

# **Application of the UM Multivariate Pseudo-Deterministic Receptor Model to Resolve Power Plant Influences on Air Quality at the CMU Supersite**

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# Outline

- Motivation
- Model Description
- Previous Application – BRACE
- Application to CMU data
- Results

## Motivation

Highly time resolved metals measurements have been made at 5 locations for at least 11 elements including useful markers of primary particle emissions of high temperature combustion sources. At this resolution, the plumes of stationary sources have been readily observed as excursions in time series profiles of the concentrations of the marker elements.

These data facilitate source attribution by

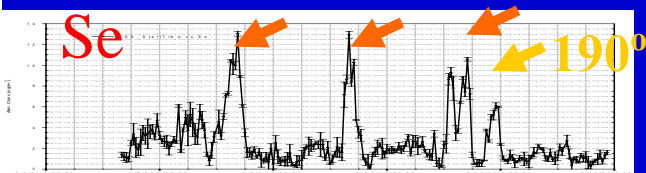
- i) reducing the number of sources affecting each measurement*
- ii) preserving directionality.*

For at least some sources, this could obviate the need for in-stack measurements for development of emission inventories.

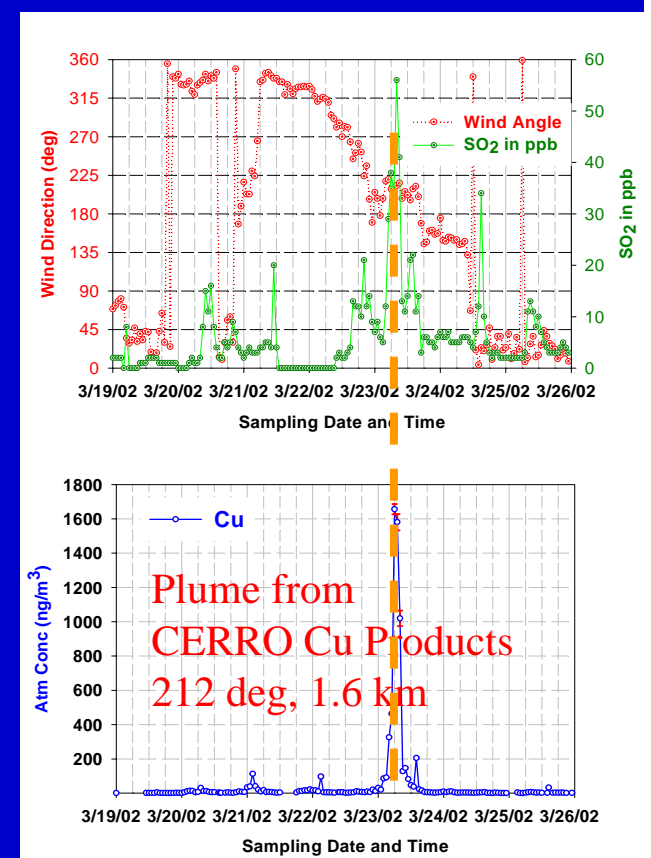
# Highly time resolved data are available for many species

Al, As, Cd, Cr, Cu, Fe, Mn, Ni, Pb, Se, Zn  
 Baltimore, Pittsburgh, St. Louis, Tampa, College Park

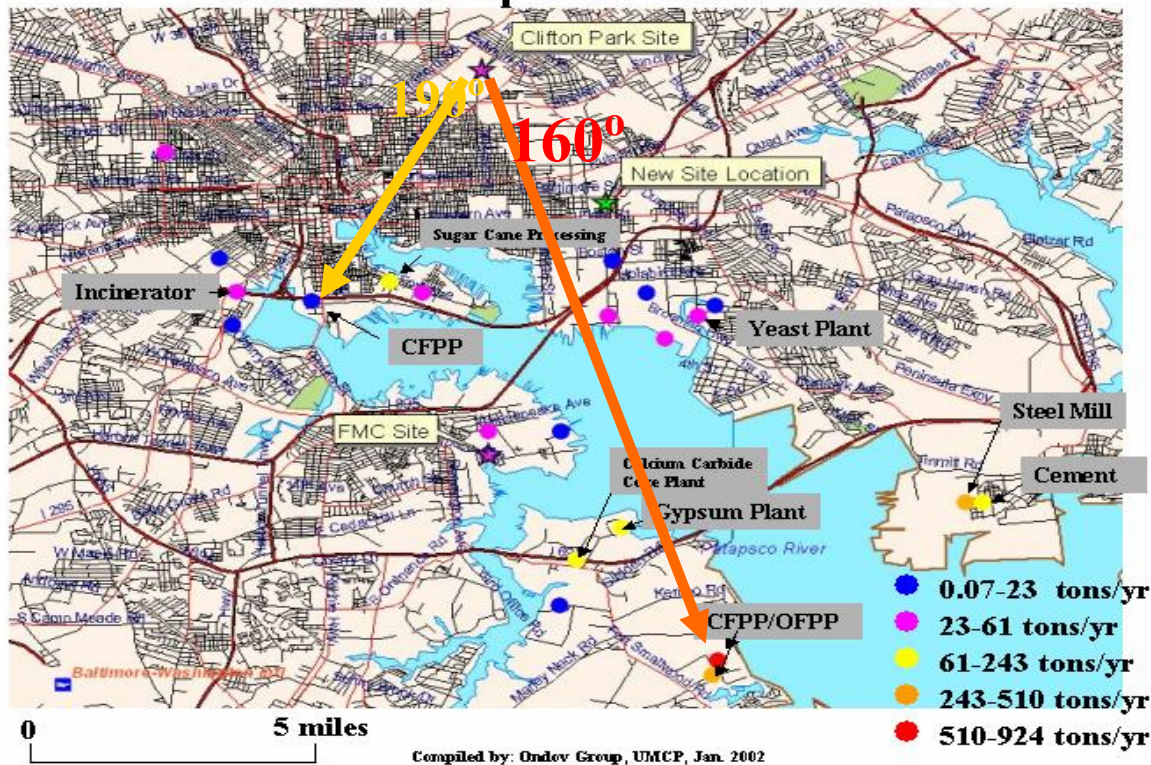
coal-fired power plants



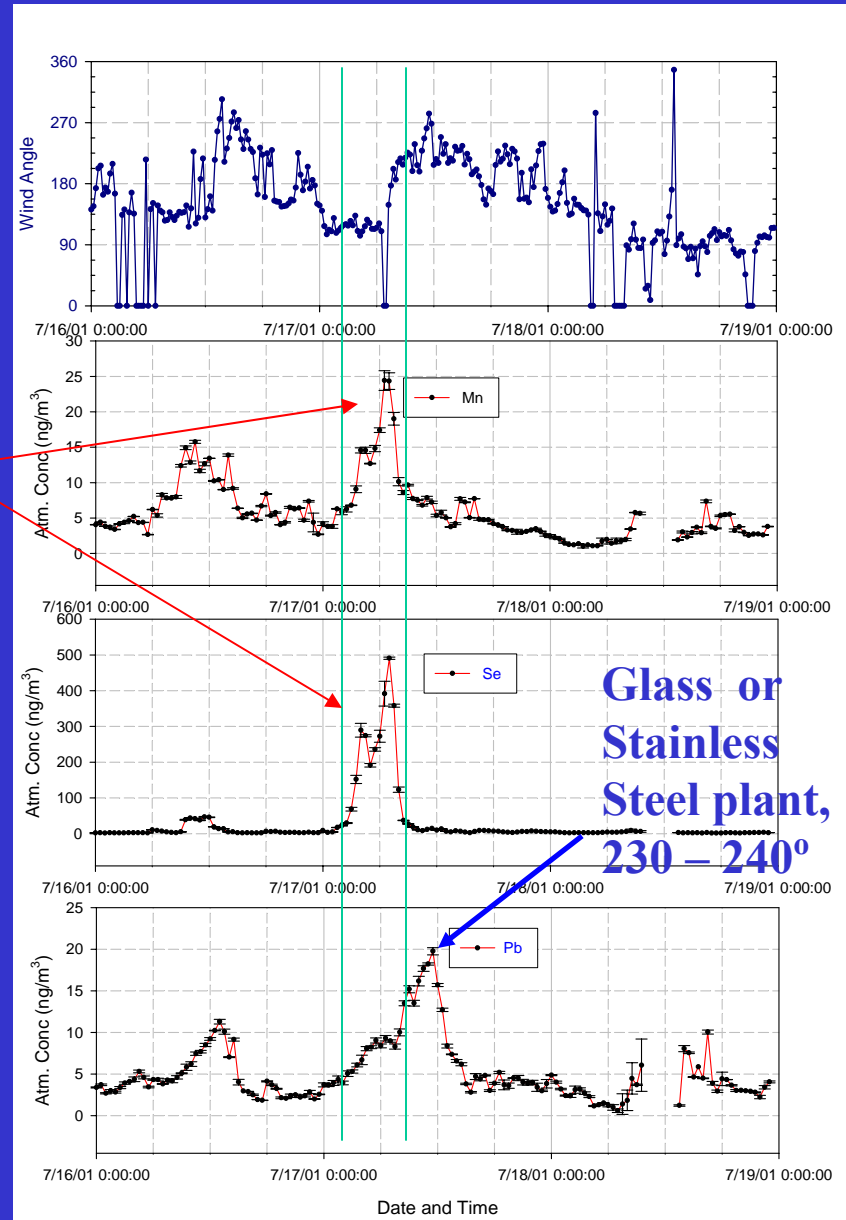
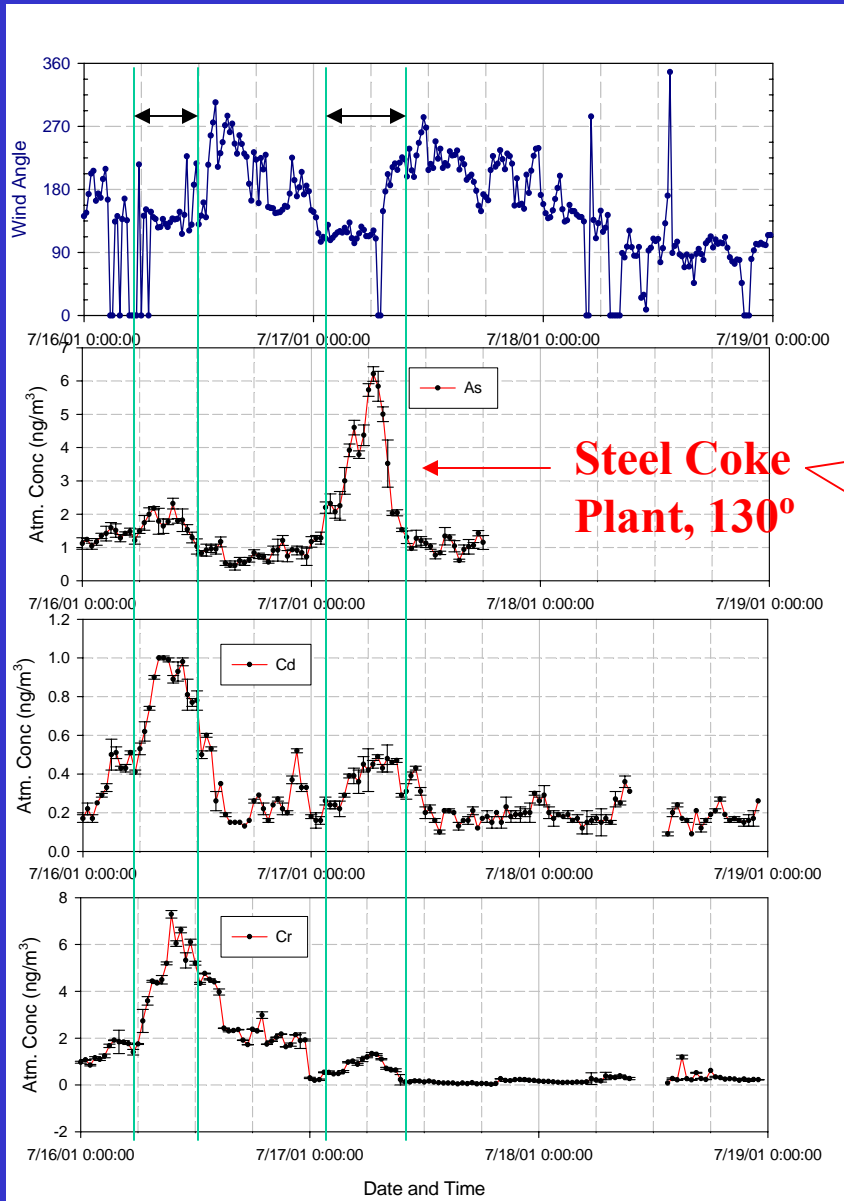
Zn emissions from Big River Zn plant



## Baltimore Supersite PM<sub>10</sub> Sources

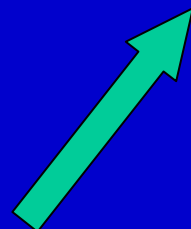
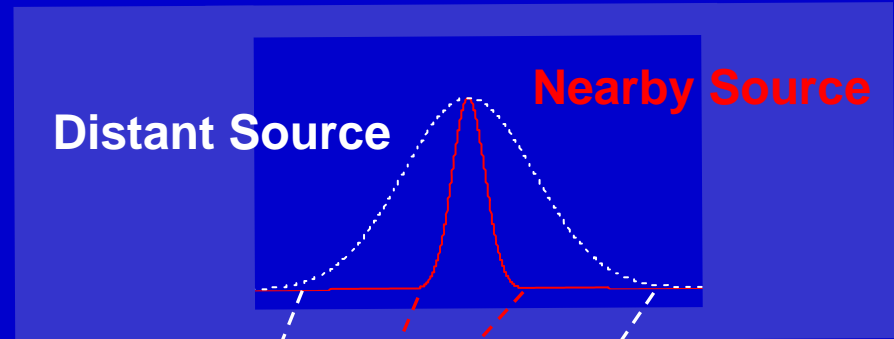
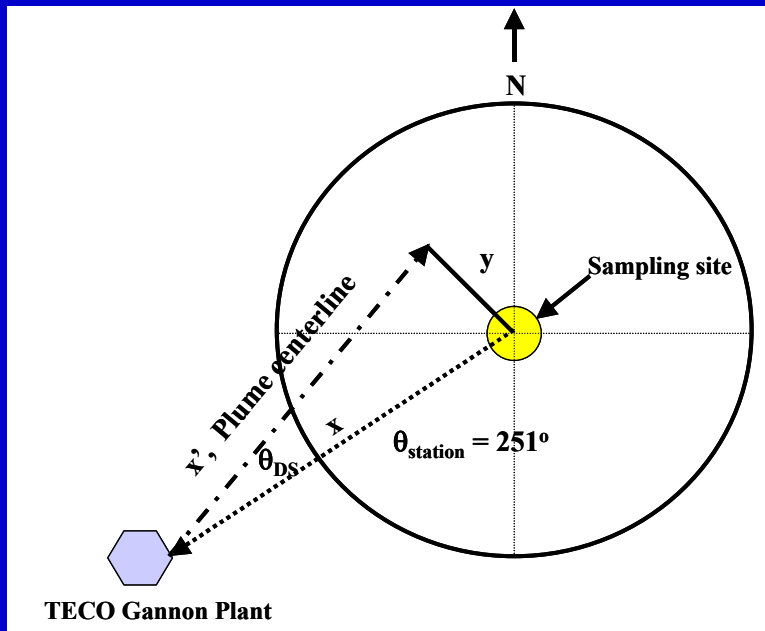


# Pittsburgh Supersite: July 16, 17, 18 – Data show 3 major influences



# These inherently contain information on source location and distance

*Directionality* and *Plume width* =  
powerful constraints exploitable with highly time-resolved data



$$y = \sin \theta_{DS} \cdot x$$

$$\theta_{DS} = \theta_{station} - 180^\circ - \theta_{wind} - \theta_{Ekman}$$

(16)

# Pseudo-Deterministic Multivariate Receptor Model

Determines emission rates of species, *i*, from *j* known sources, using highly time-resolved concentration measurements:

$$[E_i]_t = \sum_{j=1}^n ER_{i,j} \cdot \chi/Q_{j,t} \quad \text{Eq. 1}$$

where Eq 3 is expressed as a constraint, i. e.,

$$(X/Q)_{j,t} \text{ Eq. 1} = C_j (X/Q)_{j,t}^{\text{Met}} \quad \text{where} \quad 0.1 < C_j < 2 \quad \text{Eq. 2}$$

$$(\chi/Q)^{\text{Met}} = \frac{1}{\pi \sigma_y \sigma_z u} \exp\left[-\frac{1}{2} \frac{y^2}{\sigma_y^2}\right] \cdot \exp\left[-\frac{1}{2} \frac{H^2}{\sigma_z^2}\right] \quad \text{Eq. 3}$$

Minimize

$$FUN = \sum_{i=1}^l \sum_{t=1}^m \sum_{j=1}^n \left( \overline{ER_{i,j}} (\chi/Q)_{j,t} - C_{i,t} \right)^2 \quad \text{Eq. 4}$$

$[E]_{i,t}$  = Ambient conc. species *i* at time (sample) *t*,  $\mu\text{g}/\text{m}^3$   
(SO<sub>2</sub>, Se, As, Ni, Pb, Zn, Cd, Cu, Cr, Al, Fe, Mn)

$ER_{i,j}$  = *Average* Emission Rate of species *i* from source *j*, over *t* periods,  $\mu\text{g}/\text{s}$

$X/Q_{j,t}$  = Dispersion Factor for each source *j* at time *t*,  $\text{s}/\text{m}^3$

## 2. Estimate Atmospheric Dispersion (incorporates directionality and estimate of plume width)

The concentration,  $X$ , of gas or aerosols at  $x, y, z$  from a continuous source with an effective emission height,  $H$ , is given by equation, at ground level, i.e.,  $z=0$ .

$$\left(\frac{X}{Q}\right)^{Met} = \frac{1}{\pi \sigma_y \sigma_z u} \exp\left[-\frac{1}{2} \frac{y^2}{\sigma_y^2}\right] \cdot \exp\left[-\frac{1}{2} \frac{H^2}{\sigma_z^2}\right] \quad (2)$$

where

$y$  = the displacement of the site from the plume centerline, m

$H$  = Plume height, m

$\sigma_y, \sigma_z$  = Horizontal and vertical standard deviations of plume width, m

$u$  = Transport velocity, m/s

$u, \sigma_y, \sigma_z, H$  – estimated from formulae & micromet. data.

$y$  - estimated from wind and “station” angles.

Inputs:  $x$  (distance to source), stack heights, exit velocities,  $u, v, w$ ,  
 $U, S, T$ , cloud cover,





# PDRM was applied to Tampa BRACE data to resolve

- 6 Stationary sources, 15 to 41 km, 170-270° quadrant,  
*4 coal or oil Power Plants, Fertilizer plant, Battery recycling plant*  
*Flat Terrain, fairly simple Air shed*

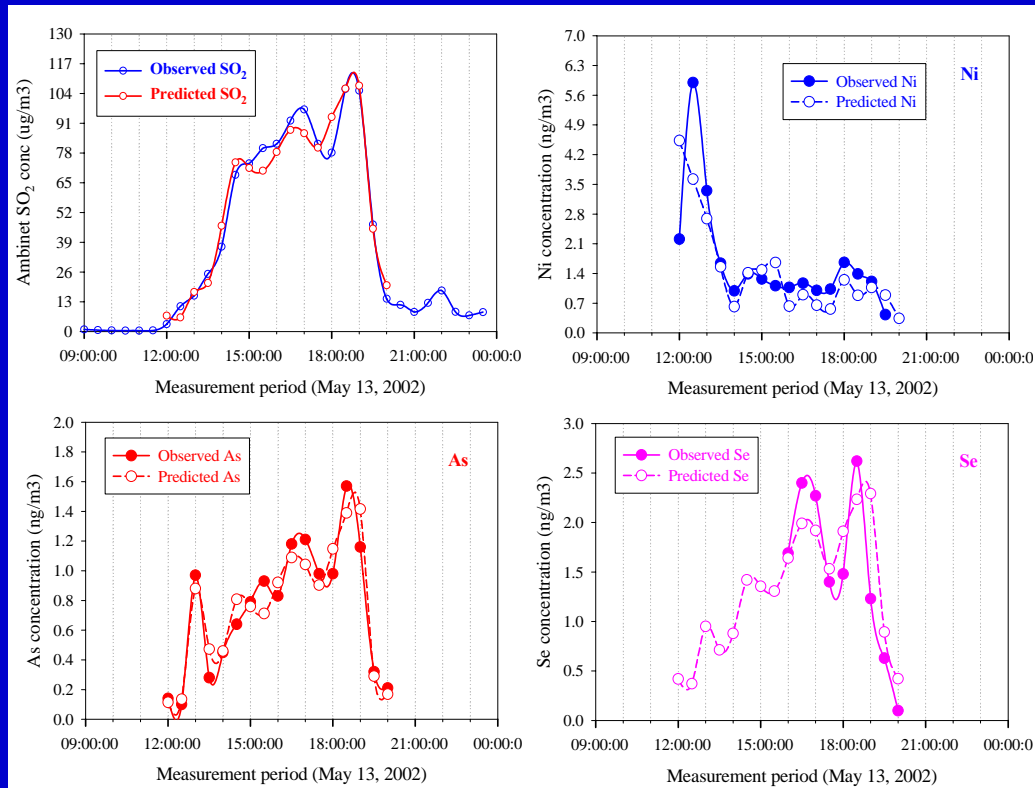


⊘ plant off-line

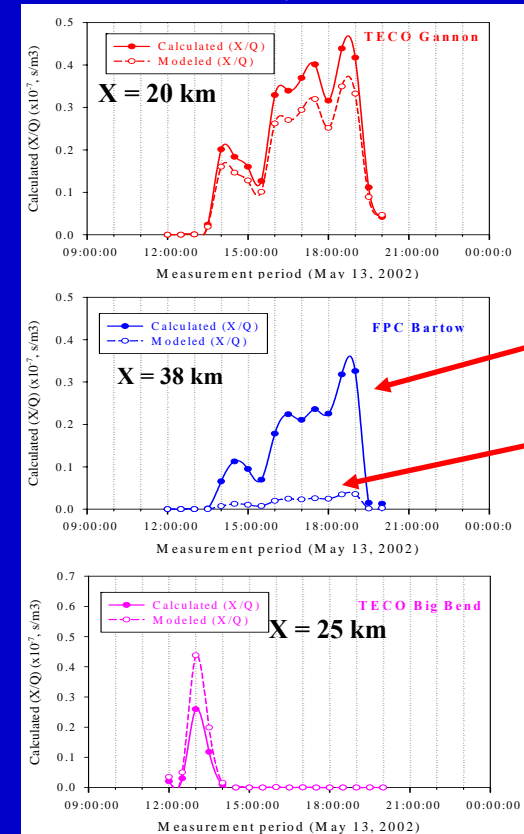


# PDRM BRACE Results: Ambient fits, SO<sub>2</sub> & Metal ERs, x/Qs

## Fits



## X/Qs



Met  
PDRM

ERs	Unit	Gannon 20 km	Big Ben 25 km	Bartow 38 km	Manatee 41 km	Cargill 20 km	Gulf Coast 15 km
SO <sub>2</sub> (obs.) <sup>1</sup>	g/s	2,600	300	1,140	1,110 <sup>3</sup>	40 <sup>2)</sup>	25 <sup>2)</sup>
SO <sub>2</sub> (pre.)	g/s	2,510	290	1,130	1045	49	31

# Study Area: Carnegie-Mellon (EPA) Supersite, April 1 2002

- **Mountainous terrain**
- **Several small (no CEMs) coal boilers operating N. W. of CMU**
- **Dataset**  
**SO<sub>2</sub> and 30 min. PM elements by UM SEAS**  
**(Al, As, Cd, Cr, Cu, Fe, Mn, Ni, Pb, Se, and Zn)**

**12.5-hr period on April 1st, when winds blew from direction of 290-330° in which six small, non-utility SO<sub>2</sub> emitting coal-boilers are situated.**

**Belfield Steam plant (286°, 0.8 km)**

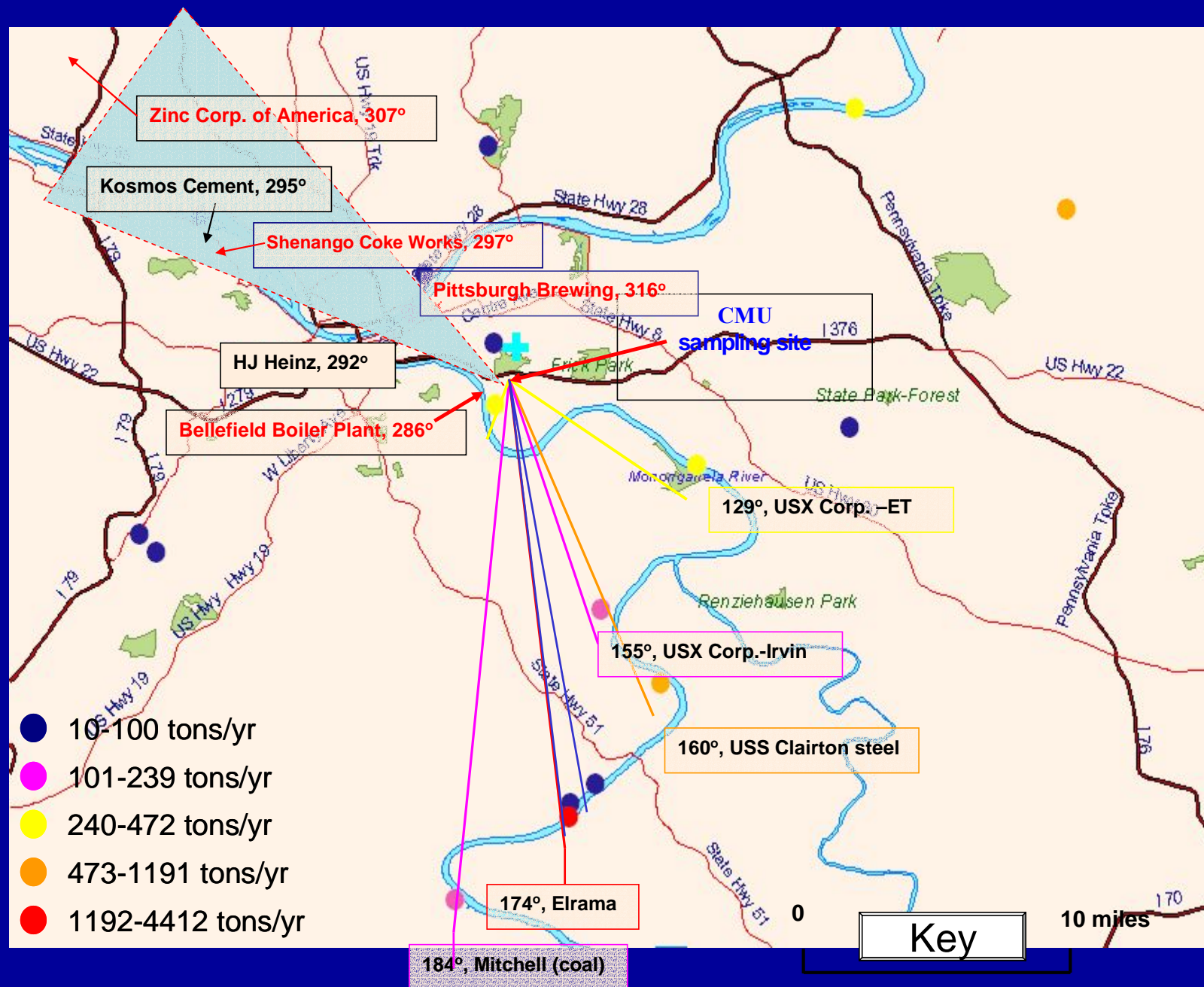
**Pittsburgh Brewing Co. (316°, 3.4 km)**

**Shenago Coke Works (297°, 13 km)**

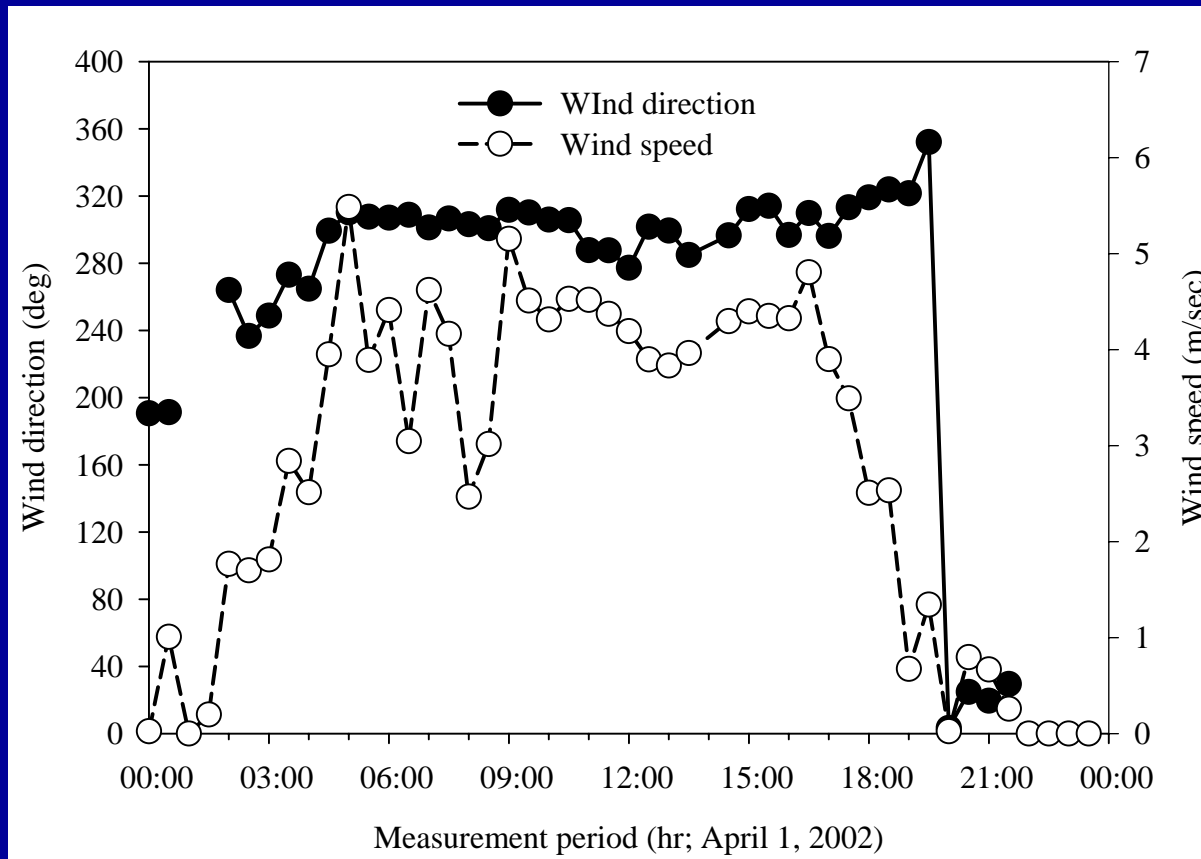
**Zinc Corporation of America - 110 MW(e) coal-fired power plant, 307°, 49 km**

**J. Heintz Co., and Kosmos Cement Co. not required for fit.**

# Location of CMU Supersite and Modeled Sources



**During the 12.5 hr study period, hourly average wind speeds were 2.5 to 5.2 m/s; hourly maxima ranged from 5.2 to 8.2 m/s and the mixing height remained between 1960 and 2010 m.**



## Information for Emission Sources (Inputs)

Four sources in the region of interest, April 1 data set

Facility Name	Control devices	Distance (km)	Station angle (deg)	PM <sub>2.5</sub> (ton/yr)	SO <sub>2</sub> (ton/yr)	Industry type	Category
<b>Bellefield boiler plant</b>	none	<b>0.8</b>	286	94	745	Steam supply	Coal fired steam
<b>Pittsburgh brewing co.</b>	none.	<b>3.4</b>	316	9	106	Food, agricultural, & beer	Coal fired steam
<b>Shenango Coke Works</b>	Fabric filter	<b>13.0</b>	297	79	2450	Blast furnace and steel mill	Coke
<b>Zinc Corp of America</b>	none	<b>41.9</b>	307	678	8641	Coal-fired boiler/industrial processes	Primary non-ferrous metals

# Meteorological Data for Dispersion Estimates (Inputs)

## Estimated from commonly available data

Parameters needed for estimation of  $S_y$ ,  $S_z$ :

$u^*$ ,  $L$ ,  $w^*$  (friction vel., Monin-Obukov length, convective vel. Scale)

$H$  (sensible heat flux)

Mixing Height

$W^* = f(\text{Mix. Hgt.}, \text{Surface heat flux}, T)$

$L = f(u^*, H)$

$U^*$ ,  $H$  calculated from 3 hrly 80 km NOAA data

<http://www.arl.noaa.gov/ready/amet.us.html>

Mixing Height – from sonde data at Pittsburgh Airport

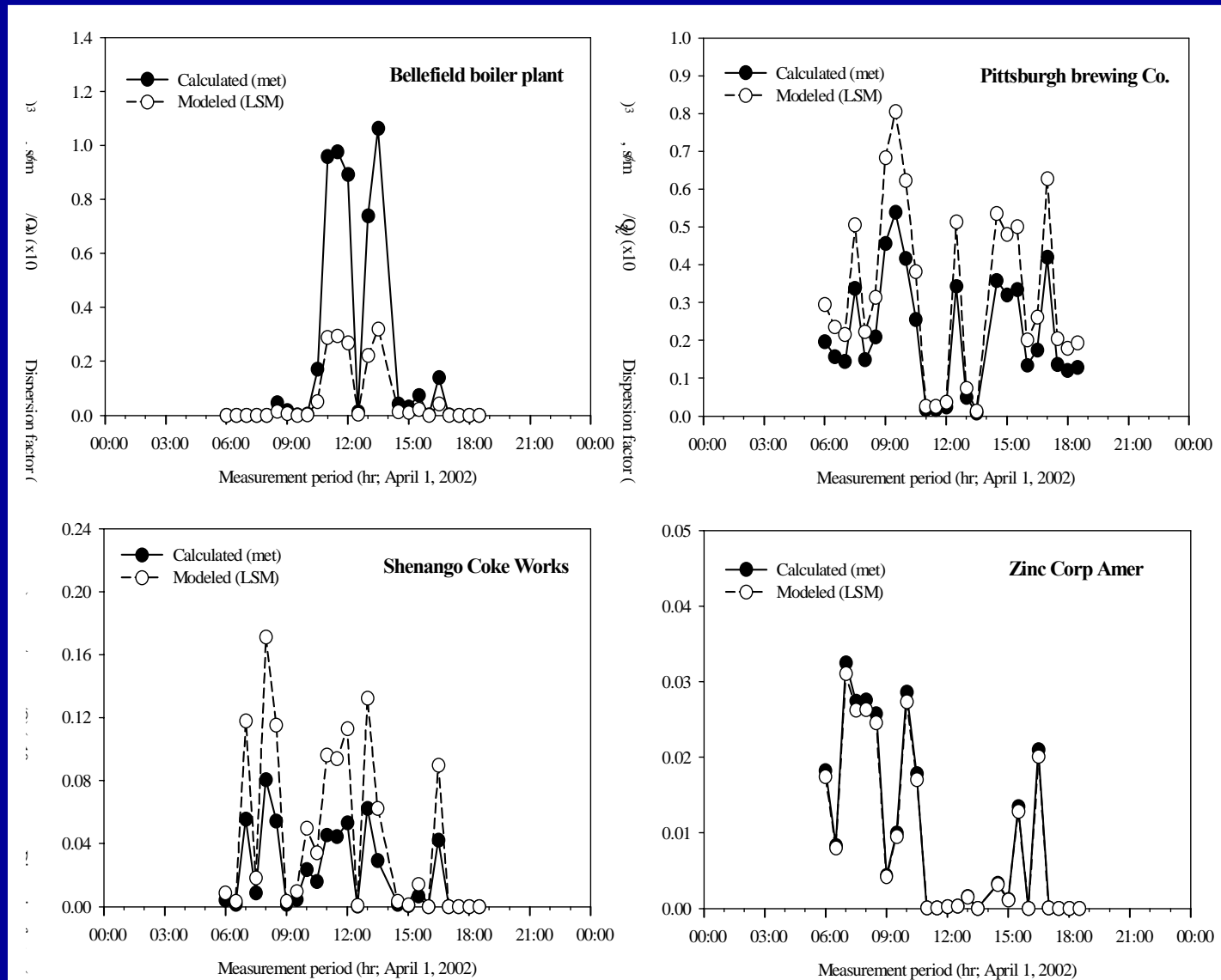
- used Holzworth method

Stability Class: Pasquill Gifford Stability Class, Turner method

$f(\text{solar flux}, w_s, \text{cloud cover})$

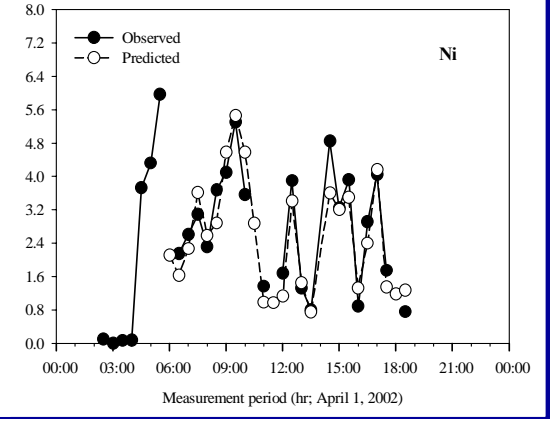
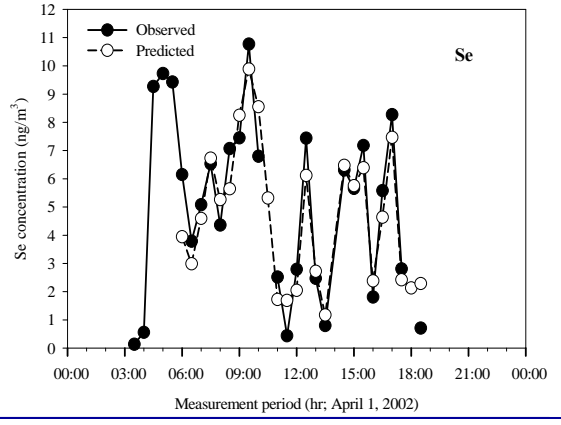
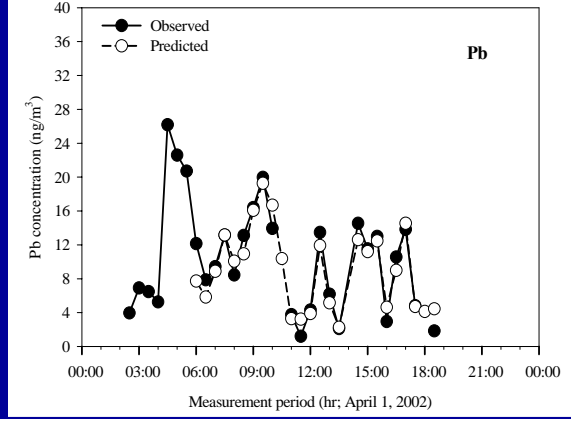
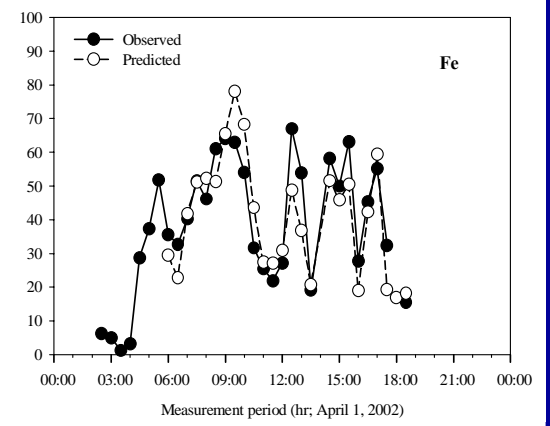
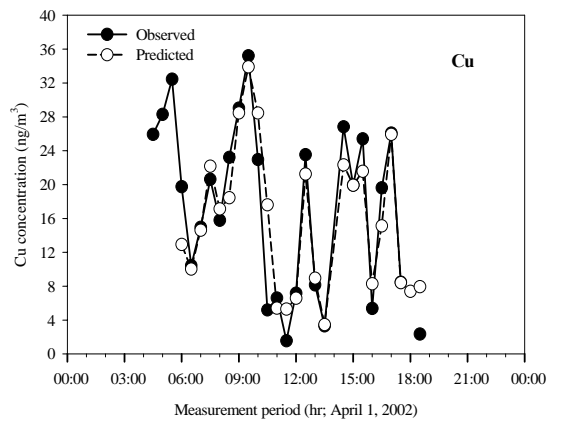
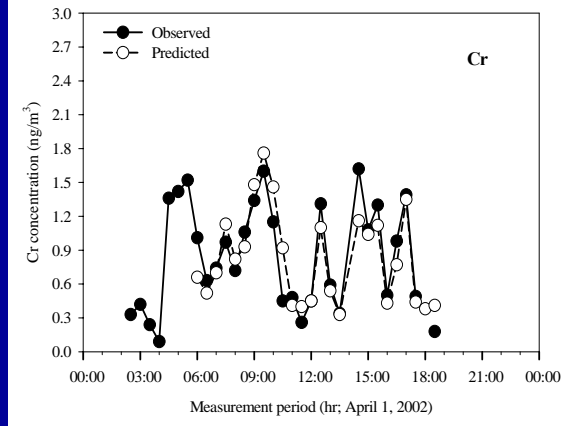
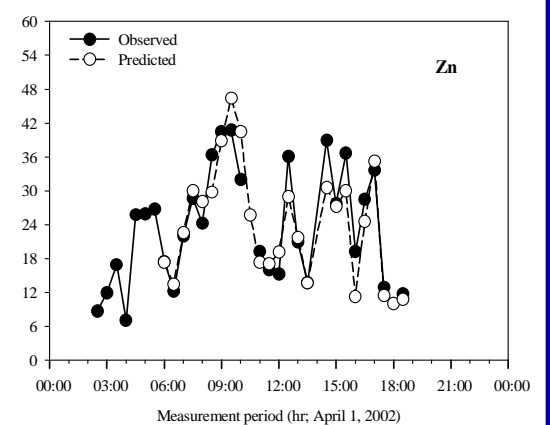
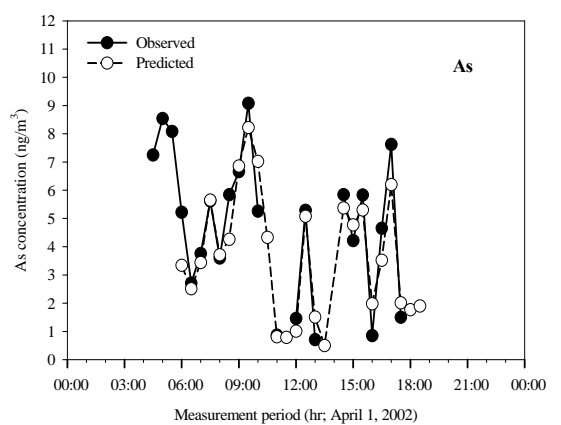
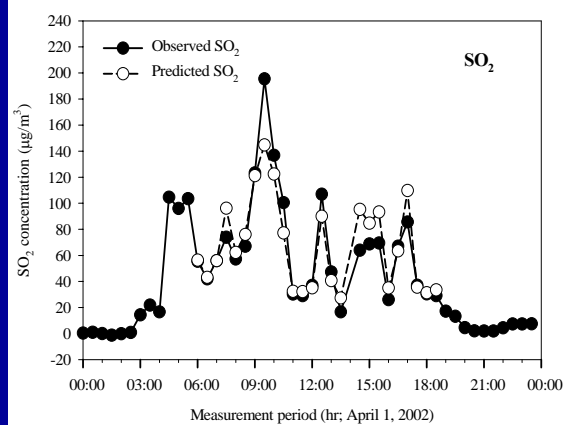
Smithsonian Tables, Pittsburgh Apt. data

# Results: PDRM corrects for error in Gaussian plume model!

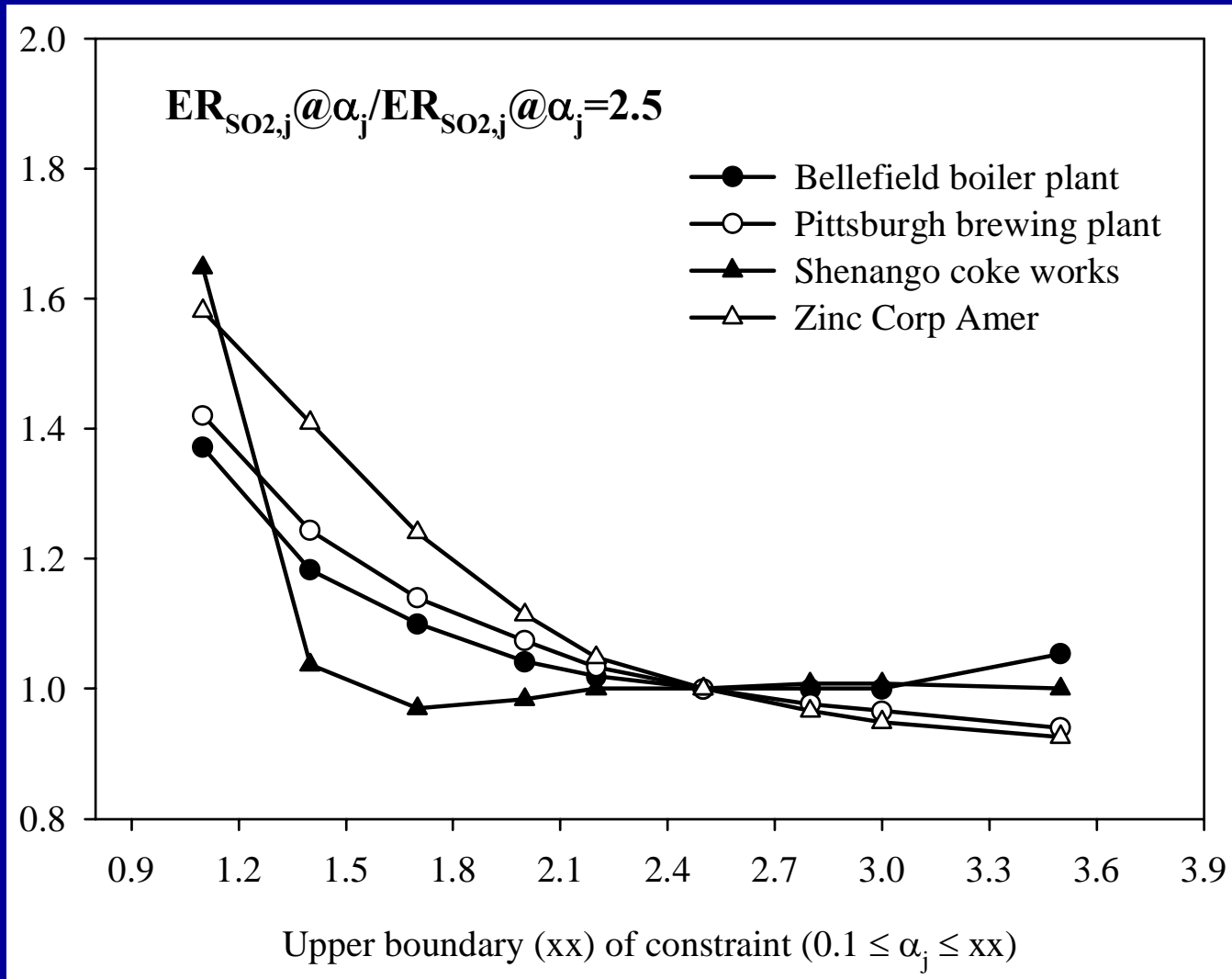




# PDRM Results: Good fits to ambient data with 4 source model



# Model is relatively insensitive to constraint upper bound for $UB > 2.2$



**Predicted emission rates for SO<sub>2</sub> and metals for each of 4 sources during measurement period (units: g/s)\***

Species	Bellefield boiler plant	Pittsburgh brewing plant	Shenango Coke Works	Zinc Corp Amer
SO <sub>2</sub>	48	176	123	176
Al	0.0336	0.0800	0.1203	0.1453
As	0.0012	0.0105	0.0046	0.0009
Cr	0.0006	0.0021	0.0017	0.0020
Cu	0.0007	0.0408	0.0402	0.0480
Fe	0.0365	0.0926	0.1610	0.1130
Mn	0.0038	0.0032	0.0038	0.0010
Ni	0.0016	0.0065	0.0062	0.0070
Pb	0.0010	0.0232	0.0236	0.0369
Se	0.0005	0.0119	0.0126	0.0184
Zn	0.0299	0.0554	0.0807	0.0633

**\*Annual average SO<sub>2</sub> emission rates are reported to be 21, 3.1, 70, and 249 g/s**

# Regressions: elements vs. Se (ng m<sup>-3</sup>)

## Se is an excellent tracer of coal combustion aerosol

Species	Regression equation	R	ER_ratio from modeling results <sup>2)</sup>			
			Bellefield boiler plant	Pittsburgh brew. plant	Shenango coke works	Zinc Corp America
	CMU measurement site					
SO <sub>2</sub>	SO <sub>2</sub> <sup>1)</sup> = (11.237±1.886) <sup>***</sup> Se + (11.815±12.723)	0.772	96.0 <sup>3)</sup>	14.790 <sup>3)</sup>	9.762 <sup>3)</sup>	9.565 <sup>3)</sup>
Al	Al = (3.023±0.750) <sup>*</sup> Se + (22.691±5.058) <sup>**</sup>	0.635	67.2	6.723	9.548	7.897
As	As = (0.987±0.033) <sup>***</sup> Se + (-1.152±0.219) <sup>***</sup>	0.987	2.4	0.882	0.365	0.049
Cr	Cr = (0.140±0.010) <sup>***</sup> Se + (0.226±0.067) <sup>*</sup>	0.944	1.2	0.176	0.135	0.109
Cu	Cu = (3.311±0.160) <sup>***</sup> Se + (0.353±1.076)	0.973	1.4	3.429	3.190	2.609
Fe	Fe = (3.333±0.786) <sup>**</sup> Se + (29.633±5.300) <sup>***</sup>	0.655	73.0	7.782	12.778	6.141
Mn	Mn = (0.029±0.033) Se + (1.912±0.222) <sup>***</sup>	0.177	7.6	0.269	0.302	0.054
Ni	Ni = (0.479±0.038) <sup>***</sup> Se + (0.422±0.258)	0.939	3.2	0.546	0.492	0.380
Pb	Pb = (2.177±0.136) <sup>***</sup> Se + (-0.799±0.919)	0.956	2.0	1.950	1.873	2.005
Zn	Zn = (2.455±0.474) <sup>***</sup> Se + (15.039±3.200) <sup>***</sup>	0.726	59.8	4.655	6.405	3.440

Note) \*: p<0.01, \*\*: p<0.001; \*\*\*: p<0.0001

<sup>1)</sup> Unit is in µg m<sup>-3</sup>; <sup>2)</sup> ER\_ratio means ratio of emission rate for each species to emission rate of Se; <sup>3)</sup> indicates the ratio divided by 1000

# Conclusions

- **PDRM successfully fit ambient concentrations measured on the CMU campus in Pittsburgh, i.e., in a region characterized by rough terrain. Average SO<sub>2</sub> emission rates predicted for the 12-hr modeling period for three of the plants are comparable to reported ambient emission rates. Those predicted for the Pittsburgh Brewing plant were 50-fold larger than the reported annual emission.**
- **Fits for most of the elements were, likewise, good, within  $\pm 10\%$  overall, suggesting that the four source model was appropriate. However, Mn correlates poorly with Se, suggesting another source of Mn is important.**
- **Timely emission data for the study period, however, prevented verification**

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