Chapter 1
Use of Air Quality Modeling Results in Health Effects Research

Armistead Russell, Heather Holmes, Mariel Friberg, Cesunica Ivey, Yongtao Hu, Siv Balachandran, James Mulholland, Paige Tolbert, Jeremy Sarnat, Stefanie Sarnat, Matt Strickland, Howard Chang, and Yang Liu

Abstract The most recent Global Burden of Disease study (Lim SS et al, Lancet 380(9859):2224–2260, 2012), for example, finds that combined exposure to ambient and indoor air pollution is one of the top five risks worldwide. Of particular concern is particulate matter (PM). Health researchers are now trying to assess how this mixture of air pollutants links to various health outcomes and how to tie the mixture components and health outcomes back to sources. This process involves the use of air quality models. As part of an EPA Clean Air Research Center, the Southeastern Center for Air Pollution and Epidemiology (SCAPE), a variety of air quality models are being developed and applied to provide enhanced temporal and spatial resolution of pollutant concentrations for use in epidemiologic analysis. Air quality models that are being further developed and used as part of the center include Bayesian-based ensemble methods and hybrid chemical transport-chemical mass balance modeling. The hybrid method uses knowledge of the emissions, modeling and measurement uncertainties, and can provide spatially and temporally complete pollutant fields.

1.1 Introduction

Evidence continues to grow that exposure to ambient air pollutants impacts health. The most recent Global Burden of Disease study [11], for example, finds that combined exposure to ambient and indoor air pollution is one of the top five risks worldwide. This study, as well as similar ones conducted for more limited

A. Russell (✉) • H. Holmes • M. Friberg • C. Ivey • Y. Hu • S. Balachandran • J. Mulholland
School of Civil and Environmental Engineering, Georgia Institute of Technology, Atlanta, GA 30332, USA
e-mail: ted.russell@ce.gatech.edu; heather.holmes@ce.gatech.edu

P. Tolbert • J. Sarnat • S. Sarnat • M. Strickland • H. Chang • Y. Liu
Rollins School of Public Health, Emory University, Atlanta, GA 30322, USA

D. Steyn and R. Mathur (eds.), *Air Pollution Modeling and its Application XXIII*, Springer Proceedings in Complexity, DOI 10.1007/978-3-319-04379-1_1,

domains (e.g., by country), relies on results from epidemiologic studies that quantify exposure-health effect relationships (e.g., by calculating concentration-response functions). Traditionally, epidemiologic studies associate observed pollutant concentrations with observed health endpoints (e.g., hospital admissions or deaths). However, air pollutant observations are limited spatially, temporally, and chemically, and do not directly identify source contributions to pollution and, thus, health. Air quality models, both receptor-based and chemical transport models, are now being used to address the limitations of using observations alone. However, air quality models also have limitations, in particular uncertainties and biases that arise from errors in the inputs (e.g., emissions timing, speciation and magnitude and meteorological) and model parameters and structure (e.g., grid resolution).

1.2 Methods and Results

Air pollution is a mixture of a variety of pollutants. Historically, the related health effects have been tied to individual pollutants, though a question of current interest is how the "mixture" of pollutants plays a role. Past studies have found that particulate matter (PM) is the primary air pollutant of concern when considering premature death or disability adjusted life-years [11], while ozone is of concern for respiratory diseases, such as asthma [15]. Identifying the sources of those two pollutants is challenging. Ozone is a secondary pollutant, and is formed by a series of non-linear chemical reactions involving emissions from a variety of sources. PM formation and morphology is more complicated, being composed of thousands of different compounds which can be both secondary and primary in origin on differently sized particles. Health researchers are now trying to assess how this mixture of air pollutants links to various health outcomes and how to tie the mixture components and health outcomes back to sources. This process involves the use of air quality models. Various methods of identifying sources of ozone using chemical transport air quality models have been used, including both "brute force" and direct sensitivity (e.g., DDM and adjoint) approaches [4, 5, 7, 16]. Identifying source impacts on PM (e.g. PM2.5, PM with aerodynamic diameters less than 2.5 μm) have utilized both receptor models (e.g., [13]) and chemical transport models (e.g. [3, 6, 10]). Marmur et al. [12] examined the use of various types of air quality models for use in epidemiologic research and found that source apportionment models based on chemical transport models tend to reduce day-to-day variability in source impact estimates (e.g., due to reducing variability in temporal and spatial source emissions and missing sub-synoptic scale meteorological variability), while receptor models can increase variability. More recently, Balachandran et al. [1] applied a number of source apportionment models to assess model differences and uncertainties and also found increased variability in receptor model results, and that the various air quality models, including receptor and chemical transport models, had similar uncertainties in their results. As part of an EPA Clean Air Research Center, the Southeastern Center for Air Pollution and Epidemiology (SCAPE), a variety of air quality models are being developed and applied to provide enhanced temporal and

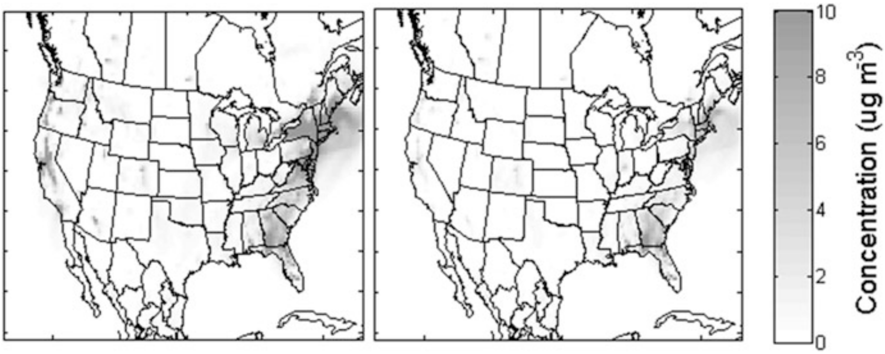

Fig. 1.1 Spatial fields of biomass burning impacts on January 4, 2004, as simulated by CMAQ (original, *left*) and a hybrid CTM-RM model (refined, *right*). Spatial fields are generated for a 36-km resolution grid. Biomass burning fields include impacts from agricultural burning, lawn waste burning, open fires, prescribed burning, wildfires, wood fuel burning, and woodstoves

spatial resolution of pollutant concentrations for use in epidemiologic analysis. The Center is also assessing how pollutant mixtures and the sources of these mixtures are linked to various health endpoints. In particular, two hybrid approaches that use both observations and air quality models address many of the limitations identified in the direct use of measured or modeled concentrations. One method, the Bayesian Ensemble approach [2], uses results of multiple models to develop an ensemble simulated source impact and then used with observed air quality to develop an improved estimate of the composition of source emissions. With the updated source compositions, a Bayesian approach is used to get improved estimates of air quality impacts and uncertainties.

A second set of methods use results of a chemical transport model (CMAQ) to provide simulated species concentrations and source impacts based on estimated emissions and modeled meteorology. In one approach, simulated species concentrations are fused with observations to develop spatial pollutant fields that are coherent with observations but use the air quality model to provide spatial gradients [8, 14]. This does not link the pollutant fields to individual sources, but does provide a spatially and temporally complete data set of pollutant fields for use in health assessments. In a more involved approach used to link the pollutants to sources, observed concentrations of individual pollutant species (e.g., single elements and gaseous compounds) are used to adjust source impacts to better match observations. This is done in a manner similar to the Chemical Mass Balance Method. However, the method involves using knowledge of the emission uncertainties and can be used to quantify many more source impacts. These results are then used to develop spatially and temporally complete fields for epidemiologic analysis using kriging [9] (Fig. 1.1).

Chemical transport model pollutant fields can also be used with satellite and ground-based observations and land-use information to develop finer scale (e.g., sub-grid scale) pollutant concentration estimates.

Acknowledgments This work was made possible in part by USEPA STAR grants R833626, R833866 and R834799 and by NASA project SV6-76007 under grant NNG04GE15G. Its contents are solely the responsibility of the grantee and do not necessarily represent the official views of the USEPA and NASA. Further, neither USEPA nor NASA endorses the purchase of any commercial products or services mentioned in the publication. We also acknowledge the Southern Company for their support and thank Eric Edgerton of ARA, Inc. for access to the SEARCH data.

References

1. Balachandran S, Pachon JE, Hu Y, Lee D, Mulholland JA, Russell AG (2012) Ensemble-trained source apportionment of fine particulate matter and method uncertainty analysis. Atmos Environ 61:387–394
2. Balachandran S, Chang HH, Pachon JE, Holmes HA, Mulholland JA, Russell AG (2013) A Bayesian–based ensemble technique for source apportionment of PM2.5. Environ Sci Technol 47(23):13511–13518
3. Boylan JW, Odman MT, Wilkinson JG, Russell AG, Doty KG, Norris WB, McNider RT (2002) Development of a comprehensive, multiscale "one-atmosphere" modeling system: application to the Southern Appalachian Mountains. Atmos Environ 36(23):3721–3734
4. Dunker AM (1981) Efficient calculation of sensitivity coefficients for complex atmospheric models. Atmos Environ 15(7):1155–1161
5. Hakami A, Odman MT, Russell AG (2003) High-order, direct sensitivity analysis of multidimensional air quality models. Environ Sci Technol 37(11):2442–2452
6. Held T, Ying Q, Kleeman MJ, Schauer JJ, Fraser MP (2005) A comparison of the UCD/CIT air quality model and the CMB source-receptor model for primary airborne particulate matter. Atmos Environ 39(12):2281–2297
7. Henze DK, Hakami A, Seinfeld JH (2007) Development of the adjoint of GEOS-Chem. Atmos Chem Phys 7(9):2413–2433
8. Holmes H et al (2013) Improved spatiotemporal air pollutant mixtures characterization for health studies. In: NATO/SPS international technical meeting on air pollution modelling and its application, Miami
9. Ivey C, Holmes H, Hu Y, Russell A, Mulholland J (2013) Spatial and temporal extension of a novel hybrid source apportionment model. Paper presented at NATO/SPS international technical meeting on air pollution modelling and its application, Miami
10. Koo B, Dunker AM, Yarwood G (2007) Implementing the decoupled direct method for sensitivity analysis in a particulate matter air quality model. Environ Sci Technol 41(8):2847–2854
11. Lim SS et al (2012) A comparative risk assessment of burden of disease and injury attributable to 67 risk factors and risk factor clusters in 21 regions, 1990–2010: a systematic analysis for the Global Burden of Disease Study 2010. Lancet 380(9859):2224–2260
12. Marmur A, Park SK, Mulholland JA, Tolbert PE, Russell AG (2006) Source apportionment of PM2.5 in the southeastern United States using receptor and emissions-based models: conceptual differences and implications for time-series health studies. Atmos Environ 40(14):2533–2551
13. Seigneur C (2001) Current status of air quality models for particulate matter. J Air Waste Manage Assoc 51(11):1508–1521
14. Sororian S, Holmes H, Friberg M, Ivey C, Hu Y, Mulholland J, Russell A, Strickland M, Chang H (2013) Temporally and spatially resolved air pollution in Georgia using fused ambient monitoring data and chemical transport model results. In: NATO/SPS international technical meeting on air pollution modelling and its application, Miami
15. US EPA (2011) The benefits and costs of the Clean Air Act from 1990 to 2020. US EPA, Washington, DC
16. Yang YJ, Wilkinson JG, Russell AG (1997) Fast, direct sensitivity analysis of multidimensional photochemical models. Environ Sci Technol 31(10):2859–2868

Questions and Answers

Questioner Name: Heinke Schlunzen

Q: Is the outdoor air quality really relevant for epidemiology and human health since most people spend most of their time indoors?

A: While much of the time is spent indoors, the air indoors is strongly impacted by outdoor air. Epidemiologic studies continue to find associations between outdoor air quality and health. The Global Burden of Disease study finds ambient PM exposure to be one of the top ten contributors to premature death. Exposure to outdoor air continues to be a serious, and apparently growing, contributor to adverse health outcomes.

Questioner Name: Clemens Mensink

Q: You focus on source impacts on health. The fact is that it's difficult to obtain statistical significant results. Does that say something about the relevance of background conditions.?

A: Background concentrations are relevant, but multiple epidemiological, animal and mechanistic studies strongly support that air pollution, above the background, has a significant impact on health. It is true that any one study may not (many are) be statistically significant, but that is due not only to the influence of background concentrations, but other confounders and small sample sizes. Using models to isolate source impacts can help identify which sources and components of the air pollution mixture are of greatest concern and then help direct control efforts.

Questioner Name: Stefano Galmarini

Q: Did you consider the non-independence of your modeling tools and that the results cluster about the truth may be accidental?

A: First, the ensembled methods have a variety of different inputs, and while some are less independent than others (e.g., PMF and CMB-LGO that use similar, but not the same inputs), others use rather different inputs, e.g., CMB-molecular markers is driven by detailed organic chemical speciation that is not used in PMF or CMB-LGO, and CMAQ does not use observations at all, except for initialization, which has little impact on the simulated values during the modeled period. Still, we were concerned about demonstrating that the ensemble results are an improvement over any one method because you can not measure source impacts directly. To provide further support, we took independent data for water soluble organic compounds (WSOC) that can be used as a marker for SOA, and levoglucosan (though for a period not used in the ensemble development), and compared the ensemble results to those, and found better agreement than any one method.