Chemical transport models for exposure assessment

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Modeling Atmospheric Scales

**Regional**
- Mobile (µg m⁻³)
- Zhai et al., 2018
- >400km

**Neighborhood**
- Mobile (µg m⁻³)
- Zhai et al., 2016
- ~1-100km

**Roadway**
- Mobile (µg m⁻³)
- Brown et al., 2020
- <100m

**Chemical Transport Model**
- Atmospheric chemistry
- Transport processes
- All pollutants simulated!

**Dispersion (or CFD)**
- *Some* turbulence
- Single pollutant
- No chemistry
Spatial Resolution of Health Studies

**County** - uniform throughout state
  - GA county resolution ~15-40km

**Zip code** - based on population density
  - Downtown ATL ~4km, ATL MSA ~13km, rural GA ~25km

**Census tract** - based on population density
  - Downtown ATL ~1.5km, ATL MSA ~15km, rural GA ~30km

**Increased spatial resolution** for health analysis
  - Location of residents, gridded data (250m)

*Spatial resolution of exposure estimates = health resolution!*
Source Impacts (Chemical Mass Balance)

\[ C_i = \sum_{i} f_{ij} \cdot S_j + e_i \]

Inputs:

- \( C_i \)
- \( f_{ij} \)

Result:

- \( S_j \)
Georgia Source Apportionment

- Average CMB results, 11 monitors 2002 to 2010
- Higher mobile contributions in urban area

Zhai et al., 2017
Ground Observations and AQ Model

Environmental Protection Agency (EPA)
Ground Based Stations
Surface PM$_{2.5}$ Concentrations

National Aeronautics and Space Administration (NASA)
Chemical Transport Modeling
Global Aerosol Concentrations

http://gmao.gsfc.nasa.gov/research/aerosol/modeling/nr1_movie/aerosols_geos5.mp4
Numerical Weather Prediction

• Weather Research & Forecasting (WRF) Model
  – Late 1990’s, National Center for Atmospheric Research (USA)

• Numerical Simulation of Atmospheric Flows
  – Meters to Hundreds of Kilometers
  – Navier-Stokes Equations
  – **Inputs:** Terrain, Land Use, Observations
  – **Outputs:** Atmospheric Physics, Moisture, Temperature, Precipitation, Radiation

Wind Speed - U (m/s)

Numerical Simulation of Physical Processes and Meteorology
Emissions Modeling

• National Emissions Inventory (NEI)
  – USA Environmental Protection Agency (EPA)
  – States report annual average by county
• Sparse Matrix Operator Kernel Emissions (SMOKE)
  – Model spatial and temporal patterns
  – Area, biogenic, mobile, point source emissions
  – Emissions factors for each source, species

Hourly Speciated Emissions Rate for Each Grid Cell
Chemical Transport Modeling (CTM)

- Community Multiscale Air Quality (CMAQ) Model
  - USA-EPA Model, Regulatory & Research Applications

CTM

Meteorology
- Advection
- Diffusion
- Plume in Grid

Emissions
- Gas-phase Chemistry
- Aerosol
- Cloud Process
- Photolysis

Concentrations, Transport Processes, Secondary Pollutant Formation
CMAQ Sensitivity to Emissions Perturbations
36km Resolution, Contiguous USA Domain

Simulated 24-hr PM$_{2.5}$ Concentration

Sensitivity of 24-hr PM to Power Plants
Spatial Source Apportionment Model

**Receptor Models**
- PMF, CMB, CMB-GC
  - Monitoring network data
  - Spatially limited
  - Different results for each method

**Source Oriented**
- CMAQ-DDM
  - Spatiotemporal source impacts
  - Atmospheric processes modeled
  - Results do not match observations

**Novel SA Method**
- Hybrid CTM-RM
  - Daily and Spatial Field
The hybrid source- and receptor-oriented (SH) approach is being developed both to develop spatially accurate source impact fields that are consistent with source-receptor relationships. SH results are also subject to potential systematic bias from the optimization and kriging statistical approaches. Statistical optimization, instead of re-running CMAQ–DDM sensitivity approaches, may not capture all nonlinearities in the PM spatial fields.

The spatial hybrid model is an effective approach for reducing the error in simulated source impact spatial fields through a widespread adjustment to biomass burning and dust impacts. There are several points of uncertainty, SH source apportionment can provide daily, spatially complete source impacts across a large domain over a long time period. The SH technique does not necessarily isolate specific atmospheric processes, as it is a complex undertaking. Also, first-order processes in CMAQ–DDM are uncertain as modeling atmospheric behavior is a complex undertaking. Also, first-order processes in CMAQ–DDM are uncertain as modeling atmospheric behavior is a complex undertaking. Also, first-order processes in CMAQ–DDM are uncertain as modeling atmospheric behavior is a complex undertaking.
CTM Modeling for Exposure Estimates

Community Multiscale Air Quality (CMAQ) Model
Species Concentrations, No Metals (CMAQ)
  • 12km Eastern USA, 8 years: 2001-2010
  • 4km Georgia, 5 years: 2007-2012

Source Impacts (CMAQ-DDM)
  • 36km Continental USA, 3 years: 2005-2007
  • 20 source categories

Un-bias Numerical Results for Health Assessments
CMAQ Concentrations Adjusted to Observations
  • Species Concentrations
    CMAQ Data Fusion Model \((Friberg\ et\ al.,\ 2016\ &\ 2017)\)
  • Source Apportionment
    CMAQ-DDM Hybrid \((Hu\ et\ al.,\ 2014;\ Ivey\ et\ al.,\ 2015,\ 2016,\ &\ 2017)\)
We found from the single-source model that IQR increases in metals (OR = 1.016, 95%CI: 1.010, 1.022), natural gas (OR = 1.014, 95%CI: 1.002, 1.027), non-road mobile diesel (OR = 1.022, 95%CI: 1.014, 1.029), and all other sources (OR = 1.021, 95%CI: 1.010, 1.032) were associated with increases in acute URI ED visits (Fig. 4, Table S7). ORs remained elevated after adjusting for other sources in the multi-source model (Table S7); as was the case for the other outcomes, the relative differences in the magnitude of the associations across sources was more prominent when associations were scaled to a 1 g/m³ increase in pollution (Table S8). We also extended the lag period to 7 days (average of lag0-lag6) for all 12 sources using the same models as in our primary analysis. For the 7-day lag period, most associations (per 1 g/m³ increase) were of greater magnitude compared to the associations based on the 3-day lag period, with the exception of biogenic and on-road gasoline for asthma; metals, natural gas, and gasoline source for pneumonia; and biogenic, dust, and on-road gasoline for acute URI. However, the relative differences in effect size across sources and outcomes were similar to those obtained using a 3-day average (Fig. S1, Tables S12–S14). Sensitivity analyses excluding patients aged < 2 years caused only slight changes in the OR estimates (Tables S9–S11).

4. Discussion

Using PM$_{2.5}$ source apportionment data from a bias-corrected CTM-RM hybrid model fused with ground measurements that apportioned both the primary and secondary PM$_{2.5}$ allowed us to estimate health associations for more source categories than previous studies (Atkinson et al., 2014; Dominici et al., 2006). In addition, the source apportionment estimates that we used have daily temporal resolution and improved spatial coverage compared to competing methods that only apportion PM$_{2.5}$ at stationary monitors (Krall et al., 2016; Mar et al., 2010; Bell et al., 2014). Our study found that metals, natural gas and all other sources were positively associated with pediatric ED visits for asthma, pneumonia and acute URI. PM$_{2.5}$ from non-road mobile diesel combustion was associated with increased pneumonia and acute URI ED visits. In addition, coal and dust were positively associated with asthma ED visits. Metals, natural gas, non-road diesel and all other sources have consistently elevated risks of the three respiratory outcomes. Heterogeneity in odds ratios across sources and outcomes could reflect differences in the importance of sources in triggering respiratory outcomes due to differences in compositional makeup of emissions sources. Because the hybrid CTM-RM has uncertainties in the emissions and meteorology inputs and in the modeling of atmospheric processes (e.g., atmospheric chemistry), such conclusions are tentative.

In line with our findings, previous studies focusing on metals in ambient particulate matter suggested that exposure to metals might be associated with adverse respiratory outcomes (Dunea et al., 2016; Hou et al., 2017).
Huang et al., 2019

Georgia Pediatric Asthma by Source

ZIP code ED visits for 0-18 years of age

M. Huang, et al.

Huang et al., 2019

www.haholmes.wordpress.com
CTMs for Non-tailpipe Exposures

Strengths

• Transport due to changing wind and meteorology conditions
• Secondary pollutant formation
• Model exposure for pollutant mixtures
• Increased number of source categories (e.g., 20+ vs. ~6)
• Improved source apportionment for secondary species

Limitations

• Near roadway gradients need smaller grid cells (~100m)
• Turbulence at small scales difficult to simulate in CTM
• Resolution depends on modeled emissions
• CPU intensive, especially CMAQ-DDM


