Integrated Source-to-Dose Assessments for Population Exposures to Co-occurring Ozone, PM, and Air Toxics: Applications to Philadelphia, PA and Camden, NJ.

Presented at the Ozone Research Center Science Workshop
Piscataway, NJ • December 17, 2003

by

Sheng-Wei Wang, Sastry Isukapalli, Qing Sun, Sai Tong, Pamela Shade, Vikram Vyas, and Panos G. Georgopoulos

Computational Chemodynamics Laboratory (CCL)
Environmental and Occupational Health Sciences Institute (EOHSI)
170 Frelinghuysen Road, Piscataway, NJ 08885
Modeling Steps in the Source-to-Dose Analysis

- Estimation of ambient levels of ozone, PM2.5, and air toxics
  - Geostatistical analysis of fixed monitor data
  - Emission-based, regional air quality modeling with Models-3/CMAQ
- Estimation of local outdoor levels of ozone, PM2.5, and air toxics at census tract level
  - Spatial and temporal interpolation (STRF and BME)
- Estimation of ozone, PM2.5, and air toxics levels in microenvironments
  - Observed indoor/outdoor relationships
  - Microenvironmental modeling through mass-balance
- Development of activity event sequences for each member of the sample population
  - Matching Consolidated Human Activity Database (CHAD) records with essential demographics of the population in the study area
Modeling Steps in the Source-to-Dose Analysis (Contd.)

• Calculation of age, gender, activity dependent inhalation rates for the members of the sample population

• Combination of inhalation rates and microenvironmental concentrations for each activity event to assess exposures

• Averaging of exposure estimates over time-units (e.g. 1-hour average, 8-hour running average, etc.) to characterize the exposure metrics of concern
Domain for Regional Meteorological and Air Quality Modeling

Camden, NJ

Philadelphia, PA
The Modeling Domains for the Exposure/Dose Case Studies

- The case studies focus on a two-week episode between 11 July 1999 and 24 July 1999
- 482 census tracts were selected in and adjacent to City of Philadelphia, PA
- 140 census tracts were selected in Camden, NJ
Calculate of Ambient Outdoor Concentrations

- US EPA’s Community Multiscale Air Quality (CMAQ) model was used to simulate spatial and temporal levels of ozone, PM2.5, and air toxics for the 36km, 12 km and 4km resolution domains.
- The meteorological inputs were obtained from MM5 simulation.
- The emissions data were processed from the National Emissions Trends (NET) inventory using the Sparse Matrix Operator Kernel Emissions (SMOKE) modeling system.
Predicted Ozone Daily Maximum Concentrations (ppb) for 7/19/1999 for the 12 km resolution (left) and 4 km resolution (right) domains.
Predicted PM2.5 24 Hour Averaged Concentrations (μg/m³) for 7/19/1999 for the 12 km resolution (left) and 4 km resolution (right) domains
Comparisons of 4km Resolution CMAQ Ozone and PM2.5 Predictions with Observation Data for the NE-OPS Baxter Site in Northern Philadelphia

![Graphs showing comparisons of CMAQ predictions with observations for ozone and PM2.5 concentrations over time.](image-url)
Comparisons of 4km Resolution CMAQ Ozone and PM2.5 Predictions with Observation Data for the AIRS Site in Camden, NJ

CAMDEN, NEW JERSEY, Monitor ID: 340070003442011

CAMDEN, NEW JERSEY, Monitor ID: 340070003811041
Spatiotemporal Interpolation for Obtaining Census-Tract Level Outdoor Concentrations

• The “Spatio-Temporal Random Field” (STRF) approach interpolates modeling output or monitor data in both space and time simultaneously

• The “Bayesian Maximum Entropy” (BME) method use prior information of hard data (measurements or modeling outputs), probability law descriptions, interval information, and physical laws
Interpolated Outdoor Concentrations of PM2.5 and O₃ for 482 Census Tracts in Urban Philadelphia for 1:00 PM EDT, 19 July 1999 (using the STRF method)

PM2.5

Ozone
Interpolated Outdoor Concentrations of PM2.5 and O₃ for 140 Census Tracts in Camden for 1:00 PM EDT, 19 July 1999 (using the STRF method)
Interpolated Outdoor Concentrations of Formaldehyde for Philadelphia and Camden for 1:00 PM EDT, 19 July 1999 (using the STRF method)

Philadelphia, PA

Camden, NJ
Interpolated Outdoor Concentrations of Toluene and Xylene for 140 Census Tracts in Camden for 1:00 PM EDT, 19 July 1999 (using the STRF method)
Calculation of Microenvironmental Concentrations - PM2.5

- For the indoor **non-residential** microenvironments, PM2.5 concentrations are determined by using observed indoor/outdoor relationships.
- For the indoor **residential** microenvironment, a single compartment, *steady-state mass balance equation* (Ozkaynak et. al., 1996) is used:

\[
C_{\text{residential}} = (P \ast ach/(ach + k)) \ast C_{\text{ambient}} + \frac{(E_{\text{smk}} \ast N_{\text{cig}} + E_{\text{cook}} \ast t_{\text{cook}} + E_{\text{others}} \ast T))/((ach + k) \ast V \ast T)}
\]

where:
- \(C_{\text{ambient}}\) = ambient outdoor PM concentration (\(\mu g/m^3\))
- \(P\) = penetration factor (unitless)
- \(k\) = deposition rate (\(h^{-1}\))
- \(ach\) = air exchange rate (\(h^{-1}\))
- \(E_{\text{smk}}\) = emission rate for smoking (\(mg/cig^{-1}\))
- \(N_{\text{cig}}\) = number of cigarettes smoked during model time step
- \(E_{\text{cook}}\) = emission rate for cooking (\(mg/min^{-1}\))
- \(t_{\text{cook}}\) = time spent cooking during model time step (min)
- \(E_{\text{others}}\) = emission rate for other source (\(mg/h^{-1}\))
- \(T\) = model time step (\(h\))
- \(V\) = residential volume (\(m^3\))
The estimation of O$_3$ concentrations in microenvironments are based on the **general mass balance equation**:

\[ \frac{dC_{in}}{dt} = (F_p)(v)(C_{out}) + S/V - (v + F_d)(C_{in}) \]

- $C_{in}$: indoor concentration (mass/volume)
- $F_p$: penetration factor (dimensionless fraction)
- $v$: air exchange rate (1/time)
- $C_{out}$: outdoor concentration (mass/volume)
- $S$: indoor generation rate (mass/time)
- $V$: indoor volume (volume)
- $F_d$: O$_3$ decay rate (1/time)
The estimation of air toxics concentrations in microenvironments is based on microenvironmental (ME) factors:

\[ ME(i, j, t) = ADD(i) + [PROX(i)][PEN(i)][AMB(j, t)] \]

- where \( ME(i,j,t) \) : concentration in microenvironment \( i \) located in census tract \( j \) at time \( t \),
  
  \( ADD(i) \) : additive factor for microenvironment \( i \),
  
  \( PROX(i) \) : proximity factor for microenvironment \( i \),
  
  \( PEN(i) \) : penetration factor for microenvironment \( i \), and
  
  \( AMB(j,t) \) : ambient concentration for census tract \( j \) at time \( t \)
Calculation of Inhalation Rates and Doses

Example: Dependence of inhaled fine PM dose on gender, age, and activity (MET= Metabolic Equivalent of Tasks)
Calculated PM2.5 Dose Distributions for Philadelphia, PA

Cumulative Distribution of PM2.5 Doses for 482 Census Tracts in Philadelphia

95th Percentiles of 24 Hour Aggregated Total PM2.5 Doses from All Sources for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Calculated O3 Dose Distributions for Philadelphia, PA

Cumulative Distribution of Ozone Doses for 482 Census Tracts in Philadelphia

95th Percentiles of 24 Hour Aggregated Total Ozone Doses for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Calculated Formaldehyde Dose Distributions for Philadelphia, PA

Cumulative Distribution of Formaldehyde Doses for 482 Census Tracts in Philadelphia

95th Percentiles of 24 Hour Aggregated Total Formaldehyde Doses for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Calculated PM2.5 Dose Distributions for Camden, NJ

Cumulative Distribution of PM2.5 Doses for 140 Census Tracts in Camden

95th Percentiles of 24 Hour Aggregated Total PM2.5 Doses from All Sources for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Calculated O3 Dose Distributions for Camden, NJ

Cumulative Distribution of Ozone Doses for 140 Census Tracts in Camden

95th Percentiles of 24 Hour Aggregated Total Ozone Doses for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Calculated Formaldehyde Dose Distributions for Camden, NJ

Cumulative Distribution of Formaldehyde Doses for 140 Census Tracts in Camden

95th Percentiles of 24 Hour Aggregated Total Formaldehyde Doses for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Calculated Toluene Dose Distributions for Camden, NJ

Cumulative Distribution of Toluene Doses for 140 Census Tracts in Camden

95th Percentiles of 24 Hour Aggregated Total Toluene Doses for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Calculated Xylene Dose Distributions for Camden, NJ

Cumulative Distribution of Xylene Doses for 140 Census Tracts in Camden

95th Percentiles of 24 Hour Aggregated Total Xylene Doses for 19 July 1999 (based on CMAQ outputs and STRF interpolation)
Comparison of Cumulative Distributions of Daily Aggregated Doses between Philadelphia and Camden

Species of Concern:
- PM2.5 (above)
- Ozone (up right)
- Formaldehyde (bottom right)
Conclusions

• This study demonstrated the feasibility of developing population exposure and dose assessments, for co-occurring ozone, PM2.5, and air toxics, using an integrated and mechanistically consistent source-to-dose framework

• Indoor PM2.5 sources dominate the contributions to the total PM2.5 doses for the upper percentiles in both Philadelphia and Camden

• Cumulative distributions of daily aggregated doses for PM2.5 and ozone are similar in Philadelphia and Camden, while the distribution of formaldehyde doses is higher in Camden than Philadelphia
Future Work

- Application of this comprehensive source-to-dose modeling framework to
  - Longer time periods (annual assessment)
  - Additional air toxics
- Further improvements of the framework (commuting patterns, etc.)
Acknowledgments

• U.S. EPA funded Center for Exposure and Risk Modeling (CERM) at EOHSI (EPAR-827033)
• NJ DEP funded Ozone Research Center (ORC) at EOHSI
• U.S. EPA funded NorthEast Oxidant and Particle Study (NE-OPS) University Consortium (EPA-TPSU-UMDNJ -826373-14)