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

cal-fired power plants

Zn emissions from Big River Zn plant

Baltimore Supersite PM10 Sources

Plume from CERRO Cu Products 212 deg, 1.6 km
Pittsburgh Supersite: July 16, 17, 18 – Data show 3 major influences

- Steel Coke Plant, 130°
- Glass or Stainless Steel plant, 230 – 240°
These inherently contain information on source location and distance

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

\[ y = \sin \theta_{DS} \cdot x \]
\[ \theta_{DS} = \theta_{station} - 180^\circ - \theta_{wind} - \theta_{Ekman} \]
Pseudo-Deterministic Multivariate Receptor Model

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

\[
[E]_{i,t} = \sum_{j=1}^{n} ER_{i,j} \cdot \chi/Q_{j,t}
\]

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

\[
(X/Q)_{j,t} = C_j (X/Q)_{j,t}^{Met} \quad \text{where} \quad 0.1 < C_j < 2
\]

\[
(\chi/Q)^{Met} = \frac{1}{\pi \sigma_y \sigma_z t} \exp\left[-\frac{y^2}{2 \sigma_y^2}\right] \cdot \exp\left[-\frac{H^2}{2 \sigma_z^2}\right]
\]

Minimize

\[
FUN = \sum_{i=1}^{l} \sum_{t=1}^{m} \sum_{j=1}^{n} \left[ ER_{i,j}(\chi/Q)_{j,t} - C_{i,t} \right]^2
\]

\[
[E]_{i,t} = \text{Ambient conc. species } i \text{ at time (sample) } t, \ \mu g/m^3
\]

\[
(SO_2, \text{Se, As, Ni, Pb, Zn, Cd, Cu, Cr, Al, Fe, Mn})
\]

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

\[
X/Q_{j,t} = \text{Dispersion Factor for each source } j \text{ at time } t, \ s/m^3
\]
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., $z=0$.

$$\left(\frac{\chi}{Q}\right)_{Met} = \frac{1}{\pi \sigma_y \sigma_z t \lambda} \exp\left[-\frac{1}{2} \frac{y^2}{\sigma_y^2}\right] \cdot \exp\left[-\frac{1}{2} \frac{H^2}{\sigma_z^2}\right]$$

(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
PDRM BRACE Results: Ambient fits, SO$_2$ & Metal ERs, x/Qs

### Fits

- **SO$_2$**
  - Observed: Red line
  - Predicted: Blue line

- **As**
  - Observed: Red line
  - Predicted: Blue line

- **Se**
  - Observed: Red line
  - Predicted: Blue line

Measurement period (May 13, 2002)

### X/Qs

- **X = 20 km**
- **X = 38 km**
- **X = 25 km**

- **Calculated (X/Q)**
- **Modeled (X/Q)**

Measurement period (May 13, 2002)

### Data Table

<table>
<thead>
<tr>
<th>ERs</th>
<th>Unit</th>
<th>Gannon 20 km</th>
<th>Big Ben 25 km</th>
<th>Bartow 38 km</th>
<th>Manatee 41 km</th>
<th>Cargill 20 km</th>
<th>Gulf Coast 15 km</th>
</tr>
</thead>
<tbody>
<tr>
<td>SO$_2$ (obs.)$^1$</td>
<td>g/s</td>
<td>2,600</td>
<td>300</td>
<td>1,140</td>
<td>1,110$^3$</td>
<td>40$^2$</td>
<td>25$^2$</td>
</tr>
<tr>
<td>SO$_2$ (pre.)</td>
<td>g/s</td>
<td>2,510</td>
<td>290</td>
<td>1,130</td>
<td>1045</td>
<td>49</td>
<td>31</td>
</tr>
</tbody>
</table>

$^1$ Ambient fits, $^2$ Met, $^3$ PDRM
Study Area: Carnegie-Mellon (EPA) Supersite, April 1 2002

- Mountainous terrain
- Several small (no CEMs) coal boilers operating N. W. of CMU
- Dataset
  SO₂ 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 SO₂ 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

Key

- Zinc Corp. of America, 307°
- Kosmos Cement, 295°
- Shenango Coke Works, 297°
- Pittsburgh Brewing, 316°
- CMU sampling site
- HJ Heinz, 292°
- Bellefield Boiler Plant, 286°
- 129°, USX Corp., ET
- 155°, USX Corp., Irvin
- 160°, USS Clairton steel
- 174°, Elrama
- 184°, Mitchell (coal)

- 10-100 tons/yr
- 101-239 tons/yr
- 240-472 tons/yr
- 473-1191 tons/yr
- 1192-4412 tons/yr

0 10 miles
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

<table>
<thead>
<tr>
<th>Facility Name</th>
<th>Control devices</th>
<th>Distance (km)</th>
<th>Station angle (deg)</th>
<th>PM$_{2.5}$ (ton/yr)</th>
<th>SO$_2$ (ton/yr)</th>
<th>Industry type</th>
<th>Category</th>
</tr>
</thead>
<tbody>
<tr>
<td>Bellefield boiler plant</td>
<td>none</td>
<td>0.8</td>
<td>286</td>
<td>94</td>
<td>745</td>
<td>Steam supply</td>
<td>Coal fired steam</td>
</tr>
<tr>
<td>Pittsburgh brewing co.</td>
<td>none.</td>
<td>3.4</td>
<td>316</td>
<td>9</td>
<td>106</td>
<td>Food, agricultural, &amp; beer</td>
<td>Coal fired steam</td>
</tr>
<tr>
<td>Shenango Coke Works</td>
<td>Fabric filter</td>
<td>13.0</td>
<td>297</td>
<td>79</td>
<td>2450</td>
<td>Blast furnace and steel mill</td>
<td>Coke</td>
</tr>
<tr>
<td>Zinc Corp of America</td>
<td>none</td>
<td>41.9</td>
<td>307</td>
<td>678</td>
<td>8641</td>
<td>Coal-fired boiler/industrial processes</td>
<td>Primary non-ferrous metals</td>
</tr>
</tbody>
</table>
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

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

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

http://www.arl.noaa.gov/ready/ametus.html

Mixing Height – from sonde data at Pittsburgh Airport
- used Holzworth method

Stability Class: Pasquil Gifford Stability Class, Turner method

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

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

The diagram illustrates the relationship between the upper boundary (xx) of the constraint (0.1 ≤ α_j ≤ xx) and the ratio of $ER_{SO_2,j}@\alpha_j/ER_{SO_2,j}@\alpha_j=2.5$. The upper boundary is represented on the x-axis, and the ratio is on the y-axis. The data points for the Bellefield boiler plant, Pittsburgh brewing plant, Shenango coke works, and Zinc Corp Amer are plotted with different markers and line styles.
Predicted emission rates for SO$_2$ and metals for each of 4 sources during measurement period (units: g/s)*

<table>
<thead>
<tr>
<th>Species</th>
<th>Bellefield boiler plant</th>
<th>Pittsburgh brewing plant</th>
<th>Shenango Coke Works</th>
<th>Zinc Corp Amer</th>
</tr>
</thead>
<tbody>
<tr>
<td>SO$_2$</td>
<td>48</td>
<td>176</td>
<td>123</td>
<td>176</td>
</tr>
<tr>
<td>Al</td>
<td>0.0336</td>
<td>0.0800</td>
<td>0.1203</td>
<td>0.1453</td>
</tr>
<tr>
<td>As</td>
<td>0.0012</td>
<td>0.0105</td>
<td>0.0046</td>
<td>0.0009</td>
</tr>
<tr>
<td>Cr</td>
<td>0.0006</td>
<td>0.0021</td>
<td>0.0017</td>
<td>0.0020</td>
</tr>
<tr>
<td>Cu</td>
<td>0.0007</td>
<td>0.0408</td>
<td>0.0402</td>
<td>0.0480</td>
</tr>
<tr>
<td>Fe</td>
<td>0.0365</td>
<td>0.0926</td>
<td>0.1610</td>
<td>0.1130</td>
</tr>
<tr>
<td>Mn</td>
<td>0.0038</td>
<td>0.0032</td>
<td>0.0038</td>
<td>0.0010</td>
</tr>
<tr>
<td>Ni</td>
<td>0.0016</td>
<td>0.0065</td>
<td>0.0062</td>
<td>0.0070</td>
</tr>
<tr>
<td>Pb</td>
<td>0.0010</td>
<td>0.0232</td>
<td>0.0236</td>
<td>0.0369</td>
</tr>
<tr>
<td>Se</td>
<td>0.0005</td>
<td>0.0119</td>
<td>0.0126</td>
<td>0.0184</td>
</tr>
<tr>
<td>Zn</td>
<td>0.0299</td>
<td>0.0554</td>
<td>0.0807</td>
<td>0.0633</td>
</tr>
</tbody>
</table>

*Annual average SO2 emission rates are reported to be 21, 3.1, 70, and 249 g/s
Regressions: elements vs. Se (ng m\(^{-3}\))
Se is an excellent tracer of coal combustion aerosol

<table>
<thead>
<tr>
<th>Species</th>
<th>Regression equation</th>
<th>R</th>
<th>ER_ratio from modeling results(^{2)})</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>CMU measurement site</td>
<td></td>
<td>Bellefield boiler plant</td>
</tr>
<tr>
<td>SO(_2)</td>
<td>SO(_2)(^1)) = (11.237±1.886)***Se + (11.815±12.723)</td>
<td>0.772</td>
<td>96.0(^3)</td>
</tr>
<tr>
<td>Al</td>
<td>Al = (3.023±0.750)<strong>Se + (22.691±5.058)</strong></td>
<td>0.635</td>
<td>67.2</td>
</tr>
<tr>
<td>As</td>
<td>As = (0.987±0.033)<em><strong>Se + (-1.152±0.219)</strong></em></td>
<td>0.987</td>
<td>2.4</td>
</tr>
<tr>
<td>Cr</td>
<td>Cr = (0.140±0.010)**<em>Se + (0.226±0.067)</em></td>
<td>0.944</td>
<td>1.2</td>
</tr>
<tr>
<td>Cu</td>
<td>Cu = (3.311±0.160)***Se + (0.353±1.076)</td>
<td>0.973</td>
<td>1.4</td>
</tr>
<tr>
<td>Fe</td>
<td>Fe = (3.333±0.786)<em><strong>Se + (29.633±5.300)</strong></em></td>
<td>0.655</td>
<td>73.0</td>
</tr>
<tr>
<td>Mn</td>
<td>Mn = (0.029±0.033) Se + (1.912±0.222)***</td>
<td><strong>0.177</strong></td>
<td>7.6</td>
</tr>
<tr>
<td>Ni</td>
<td>Ni = (0.479±0.038)***Se + (0.422±0.258)</td>
<td>0.939</td>
<td>3.2</td>
</tr>
<tr>
<td>Pb</td>
<td>Pb = (2.177±0.136)***Se + (-0.799±0.919)</td>
<td>0.956</td>
<td>2.0</td>
</tr>
<tr>
<td>Zn</td>
<td>Zn = (2.455±0.474)<em><strong>Se + (15.039±3.200)</strong></em></td>
<td>0.726</td>
<td>59.8</td>
</tr>
</tbody>
</table>

Note) *: p<0.01, **: p<0.001; ***: p<0.0001
\(^{1)\) Unit is in µg m\(^{-3}\); \(^{2)\) ER_ratio means ratio of emission rate for each species to emission rate of Se; \(^{3)\) 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$_2$ 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 ±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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  Jay Turner, Meg Yu – Washington Univ.
- Pittsburgh Supersite Project
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