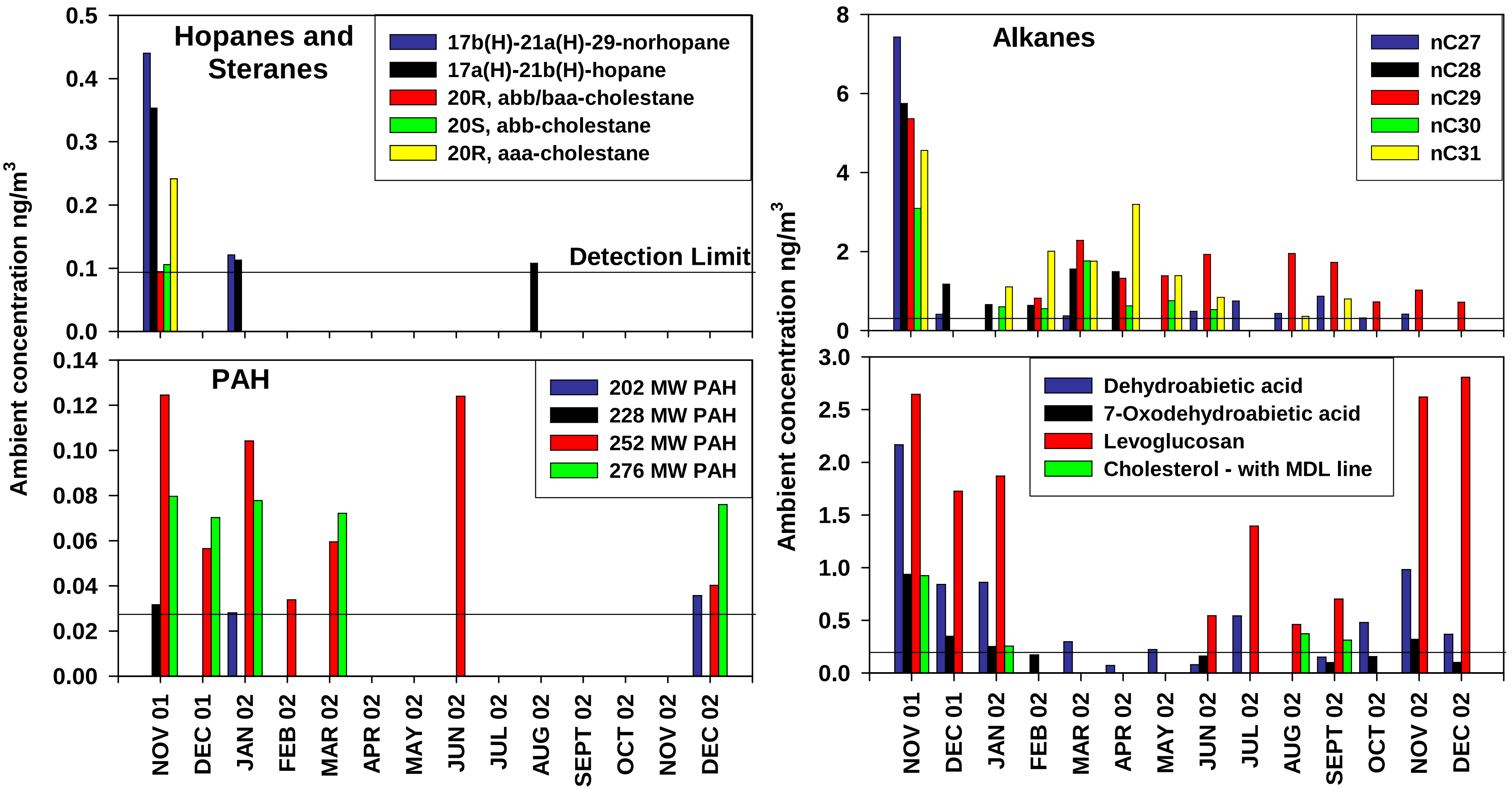

Influence of Iron on Soil Component of PM2.5
Reconstructed Mass
Conc.
3
2
1
0
Soil
Non-Fe Soil
Luna Pier
Ypsilanti
Allen Park
Dearborn
E. 7 Mile
Southfield

Molecular Markers for Source Apportionment

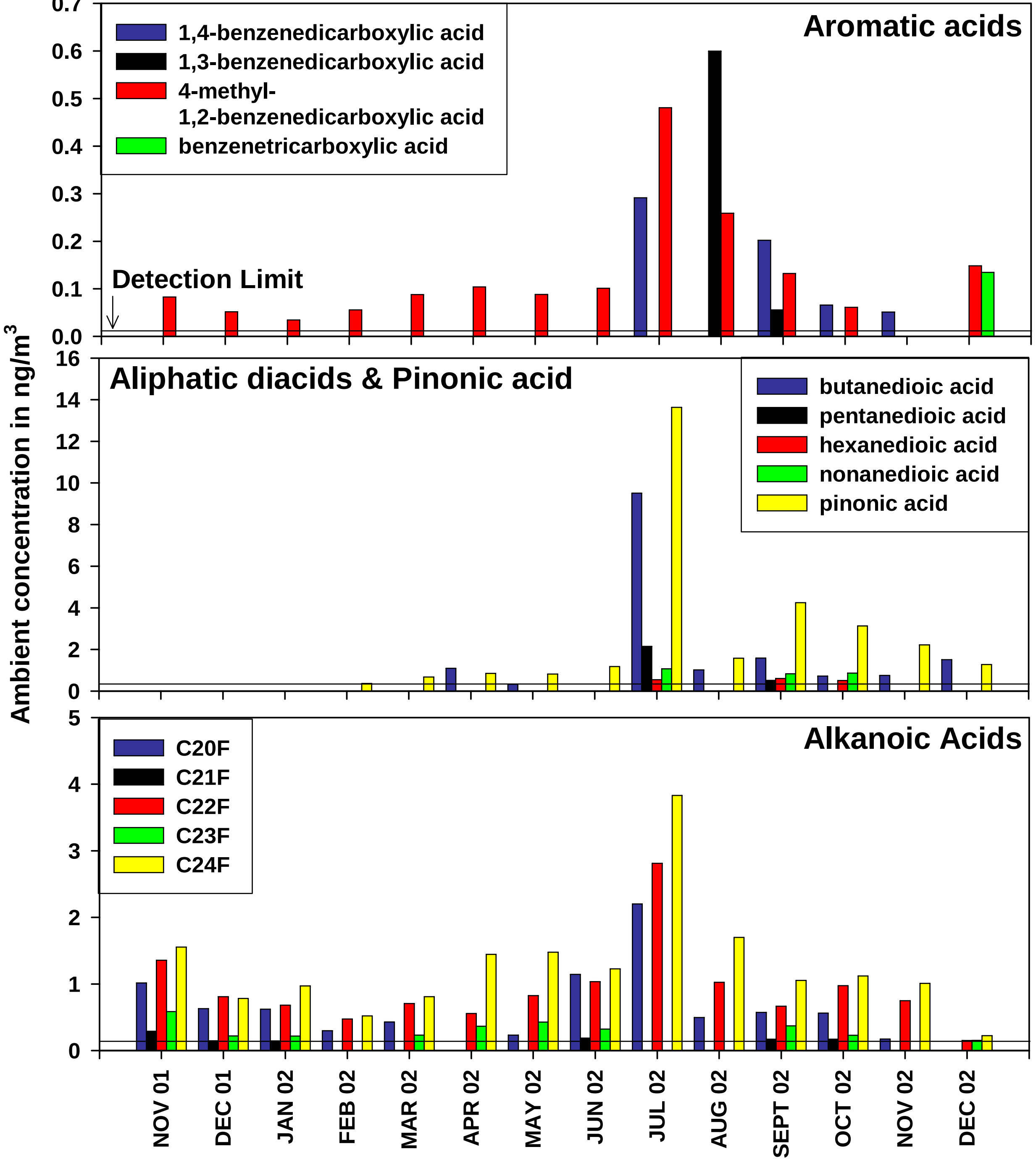
- *Molecular Markers*: Compounds present in the emissions from an air pollution source that are relatively unique to that source
- Used to understand the contributions of primary sources to the organic aerosol and PM concentrations
- Molecular Marker CMB models incorporating primary emission tracers have been reasonably well developed
- The organic compounds that make up SOA are different than the organic compounds in primary particulate matter emissions
- Recent work to identify anthropogenic and biogenic SOA markers and ratios to OC mass through smog chamber experiments


Minnesota
Wisconsin
Lake Michigan
Michigan
Lake Huron
Iowa
Northbrook , 4201
Detroit, MI 0001
Lake Erie
Illinois
Bondville, IL 1001
Indiana
Indianapolis, 0078
Ohio
Cincinnati, O 0040
St. Louis, MO 7003
Missouri
Kentucky
West Virginia
Virginia
Tennessee
0 25 50 100 150 Miles

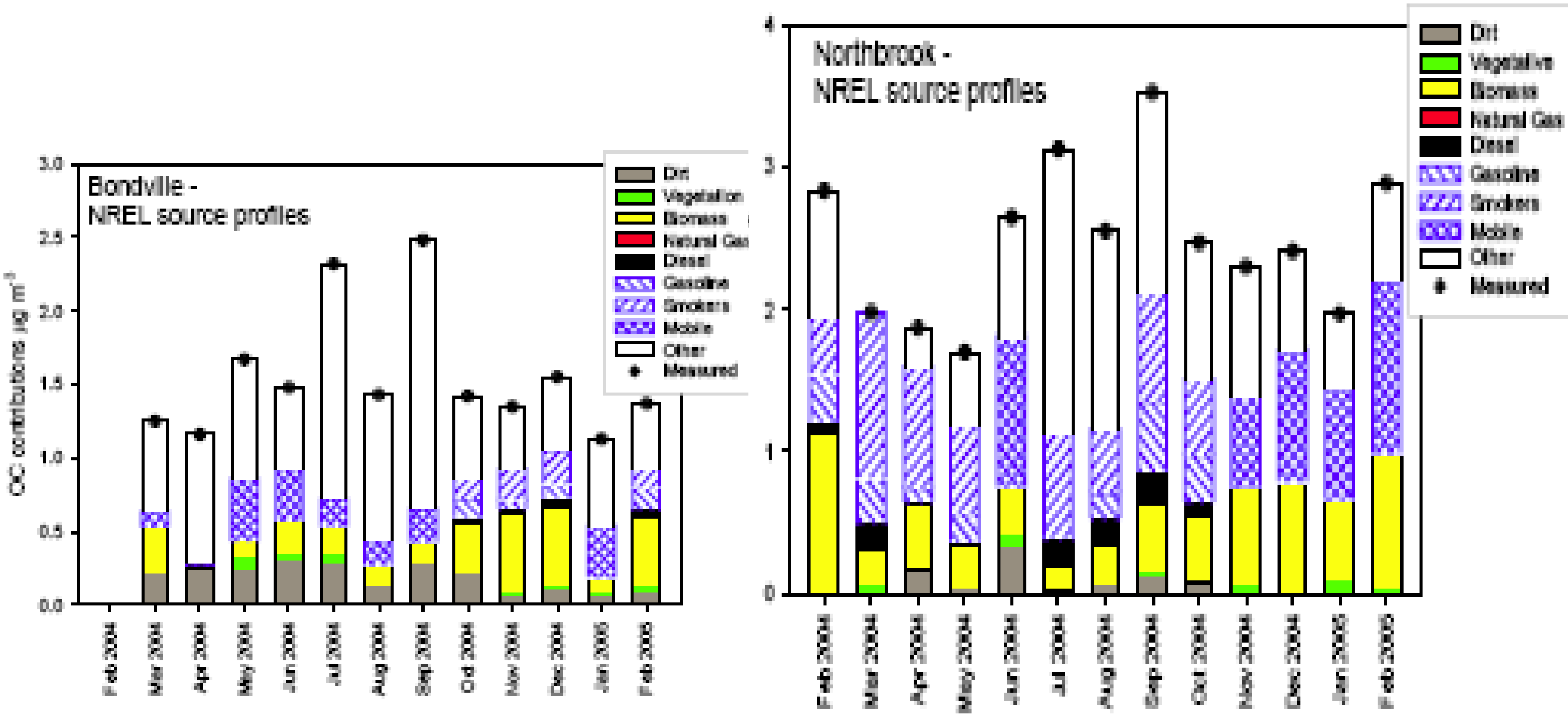
Primary emission tracers



Secondary OC tracers



(b)


Bondville -
NREL source profiles
OC contributions μg m-3
0.0
0.5
1.0
1.5
2.0
2.5
3.0
Dirt
Vegetation
Biomass
Natural Gas
Diesel
Gasoline
Smokers
Mobile
Other
Measured
Feb 2004
Mar 2004
Apr 2004
May 2004
Jun 2004
Jul 2004
Aug 2004
Sep 2004
Oct 2004
Nov 2004
Dec 2004
Jan 2005
Feb 2005
Northbrook -
NREL source profiles
0
1
2
3
4
Dirt
Vegetative
Biomass
Natural Gas
Diesel
Gasoline
Smokers
Mobile
Other
Measured
Feb 2004
Mar 2004
Apr 2004
May 2004
Jun 2004
Jul 2004
Aug 2004
Sep 2004
Oct 2004
Nov 2004
Dec 2004
Jan 2005
Feb 2005

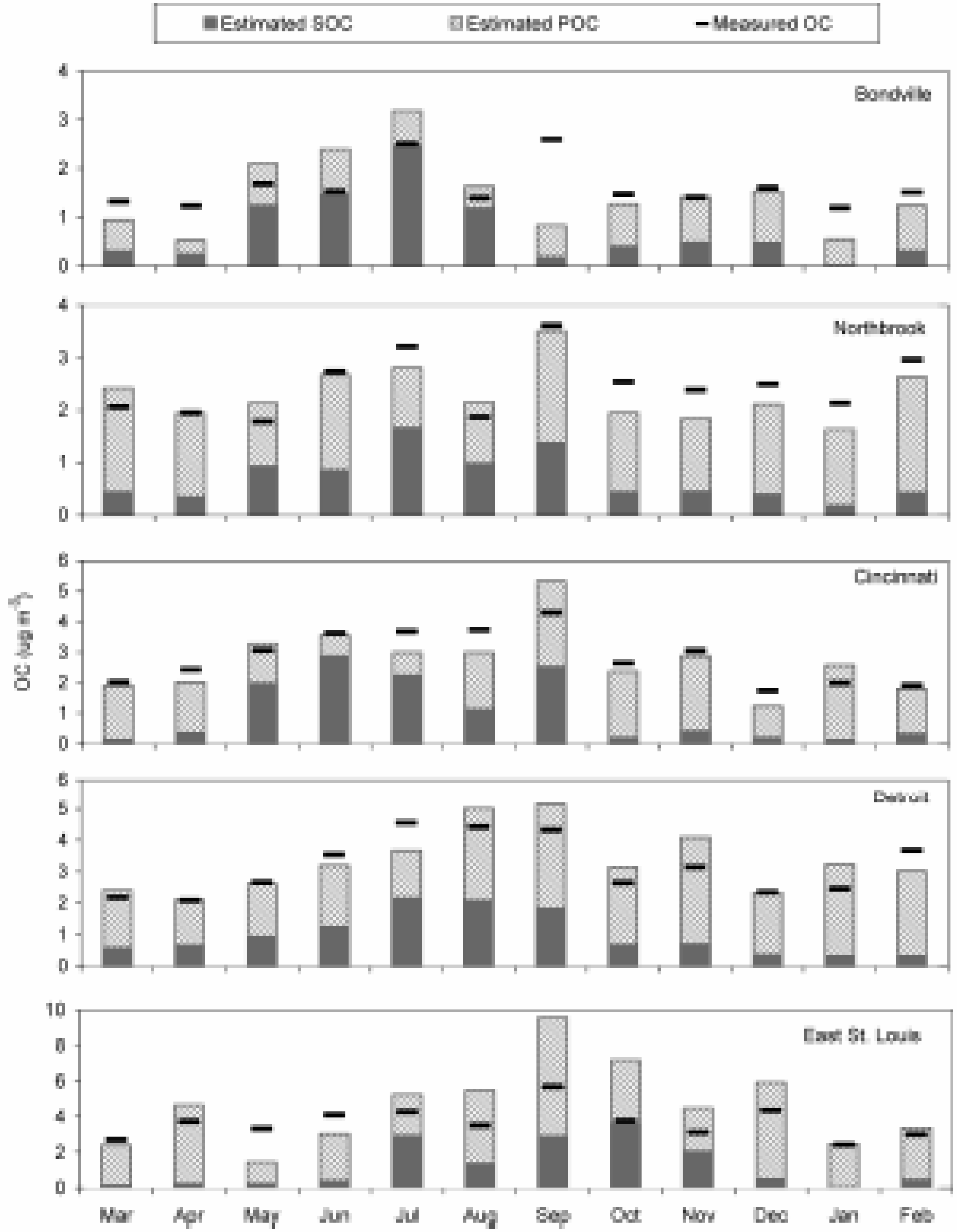


FIGURE 1. Estimated primary and secondary contributions compared with measured organic carbon for March 2004 through February 2005.

Source: Lewandowski et al, ES&T, 2008

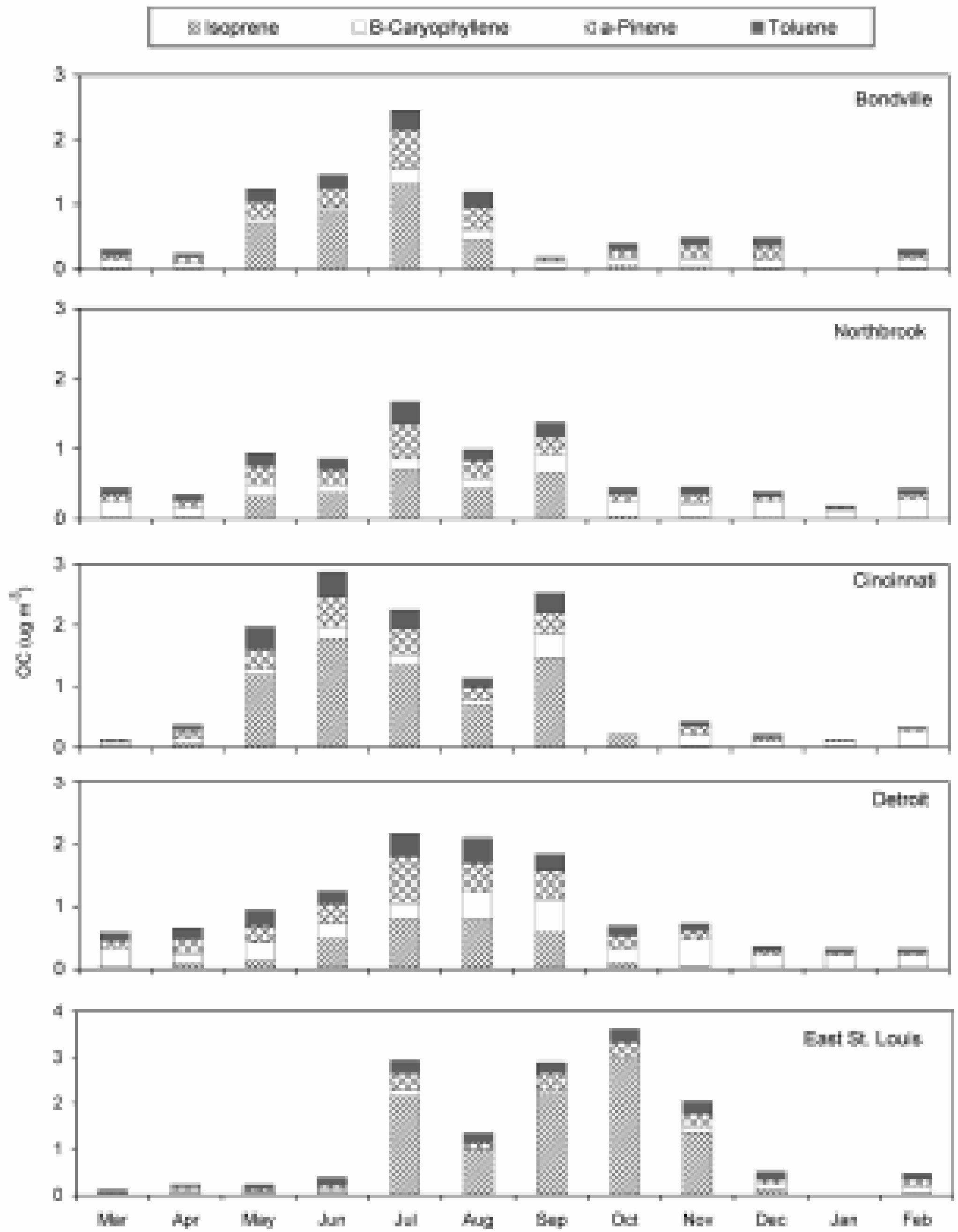


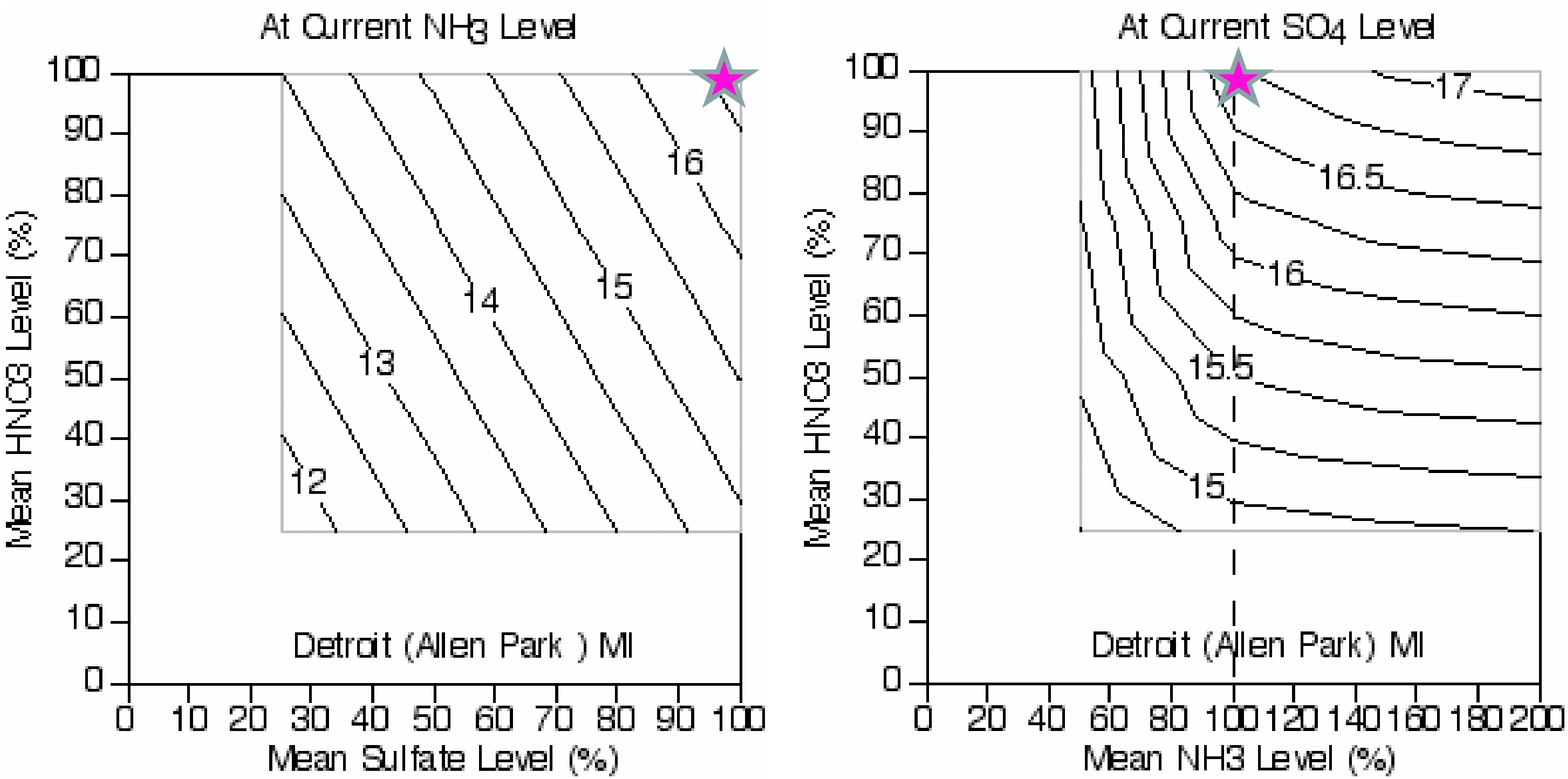
FIGURE 2. Detailed secondary contributions to ambient $PM_{2.5}$ in Bondville, Northbrook, Cincinnati, Detroit, and East St. Louis for March 2004 through February 2005.

Source: Lewandowski et al, ES&T, 2008

Thermodynamic Models—ISORROPIA and SCAPE2

- Thermodynamic models predict the partitioning of PM species between gas and particle phases, based on concentration, temperature, and RH
- Using measured NH3, HNO3, NH4, NO3, and SO4, systematically vary concentrations from starting (ambient) conditions and calculate new equilibrium concentrations
- Resulting isopleths tell us how sensitive PM is to changes in precursors
- SO4 and NO3 – 25, 50, 75, 100% of current
- NH4 – 50, 100, 150, 200% of current

Predicted $PM_{2.5}$ Concentrations

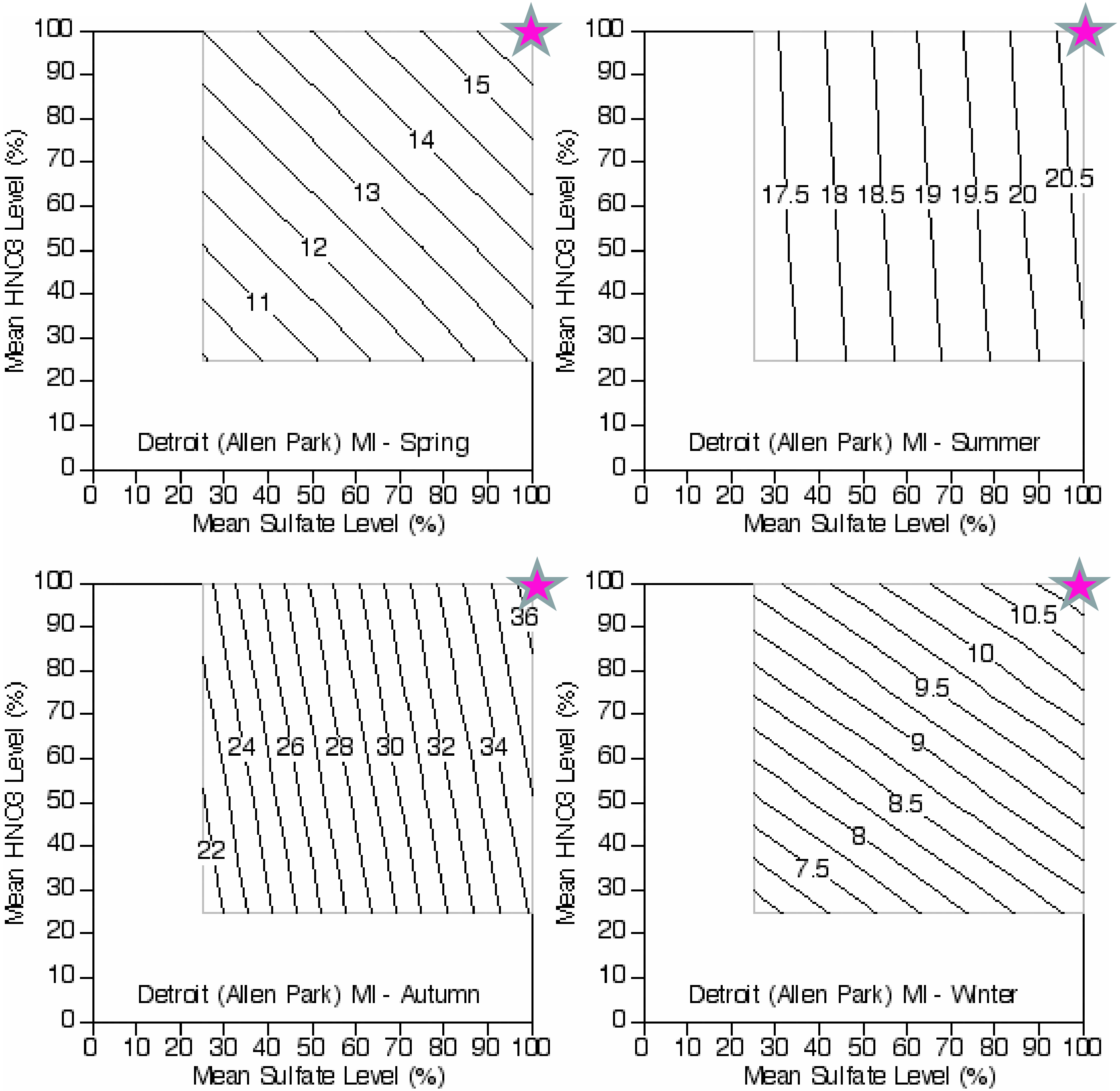


PM is about equally sensitive to reductions in SO4 and NO3

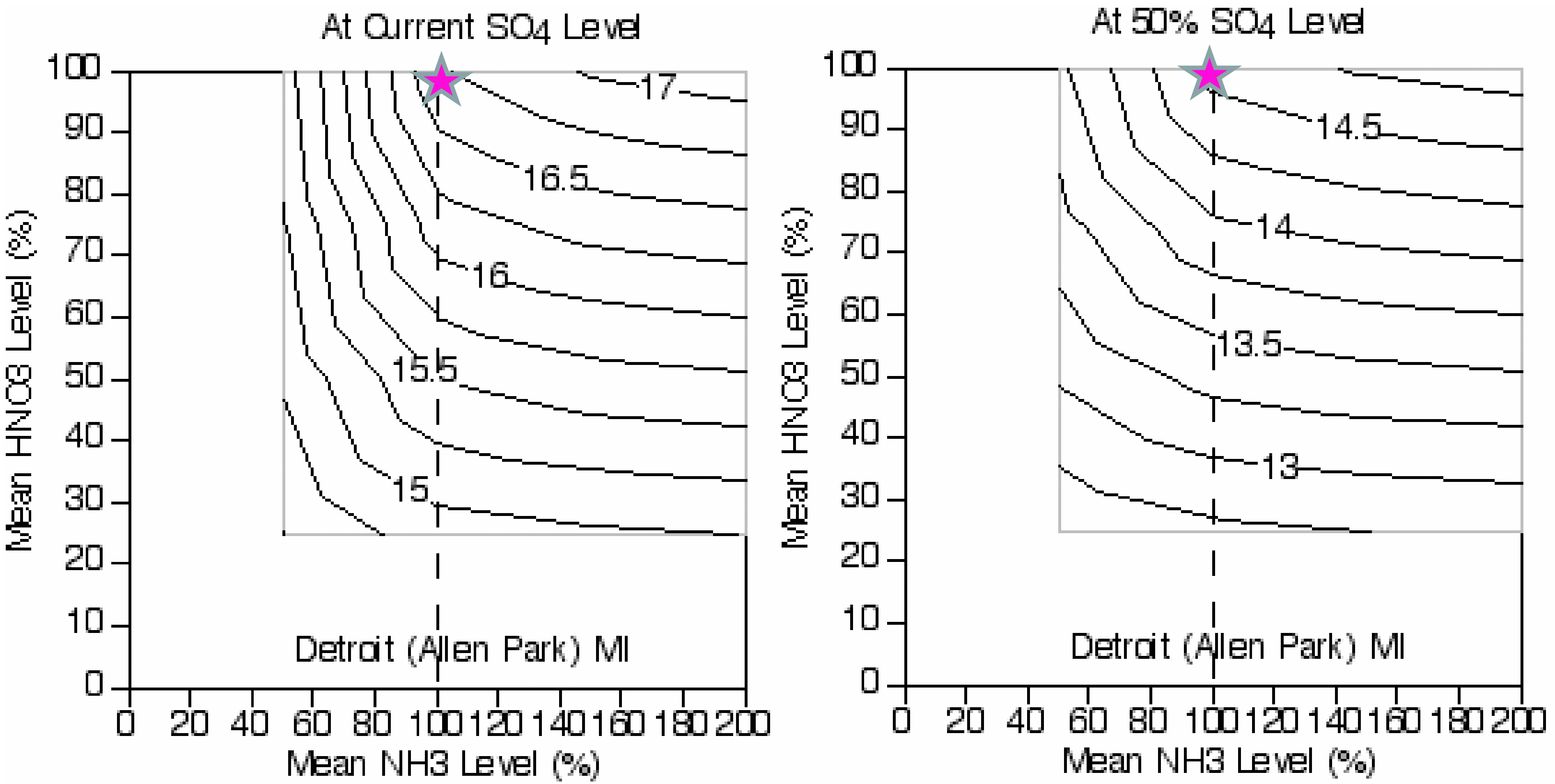
PM is slightly more sensitive to NH3 reductions than to HNO3

Seasonal $PM_{2.5}$ Concentrations

PM is most responsive to NO3 in the winter; response to sulfate is similar year-round.



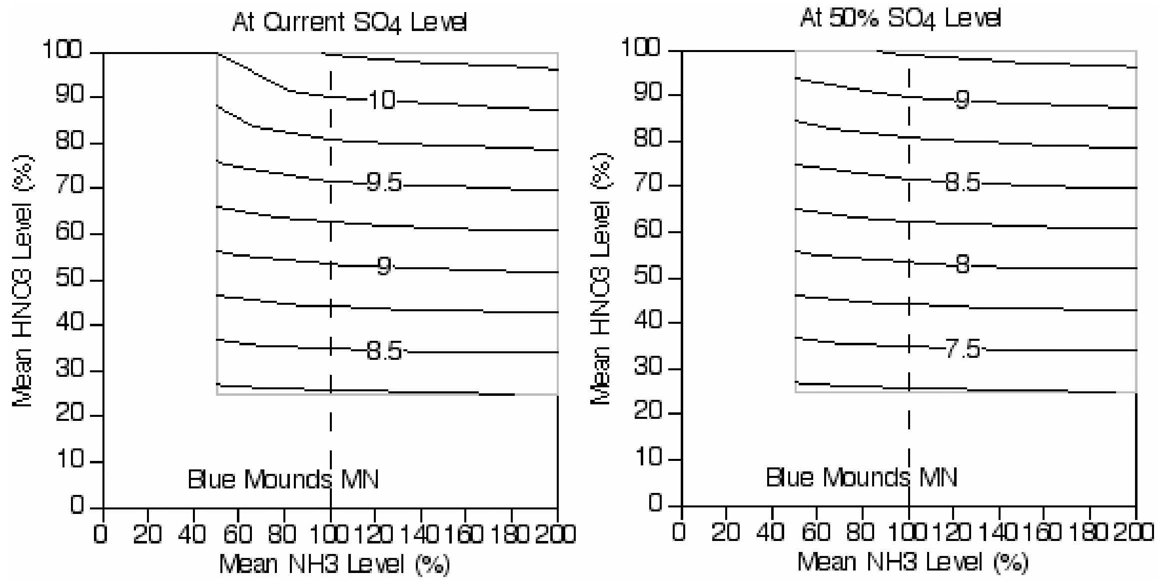
Predicted $PM_{2.5}$ Concentrations



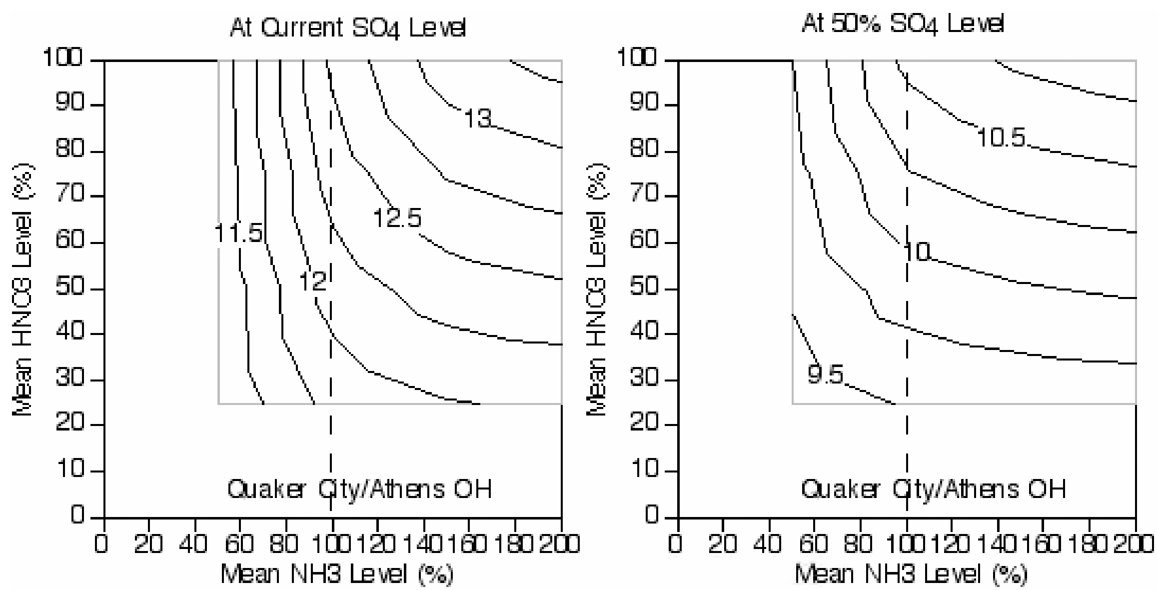
Expected reductions in SO4 may lead to PM being less responsive to reductions in ammonia

Geographic extremes

Blue Mounds, MN: Least sensitive to NH3; farthest north, and highest NH3 site

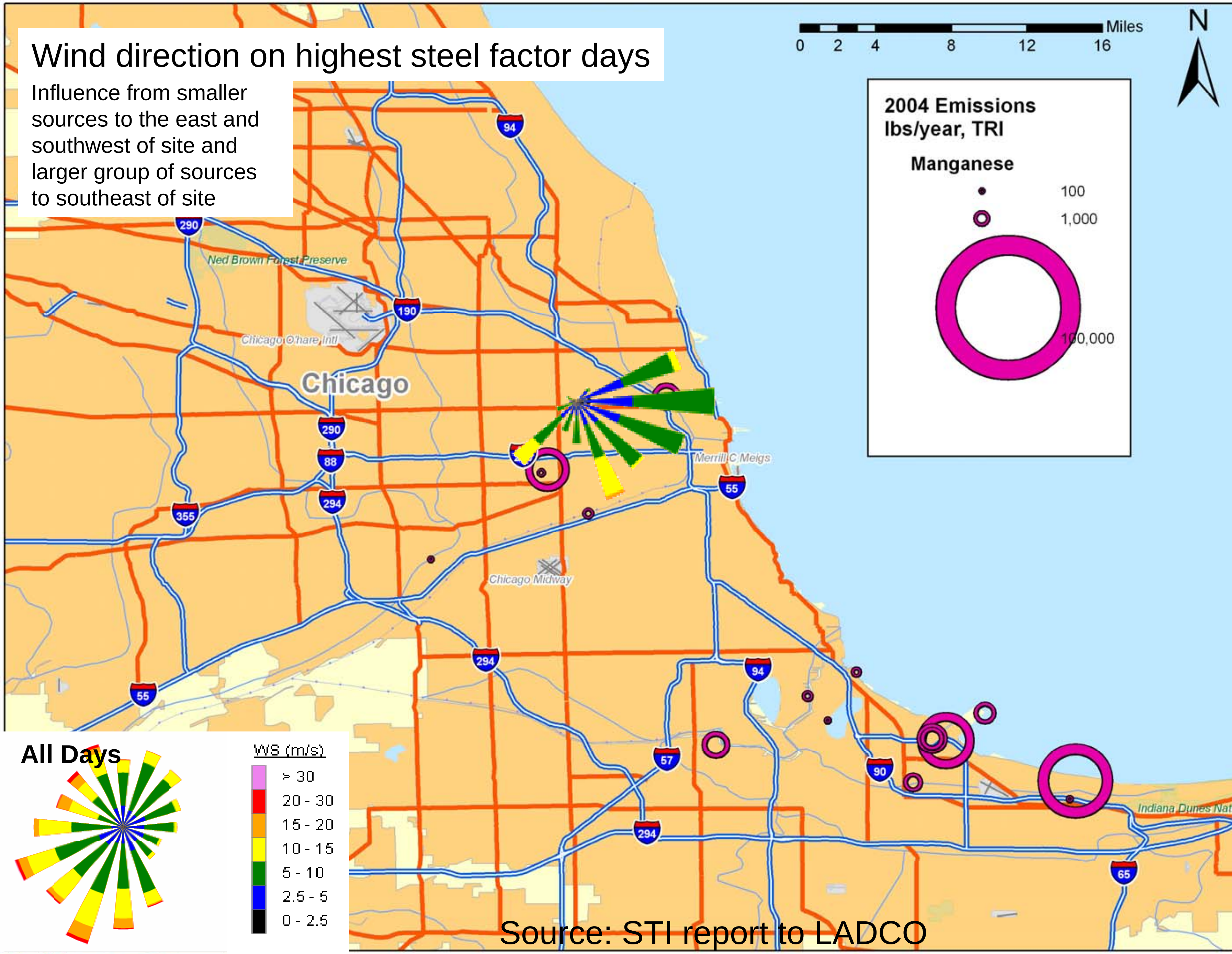


Athens, OH: Most sensitive to NH3; farthest east, lowest NH3 site



Where are the sources of interest?

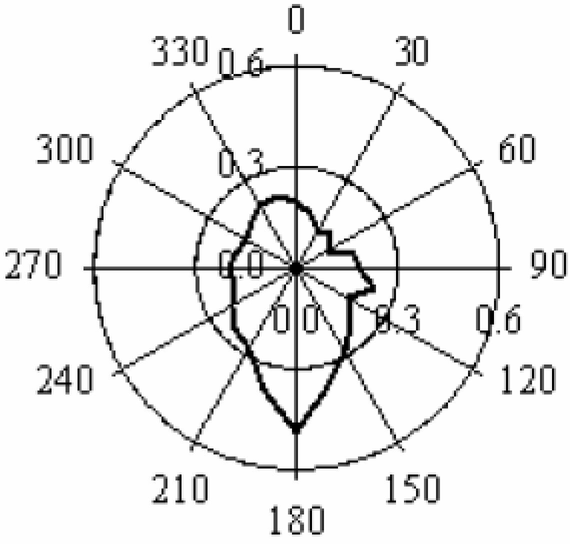
- Met data can help identify where the important local sources are
- Tools: wind roses, pollution roses, conditional probability functions, trajectory analysis, nonparametric regression



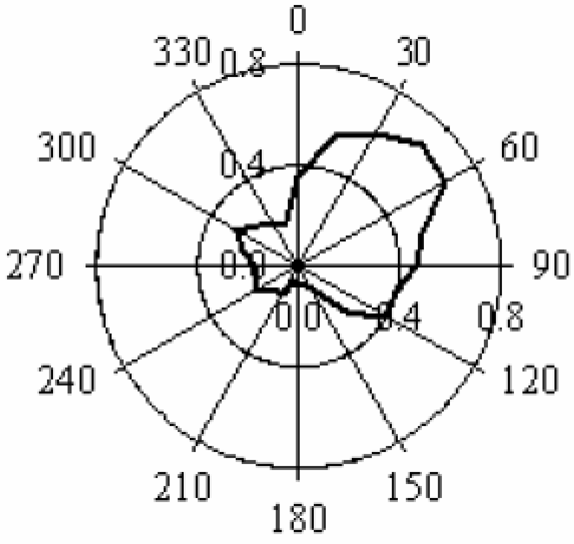
Wind direction on highest steel factor days
Influence from smaller sources to the east and southwest of site and larger group of sources to southeast of site
Miles
0 2 4 8 12 16
N
2004 Emissions
lbs/year, TRI
Manganese
100
1,000
100,000
Ned Brown Forest Preserve
Chicago O'hare Intl
Chicago
Merrill C Meigs
Chicago Midway
94
290
190
88
294
355
55
57
90
65
All Days
WS (m/s)
> 30
20 - 30
15 - 20
10 - 15
5 - 10
2.5 - 5
0 - 2.5
Source: STI report to LADCO

Conditional Probability Function

Gasoline Vehicles



Diesel Vehicles



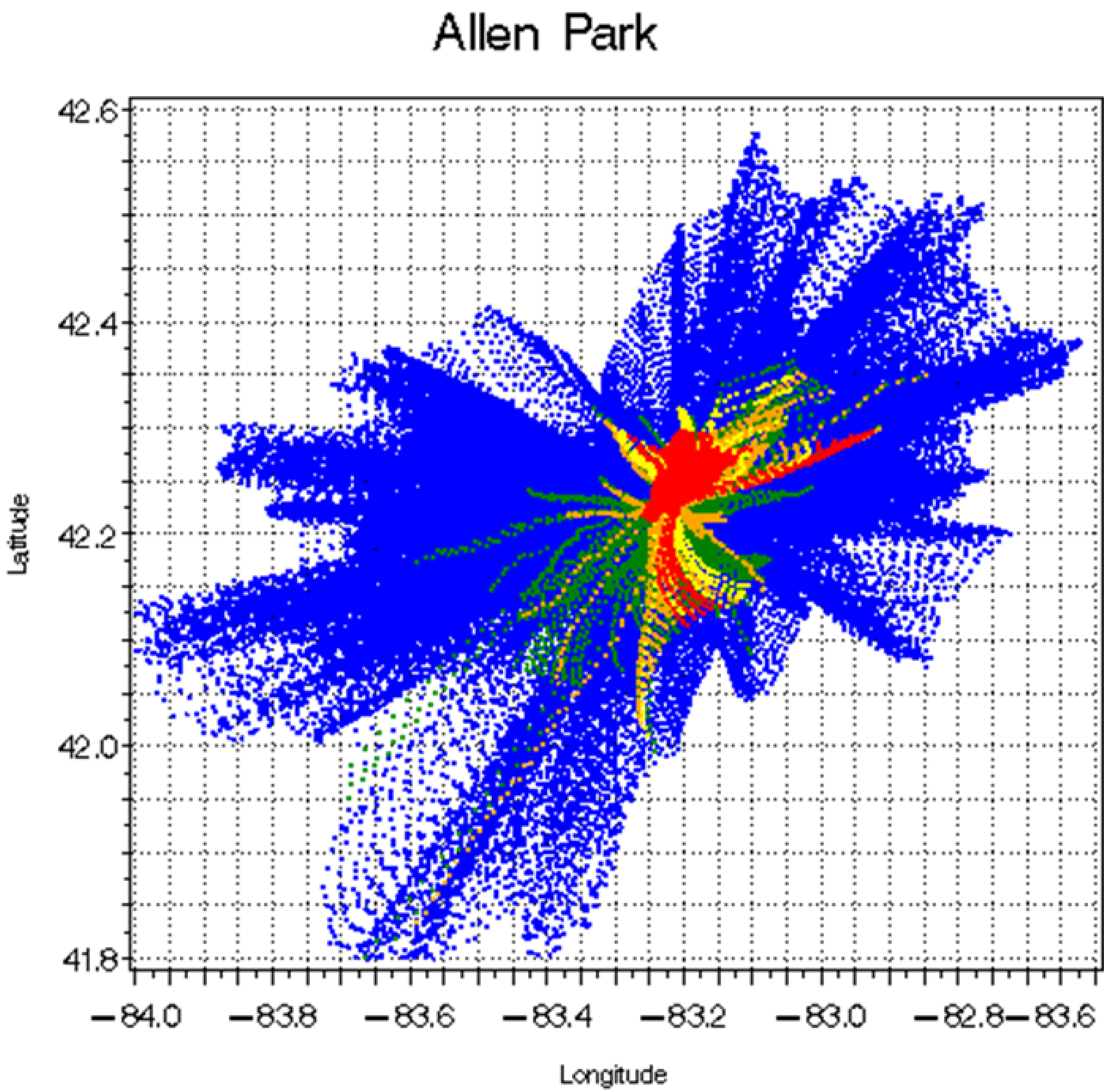
CPF = Probability that source contribution from a given wind direction
will exceed the 75th percentile

Nonparametric Regression

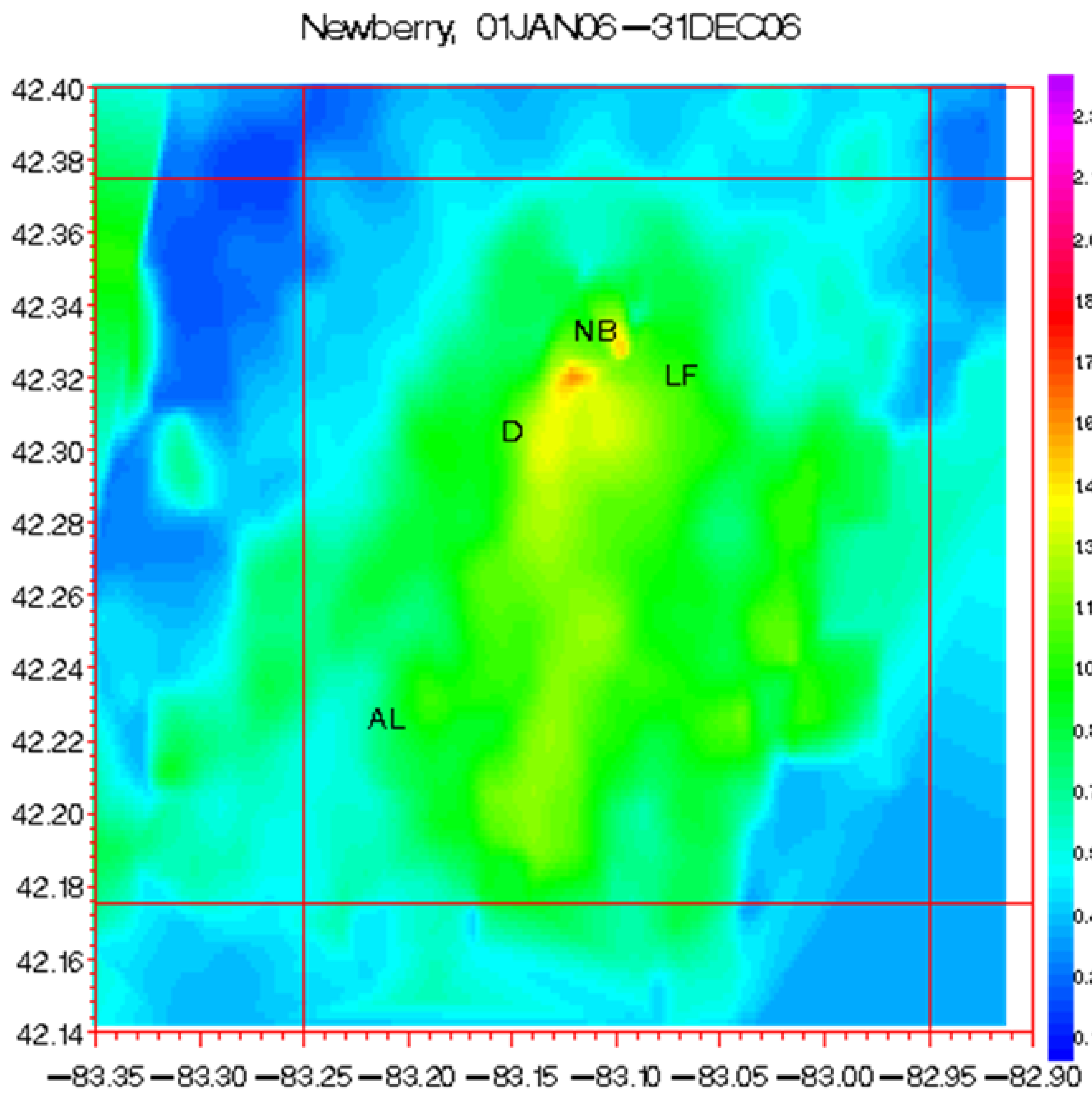
- Model regresses concentration on wind direction and speed (as x,y vectors) to locate areas associated with peak concentrations (i.e., source locations)
- Kernel density estimate, weighted by no. of observations
- Like a moving average, but with a smoothing parameter

$$\overline{C}(X_i, Y_j) = \frac{\sum_k K\left(\frac{(X_j - x_k)}{h}\right) K\left(\frac{(Y_j - y_k)}{h}\right) c_k}{\sum_k K\left(\frac{(X_j - x_k)}{h}\right) K\left(\frac{(Y_j - y_k)}{h}\right)}$$

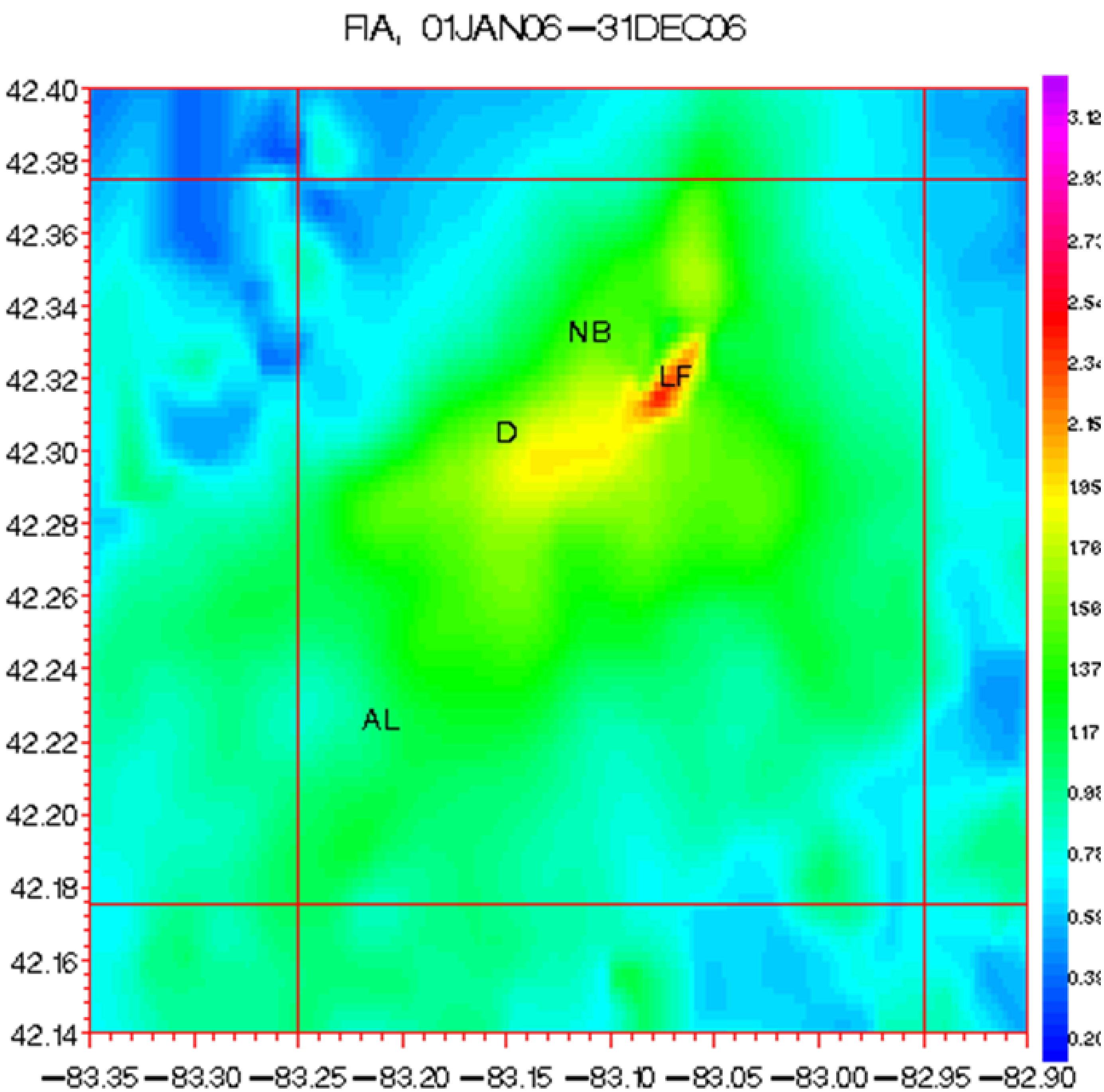
Where K is the Epanechnikov kernel (or Gaussian) and h is the smoothing parameter



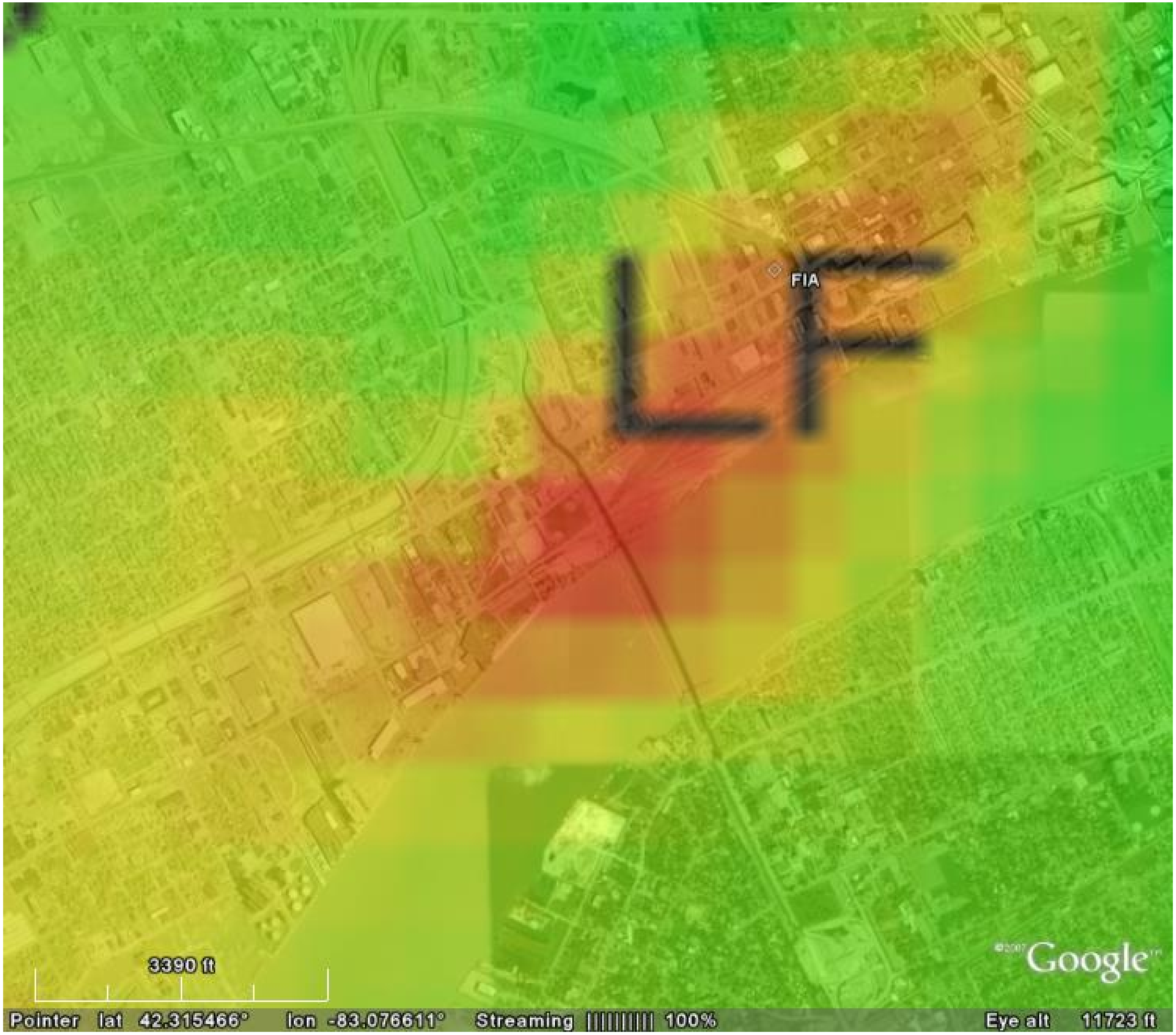
Allen Park
42.6
42.4
42.2
42.0
41.8
Latitude
−84.0
−83.8
−83.6
−83.4
−83.2
−83.0
−82.8
−83.6
Longitude


Newberry, 01JAN06—31DEC06
NB
LF
D
AL
42.40
42.38
42.36
42.34
42.32
42.30
42.28
42.26
42.24
42.22
42.20
42.18
42.16
42.14
—83.35
—83.30
—83.25
—83.20
—83.15
—83.10
—83.05
—83.00
—82.95
—82.90

Newberry aethalometer data – points very specifically to intermodal freight terminal (1 hr data, 2006)



FIA, 01JAN06—31DEC06
NB
LF
D
AL
42.40
42.38
42.36
42.34
42.32
42.30
42.28
42.26
42.24
42.22
42.20
42.18
42.16
42.14
—83.35 —83.30 —83.25 —83.20 —83.15 —83.10 —83.05 —83.00 —82.95 —82.90
1.95
1.76
1.56
1.37
1.17



FIA aethalometer data points very specifically to Ambassador Bridge (1-hr data, 2006 annual)

Conclusions

- Routine monitoring data not always sufficient to answer questions about sources and interactions of pollutants; special study data very helpful
- Gases, particles, and toxics all share sources; need to use multiple approaches and methods to assess impacts
- Each method and model has associated uncertainties; no single ‘right’ answer