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Georgia Tech
Southeastern Center for Air Pollution & Epidemiology
This research is funded by U.S. EPA - Science To Achieve Results (STAR) Program
Grant # R834799

Chemical transport models for exposure assessment

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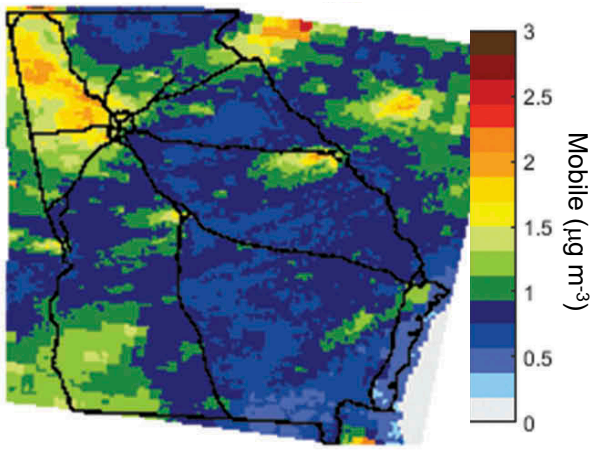
13 November 2020
HEI Brake and Tire Wear PM Emissions and Exposure Workshop

Modeling Atmospheric Scales

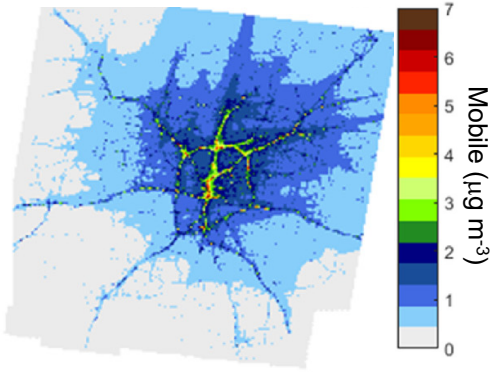
Regional



Zhai et al., 2018

>400km

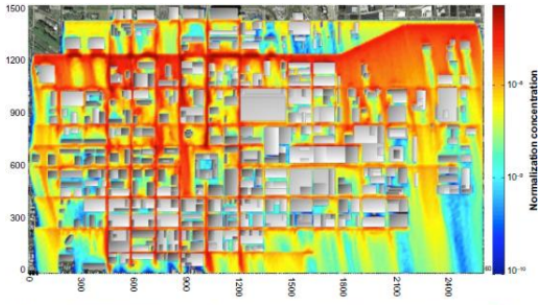
Neighborhood



Zhai et al., 2016

~1-100km

Roadway



Brown et al., 2020

<100m

Decreasing Spatial Resolution

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)

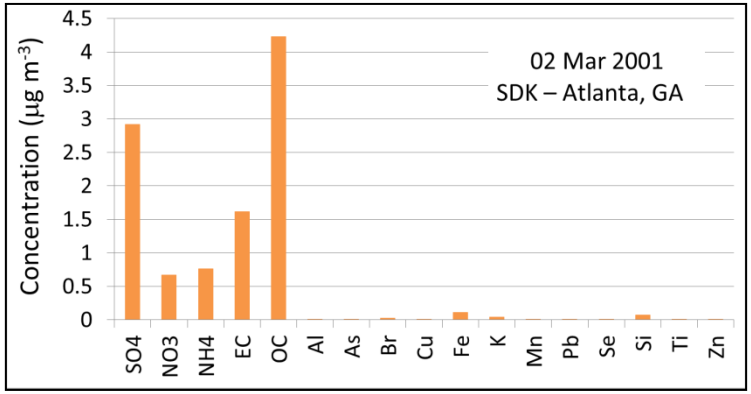
Spatial resolution of exposure estimates = health resolution!

Source Impacts (Chemical Mass Balance)

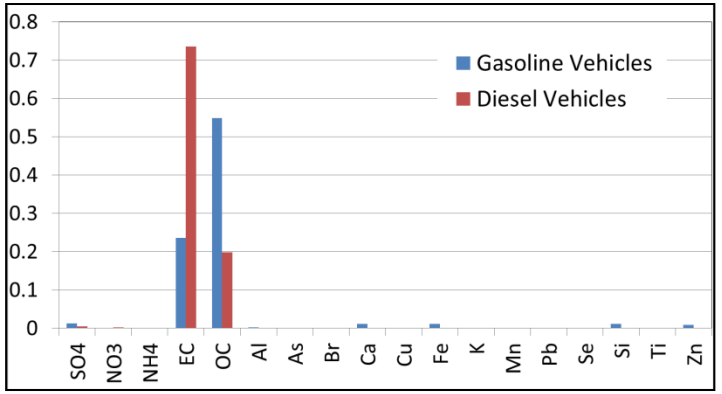
$$C_i = \sum_{i}^{I} f_{ij} \cdot S_j + e_i$$

Inputs:

C_i

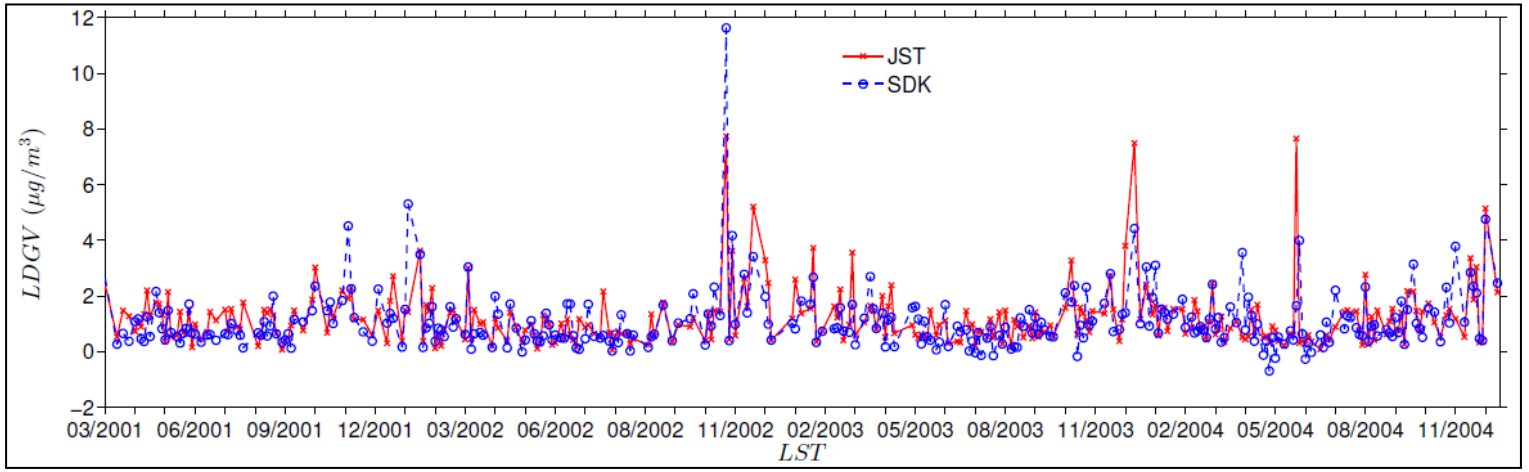


f_{ij}



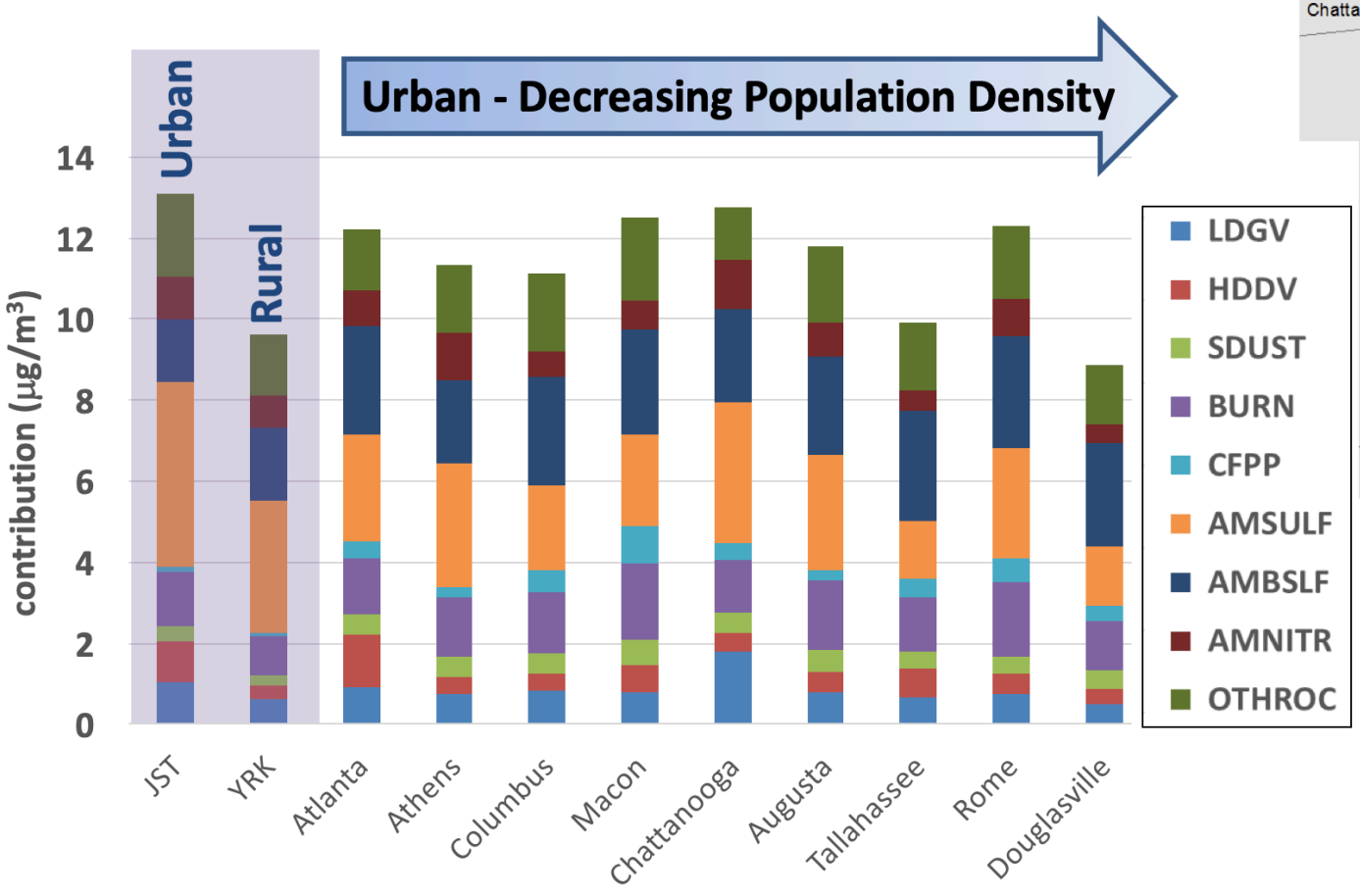
Result:

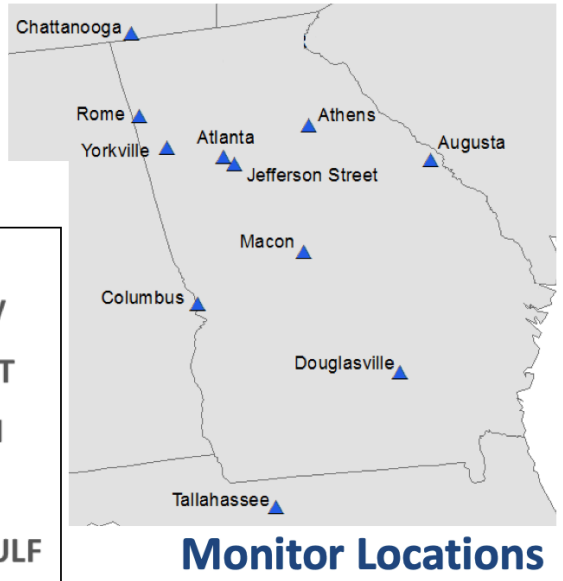
S_j



Georgia Source Apportionment

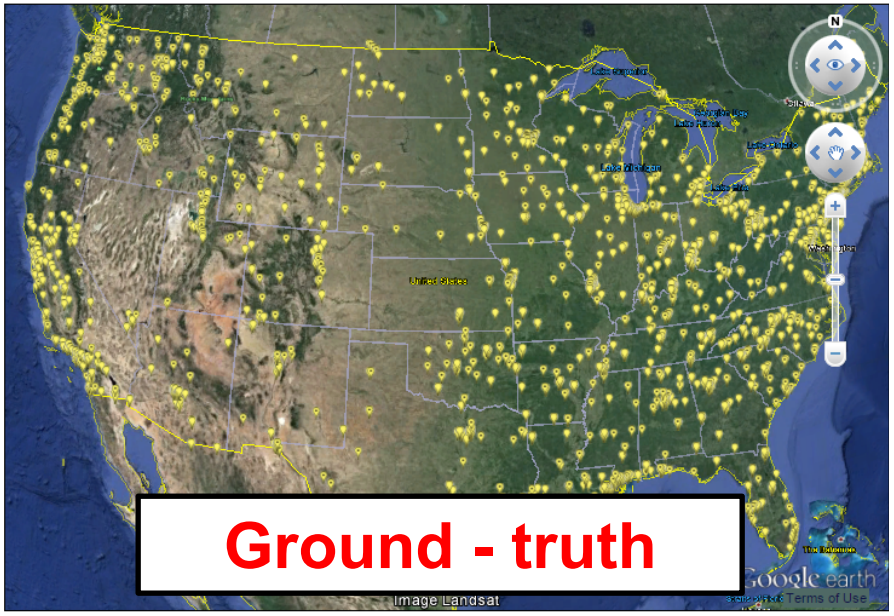
- Average CMB results, 11 monitors 2002 to 2010
- Higher mobile contributions in urban area



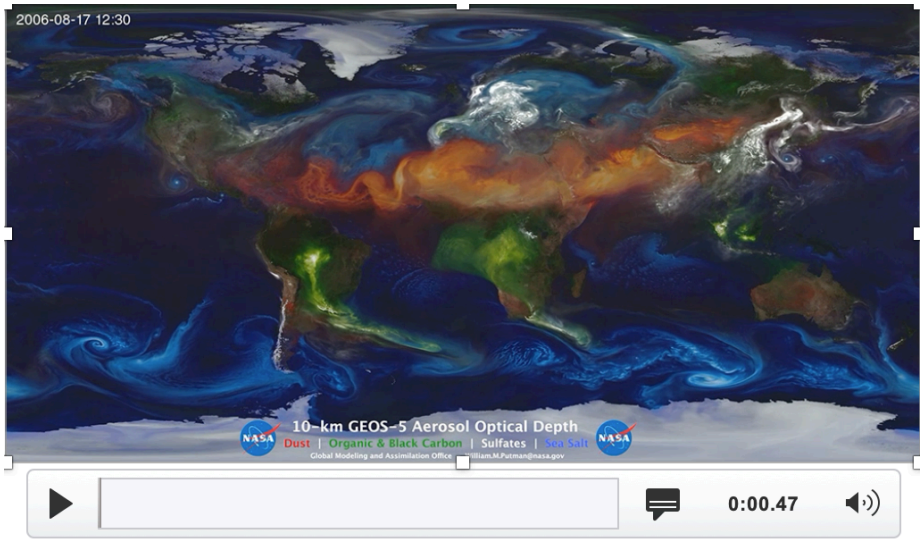


Zhai et al., 2017

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

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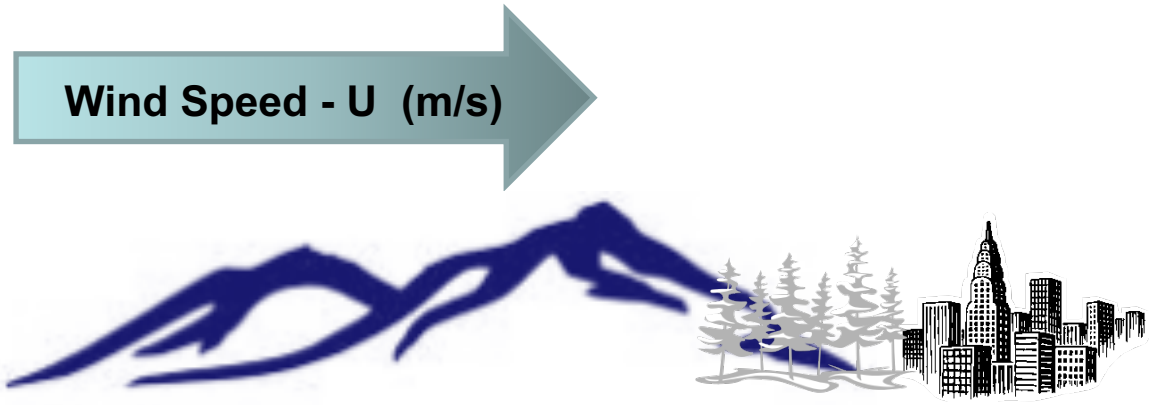
Numerical Weather Prediction

- **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



Numerical Simulation of Physical Processes and Meteorology

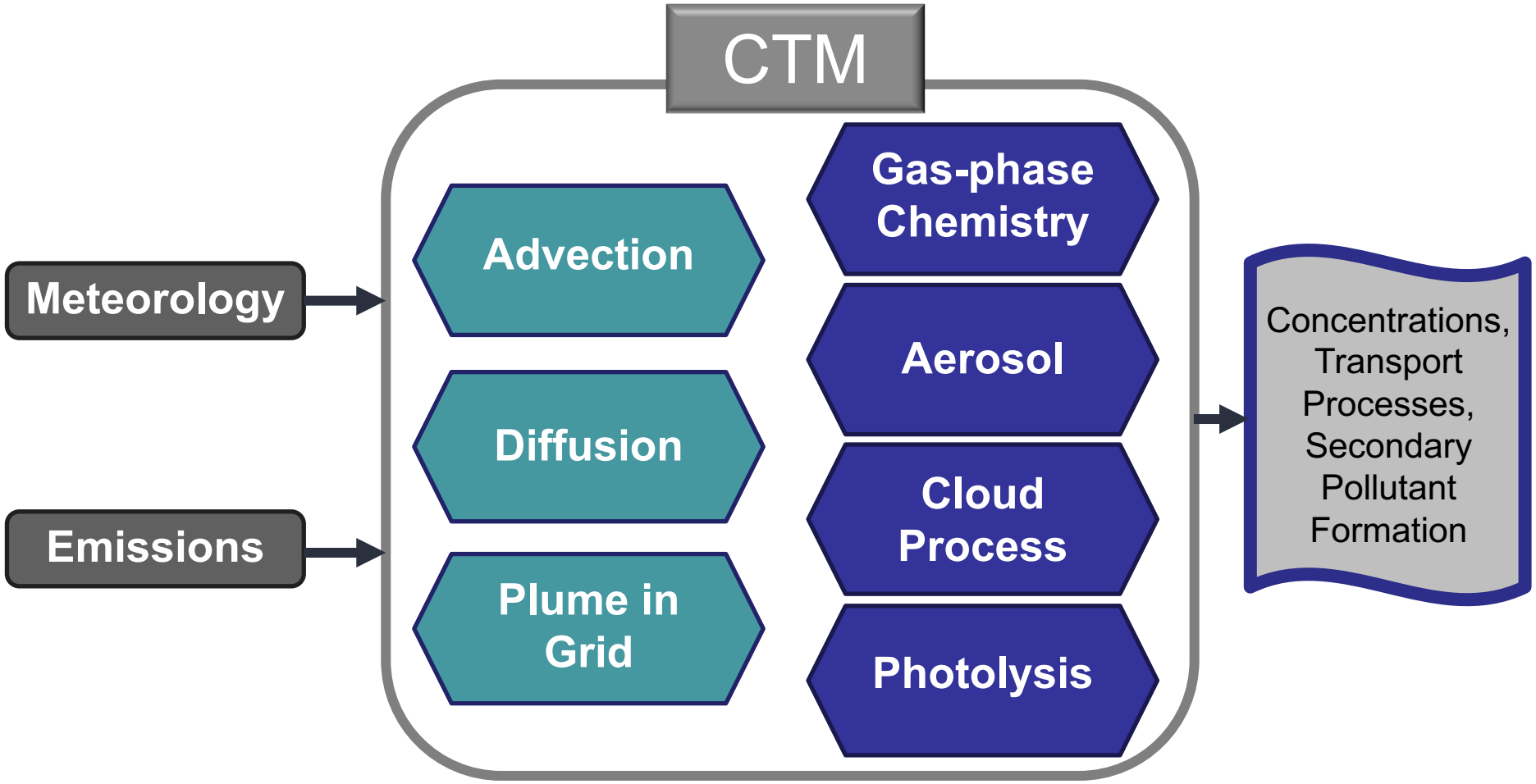
Emissions Modeling

- **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)

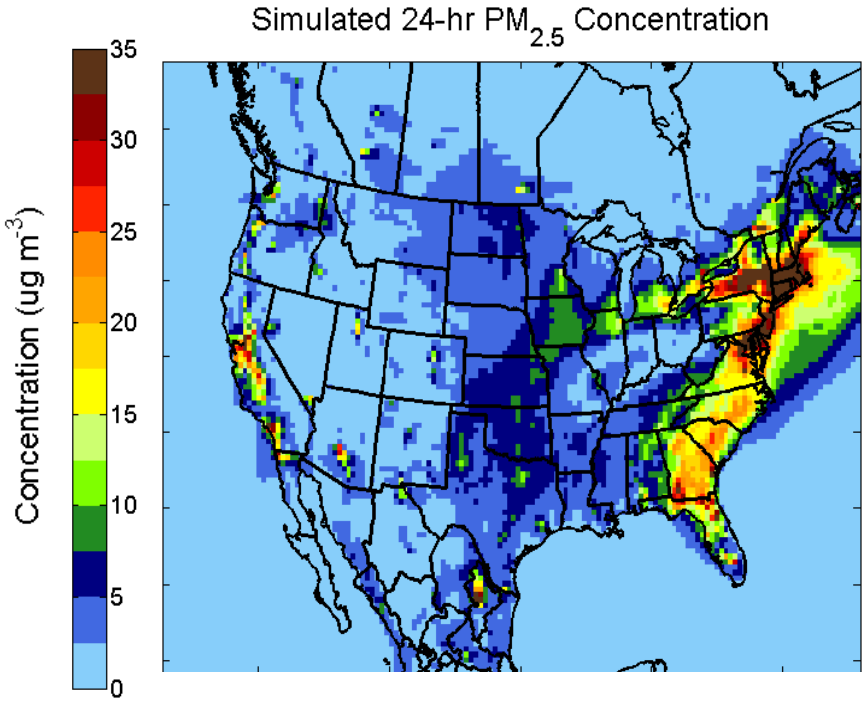
- **Community Multiscale Air Quality (CMAQ) Model**
  - USA-EPA Model, Regulatory & Research Applications

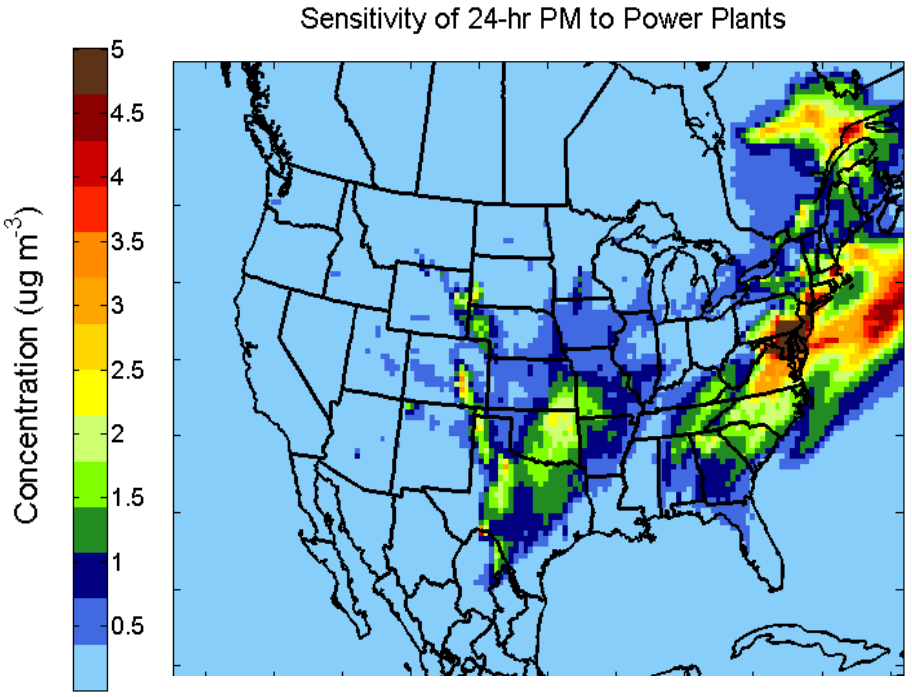


CMAQ-Direct Decoupled Method (DDM)

CMAQ Sensitivity to Emissions Perturbations

36km Resolution, Contiguous USA Domain





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

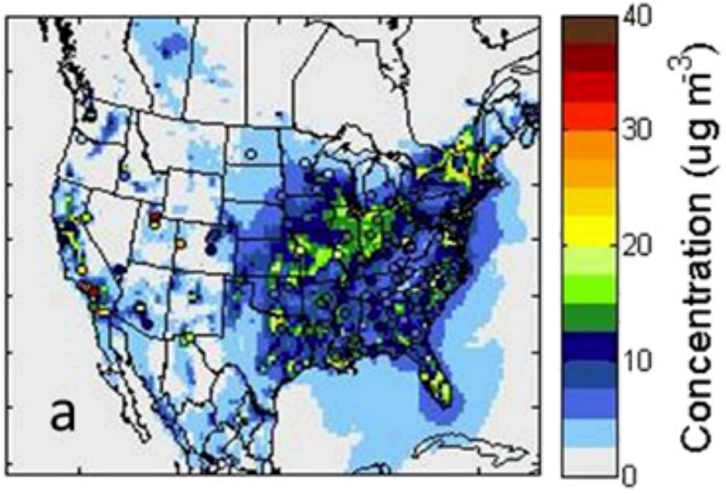
Novel SA Method

Hybrid CTM-RM

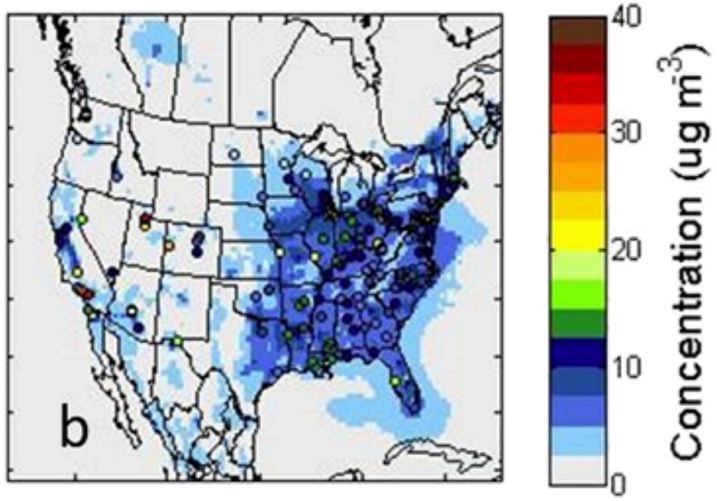
Daily and Spatial Field

Spatial Source Apportionment Model

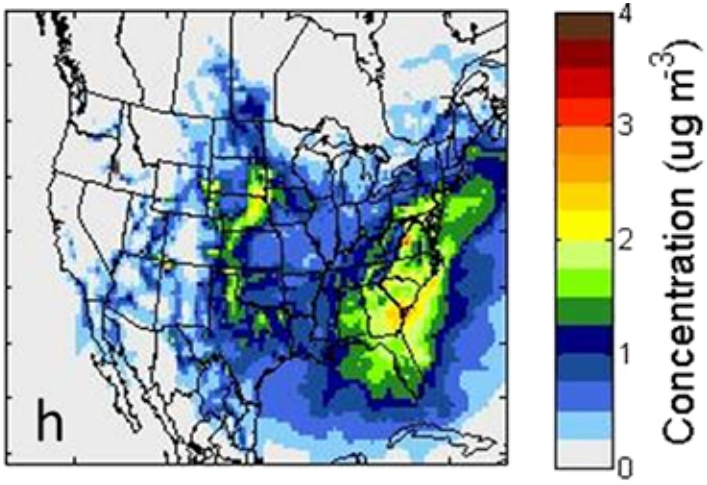
CMAQ-DDM $PM_{2.5}$



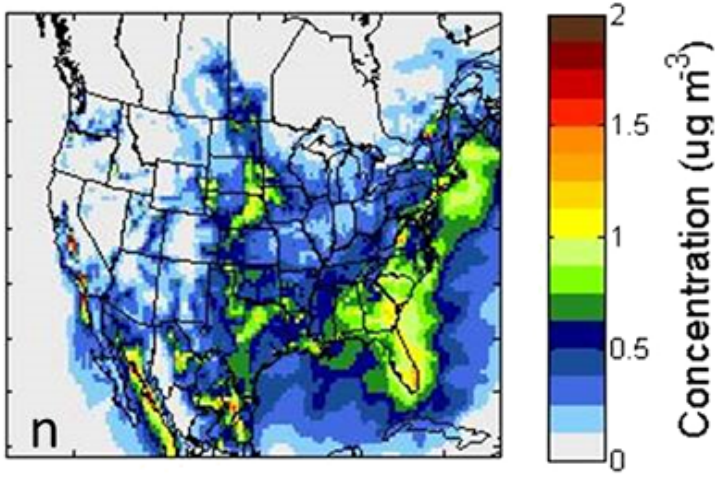
Hybrid CTM-RM $PM_{2.5}$



Traffic Related $PM_{2.5}$



Metals Processing $PM_{2.5}$



Ivey et al., 2015

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

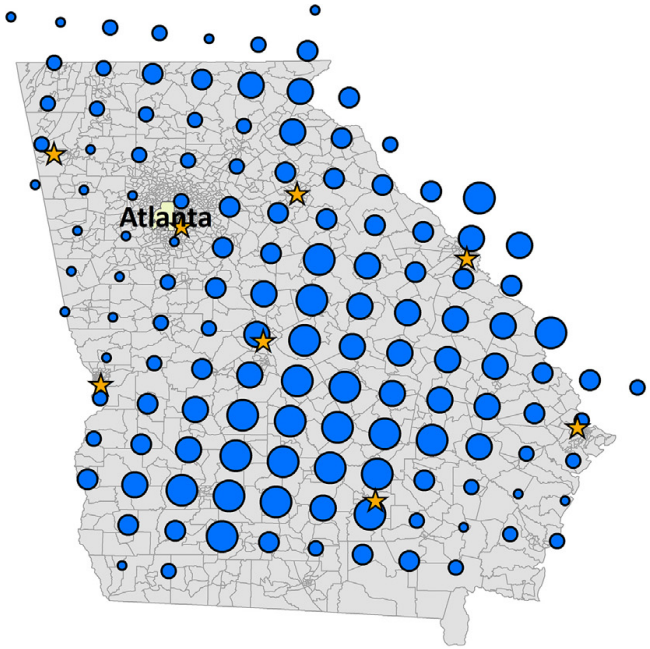
Un-bias Numerical Results for Health Assessments

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)*

Georgia Hybrid CTM-RM Sources

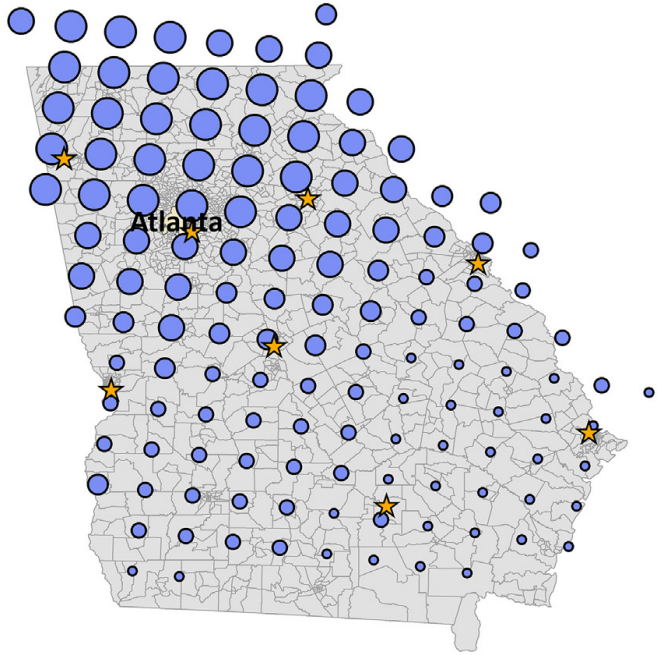
Annual Average Dust



Dust

- 0.30 - 0.44
- 0.45 - 0.57
- 0.58 - 0.71
- 0.72 - 0.86
- 0.87 - 1.09

Annual Average On-road Diesel



On-road diesel

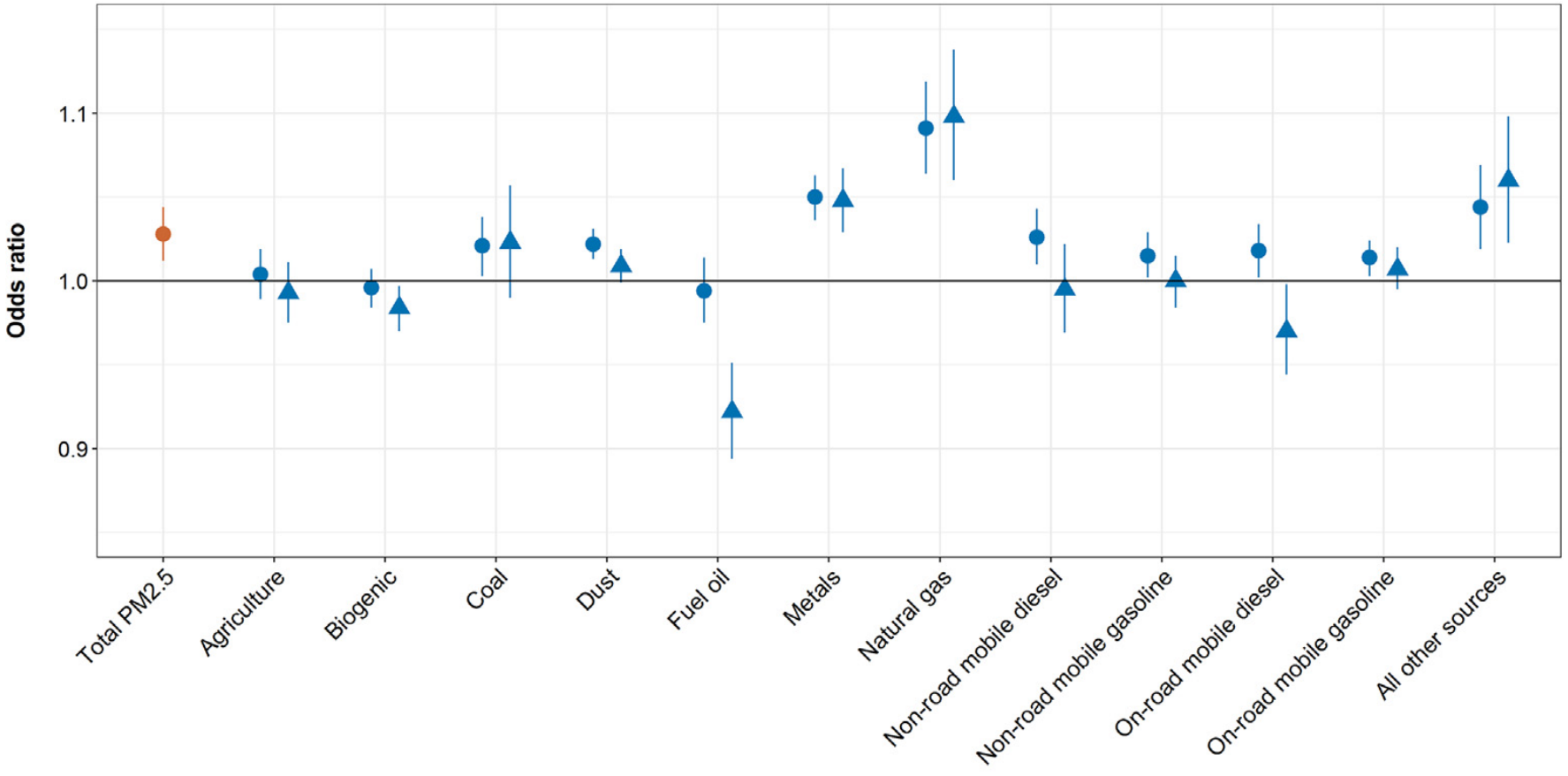
- 0.44 - 0.53
- 0.54 - 0.62
- 0.63 - 0.73
- 0.74 - 0.91
- 0.92 - 1.23

0 37.5 75 150 225 300 Miles

Huang et al., 2019

Georgia Pediatric Asthma by Source

ZIP code ED visits for 0-18 years of age



Huang et al., 2019

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

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References

1. Brown, M. J., Williams, M. D., Nelson, M. A., & Werley, K. A. (2015). QUIC transport and dispersion modeling of vehicle emissions in cities for better public health assessments. *Environmental Health Insights*, 9, EHI-S15662.
2. Friberg, M. D., Zhai, X., Holmes, H. A., Chang, H. H., Strickland, M. J., Sarnat, S. E., Tolbert, P. E., Russell, A. G., & Mulholland, J. A. (2016). Method for fusing observational data and chemical transport model simulations to estimate spatiotemporally resolved ambient air pollution. *Environmental Science & Technology*, 50(7), 3695-3705.
3. Friberg, M. D., Kahn, R. A., Holmes, H. A., Chang, H. H., Sarnat, S. E., Tolbert, P. E., Russell, A. G., & Mulholland, J. A. (2017). Daily ambient air pollution metrics for five cities: Evaluation of data-fusion-based estimates and uncertainties. *Atmospheric Environment*, 158, 36-50.
4. Hu, Y., Balachandran, S., Pachon, J. E., Baek, J., Ivey, C., Holmes, H., Odman, M. T., Mulholland, J. A., & Russell, A. G. (2014). Fine particulate matter source apportionment using a hybrid chemical transport and receptor model approach. *Atmospheric Chemistry & Physics*, 14(11), 5415-5431.
5. Huang, M., Ivey, C., Hu, Y., Holmes, H. A., & Strickland, M. J. (2019). Source apportionment of primary and secondary PM2. 5: Associations with pediatric respiratory disease emergency department visits in the US State of Georgia. *Environment International*, 133, 105167.
6. Ivey, C. E., Holmes, H. A., Hu, Y. T., Mulholland, J. A., & Russell, A. G. (2015). Development of PM 2.5 source impact spatial fields using a hybrid source apportionment air quality model. *Geoscientific Model Development*, 8(7).
7. Ivey, C. E., Holmes, H. A., Hu, Y., Mulholland, J. A., & Russell, A. G. (2016). A method for quantifying bias in modeled concentrations and source impacts for secondary particulate matter. *Frontiers of Environmental Science & Engineering*, 10(5), 14.
8. Ivey, C., Holmes, H., Shi, G., Balachandran, S., Hu, Y., & Russell, A. G. (2017). Development of PM2.5 source profiles using a hybrid chemical transport-receptor modeling approach. *Environmental Science & Technology*, 51(23), 13788-13796.
9. Zhai, X., Russell, A. G., Sampath, P., Mulholland, J. A., Kim, B. U., Kim, Y., & D'Onofrio, D. (2016). Calibrating R-LINE model results with observational data to develop annual mobile source air pollutant fields at fine spatial resolution: Application in Atlanta. *Atmospheric Environment*, 147, 446-457.
10. Zhai, X., Mulholland, J. A., Russell, A. G., & Holmes, H. A. (2017). Spatial and temporal source apportionment of PM2. 5 in Georgia, 2002 to 2013. *Atmospheric Environment*, 161, 112-121.
11. Zhai, X., Mulholland, J. A., Friberg, M. D., Holmes, H. A., Russell, A. G., & Hu, Y. (2019). Spatial PM2. 5 mobile source impacts using a calibrated indicator method. *Journal of the Air & Waste Management Association*, 69(4), 402-414.