Enhanced Air Pollution Health Effects Studies Using Source-oriented Chemical Transport Models

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Motivation

- Fewer sites provide detailed PM chemical component measurements than total PM$_{2.5}$ mass.
- Are central monitors providing poor exposure estimates that are masking the more detailed associations?

- Epidemiological and toxicological studies have shown positive associations between exposure to atmospheric particulate matter and adverse health effects.
  - Can we target a specific set of sources / components / size fractions for less cost than the current PM2.5 control program?

Figure Source: DOCKERY DW, et al., 1993.
Population Exposure

• Strong spatial heterogeneity in concentrations and population

• Use one or a few monitor sites to represent an entire county/air basin could lead to exposure misclassification

• Population weighted concentrations (PWC)

\[
PWC = \frac{\sum_i C_i \times P_i}{\sum_i P_i}
\]

Reference: Ostro et al., *EHP*, 2015
Source-Oriented Air Quality Models

Source apportionment using Source-oriented air quality models

- Tag precursors from different sources
- Track the sources directly through all atmospheric processes
- Need to expand the gas and aerosol mechanisms
Central Site Concentrations vs. Population Weighted Concentrations of Total EC and Mass Concentrations

Reference: Hu et al., Environmental Science & Technology, 2014
95% CIs when Choosing Different Spatial Representativeness of Central Monitors
95% CIs for PM$_{2.5}$ Components with a 12 km buffer
95% CIs for PM$_{2.5}$ Components in Warm (Apr-Sept) vs. Cold (Oct-Mar) Seasons

![Graphs showing CI of PWC/CMC ratio vs. distance from monitors for Los Angeles and Fresno.](image)
PWC/CMC ratios for Primary PM$_{2.5}$ Sources

One Year Simulation in China
Summary

• Strong spatial heterogeneity in concentrations in PM$_{2.5}$ components, sources and in different seasons.

• Population weighted concentrations of PM emitted from various sources calculated using the model spatial information differed from the central monitor estimates.

• CTMs provide more detailed information to help improve exposure assessment for health effect studies.
Acknowledgements

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Data Availability: http://faculty.engineering.ucdavis.edu/kleeman/.
Supporting Slides
95% CIs for PM$_{2.5}$ Mass at Different Locations

![Graph showing 95% CIs for PM$_{2.5}$ Mass at different locations along the distance from monitors in kilometers.](image)
95% CIs of PWC/CMC ratios for $\text{PM}_{2.5}$ vs. $\text{PM}_{0.1}$

- Calculation is based on the distance from monitors of 8km.
- $\text{PM}_{0.1}$ shows greater spatial variations of CIs than $\text{PM}_{2.5}$.
Chemical Transport Model (CTM): UCD/CIT

- **Observation Data**
- **Model Gridded Data**
- **Terrestrial Data**
- **Meteorological Modeling by WRF**

Emissions Inventory
- **Emissions Modeling UCD**
- **Biogenic Emissions**
- **Wildfire Emissions**
- **Source Profiles from Emission Tests**

**UCD/CIT Air Quality Model**

\[
\frac{\partial C_i}{\partial t} + \nabla \cdot (u C_i) =
\nabla K \nabla C_i + E_i - S_i + R_i^{gas}(C) + R_i^{part}(C) + R_i^{phase}(C)
\]

- **Gas Pollutants** (O\textsubscript{3}, NO, NO\textsubscript{2}, NH\textsubscript{3}, SO\textsubscript{2}, CO, HCHO, PAN, ISOP, etc.)
- **Particulate Matter** (EC, OC, SO\textsubscript{4}\textsuperscript{2-}, NO\textsubscript{3}-, NH\textsubscript{4}\textsuperscript{+}, Cl\textsuperscript{-}, Na\textsuperscript{+}, Ca\textsuperscript{2+}, Fe, Cu, Mn, etc.)
- **Particulate Size Distributions** (PM\textsubscript{0.1}, PM\textsubscript{2.5}, PM\textsubscript{10})
- **Source Apportionment Information**
Predicted Regional Distribution of PM$_{2.5}$ Sources

- on-road mobile sources
- off-road mobile sources
- wood burning sources
- shipping sources

Reference: Hu et al., Identifying Primary PM2.5 and PM0.1 Sources for Epidemiological Studies in California. ES&T, 2014.
Model Configuration for California 2000-2008

• **Meteorology**
  – WRFv3.1 with FDDA
  – Hourly average outputs
  – Increased surface friction velocity (u*) by 50% (Mass CF, 2010)

• **Emissions**
  – Emissions inventory from California Air Resources Board
  – EMFAC2007 for mobile emissions
  – 1kmX1km satellite wildfire emissions ([http://bai.acd.ucar.edu/Data/fire/](http://bai.acd.ucar.edu/Data/fire/), Wiedinmyer C. et al., Geosci. Model Dev. Discuss., 3, 2439-2476, 2010)

• **UC-Davis_Primary (UCD_P)**
  – ~900 sources of primary PM

• **UCD/CIT**
  – gaseous pollutants,
  – secondary inorganic aerosols (nitrate, sulfate, ammonium, etc.)
  – secondary organic aerosol from
  – 10 sources
    • onroad/offroad gasoline, onroad/offroad diesel, wood burning, meat cooking, high sulfur content fuel combustion, other anthropogenic sources, biogenic sources, and IC/BCs

Predicted vs. Measured $O_3$ and PM$_{2.5}$

Predicted vs. Measured
Nitrate and Total Organic Compounds

Mean Fractional Bias

Mean Fractional Error

Mean Fractional Bias

Mean Fractional Error

Model Evaluation: MFB(numbers) and R (colors) of Monthly Average EC and Trace Elements at Individual Sites

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R values range from 0.8 to -1.9. The table uses colors to indicate the magnitude of the correlation coefficients, with yellow indicating positive correlation and red indicating negative correlation.
Predicted Regional Distribution of PM$_{2.5}$ Components

- Model performance provides confidence in CTM predictions at locations with no measurement

1 - Predicted
2 - measured

- 9-year average concentrations of PM2.5 total mass (a), EC (b), OC (c), nitrate (d), sulfate (e), and ammonium (f)