USE OF INVERSE MODELING IN AIR QUALITY MANAGEMENT

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USE OF INVERSE MODELING IN AIR QUALITY MANAGEMENT

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In the name of Allah,
the Merciful, the Compassionate

To my parents and brother

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LIST OF SYMBOLS AND ABBREVIATIONS

Anthropogenic Volatile Organic Compounds	AVOC
AQM	Air Quality Models
CAIR	Clean Air Interstate Rule
CMAQ	Community Multiscale Air Quality model
CV	Compensating Variation
DDM-3D	Direct Decoupled method in three dimensions
FAQs	Fall Line Air Quality Study
LPO_3	Locally produced ozone concentrations
MB	Marginal Costs
MC	Marginal Benefits
NAAQS	National Ambient Air Quality Standards
NH_3	Ammonia
NO_x	Oxides of nitrogen
$PM_{2.5}$	Particulate Matter with aerodynamic diameter of less than 2.5microns
ppb	Part per billion
ppm	Part per million
Q	Level of desired air quality
SIP	State Implementation Plan
SMARTRAQ	Strategies for Metropolitan Atlanta's Regional Transportation and Air Quality
SO_2	Sulfur dioxide
SOA	Secondary Organic Aerosol
U.S EPA	United States Environmental Protection Agency

SUMMARY

Inverse modeling has been used in the past to constrain atmospheric model parameters, particularly emission estimates, based upon ambient measurements. Here, inverse modeling is applied to air quality planning by calculating how emissions should change to achieve desired reduction in air pollutants. Specifically, emissions of nitrogen oxides (NO_x = NO + NO_2) are adjusted to achieve reductions in tropospheric ozone, a respiratory irritant, during an historic episode of elevated concentrations in urban Atlanta, GA. Understanding how emissions should change in aggregate without specifying discrete abatement options is particularly applicable to long-term and regional air pollution management. Using a cost/benefit approach, desired reductions in ozone concentrations are found for a future population in Atlanta, GA. The inverse method is applied to find NO_x emission adjustments to reach this desired reduction in air pollution. An example of how emissions adjustments may aid the planning process in two neighborhoods is demonstrated using urban form indicators from a land use and transportation database. Implications of this method on establishing regional and market-based air quality management systems in light of recent legal decisions are also discussed.

Both ozone and secondary particulate matter with diameters of less than 2.5μm ($PM_{2.5}$) are formed in the atmosphere from common precursor species. Recent assessments of air quality management policies have stressed the need for pollutant abatement strategies addressing these mutual sources. The relative contribution of several important precursor species (NO_x, sulfur dioxide, ammonia, and anthropogenic volatile

organic compounds) to the formation of ozone and secondary $PM_{2.5}$ in Atlanta during May 2007–April 2008 is simulated using CMAQ/DDM-3D. This sensitivity analysis is then used to find adjustments in emissions of precursor species to achieve goal reductions for both ozone and secondary $PM_{2.5}$ during a summertime episode of elevated concentrations. A discussion of the implications of these controls on air pollutant concentrations during the remaining year follows.

CHAPTER 1

INTRODUCTION

1.1 Overview of air quality management in the United States

The Clean Air Act gives the United States Environmental Protection Agency (U.S. EPA) the responsibility to set National Ambient Air Quality Standards (NAAQS) to promote public health and protect ecological and environmental well being (42 U.S.C. §7409). Metropolitan areas with air pollution concentrations above the NAAQS are classified as non-attainment areas. Under the Clean Air Act, states or tribal lands with non-attainment areas are required to develop State or Tribal Implementation Plans (hereafter referred in short as SIP). These plans contain three elements (NRC 2004):

- An inventory of major emission sources of air pollution in the non-attainment area
- An analysis using air quality models and observation studies to find the required reductions in emissions needed to bring the non-attainment area into compliance with the NAAQS within the Clean Air Act's deadlines
- Specific emission control measures which will be implemented

The success of the SIP framework has been mixed. The number of nonattainment areas for lead, sulfur dioxide, carbon monoxide and nitrogen dioxide has been greatly reduced, and national averages of air pollution concentrations in nonattainment areas have decreased. However, the SIP process has not been as successful in areas with severe

ozone and particulate matter concentrations (U.S. Environmental Protection Agency 2003).

In their critical discussion of the SIP process, the National Research Council of the National Academies (2004) criticized how air quality models are used to demonstrate attainment of the NAAQS (in bullet point two of the list above). Though they noted that air quality models are vital in finding the magnitude of emissions reductions that are necessary to attain the standards, they found state agencies too often base air quality attainment demonstrations on a "one-time robust prediction of how air quality in a given areas will evolve over a multiple-year or decadal time scale and does not take into account the significant modeling, socioeconomic, and control-technology uncertainties implicit in such a process" (NRC 2004). The National Research Council proposed replacing the existing SIP process with an integrative approach which would allow state and local agencies to update air quality management plans on an ongoing basis. In such a system, air quality modeling is separated from emission control strategy design. Air quality modeling is used only to find emission reduction targets that achieve air quality goals without specifying emission growth or control methods. Knowing the amount of emission changes needed, agencies can then design and implement emission abatement strategies based upon current socioeconomic conditions and available control methods. In this thesis, a method is developed for finding emission reduction targets and applied to several current problems in air quality management.

1.2 Inverse Air Quality Modeling for Air Quality Management

Variables such as population and economic growth, changes in social and cultural norms, advances in technology, and the whims of local, national and global politics are but a few of the unpredictable factors that will affect future air quality. A typical forecasting approach in the development of a SIP would require one to predict changes in the independent variables—e.g. population, vehicle miles of travel, and energy production—to predict the dependent variable, air quality. By defining a desired air quality goal and using an inverse approach, we can identify the minimum changes in emissions needed, relative to the present, to achieve the established outcome. In so doing, the air quality objective becomes the independent variable, and the factors required to achieve the goal are derived from the variable.

"Desired air quality" is a subjective value. Stakeholders ranging from the mothers of asthmatic children to business executives and their stockholders all have their own concept of desired air quality. Rather than requiring consensus *a priori*, multiple levels of air pollution may be modeled and the required emissions changes can inform these stakeholders as they participate in the policy debate on air quality management strategies. Application of this method allows planners to shift their focus from the details of forecasting future emissions growth to the management of ongoing emissions growth.

1.3 Scope

In this thesis, inverse modeling is applied to a variety of concerns in current air quality management. First, I apply inverse methods to a case study in Atlanta, GA exploring how a range of desired air quality levels will affect how emissions are adjusted.

The inverse model is then applied in a long term air quality planning framework. Discussions on how to estimate future desires of air pollution and how urban planning may be leveraged to achieve air quality goals is included. Inverse modeling is used to find emission adjustments which can be used to address concerns on recently proposed regional emissions trading programs (Tong and Mauzerall 2008; D.C. Cir. 2008). Understanding and addressing the effects of emissions on multiple pollutants is seen as a critical next step in air quality management (NRC 2004; U.S. Environmental Protection Agency 2008). I conducted an inter-seasonal study of the response of ambient pollutants to common precursors, and investigated how multiple pollutants may be controlled using a single emissions abatement plan by applying inverse modeling.

The thesis is organized as follows:

Chapter 2: An inverse modeling approach to air quality planning. Air quality modeling is used to find the most effective control strategies to reach compliance with air quality standards. The typical modeling approach is extended using inverse methods to estimate the minimum change in emissions needed to achieve a desired air quality goal. The inverse method is described and applied to the management of NO_x emissions to reduce concentrations during an historical high ozone episode in Atlanta, GA.

Chapter 3: A method to prescribe air quality in 2050: Optimizing air pollutant emissions towards long-term air quality goals. An economic cost benefit analysis is used to predict the desired air quality level of a future population in Atlanta, GA. Minimum adjustments to current emissions to achieve this desired air quality level are

calculated using inverse modeling techniques. I discuss how these adjustments may inform the decisions on the urban form of two neighborhoods.

Chapter 4: Application of inverse modeling in regional trading programs: Cost optimization of future growth. To address air pollution in the eastern United States, the Environmental Protection Agency recently proposed a regional emissions cap-and-trade system, Clean Air Interstate Rule (CAIR). However, the U.S. Appeals Court for the District of Columbia ruled that the EPA's implementation of the CAIR did not meet the requirements of the Clean Air Act. Inverse methods are used to address these concerns by developing emission allocations for states based upon their downwind effects during an August 1999 episode. Two emission allocation cases are presented; one solely based upon interstate transport of pollutants and the other weighted by the costs for emission reductions in each state.

Chapter 5: Multiple Pollutant Responses from Multi-Seasonal Emission Controls. Both ozone and secondary particulate matter are formed in the atmosphere from common precursor species. To understand the response of emission controls on these pollutants, sensitivity modeling was conducted for a full year (May 2007-April 2008) in Atlanta, GA. Inverse modeling is used to find a common emission abatement strategy to reduce ozone and secondary particulate matter for a summertime period of elevated air pollution. The effect of these controls in other seasons is evaluated.

Chapter 6: Conclusions and future work

1.4 References

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CHAPTER 2

USE OF INVERSE MODELING IN AIR QUALITY PLANNING

2.1 Introduction

The Clean Air Act requires states, air quality management districts, and tribes to create plans for addressing air pollution in areas that fail to meet the National Ambient Air Quality Standards (NAAQS) (42 UCS 7410). To aid in developing plans to meet these standards, the United States Environmental Protection Agency (U.S. EPA) provides modeling guidance that describes the acceptable use of emissions based air quality modeling for testing strategies and for demonstrating attainment of the NAAQS (U.S. Environmental Protection Agency 1997; U.S. Environmental Protection Agency 1999). Beyond the basic approach outlined by the U.S. EPA, some have applied air quality modeling to conduct a sensitivity analysis to determine the response of ambient air pollution to emissions abatement options (Liu and Trb 2003; Cohan, Hakami et al. 2005; Chestnut, Mills et al. 2006; Cohan, Tian et al. 2006; Cohan, Boylan et al. 2007; Gilliland, Hogrefe et al. 2008). Here, we use a sensitivity analysis in an inverse modeling application to find the minimum emission controls required to achieve a desired air quality level.

In forward applications of atmospheric chemical transport models, parameterizations of emissions, meteorology, and other variables are used to simulate ambient concentrations of pollutants and other constituents of interest. Conversely, in

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inverse applications, the pollutant concentrations determine one or more of the input variables. The inverse methods employed here build upon past work that adjusted emissions rates to minimize the differences between modeled pollutant concentrations and ambient pollutant measurements. In previous studies, inverse methods were used to improve model estimates of regional and global atmospheric gases (Hartley and Prinn 1993; Mulholland and Seinfeld 1995; Chang, Hartley et al. 1996; Gilliland, Dennis et al. 2003) and to quantify errors in emissions inventories (Mendoza-Dominguez and Russell 2000; Hakami, Henze et al. 2005; Napelenok, Pinder et al. 2008) In the application here, a desired air quality outcome replaces ambient pollutant measurements as inputs into the inverse model. The emission changes necessary to achieve the desired air quality outcome are then calculated based upon the simulated chemical and physical transport of pollutants in the atmosphere.

Given how air quality can vary in space and time, determining optimal air quality is challenging under the inverse framework. The model may identify targets for emission reduction for any level of desired air quality, including the NAAQS. In so doing, stakeholders and decision-makers are able to better understand the changes that are required to achieve their desired air quality state. Some of these possibilities are explored herein through a case study application of the method in Atlanta, Georgia.

2.2 Method

2.2.1 The Iterative-Inverse Model

Mendoza-Dominguez and Russell (2000; Mendoza-Dominguez and Russell 2001) used a hybrid forward/inverse model to calculate corrections for emission inventories in Atlanta, GA. Our method follows a similar approach here, alternating between an

emissions based-forward model which simulates concentrations and sensitivities and an inverse method which calculates adjustments to the emissions inputs to minimize the difference between the simulated concentrations and the desired levels. The iterative process repeats until simulated pollutant concentrations sufficiently agree with the desired goal. A diagram of the procedure is shown in Figure 2.1. The emissions-based modeling application is described below and followed by a derivation of the inverse method.

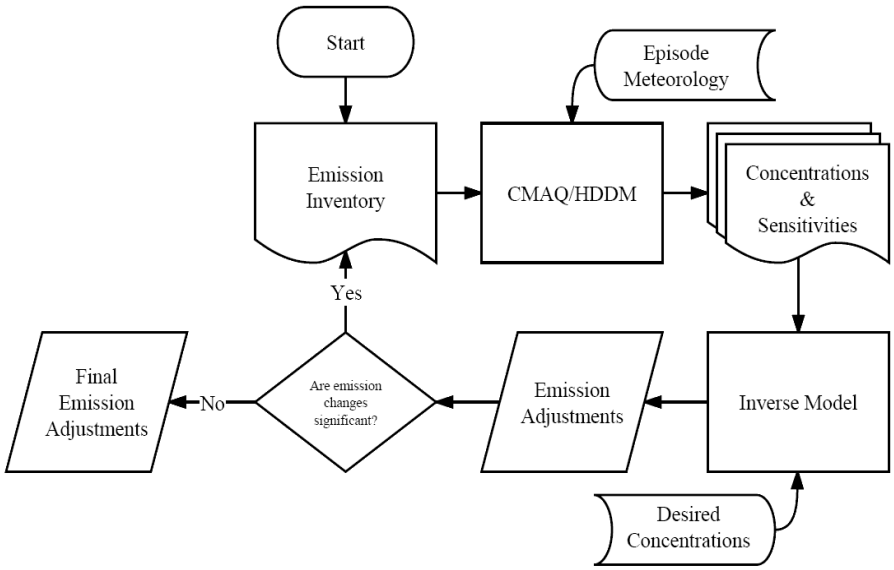

Figure 2.1: Hybrid model schematic. First, the initial concentration and sensitivities are found for the base case. These files are then read into the inverse model and initial adjustments to the emission inventory are found. These adjustments are applied to the emission files, and CMAQ/DDM-3D is rerun to calculate new concentrations and sensitivities. These new concentrations are again compared with the desired concentrations using the inverse method. This process continues to iterate until the predicted change in emission rate is less than 10% of the original emission rate.

2.2.1.1 Description of the Emissions-based Model Application

In the forward modeling step, an emissions based model is used to simulate pollutant concentrations and calculate pollutant sensitivities used in the inverse method. Sensitivities describe the change in pollutant concentrations due to a change in precursor emissions. In past inverse method applications, indirect brute force methods were used to find sensitivities by running the air quality model for two sets of emissions to find the change in concentrations due to the known change in emissions (Cunnold, Prinn et al. 1983; Hartley and Prinn 1993; Mulholland and Seinfeld 1995; Chang, Hartley et al. 1996; Chang, Hartley et al. 1997; Gilliland and Abbitt 2001; Gilliland, Dennis et al. 2003). Here, the sensitivities are calculated using the Direct, Decoupled Method in three dimensions (DDM-3D) which directly calculates sensitivities using the chemistry and transport equations of the air quality model. Sensitivities calculated using DDM-3D have been shown to be comparable with indirect brute force methods even as the calculation time for the sensitivity of multiple pollutant/source relationships requires less computational time (Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006).

The Community Multiscale Air Quality model extended by the Direct Decoupled Method in three Dimensions (CMAQ/DDM-3D) (Cohan, Hakami et al. 2005; Byun and Schere 2006; Napelenok, Cohan et al. 2006) is applied for an historical episode of elevated ozone concentrations, August 3-8, 1999, on a 4km domain covering the 13-county Atlanta, GA metropolitan area (Figure 2.2). The base emissions inventory and meteorological modeling were undertaken as a part of the Fall Line Air Quality Study and is extensively documented elsewhere (Chang 2004). The first 36 hours of the simulation is discarded to reduce the impact of initial concentrations after emission

adjustments. The inverse method is programmed in Matlab (The Mathworks 2007) and directly imports the concentrations and sensitivities from the CMAQ-DDM output files using the SNCTools and Mexnc tools (Evans 2007).

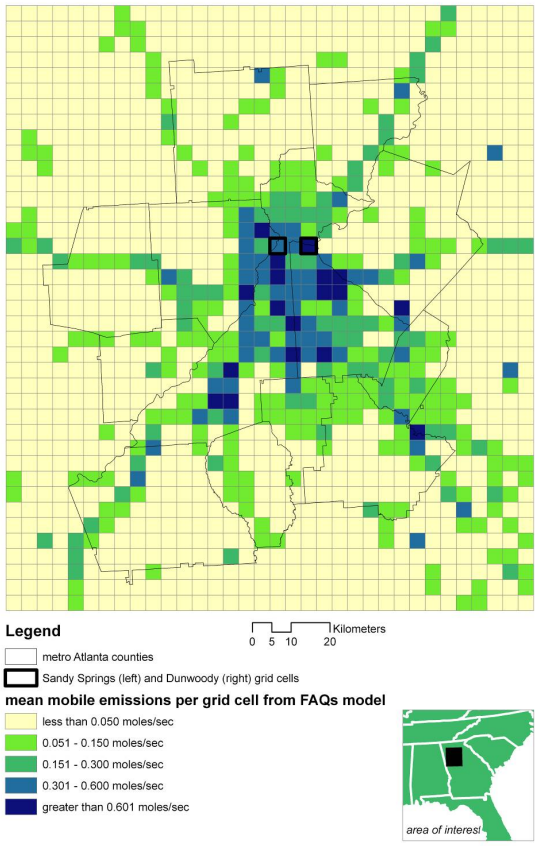

Figure 2.2: Mean mobile source NO_x emissions in the 4km modeling domain. The county lines represent the 13-county Atlanta1999 ozone nonattainment area. Map courtesy of Ann Carpenter.

2.2.1.2 Derivation of the Inverse Method

We begin our derivation of the inverse method by describing the relationship between precursor emissions and pollutant concentrations. Conceptually, concentrations of atmospheric species are a function of meteorology and emissions. For a modeled meteorological episode, the relationship between concentrations and emissions may be approximated in its simplest form by a linear function using a sensitivity parameter, *S*. Using the calculated sensitivities from the forward modeling step, we approximate the concentration species *i* at receptor *r* after a perturbation in emissions of species *j* from source type and location defined by parameter *p* by the first-order Taylor series (time indices are dropped for convenience):

$$C_{i,r}^{k+1} = C_{i,r}^{k} + S_{E_{j,p}}^{i,r,k} \cdot \Delta E_{j,p}^{k} + \delta_{i,r}^{k} \quad (2.1)$$

$where$:

$C_{i,r}^{k+1}$ = *estimated concentration of species i at receptor r after perturbation in emissions of species j from source parameter p*

$C_{i,r}^{k}$ = *initial concentration of species i at receptor j for iteration k*

$E_{j,p}^{k}$ = *emissions of precursor species j from source parameter p for iteration k*

$S_{\Delta E_{j,p}}^{i,r,k} = {\partial C_{i,r}}/{\partial E_{j,p}}$ = *change in* $C_{i,r}^{k}$ *due to a perturbation in* $E_{j,p}^{k}$

$\delta_{i,r}^{k}$ = *residual error of the linear approximation*

For small changes in emissions, the linear approximation using DDM-3D sensitivities is assumed to accurately model the effects of emission changes on air pollutants (Cohan, Hakami et al. 2005). The magnitude and spatial distribution of the sensitivity parameters change as emissions sources are adjusted. Since sensitivities used

in the inverse method are recalculated using DDM-3D during the forward modeling portion of the iteration, nonlinear relationships between precursor emissions and pollutant concentrations are captured (Mendoza-Dominguez and Russell 2000). Therefore, the residual error from Equation 2.1 is dropped, i.e. $\delta_{i,r}^{k} = 0$.

While the spatial and temporal distribution of emissions will likely change over time, in the near term, the spatial change in emissions will be limited by the cost of replacing existing infrastructure. The problem is the opposite in the long-term; the number of possible emission scenarios is limitless or, at least, difficult to constrain beyond basic physical limits. To constrain emissions for these cases and to maintain the linear assumption of Equation 2.1, future emissions are assumed to be a scaled product of current emission rates. The emissions adjustment factor for a species *j* from a source parameter *p* is defined as $\chi_{j,p}$.

The sensitivity term, *S*, in Equation 2.1 is defined in terms of the change in pollutant concentration due to a small perturbation in the emissions strength of the parameter. *S* can be put into terms of χ by multiplying *S* by the total emissions strength, E, from the source parameter:

$$S_{E_{j,p}}^{i,r,k} \cdot E_{j,p}^{k} = \frac{\Delta C_{i,r}^{k}}{\Delta E_{j,p}^{k} / E_{j,p}^{k}} = \frac{\Delta C_{i,r}^{k}}{\chi_{j,p}} = P_{E_{j,p}}^{i,r,k} \tag{2.2}$$

where:

$P_{E_{j,p}}^{i,r,k}$*= sensitivity of the concentration of species i at receptor r to a percent change in emissions of species j from parameter p*

$\chi_{j,p} = \Delta E_{j,p}^{k} / E_{j,p}^{k}$*= unitless emissions adjustment factor for species j from parameter p*

The scaled sensitivity term *P* may be seen as the contribution to the pollutant concentration at a receptor due to χ percent of emissions from a source parameter. Equation 2.1 may be then rewritten in terms of a relative change in emissions from the base case emissions (with terms as defined above):

$$C_{i,r}^{k+1} = C_{i,r}^{k} + P_{E_{j,p}}^{i,r} \cdot \chi_{j,p} \tag{2.3}$$

The minimal percent changes in the emissions, $\chi_{j,p}$, in order to achieve a desired air quality distribution are found using a weighted least squares method. First, the simulated concentrations, $C_{i,r}^{k+1}$, from Equation 2.3 can be compared with the desired concentrations:

$$C_{i,r}^{desired} = C_{i,r}^{k+1} + \varepsilon_{i,r}^{k} = C_{i,r}^{k} + P_{E_{j,p}}^{i,r} \cdot \chi_{j,p} + \varepsilon_{i,r}^{k} \tag{2.4}$$

where:

$C_{i,r}^{desired}$*= the desired concentration of species i at receptor r after emission control*

$\varepsilon_{i,r}^{k}$ *= difference between estimated concentrations,* $C_{i,r}^{k+1}$*, and desired concentration*

The number of source parameters is limited by the computational cost of calculating sensitivities. Since the number of receptors is only limited by the number of simulated grid cells and the definition of the desired concentrations, the inverse problem outlined here is highly over-determined (i.e. the error between the simulated and desired concentrations at each receptor cannot be brought into perfect agreement by adjusting the emission strengths of the source parameters) (Mendoza-Dominguez and Russell 2000). Instead, the error between the simulated and desired concentrations is minimized while keeping the size of the emission adjustments within a physically meaningful range. We use a weighted least squares method to find a solution for the two unknown variables in

Equation 2.4 ($\varepsilon_{i,r}$and$\chi_{j,p}$). The following weighted least squares cost function, J, is written for these variables in matrix form (Mendoza-Dominguez and Russell 2000):

$$\boldsymbol{J = \mathbf{x}_{k+1}^{T} \mathbf{W}_x \mathbf{x}_{k+1} + \mathbf{e}_k^{T} \mathbf{W}_e \mathbf{e}_k} \quad (2.5)$$

where:

$\mathbf{x}_{k+1}^{T} = \left[\chi_1^{k+1} \ldots \chi_p^{k+1}\right]$ = *vector of emission adjustment factors*

$\mathbf{e}_k^{T} = \left[\varepsilon_{i,1}^{k} \ldots \varepsilon_{i,r}^{k}\right]$ = *vector of differences between modeled and desired concentrations*

$\mathbf{W_x}$ = *weighting matrix of the scaling factors*

$\mathbf{W_e}$ = *weighting matrix of the modeled differences*

This function is minimized when $\partial J / \partial \chi = 0$ and may be reduced using Equation 2.4 to (Mendoza-Dominguez and Russell 2000):

$$\mathbf{x_{k+1}} = (\mathbf{P_k^T W_x P_k} + \mathbf{W_e})^{-1} \mathbf{P_k^T W_x e_k} \quad (2.6)$$

where:

$\mathbf{P_k} = \begin{bmatrix} P_{E_{j,1}}^{i,1,k} & \cdots & P_{E_{j,p}}^{i,1,k} \\ \vdots & \ddots & \vdots \\ P_{E_{j,1}}^{i,r,k} & \cdots & P_{E_{j,p}}^{i,r,k} \end{bmatrix}$ = *matrix of sensitivity at each receptor to emissions from each parameter*

Estimates of $\mathbf{x_{k+1}}$ found using Equation 2.6 are used to scale the emission inputs into the next forward model simulation of the concentrations and sensitivities (See section 2.2.1.3 for a description of the iterative process).

The weighting matrix of the adjustment factors, $\mathbf{W_x}$, controls the degree to which the emissions from a certain source may vary. For example, if a source cannot be changed, then $\mathbf{W_x} = \mathbf{0}$, and inverse optimization equation is reduced to $\mathbf{x_{k+1}} = \mathbf{0}$ (Welch 2004). By setting relative weights between source parameters, sources that are unlikely to change may be held relatively constant and others which are foreseen to have high

variability in future emissions may be allowed to change freely. Additionally, physical, social and economic constraints may be included in this weighting system. For example, in the case for a large point source such as a power plant, this weighting matrix may be used to limit the emission adjustments to the amount of reductions expected from available controls.

In our application, this matrix is used to ensure that the emission adjustment factors are within an acceptable range of values. Two sets of criteria define the acceptable range for the adjustment factors. First, emissions must remain within expected limitations of possible emission changes. For the application here, the upper limit of this range is the current emissions rate, i.e. emissions are not allowed to increase from current levels. The lower limit for this range is zero, as negative sources have no physical meaning. The second set of criteria is designed to uphold the linearity assumption of Equation 2.1. In the results shown here, sources are not allowed to change by more than ±30% in a single iteration, the range for which our assumption of linear sensitivities is valid (Cohan, Hakami et al. 2005). In tests, larger ranges proved to be unstable. Initially, the $\mathbf{W_x}$ matrix is set to weight each source parameter equally and independently. If an adjustment factor for a source is predicted to be outside the acceptable range, the corresponding term in the weighting matrix for that source is reduced. This correction inhibits changes to the source parameter relative to changes in the other sources. This process is repeated until all the scaling factors fall within the acceptable range.

The second weighting matrix**,** $\mathbf{W_e}$, governs the degree of agreement between the desired concentrations and the simulated concentrations. In the case of desired concentrations, the matrix allows for ambiguity in the future populations' desired air

quality. Without this factor, the inversion may become unstable if there is perfect agreement to the desired air quality concentrations ($\mathbf{W_e} = \mathbf{0}$). In this situation, the optimization equation is reduced to the simple case $\mathbf{x_{k+1}} = \mathbf{P_k e_k}$ (Welch 2004). Under such assumptions, the $\mathbf{W_x}$ matrix is also dropped leading to no control over **x** and the inversion may predict unrealistic changes in emissions. Here, given how the desired concentrations are defined (See Section 2.2.2), the $\mathbf{W_e}$ matrix is constant for all receptors.

2.2.1.3 Iterative Procedure

The initial emission adjustments are found by setting $\mathbf{e_k}$ to the difference between the base concentrations and the desired concentrations. In each subsequent iteration, emission adjustments are applied to the CMAQ emission files, and the model is run to simulate new concentrations and sensitivities (Figure 2.1). As emissions are adjusted and the difference between the simulated and the desired concentrations is reduced, the change in emissions decreases. Iterations stop once the amount of predicted change in emissions from an iteration is less than 10% of the total initial emissions from the parameter, i.e. $\mathbf{x_{k+1}^T E_{j,p}^k} < (0.1)\mathbf{E_{j,p}^0}$.

2.2.2 Desired Air Quality

Reducing concentrations of tropospheric ozone, a respiratory irritant, is a challenging problem for air quality managers since it is not emitted directly from pollution sources but rather formed in the atmosphere from precursor emissions, primarily oxides of nitrogen ($NO + NO_2 = NO_x$) and volatile organic compounds (VOC) (Haagen-Smit 1952). The primary method for controlling regional ozone concentrations

in the Atlanta area has been demonstrated to be through the control of NO_x emissions (Chameides, Lindsay et al. 1988) though VOC control strategies may be effective for reducing ozone in some areas (Cohan 2004; Zavala, Lei et al. 2009),

A relative change in simulated ozone concentrations during an historical episode of elevated concentrations, C^0, is the basis for estimating the future desired air quality in the application shown here. The desired future concentrations are a scaled percent change, λ, from C^0:

$$C_{i,r}^{desired} = \lambda C_{i,r}^{0} \tag{2.7}$$

where:

λ = *the desired percent change from base case concentrations*

Here, a series of λ levels (10%, 15%, and 25%) are modeled. Grid cells with 8 hour average ozone concentrations above a threshold value, 0.06ppm, are defined as receptor cells. The receptor cells are found at every iteration after new concentrations are modeled by CMAQ/DDM-3D. The impact of the threshold value on adjusted emissions is discussed in Chapter 4.

One important consideration is the transport of ozone into the domain. The domain closely outlines the urbanized area of Atlanta (Figure 2.2), and there are significant regional sources which impact ozone concentrations inside this region. However, as only emission sources within this domain are optimized by the inverse method, ozone from these regional sources is removed in this analysis. DDM-3D was used to find the sensitivity of ozone within the domain to transport from the boundary. Locally produced ozone concentrations (LPO_3) are calculated by subtracting this sensitivity from simulated ozone concentrations. Based upon the sensitivity analysis of

ozone concentrations to ozone transported from the boundary, LPO_3 concentrations in Atlanta are approximately 70% of total ozone concentrations on average.

2.2.3 Emission source parameters

Sensitivities modeled in DDM-3D describe the response of an air pollutant to emissions from a source parameter. Emission source parameters are defined by the chemical species, a source category from the emissions inventory and a region of the model domain. Four source categories are defined (U.S. Environmental Protection Agency 2008): Point, Area, Mobile, and Non-road sources. Point sources are large stationary sources that are explicitly included in the emissions inventory by name and location. They include large industrial facilities and electrical generating units. Area sources are small stationary sources that are not explicitly included in the emissions inventory as point sources. Area sources also include diffuse sources such as wildfires and prescribed burning. Mobile sources include licensed, on-road gasoline and diesel vehicles. All other vehicular sources, including construction equipment, which are not considered as a part of the mobile source category are included as non-road sources. As noted above in the application here only NO_x sources are considered. Since the majority of the mobile NO_x emissions occur in the 13-county 1999 Atlanta ozone non-attainment region (Figure 2.2), they are included in the inverse model separately from the remaining mobile source emissions. Parameters were defined for the three remaining source categories for domain-wide NO_x emissions.

2.3 Results

To test whether the sensitivity analysis and concentration modeling in CMAQ/DDM-3D reproduces a unique response for a given change in air pollution, we performed a pseudo-data test (Hartley and Prinn 1993; Chang, Hartley et al. 1997; Mendoza-Dominguez and Russell 2000; Gilliland and Abbitt 2001). We generated pseudo-data by running the transport model with a specified perturbation of emissions. These pseudo-data were taken as the desired air quality concentrations, and the inverse method was tested to see if the resulting changes to the emission inventory were equal to the initial perturbation used to generate the pseudo-data. Since the pseudo-data were directly generated from the transport model, any discrepancy between the inverse method adjustment factors and those used to generate the pseudo-data would indicate errors from the CMAQ/DDM-3D model (Chang, Hartley et al. 1997). The five source parameters were scaled by random amounts to generate the pseudo-data. Within three iterations, the inverse model produced adjustment factors closely resembling those used to generate the goal concentrations (Table 2.1).

Table 2.1: Cumulative percent change in emissions from each iteration for the pseudo data case. The inverse procedure the adjustment factors closely resembles the initial perturbations to the emissions inventory used to generate the pseudodata. This result indicates that the errors from the linear approximations of the model based upon the CMAQ/DDM modeling do not prohibit finding a unique solution.

Iteration	Mobile Sources 13 counties	Mobile Sources Outside of 13 counties	Area Sources Whole Domain	Nonroad Sources Whole Domain	Point Sources Whole Domain
1	74.13%	84.78%	77.20%	77.35%	80.97%
2	72.17%	85.98%	88.67%	75.28%	82.96%
3	72.01%	86.00%	89.86%	75.04%	83.00%
Goal	72.00%	86.00%	90.00%	75.00%	83.00%

With the pseudo-data validation of the model complete, the iterative inverse model was run for goal cases of 10%, 15%, and 25% reductions in ozone concentrations using the iterative inverse model. The adjustment factors resulting from each reduction case are listed in Table 2.2. In the 10% and 15% cases, reductions in area and point source emissions exceeded 50%. For each of the cases, we found increasing reductions of mobile source emissions from within the 13-county region, ranging from 29.8% in the 10% case to 66.1% in the 25% case. Mobile sources outside the 13-county region and nonroad emissions were relatively unchanged for the 10% and 15% cases. In the 25% case, all source parameters were reduced by more than 50%.

Non-road sources are reduced by less than 1% in the 10% and 15% reduction cases. The Atlanta Hartsfield-Jackson Airport dominates emissions in this category and is located directly upwind of the main ozone plume during the modeled episode. Within the plume, ozone concentrations are VOC-limited. That is, ozone concentrations are dependent on the products of VOC oxidation. Since reducing NO_x concentrations would result in more VOC oxidation, the sensitivities of ozone to NO_x emissions are negative in

Table 2.2: Results for the test cases. Cumulative scaling factors are given for the final change in emissions from the optimization plan.

Goal Percent Reduction	Cumulative Percent Reduction in Emissions					Number of receptor grid cells[a]		Average Concentration[b] (ppb)			Root mean squared error[b] (ppb)	
--	Mobile, 13-county region[c]	Mobile, outside 13-county region	Area, whole domain	Nonroad, whole domain	Point, whole domain	Base	Optimized	Base	Optimized	Goal	Base	Optimized
10%	29.8%	15.4%	58.6%	0.5%	57.1%	6501	3828	66.83	60.97	60.15	6.7	2.1
15%	47.5%	9.7%	58.1%	0.7%	75.8%	6501	2629	66.83	57.18	56.80	10.0	2.5
25%	66.1%	59.7%	64.3%	54.2%	65.0%	6501	700	66.83	48.39	50.12	16.7	3.1

[a] – Defined as cells with LPO_3 greater than with concentrations greater than 60ppbv

[b] – Given for base case receptors with optimized concentrations greater than goal concentrations

[c] – Cherokee, Clayton, Cobb, Coweta, Dekalb, Douglas, Fayette, Forsyth, Fulton, Gwinnett, Henry, Paulding, Rockdale

these regions. With negative sensitivities, the inverse calculation attempts to increase emissions of NO_x to achieve the desired ozone concentration reductions. However, since an increase in emissions is not allowed by our *a priori* assumptions, the weighting value in the $\mathbf{W_x}$ matrix corresponding to the non-road source is reduced to near zero, and the final inverse optimization did not reduce emissions in this category. However, in the 25% reduction case, the plume of NO_x and ozone were reduced enough for the ozone to become NO_x limited and non-road sources were accordingly adjusted.

Increased point source emission reductions were the main difference in adjustment factors in the 15% reduction case in comparison with results from the 10% case. With the more equally distributed reductions required by the 25% reduction case, point sources were not as stringently controlled as they were in the 15% case.

Total emissions were reduced in increasing amounts as the percentage of desired concentration reductions increases (37.9%, 50.5%, and 63.3% respectively) (Figure 2.3). Moreover, as NO_x emissions are decreased, ozone concentrations become more sensitive to NO_x. The average sensitivity of LPO_3 to total NO_x emissions for each of the cases was 0.10 ppb LOP_3/ton NO_x, 0.12 ppb LOP_3/ton NO_x, and 0.19 ppb LOP_3/ton NO_x. This indicates that once NO_x emissions are reduced by ~50%, the returns in terms of ozone reduction for additional reductions of NO_x increases.

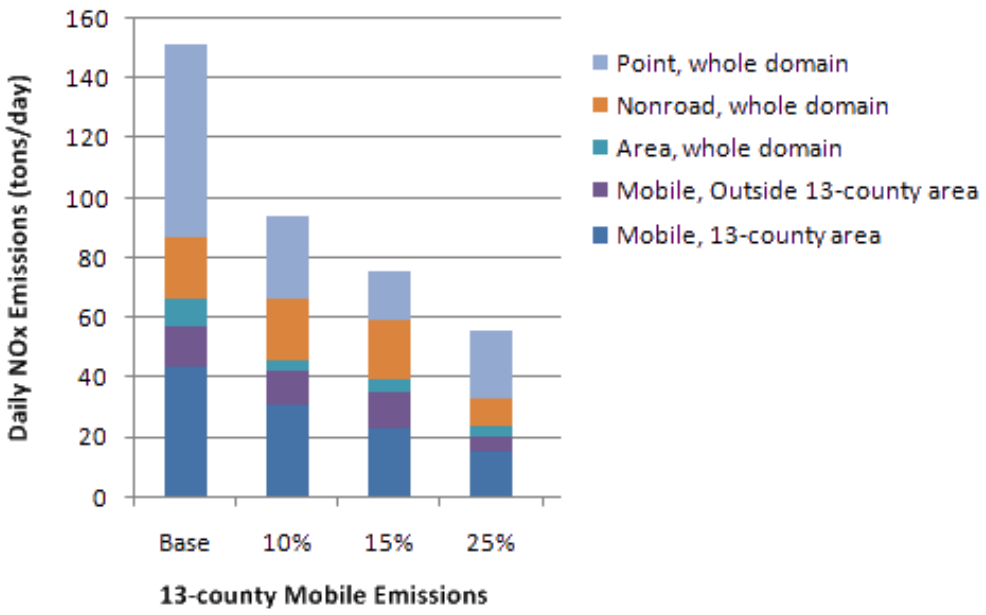

Figure 2.3: Daily NOx emissions for each case. Emissions decrease as the goal reduction case increases.

A measure for the error between the desired and simulated LPO_3 in the base case receptors (i.e. cells with initial concentrations above the threshold value), the overall root mean square error was reduced after the emissions were adjusted (Table 2.2). For all three reduction goals, the hourly average LPO_3 in the base case reduced to the desired concentrations after the emissions were adjusted (Figure 2.4). In the 25% reduction case, the average LPO_3 at these receptors are reduced below the desired LPO_3 since the majority (89%) of the grid cells fall below the 60ppb threshold in the final iteration and are no longer considered as receptors by the inversion calculation (Table 2.2). The inversion included only the higher concentrations in the final iterations, leading to reductions beyond the goal concentrations in receptors with base LPO_3 concentrations close to the threshold value.

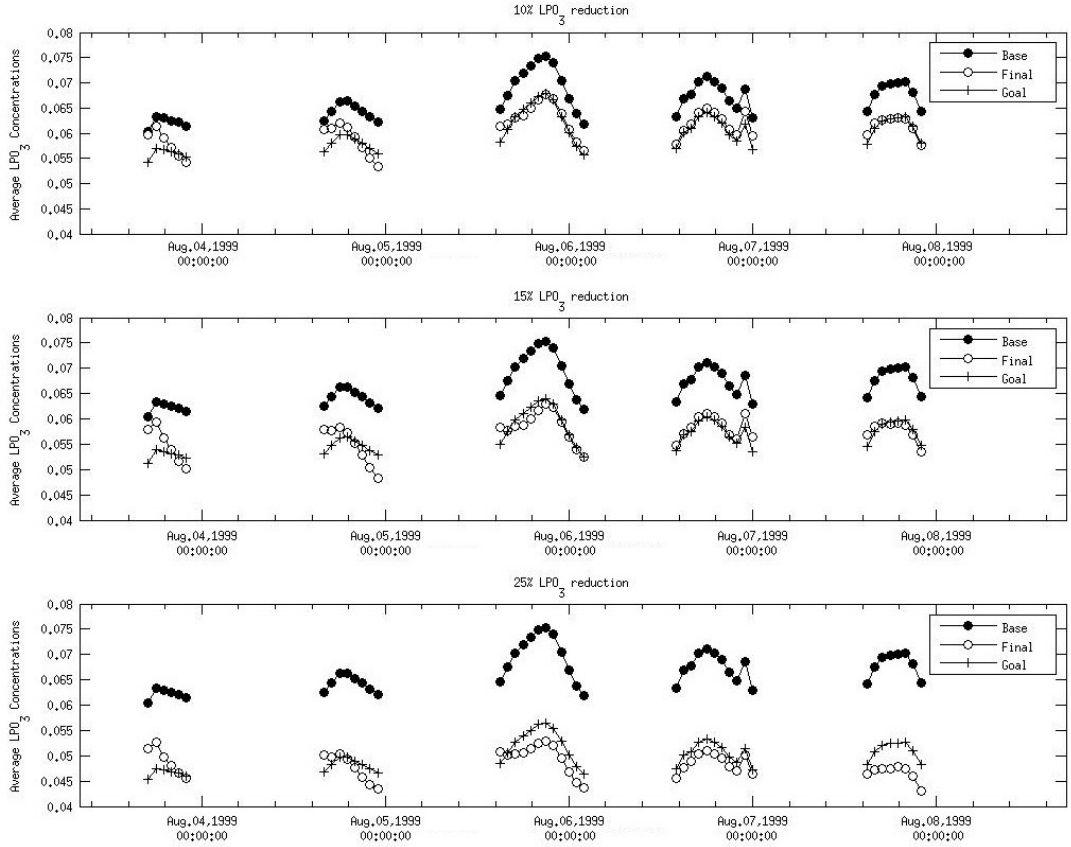

Figure 2.4: Hourly Average 8hr-average LPO_3 Concentrations in grid cells with base concentrations above the threshold level, 0.06ppm. In each case, the final modeled concentrations are nearly reduced to the goal concentrations. As concentrations fall below the threshold value, grid cells are no longer considered in the inversion model though they are included in the averages shown here.

To qualitatively observe the spatial convergence between the optimized and desired LPO_3, the episode peak hour 8 hour LPO_3 are shown in Figure 2.5. Though the spatial distribution of the final iteration simulated LPO_3 and the desired LPO_3 was not identical at each grid cell, on average, the majority of cells showed reductions comparable with the goal concentrations. This is consistent with the expectation of the method reducing the overall error between the simulated and desired concentrations but not achieving a perfect fit.

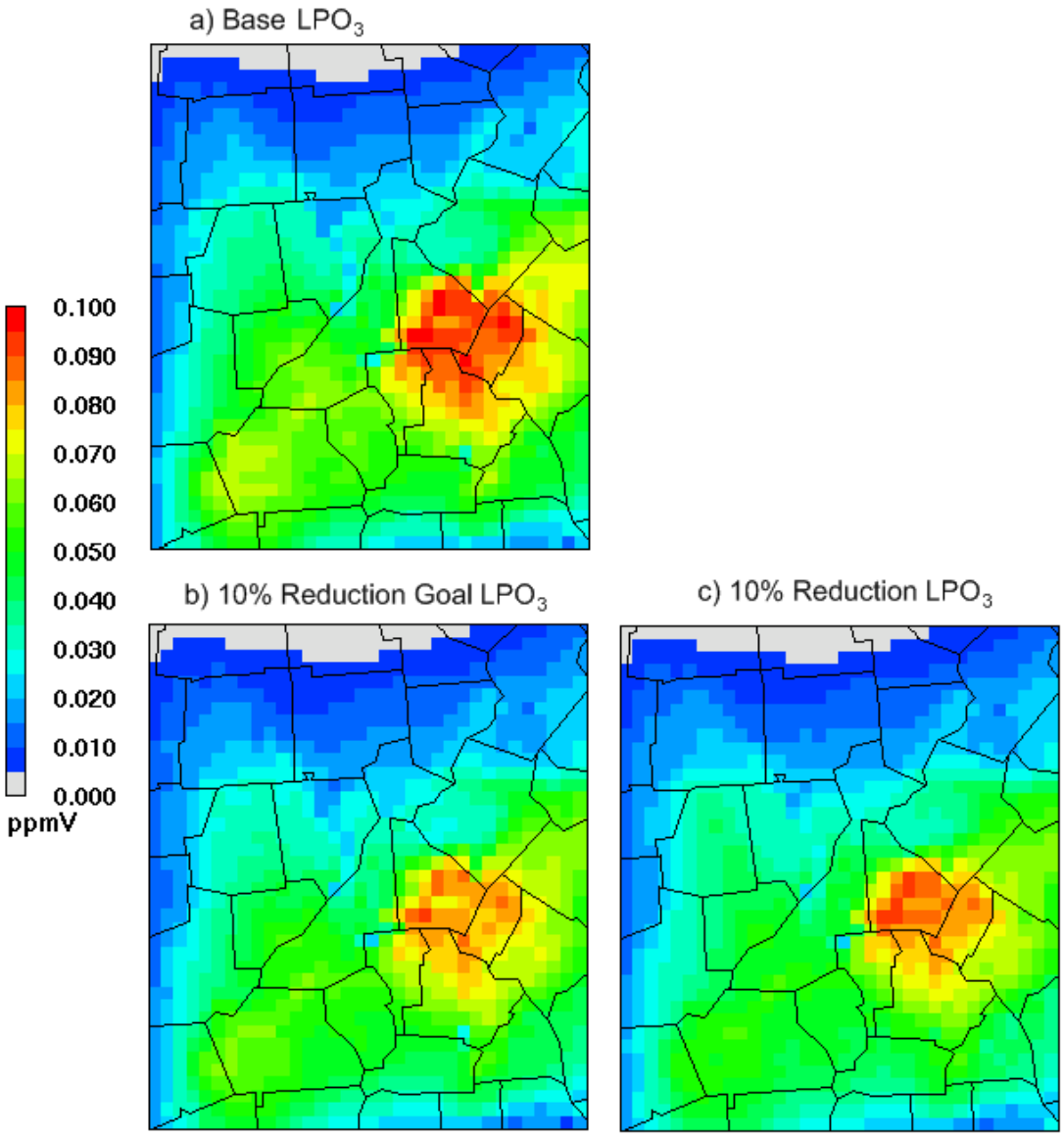

Figure 2.5: Local 8-hour average ozone concentrations at the episode peak hour (20:00 August 5, 1999). Concentrations for each reduction case are optimized to achieve the goal levels (b, d, and f). The optimized results (c, e, and g) are all reduced to levels similar to that of the goal concentrations. Since the emissions are only scaled in quantity and not changed in time and space, the optimized concentrations do not perfectly replicate the goal concentrations which are generated without regard for atmospheric chemistry or transport.

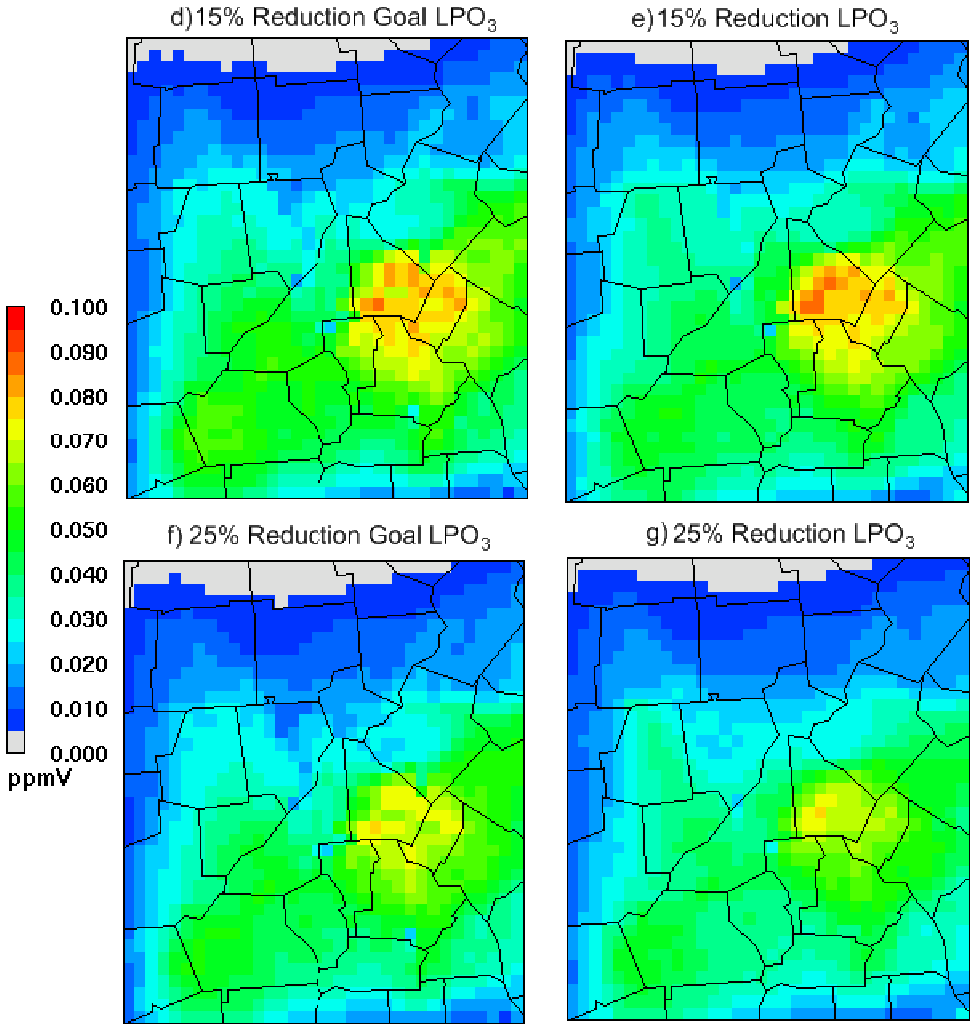

Figure 2.5 continued

2.4 Discussion

The modeling method outlined here was able to find adjustments to emissions that achieve a series of air quality goals. These general emission adjustments provide air quality managers with an understanding of how existing emissions sources should change without specifying emission control options. The method can be applied to a particular representative episode to reveal how emissions should change within a non-attainment area for compliance of the NAAQS. Using emission models that incorporate predictions of emissions growth and the impact of available emission controls, air quality managers can develop emission abatement policies for adjusting emissions to achieve compliance with the NAAQS. Because specific control options are not defined as a part of the air quality modeling process, air quality managers are free to update emission abatement policies as new emission control options become available without having to discretely model the air quality impact of each control option.

The cases modeled here assume NO_x emissions can be selectively removed without reducing emissions of any other species. This is possible with some control technologies, such as catalyst-based emission controls (Heck 1999). Control options such as decreasing vehicle miles traveled or increasing home heating and cooling efficiency, lead to ancillary reductions in other pollutants. The CMAQ-DDM system calculates the sensitivities of all pollutants to emissions of a certain precursor. Emission adjustments may be found using this method that achieves a desired reduction in a mixture of pollutants. Additionally, multiple precursor species can be defined as source parameters and included in this method to find the relative effectiveness of species-specific controls.

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CHAPTER 3

A METHOD TO PRESCRIBE AIR QUALITY IN 2050: OPTIMIZING AIR POLLUTANT EMISSIONS TOWARDS LONG-TERM AIR QUALITY GOALS

3.1 Introduction

Title I of the Clean Air Act specifies a planning and implementation phase for areas failing to meet National Ambient Air Quality Standards that typically spans a time period of 3 to 9 years for all but the most severe or extreme nonattainment areas. Recent court decisions and government findings define greenhouse gases as air pollutants (Massachusetts v. EPA 2007; U.S. Environmental Protection Agency 2009) and several studies describing the effect of climate change on air quality (Turner, Baglio et al. 1991; Liao, Tagaris et al. 2007; Tagaris, Manomaiphiboon et al. 2007; Dawson, Racherla et al. 2009; Jacob and Winner 2009) suggest that longer air quality planning horizons of 25, 50, or even 100 years into the future may be forthcoming. The array of options available to manage air quality over these longer time periods is greatly expanded over what has been possible under Title I of the Clean Air Act. However, relating decisions today to air quality in the far off future is not straightforward. Most of the previous efforts at long-term air quality planning have relied on forecasts of future emission inventories by making assumptions of future economic, technological, and population development (Nakicenovic, Alcamo et al. 2000; Woo, He et al. 2008). While such forecasts are accurate in the short-term, under long-term planning horizons, they become increasingly uncertain. In its report on emission scenarios, the International Panel on Climate Change (IPCC) noted that uncertainties in such predictions arise “from inadequate scientific

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understanding of the problems, data gaps and general lack of data to inherent uncertainties of future events in general" (Nakicenovic, Alcamo et al. 2000). To overcome these uncertainties, often multiple assumptions of future development are simulated. As the impacts of these assumptions are analyzed, a satisfactory path of development may be chosen. But at the conclusion, one is unable to determine if other plans not considered could have provided better air quality outcomes or lower costs.

Here we describe and demonstrate a method for prescribing a desirable future air quality and the minimal changes needed to attain that desired state. Changes may include the regulation of stationary and mobile sources of pollutants and pollutant precursors that are the traditional mainstays of air quality management. But given the longer time horizons, change may also include modifications to elements that, until now, have not been considered to be pliant. For example, unless told that there are explicit redevelopment plans in the offering, air quality planners have traditionally assumed that land uses that are currently industrial will remain industrial, or that the hardscaped transportation network is unyielding. As such, land use is a fixed amenity that determines air quality.

The method outlined here reverses the traditional approach. Given a desirable future state of air quality, we derive the land uses that suit it – taking into consideration that land use is already presently defined and that any changes to this state will incur costs, which can be minimized. The computed emissions changes are then linked to actual land use characteristics in a tangible way that is more readily communicated to planners and decision-makers.

3.2 Desired future air quality

From practical concerns about impacts on health or economic well being, to more ethereal qualities like altruism or aesthetics, air quality can be valued in different ways. Some studies have surveyed populations for the willingness to pay for cleaner air (Mansfield, Reed Johnson et al. 2006); others have used hedonic modeling, observing changes in wages or housing prices in response to measured air quality within a community (Dickie and Gerking 1991; Smith and Huang 1995; Chattopadhyay 1999; Zabel and Kiel 2000; Gabriel, Mattey et al. 2003; Chay and Greenstone 2005).

In our analysis regarding desirable air quality for the residents of Atlanta in the year 2050, we make no claim as to the uniqueness of the method or the truthfulness of the result. Instead, the intent of this effort is to produce a seed "air quality state" from which the demonstration of the larger inverse concept is made possible. We recognize that any arbitrary air quality state would be sufficient for the demonstration. Nonetheless, a rational approach to estimate a desirable long-term air quality state is presented here if only to avoid criticism over the selection of an arbitrary goal. The rationally derived state we provide here is intended as an abbreviated substitute for a more complex approach with extensive time for public comment that we imagine would be necessary to create a consensus around a common, future goal like air quality in Atlanta in the year 2050.

3.2.1 Partial Equilibrium Modeling

Here, we use cost-benefit analysis to determine the optimal desired future air quality (F) by maximizing the net benefit function:

$$F(Q) = B(Q) - C(Q) \quad (3.1)$$

Where B(Q) and C(Q) are the total benefits and costs for a prescribed air quality (Q). In a partial equilibrium model, the net benefit function is maximized when the marginal benefits (MB) are balanced by the marginal costs (MC) :

$$MB(Q^{eq}) = MC(Q^{eq}) \quad (3.2)$$

and the second order conditions verify that there is a global maximum at Q^{eq}. This implies that society would pay for improved air quality until the cost for the next increment of emission abatement exceeds the benefits that would result from the next incremental reduction in pollution.

As there is yet no direct market for air quality that sets prices or defines the value of a unit of air quality improvement, it is necessary to use nonmarket valuation methods (Gabriel, Mattey et al. 2003; Mansfield, Reed Johnson et al. 2006) to account for improvements in air quality. Several methods are used to estimate contemporary marginal costs and benefits of air pollution reductions which are then projected to a 2050 future.

Over the next 50 years it is likely that there will be a variety of shifts in the marginal costs and benefits of air quality leading to a Q^{eq} that will be different from today. Across this period of time, changes in a variety of factors will affect the relative value of the MC and MB, among others, population, income, technology, and tastes. A description of our future projection of each of these factors to Atlanta, GA in 2050 follows.

According to the 2000 U.S. census the population of the metropolitan area of Atlanta was 4.3 million persons and 1.6 million households. By 2030, the region's primary planning agency, the Atlanta Regional Commission, estimates that these values will grow to 6 million personse and 2.3 million households based upon the current average household size. If the 1.025% yearly growth rate predicted by the ARC continues from 2030 to 2050, 3.7 million households would be expected in metro Atlanta by 2050. The MB and MC curves are assumed to scale with population, as both marginal benefits and costs are shared by each individual equally.

The median household income level in metropolitan Atlanta was $51,654 in 2000 (U.S. Census Bureau 2007) (all dollars are given as 2000$ adjusted by the consumer price index). This is projected to the year 2050 by applying a 1.4% annual growth rate in income, a rate based on Harrison and Pearce (2000). At this rate, the (real) per household income is expected to reach $96,563 by 2050. The forecasted income for 2050 is used in the benefits transfer method described in section 3.2.3. The MC curve is assumed to be insensitive to income.

Central to estimating future marginal costs is the rate of technological growth and innovation. Since the progress in abatement technologies is closely tied to the political and economic costs of controls, they are responsive to when, how, and to what degree future stakeholders decide to control emissions. As noted earlier, long term predictions over the future development of any specific technology are understandably unreliable. In this analysis, only a general baseline for the rate of change in air pollution abatement is considered. A relatively optimistic rate of 1.5% per year (relating to the historical change in energy efficiency of central air conditioners from Newell et al. (1999)) is set here as

the technological growth rate. Lower growth rates were also studied, however, the effects were not shown to significantly change the optimal level of air quality suggested by this analysis. Breakthrough technologies which would greatly alter this rate are not considered here.

How preferences for cleaner air based on likes and dislikes will change over long time periods is difficult to predict given that they are intrinsically unobservable determinants of economic value. More akin to style than substance, the effect of future taste on desired air quality is inherently different than education or the passing of time or other prime determinants of demand for environmental protection, such as income and population, which are accounted for directly elsewhere in the model. Because, however, we have no reasonable way to predict future air quality tastes, we restrict tastes in the model to reflect the current population's preferences. That is, tastes are not assumed to change between now and 2050. However, this assumption is not a requirement. Variations in the desired air quality may be found by applying a specific segment of the population's desires (e.g. those of highly sensitive children or the elderly) as the main constraint on future desires. An example of this is presented below by basing our analysis on parents' willingness to pay for clean air.

3.2.2 Transferring marginal costs to 2050

Two baselines for marginal costs are drawn from the Fall Line Air Quality Study (FAQS) – a detailed and regionally specific study of abatement costs in central Georgia (Chang 2004). In addition to being specific to Georgia, this study uses the results of air quality sensitivity studies to relate emission abatement costs directly to improvements in air quality. Using sensitivity analysis, a list of available control options for the Macon,

GA area and the surrounding areas was sorted and ranked in order of cost effectiveness to produce MC curves.

Chang (2004) developed a MC curve that corresponds to the least-cost controls from within the Macon, GA area needed to reduce daily maximum 8-hour ozone within the city based on average sensitivities for two episodes in August 1999 and 2000. Because the 2000 episode showed a larger response in ozone concentrations to reductions in local NO_x emissions, the air quality improvements from this analysis are termed "lower cost" solutions. We assume these cost estimates to be similar to those expected with new technologies creating significant air quality improvements without large costs. An alternative MC curve is developed from the August 1999 modeling episode when modeled ozone concentrations in Macon, GA were less responsive to local controls. This can be seen as a "higher cost" MC curve where future costs increase as abatement options are exhausted.

The baseline 2005 MC curve is projected to 2050 based upon the factors identified above. This involves scaling the costs proportionally up with the population increase and also scaling them proportionally down due to technological advances. This assumes the costs of additional controls will be proportional to the population size. It also assumes the benefit from technological advances will be similarly proportional to population. The marginal cost curves for the higher cost scenario projected to 2005 and 2050 are shown in Figure 3.1.

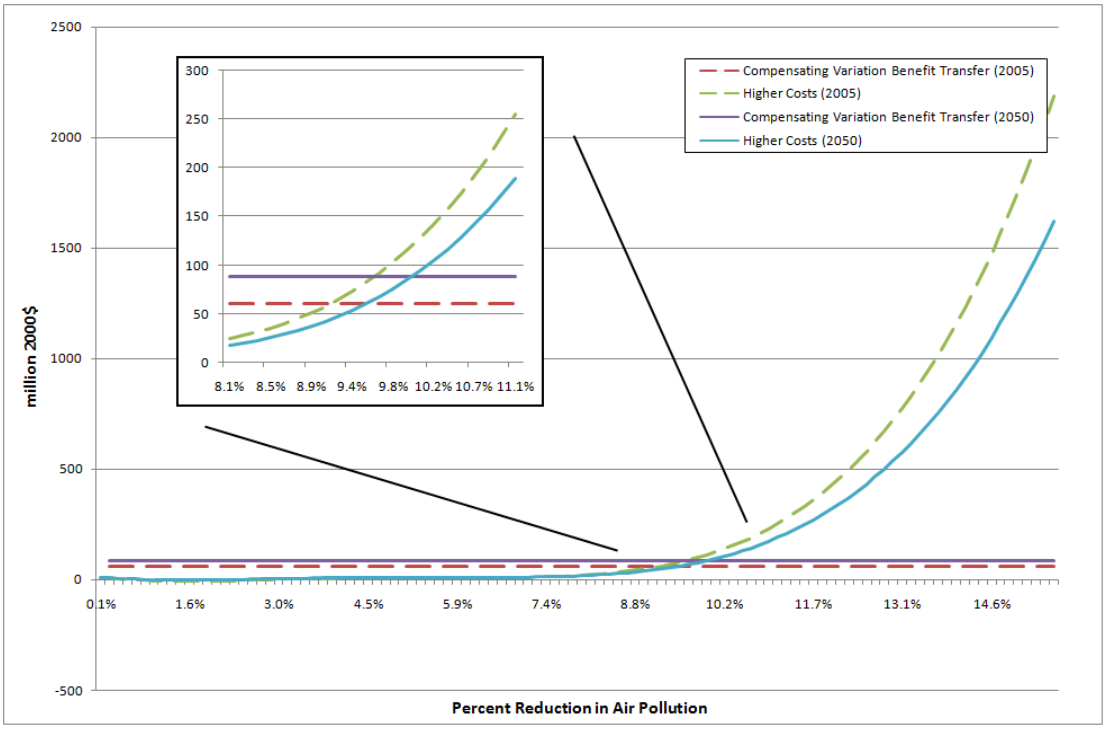

Figure 3.1: The marginal cost and benefit curves for 2005 and 2050. Marginal cost curves were developed from the modeled effects of pollution abatement options on air quality (Chang 2004) and were transferred to the future case assuming population and technology growth rates (Newell, Jaffe et al. 1999). The marginal benefit curves are based on the compensating variations analysis and are projected to an expected population size. The optimal percent reduction in air pollutions is at the intersection of each set of MB and MC curves. Currently, to maximize net benefits, emissions controls should be installed to reduce air pollution by 9.1%. This value is raised to 10.0% when the curves are shifted for our 2050 projections.

3.2.3 Transferring marginal benefits to 2050

Three methods were employed to determine the 2050 MB curve for Atlanta. The first two methods arrived at a similar result despite using different data and methods to estimate the benefit of cleaner air for the general public. The third focused on valuing air quality based upon the most sensitive members of the population which may be representative of an upper limit on the benefits from clean air. Each is described in detail below.

The first method for estimating MB relies on a cohort of 21 previous studies (listed in the footnotes of Table 3.1) which measure how much individuals are willing to pay for air quality improvement or be compensated for poor air quality. These values are elicited via surveys from individuals in carefully constructed hypothetical scenarios or "contingent" markets. The studies yielded 62 valuation estimates for a variety of air pollution species. Each of these valuations was then rendered into a comparable compensating variation (CV) measure which relates value placed on avoiding (or being compensated for) an additional increment of unspecified air pollution. Income elasticity consistent with the literature was assumed whenever the original study did not report such information. The annualized CV relied on a 5% discount rate.

To transfer the benefit estimates to the future Atlanta case, a parametric model of the variation in CV values across and within studies was devised using a random effects regression model (with errors clustered by study, for those studies with multiple valuation estimates). The regression used the following covariates: log income, log population, annual precipitation, average high temperature, ΔQ, a dummy variable for whether the study site was within the US or foreign, and ΔQ interacted with the foreign dummy variable. After restricting the sample to those observations without missing variables, the regression was based on 32 observations. All of the covariates were significant at the 10% level, except for log population and the foreign dummy variable. The R-square of the model was 0.83, suggesting that the regression explains a large amount of the variation in benefit estimates. Alternative models were estimated controlling for valuation method (CVM or not), other combinations of population and income, and other specifications for Q or ΔQ, but the best fit was achieved in the preferred model.

The benefit transfer function is linear in ΔQ, meaning that the change in CV valuation is constant across marginal changes in ΔQ. Alternative specifications were explored, but they did not fit the data in our sample of benefit estimates. Furthermore, because the specification did not include interaction between the ΔQ variable and other covariates (except for the foreign dummy), the MB (but not gross CV level) is independent of other variables such as income, population, and weather. Such interactions were tested but found insignificant. Therefore, the MB estimates are not sensitive to projections of future income. While the marginal effect of ΔQ on CV is also independent of population, the MB estimation is sensitive to population growth because the CV measure is given in per-household terms and must be scaled up to the appropriate regional population. The benefit transfer method yields an estimated MB(Q) of $88.28 million per year per ppb of ozone for the Atlanta region in 2050.

The second method focuses on empirical data instead of survey information. Gabriel et al. (2003) offers a robust application of a compensating differentials approach to determine the impact of air quality on wages and rents. We take the implicit price of $37.58 per household per year for 1 ppb of ozone improvement from this study as the MB of improvements to Q. This MB value is scaled up to the regional population of the projected Atlanta 2050 scenario, yielding a MB(Q) = $87.14 million per year. Consistent with the reported values in Gabriel et al. (2003), this value is also constant across all changes in Q, implying that the benefits of each additional increment of Q are the same, i.e. no matter how much air quality improves, people will be willing to pay the same amount for an additional increment of Q.

In the previous derivations of the MB curve, the analysis focused on establishing the benefits of clean air on the population as a whole. However, individual sensitivity to air pollution varies significantly. The third method attempts to estimate the marginal benefits of air pollution abatement to a future population that is highly sensitive to air pollution. Mansfield et al. (2006) asked parents' willingness to pay to avoid restricted outdoor activity time for their child. Since children are more sensitive to air pollution's effects, parents may value clean air more greatly than the general population. Under this case where the average resident's demand for cleaner air will be the same as that of present-day parents of asthmatic children, the MB(Q) would rise by 55% over the estimates for a typical population.

In each of these cases, MB is scaled based on the projected population size in 2050. MB curves from the first benefit transfer method, projected to 2005 and 2050 are shown in Figure 3.1.

3.2.4 Economically Optimal Reductions

In Figure 3.1, net benefits are maximized at the intersections of both sets of the MC and MB curves for 2005 and 2050. The cost curves shown in Figure 3.1 are for the higher MC scenario outlined above. The MB curves are from the compensating variations transfer analysis. In 2005, based upon our cost and benefit analysis, air pollution concentrations should be reduced by 9.1% from current concentrations. By 2050, the optimal reduction in air pollution will be 10.0% based upon projected population, income and technology growth.

The 2050 projected optimal air pollution reductions for each combination of cost and benefit assumptions are shown in Table 3.1. Using the lower MC scenario where air quality is highly sensitive to inexpensive emission controls, the desired reduction is greater than the higher MC scenario where effective abatement costs remain high as emission control options are eliminated. The MB estimates from both the compensating variations and the compensating differentials analysis are very similar. This is an unexpected coincidence, given the markedly different methods employed. Consequently, the optimal reductions in air pollution are equivalent between the benefit transfer methods. Though, by assuming that the entire future population will have tastes similar to that of contemporary sensitive populations, the estimated MB curve increases. This MB, in effect, estimates a maximum level of benefits from less air pollution, and accordingly, when these preferences are applied, more air pollution reductions are called for than with the other benefit transfer methods.

Table 3.1: Percent reduction in air pollution desired in 2050 Atlanta under different benefit valuation and cost assumptions

	Higher costs[a]	Lower costs[b]
Contingent Variation[c]	10.0%	12.3%
Compensating Differentials[d]	9.9%	12.3%
Sensitive Populations[e]	10.5%	12.6%

a – Table 3.6, Section IV, Part 2 Chang (2004)
b – Figure 3.4, Section IV, Part 2 Chang (2004)
c – 21 study cohort (Brookshire, d'Arge et al. 1982; Berger, Blomquist et al. 1987; Brucato, Murdoch et al. 1990; Dickie and Gerking 1991; Shechter 1991; Halvorsen 1996; Pearce 1996; Alberini, Cropper et al. 1997; Beron, Murdoch et al. 1999; Chattopadhyay 1999; Palmquist and Israngkura 1999; Sieg, Smith et al. 1999; Carlsson and Johansson-Stenman 2000; Kumar and Rao 2001; Kwak, Yoo et al. 2001; Srivastava and Kumar 2002; Kim, Phipps et al. 2003; Mahesh D. Pandey and Jatin S. Nathwani 2003; Li, Guttikunda et al. 2004; Rozan 2004; Dziegielewska and Mendelsohn 2005)
d – Gabriel et al. (2003)
e – Mansfield et al. (2006)

Regardless of the assumptions or methods used, the economic analysis produced optimal air pollution reductions within a relatively narrow band of 10-12%. In the next section, we select the optimal air quality reduction from the higher cost scenario to calculate emission inventory adjustments necessary to achieve a 10% reduction in air pollution

3.3 Inverse method for adjusting emission inventories

Having an air quality goal, it is the task of air pollution managers to determine a plan of action to achieve the goal. Some pollutants which are directly released into the atmosphere, such as lead or carbon dioxide, are relatively straightforward to control (though the controls still may be costly). Other pollutants such as ozone and secondary

particulate matter are more difficult to control, as they are not emitted directly into the atmosphere but instead form in the atmosphere from a mixture of precursor species under certain conditions. Air quality managers must first identify the conditions at which these pollutants form and then understand the relative importance of precursor species in order to create effective control strategies. Atmospheric modeling plays a key role in this process.

Since air quality planning is dominated by short term goals, modeling studies often focus on determining the effectiveness of immediate control solutions for reducing air pollution. However, longer term approaches like applying smart growth initiatives that affect land use or altering individual travel behavior can lead to significant gains in reducing air pollution (Kessler and Schroeer 1995; Liu and Trb 2003; Stone, Mednick et al. 2007; Stone 2008). The model outlined here does not specify control strategies. It calculates the necessary changes in emissions of precursor species to achieve the desired reductions in air pollution. By knowing how emissions must change in aggregate, managers can implement long-term solutions or challenge the marketplace of ideas for finding a solution which reduces precursor emissions to the requisite amounts.

In the economic analysis, estimates of MC and two of the three methods for estimating MB are based upon the benefits and costs of managing tropospheric ozone (the remaining MB method used the compensating variation measure and is applicable to any atmospheric pollutant). Accordingly, ozone is considered in our inverse method analysis. Ozone is a respiratory irritant and has been shown to cause and exacerbate a number of respiratory illnesses and shorten lifespans (Jerrett, Burnett et al. 2009). The primary precursors of ozone are nitrogen oxides ($NO + NO_2 = NO_x$) and volatile organic

compounds (VOCs). In the southeast United States, the majority of emissions of VOCs are derived from biogenic sources which are difficult to control (Chameides, Lindsay et al. 1988; Sillman 1999; Cohan, Tian et al. 2006). Historically, NO_x controls have been the focus of air quality managers for addressing ozone control in the southeast (Kasibhatla, Chameides et al. 1998; Cohan, Tian et al. 2006). While vegetation may change over the course of 50 years (Turner, Baglio et al. 1991; Woo, He et al. 2008) and some control options over the anthropogenic fraction of VOC emissions may be effective (Cohan, Tian et al. 2006; Zavala, Lei et al. 2009), they are not subject to our analysis here. Here, we focus on NO_x emissions reductions to reduce ozone concentrations in Atlanta, GA. Though efforts have been made for several decades to reduce ozone concentrations, Atlanta, GA has continued to be out of attainment of the National Ambient Air Quality Standard and is subject to the regulatory requirements set forth in the Clean Air Act (U.S. Environmental Protection Agency 2008).

3.3.1 Modeling Description

The approach used here is similar in form and scope to other inverse methods that have been deployed to assess emission inventories from ambient air observations (e.g. Mulholland and Seinfeld 1995; Mendoza-Dominguez and Russell 2000; Schichtel, Malm et al. 2006). That is, an air quality model, instead of entering emissions as inputs and receiving atmospheric concentrations of pollutants or pollutant precursors as output, is inverted in the sense that ambient concentrations are input and emissions are output. The difference with previous applications is that instead of observations driving the inversion, here a proposed or desired future air quality concentration state is the progenitor.

The method outlined here closely follows the method used in Mendoza-Dominguez and Russell (2000) and Napelenok et al. (2008). Though the derivation that follows is specific to the case of ozone concentrations and NO_x emissions, any pollutant/precursor combination may be substituted. A more detailed derivation of method is presented in Chapter 2.

3.3.2 Inverse model

The desired future ozone concentrations, $C^{desired}$, at receptor *r* may be seen simply as a change in the concentrations, ΔC, from the base concentrations, C^{base}.

$$C_{O_3,r}^{desired} = C_{O_3,r}^{base} + \Delta C_{O_3,r} \quad (3)$$

This change in concentrations may be described using a linear model based upon the first order sensitivity, S (Cohan, Hakami et al. 2005).

$$\Delta C_{O_3,r} = S_{E_{NO_x,p}}^{O_3,r} \cdot \Delta E_{NO_x,p} \quad (4)$$

where:

$S_{E_{NO_x,p}}^{O_3,r} = {\partial C_{O_3,r}}/{\partial E_{NO_x,p}}$ *= response of ozone concentrations at r to changes in* NO_x *emissions from a particular source parameter p*

Since future emissions within each source parameter are assumed to change from the base case emissions, E^{base}, only in magnitude and not place nor time, a relative adjustment factor, χ_p, from E^{base} is found. The sensitivities are calculated in terms of the total contribution of ozone from E^{base}, and the previous equation may be rewritten to find the adjustment factors:

$$\Delta C_{O_3,r} = P_{O_3,E_{NO_x,p}} \cdot \chi_p \quad (5)$$

where:

$P_{E_{NO_x,p}}^{O_3,r} = S_{E_{NO_x,p}}^{O_3,r} \cdot E_{NO_x,p}^{base}$ *= total contribution of ozone at receptor r due to NOx emissions from source parameter p*

$\chi_p = {\Delta E_{NO_x,p}}/{E_{NO_x,p}^{base}}$ *= relative adjustment factor for emission parameter p*

Equation 3 may be rewritten as:

$$C_{O_3,r}^{desired} = C_{O_3,r}^{base} + P_{E_{NO_x,p}}^{O_3,r} \cdot \chi_p + \varepsilon_{O_3,r} \quad (6)$$

where:

$\varepsilon_{O_3,r}$ *= the remaining difference between the desired concentration change and the simulated concentrationsnot accounted for by the linear model*

Since the number of receptor cells is greater than the number of source parameters, the inversion problem is overdetermined and no solution can be found which reduces the residual to zero at all receptors (Mendoza-Dominguez and Russell 2000). We find a solution which minimizes the residual error, however, between desired and simulated ozone concentrations in a least square sense, and produces physically meaningful emission adjustments. The following cost function, *J*, is written in matrix form (Mendoza-Dominguez and Russell 2000):

$$J = \mathbf{x}^{\mathbf{T}}\mathbf{W}_{\mathbf{x}}\mathbf{x} + \mathbf{e}^{\mathbf{T}}\mathbf{W}_{\mathbf{e}}\mathbf{e} \quad (7)$$

where:

$\mathbf{x}^{\mathbf{T}} = [\chi_1 \ldots \chi_p]$ = *vector of emission source adjustment factors*

$\mathbf{W_x}$ = *weighting matrix of the source parameters*

$\mathbf{e}^{\mathbf{T}} = [\varepsilon_{O_3,1} \ldots \varepsilon_{O_3,r}]$ = *vector of differences between modeled and desired concentrations*

$\mathbf{W_e}$ = *weighting matrix of the residual error*

This function is minimized when $\partial J / \partial \chi = 0$ and may be reduced to (Mendoza-Dominguez and Russell 2000):

$$\mathbf{x} = (\mathbf{P}^{\mathbf{T}}\mathbf{W_x}\mathbf{P} + \mathbf{W_e})^{-1}\mathbf{P}^{\mathbf{T}}\mathbf{W_x}\mathbf{e} \quad (8)$$

The model iteratively optimizes the adjustment factors by adjusting emissions and regenerating concentrations and sensitivities until the emissions adjustments converge.

The weighting of the source parameters, $\mathbf{W_x}$, limits the amount that a source may change over the course of the next 50 years. In theory, the matrix defines the future uncertainity in the emission strength of a source. Effectively, it limits emission adjustments to a phyisically meaningful amount. First, it restricts sources from increasing beyond their current emission levels and being reduced below zero. The latter condition is to prevent the creation of NO_x sinks in place of sources. While it is possible that NO_x emissions will increase in the future, the former condition restricts the model from using high NO_x emissions to titrate oxidant species in VOC-limited areas. Second, by limiting the change in emissions from any parameter in a single iteration to 30%, the weighting matrix supports the use of the first order sensitivities between ozone and NO_x (Cohan, Hakami et al. 2005). In other applications, the matrix could contain *a priori* information

of the uncertainty of future emissions changes based upon regulations, growth, or technical innovation.

For the case of desired future concentrations, the weighting of the residual error, $\mathbf{W_e}$, may be seen as measuring the consensus over what constitutes a desirable future air quality (or the lack thereof). There are significant differences of opinion over what qualifies as "clean air." As the economic analysis suggests, there is a range of possible optimal concentrations. Though as the goal concentrations are defined here, weights are assumed to be uncorrelated and constant.

3.3.3 Forward Model System and Domain

The Community Multiscale Air Quality Model (CMAQ) extended with the Direct Decoupled Method in three dimensions (DDM-3D) was used to generate the concentration and sensitivity fields (Dunker 1984; Yang, Wilkinson et al. 1997; Hakami 2003; Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006). The model was run for August 3-8, 1999 episode on a 4km domain covering the 13-county Atlanta, GA metropolitan area (Figure 3.2). Meteorology fields, emissions fields, boundary conditions and initial conditions for this domain and episode were generated and extensively studied as a part of the Fall Line Air Quality Study (Chang 2004). To remove the effect of static initial conditions after emissions were changed the first 36 hours of modeling time is discarded. Since local planners may only regulate emissions within their jurisdiction, ozone concentrations sensitive to transport into the domain are removed, leaving only the locally produced ozone (LPO_3) to be optimized. The inverse model is programmed in Matlab, and uses the SNC and Mexnc toolboxes to interact with the CMAQ-DDM output and emission input files (Evans 2007; Matlab(R) 2007).

The DDM-3D method (Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006)(Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006)(Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006)(Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006)provides spatially explicit sensitivities of an atmospheric chemical species to a specific source parameter more efficiently than by brute force methods (Dunker 1984; Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006).

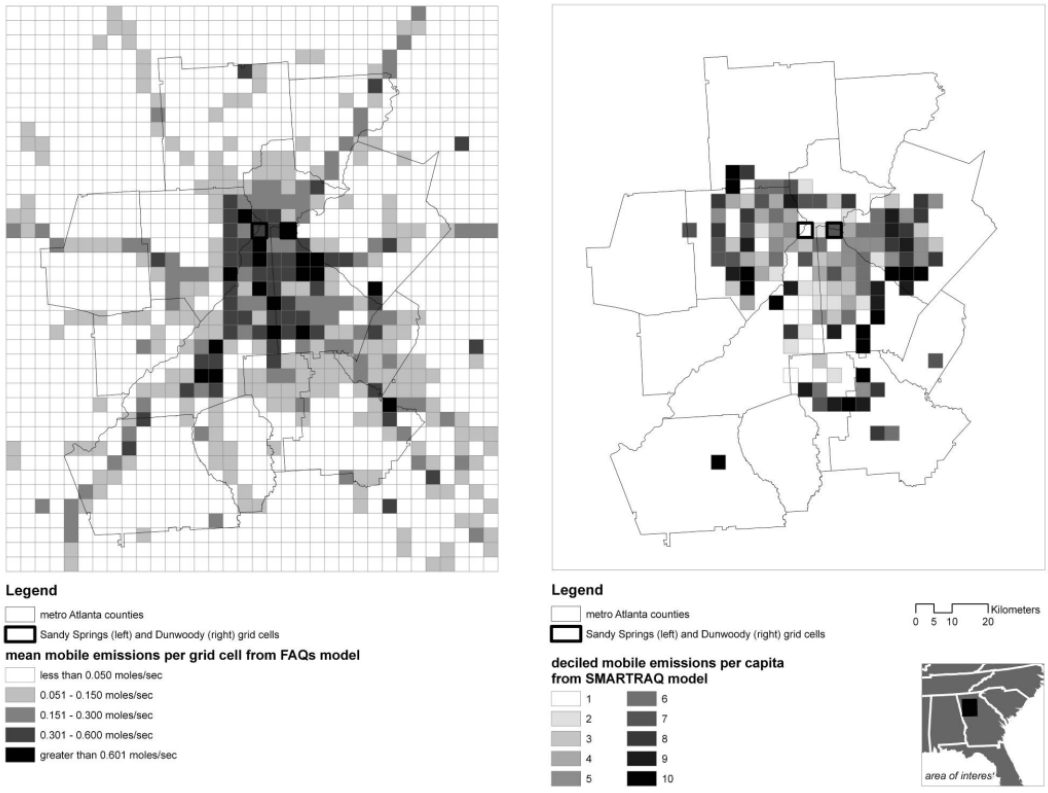

Figure 3.2: Comparison between the FAQs and SMARTRAQ emission inventory. The FAQs study assigns emissions based upon where they occur on roads (a). The SMARTRAQ study assigns emissions to the location of the responsible households (b). Both systems are measurements of mobile source emissions and must be reduced in the future case. Since the results from the inverse model are set as reductions for the entire 13 county area and the majority of trips in the SMARTRAQ database begin and end inside this region, where the emissions are assigned is irrelevant in our application. Both measures must be reduced by the same relative amount. Maps courtesy of Ann Carpenter

Source parameters are defined by three attributes: chemical species, a specific area of the domain, and the emission inventory source category. Five parameters are defined: mobile sources inside and outside the 13-county metropolitan area and emissions from the whole domain for area, nonroad, and point sources separately. A detailed description of these source categories may be found in Chapter 2. As mentioned previously, only NO_x emissions are considered in the analysis presented here.

3.3.4 Emission adjustment results

Because the desired change in air quality from our economic modeling is in terms of the relative change from present levels, any metric may be used to generate the desired, or goal, air quality concentrations. Here, the desired future ozone concentrations are generated by applying a 10% reduction in cells with LPO_3 above 60ppb. This set of cells incorporates concentrations which are currently seen as undesirable and includes elevated peak hour concentrations (Henderson 2008). The inverse model is assumed to have converged once the model does not adjust emissions beyond 10% of E^{base} in a single iteration (Figure 3.3).

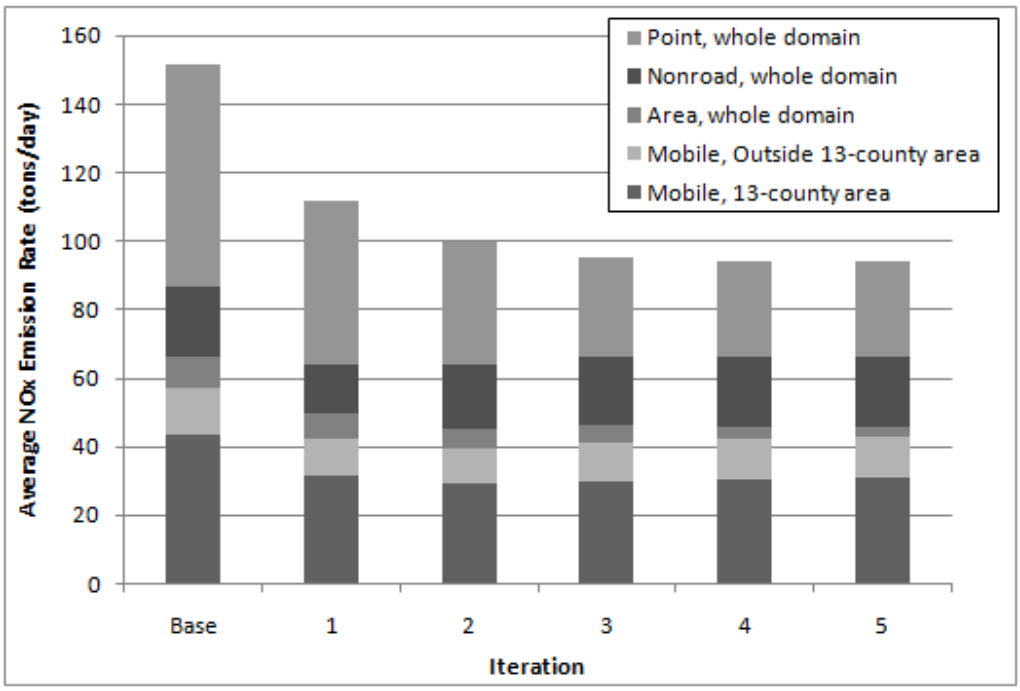

Figure 3.3: Total NO_x emissions by source type and region for each iteration. Point, non-road, and area sources include emissions domain-wide. Mobile emissions are split into two areas: 1) inside the 13-country metro area and 2) the surrounding area within the domain. While reductions are distributed across the parameters in the first iteration, after recalculating sensitivities with this new emissions distribution in the second and later iterations, the inverse method readjusted the reductions so that area and point sources are reduced further and non-road emissions reductions are relaxed. Total NO_x emissions are reduced by nearly 40% in the optimized case.

Emission adjustments for each parameter and the change in emission rates are shown in Table 3.2. Significant reductions are called for in both area and point sources while little reduction is called for from non-road sources. Since no a priori information over control costs is assumed here, the differences in the adjustment factors between source categories are solely based upon the timing and location of emissions and the fate of those emissions in the atmosphere. The non-road category is dominated by airport emissions which are largely negatively sensitive to ozone due to the airport's proximity

Table 3.2: Emission adjustment factors from the inverse analysis

	Final Percentage of Initial Emissions	**Initial Daily Average NO_x Emissions Rate (tons/day)**	**Adjusted Daily Average NO_x Emissions Rate (tons/day)**
Mobile emissions 13-county region	70.2%	43.34	30.42
Mobile emissions outside 13-county region	84.6%	13.69	11.58
Area Sources	41.4%	8.81	3.64
Non-Road Sources	99.5%	20.60	20.50
Point sources	42.9%	65.29	28.02
Total	**60.1%**	**151.73**	**94.17**

to the urban core. Therefore, the model does not reduce emissions from the non-road parameter since any reduction would result in an increase in emissions.

The total NO_x emissions reduction from all sources is 39.1%. While reductions in point sources comprise the majority of the NO_x reductions, significant reductions are also required from the mobile source category (Table 3.2). By distinguishing emissions from the 13-county core area from the rest of the domain, the results suggest that mobile source reductions (~30%) should be concentrated inside the 13-county area as opposed to the surrounding rural areas.

The emission reductions given by the inverse model largely achieve the goals set forth by the desired air concentrations. As noted above, because inversion problem is overdetermined, the desired concentrations cannot be perfectly replicated by adjusting the

source parameter emissions – the inverse method simply minimizes the residual error between the simulated and desired concentrations. With the adjusted emissions, the hourly average concentrations show good agreement with the desired concentrations, particularly for the days with the most elevated concentrations (Figure 3.4).

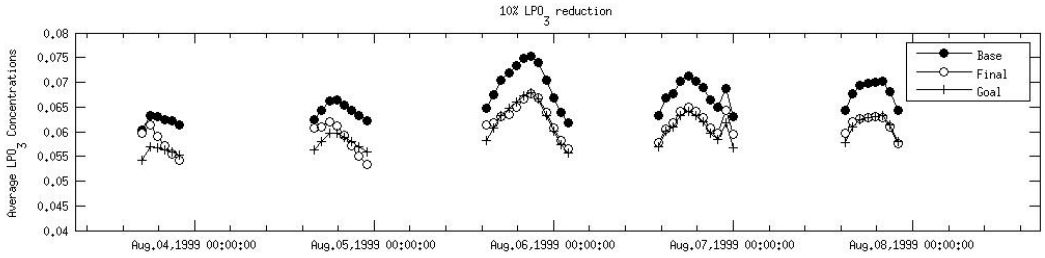

Figure 3.4: Hourly Mean Concentrations in Cells with O_3 Concentrations greater than 60ppb in the base case. Concentrations are shown for the base case, desired concentrations, and final iteration. The reduced emissions case in the final case, achieves the desired concentration reductions for most of the hours in the last 3 days, particularly on August 6th when concentrations reach their peak concentrations for the episode.

As a specific example of the change in concentration seen after emissions are adjusted, the base 8-hour average LPO_3 concentrations for the peak hour in the modeled episode are shown in Figure 3.5a. Qualitatively, the modeled ozone concentrations (Figure 3.5b) closely resemble those of the desired concentrations (Figure 3.5c) with many regions achieving a 10% reduction. The change in total 8-hour average ozone concentrations between the base and final iteration for the same hour is shown in Figure 3.6. Even including the influence of ozone transported into the domain from the boundary, ozone concentrations have been reduced in many areas.

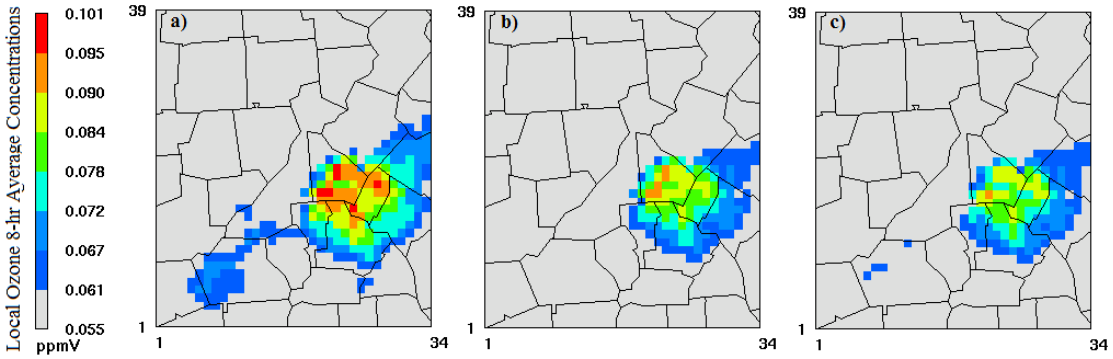

Figure 3.5: The local 8-hour ozone concentrations for the a) base case, b) final iteration, and c) desired concentrations at 20:00:00 August 5, 1999 EDT. After the emission adjustments are applied, the concentrations in iteration 5 closely resemble the desired concentrations.

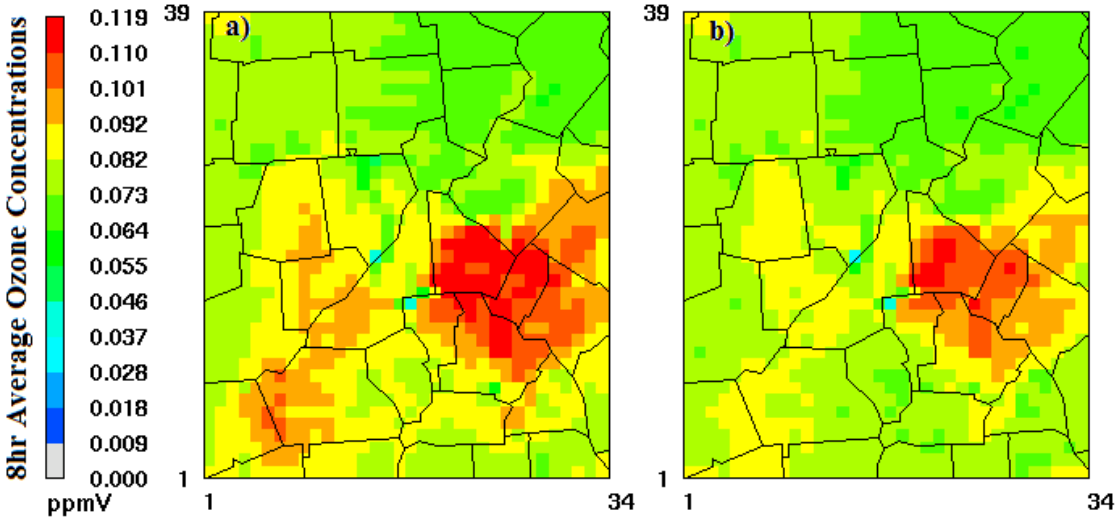

Figure 3.6: Total modeled ozone concentrations for the a) base case and b) final iteration at 20:00:00 August 5, 1999 EDT. Even including ozone transported into the area from the boundary, the majority of cells above 0.06ppm are reduced by 10%. However, reduced NOx titration of oxidant species causes ozone concentrations to increase in some regions with concentrations below 0.06ppm in the base case.

3.4 Land Use Modeling

By themselves, the aggregated changes in emissions given by the inverse method are only the starting point for planners. Aggregated changes only provide guidelines upon which planners may evaluate potential changes in emissions as to their impact on achieving future desired air quality. We apply these guidelines to indicators of urban form to understand how emission adjustments may inform the urban land use planning process.

Several studies have linked land use indicators with mobile source emissions. Chapman et al. (2004) showed that residential density, intersection density, and land use mix have a significant inverse association with per capita NO_x emissions. In addition, a single index of walkability (incorporating land use mix, street connectivity, net residential density, and retail floor area ratios) has been found to be significantly and negatively associated with per capita NO_x emissions (Frank, Sallis et al. 2006). Also, residential density has been found to have a significant negative relationship with household vehicle emissions (Frank, Stone et al. 2000). Knowing the relationship between these land use parameters and emissions, it is possible to estimate possible changes in land uses to achieve the emission reductions suggested by the inverse model.

We use the Strategies for Metropolitan Atlanta's Regional Transportation and Air Quality (SMARTRAQ) study is to understand how land use impacts mobile source emissions in the Atlanta region (Chapman and Frank 2004). Studying the 13-county Atlanta, GA area, the SMARTRAQ database contains a 1.2 million parcel land use database and the results of an 8,000 household, 17,000 person, two day travel survey

conducted in 2001-02. To compare with the inverse modeling results, the SMARTRAQ parcel information is aggregated to the same 4-km grid used here (Figure 3.2a & b).

A set of grid cells was chosen with similar locations relative to the city core and access to transportation but with different amounts of per capita NO_x emissions (Figure 3.2a, Table 3.3). The grid cells are both near the perimeter of the inner city and are accessible by the major interstates in the area (Figure 3.2b). The western cell, roughly corresponding to the city of Sandy Springs, has approximately 28% less per capita mobile NO_x emissions than the eastern cell, which contains the Chamblee neighborhood. In accordance with the results of the inverse modeling, which indicated that mobile source emissions must change by ~30%, the per capita mobile emissions in the Chamblee grid cell should change to one similar to the present day Sandy Springs grid cell. By comparing land use patterns within these grid cells, it is possible to see how different land uses may be associated with differing emissions.

Table 3.3: Mobile NOx emissions, transportation access and urban form measurements for Sandy Springs and Chamblee

	Sandy Springs	**Chamblee**
NOx per capita per weekday	19.06	26.32
Normalizing factors		
Distance to central business district	24.6 km	27.9 km
Length of highway road	0.0 km	0.0 km
Distance to nearest highway ramp	5.8 km	6.0 km
Distance to nearest rail station	6.4 km	7.2 km
Number of bus stops	3.6 stops/sq km	3.4 stops/sq km
Urban form factors		
Mixed use index	0.34[a]	0.11[a]
Net residential density	3.23 units/ac	1.41 units/ac
Intersection density	15.75 int/km^2	21.88 int/km^2

a) Ratio of residential, commercial and office land use in the area. A value of 1 means a perfectly mixed area while 0 mean only a single type category of land use is present.

There are numerous factors in each of these cells that determine per capita emission rates. Demographics, incomes, and tastes all play an important role in an individual's mobility choice and travel behavior, and we control for these factors as we consider the land use in each area. Various demographic and trip data for each grid cell is shown in Table 3.4. While the demographic data between the two cells is similar, the main difference is the length of trips made by motor vehicle. It is possible that these distances are purely due to the location of the cells in the region. Although this is unlikely since they have similar access to highways and are a similar distance from the central business district. Chapman et al. (2004) concluded that urban form is a predictor of automobile

Table 3.4 Mean demographic and travel behavior data for Sandy Springs and Chamblee based on SMARTRAQ database. The number of participants is given in parenthesis

		Sandy Springs	**Chamblee**
Demographic Data	Age	41.0 (50)	43.5 (48)
	Percent female	48.0 (50)	41.7 (48)
	Percent with driver's license (16+ yr)	97.8 (45)	100.0 (39)
	Number of persons per household	2.3 (50)	1.9 (48)
	Number of vehicles per household	2.5 (50)	2.2 (48)
	Average vehicle age (years)	6.8 (41)	6.1 (38)
Travel Behavior	Mean number of miles traveled by motor vehicle (per capita weekday)	**20.3 (46)**	**30.3 (46)**
	Mean number of trips made by motor vehicle (per capita weekday)	3.4 (46)	3.5 (46)
	Percent weekday trips by transit (all modes)	0.3 (50)	0.0 (48)
	Percent weekday trips by walking	0.0 (50)	0.0 (48)

trip length. Here, we consider three urban land use indicators: diversity of land uses, residential land use density, and intersection density.

The diverse land uses in each grid cell are grouped into three land use categories: residential, commercial, and office (including governmental buildings). We calculate an indicator of the relative amount of each land use type from square footage information from each county's circa-2000 property tax parcel database. The details of how the index is calculated is presented in detail elsewhere (Chapman and Frank 2004). A grid cell with only a single type of land use has a value of zero while a value of one represents an equally mixed cell. Increasing the mixed land uses in an area should reduce the amount of

mobile NO_x emissions as trips are shortened between land use types. Accordingly, the Sandy Springs cell has a higher mixed use index value than the Chamblee cell (Table 3.3). A hypothetical planner in Chamblee may need to increase the diversity of land use types through zoning laws or other means.

Residential land use density is measured as the number of residential units per residential acre. This data is taken from the 1999 Atlanta Regional Commission LandPro database (Atlanta Regional Commisssion 1999) and the 2000 U.S. Census (U.S. Census Bureau 2000). In general, areas with low residential density (i.e. areas with large lot sizes) result in high levels of emissions as residents are more dependent on automobiles for longer travel distances. The Sandy Springs cell has over twice the residential density of the Chamblee cell. Therefore, in addition to encouraging more diverse land use, the Chamblee planner may seek to lower mobile source emissions by encouraging higher density residential developments.

The last indicator of urban form, intersection density (the number of intersections of at least three streets per square kilometer), is also a measure of the walkability of an area. Areas with high intersection density generally create a more welcome pedestrian environment by slowing traffic, enabling more opportunities for crosswalk access and provide more direct trips for all transportation modes including cars. The intersection density is calculated using information from the Georgia Department of Transportation road network (Georgia Department of Transportation 1997). In the case of these two grid cells, the expected result that an increase in intersection density leads to a decrease in mobile NO_x emissions is not validated. This is not wholly unexpected as each area has unique properties, and solutions expected to reduce NO_x emissions may not work in all

cases. It is possible that intersection density in Chamblee and Sandy Springs have both reached a threshold level in intersection density, where further emissions reductions are dependent on adjusting the other urban form measures. Therefore, the first priority of the Chamblee planner may not be increasing the intersection density of the area. Instead, the planner's focus would be on creating dense residential areas and well mixed land uses without which the relatively high level of intersections is not as effective at reducing mobile source emissions. Moreover, even though it is considered the "goal" here, planners in Sandy Springs will need to go through a similar process for finding solutions for reducing its emissions since the 30% reductions are called for across the entire 13-county region. Increasing intersection density may be a part of a solution for reducing emissions in Sandy Springs.

This illustrates the point that there will not be a single solution to improving air quality across the 13-county region. While each of the three urban form measures was discussed individually above, their effects are intertwined and synergistic. For example, a location which only has a high density of housing, without nearby destinations and street designs which encourage walking and bicycling, or offer transit service, is not likely to encourage shorter trips and/or trips made by less polluting transportation modes. A suburban, large apartment complex located off a major arterial road is an example of this. Similarly, locations with a high degree of mixed uses in close proximity can be very unwalkable if they are separated by fences and each facility has its own entrance point. Understanding this synergy is an important consideration for any plan to reduce mobile source emissions. With the guidelines provided by the inverse modeling, solutions and

changes to these factors may be evaluated and implemented due to the unique circumstances in each area.

3.5 Discussion

With rising populations and greater awareness of the health effects of air pollution at lower concentrations, air pollution management is not going to get easier. Only with more effective solutions for air pollution abatement will a desired air pollution level be achieved. Further research into control strategies for air pollution will be central to this struggle. The process outlined here will help illustrate where the development of these technologies could be more effectively focused. Additionally, should this method be adopted broadly, there will also need to be a change in the regulatory approach of air pollution control. While the requirements of the Clean Air Act to provide clean air as quickly as possible should remain a priority, a greater awareness of the long-term trends in emissions can ensure that future emissions inventories are easier to control, or in the least, not working against future air pollution mitigation efforts.

Such a system will require communities to proactively address emission source control and incorporate air quality considerations into their development plans. In an ideal world, planners would find and implement changes to the emission distribution until the future desired air quality is realized. Realistically, planners have other costs and benefits to consider as they make decisions regarding emission sources. It is unlikely that the desired air quality will be achieved via a single path. As abatement options are proposed, they may be evaluated based on their contribution towards the community's air quality goal. Through smaller changes over a long period of time, it is possible for

planners to leverage the inevitable change in cityscape over time to move towards a desired air quality goal. As there likely will be little consensus over what future air quality level is considered desirable or which sector of emissions should be reduced first, individual stakeholders may apply the model using their own desires. The knowledge of how emissions should change to achieve their desires may inspire a more informed debate among these stakeholders over possible development options.

The case study results presented here are merely one possible application of the method. Future applications may explore other options for desired air quality outcomes, optimal emissions reduction scenarios, and development options for emissions abatement. To improve the estimates of the desired future air quality, the proposed changes in emissions may be endogenized into the economic analysis to determine how they affect the desired level of air quality. In the inverse modeling, a weighting regime to incorporate a priori information of likely areas for emissions reductions may be included or relative control costs between parameters may be included to alter the proposed emission adjustments. The results of the model may be used to inform a variety of emissions abatement options. For example, the proposed reductions in point sources may be used in a market based system to allocate emissions to various facilities and to set the eventual cap on emissions. Beyond this, such a system needs not be limited to air quality planning – applications may be made to various other long-term environmental problems such as climate change or water resource use.

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CHAPTER 4

APPLICATION OF INVERSE MODELING IN REGIONAL TRADING PROGRAMS: COST OPTIMIZATION OF FUTURE GROWTH

4.1 Introduction

Noting the need for regional reductions in air pollutant precursor emissions and the success of the acid rain emissions trading program under Title IV of the Clean Air Act, the U.S. Environmental Protection Agency (US EPA) proposed an emissions trading system for the Eastern United States under the Clean Air Interstate Rule (CAIR) (U.S. Environmental Protection Agency 2008). When implemented, the EPA predicted that CAIR would lead to significant reductions of sulfur dioxide (SO_2) and nitrogen oxides (NO_x) at less cost than the traditional command and control method. CAIR sets a region-wide cap on SO_2 and NO_x emissions and distributed emission allowances to sources throughout the region. If a source does not have enough emission allowances to cover its emissions, it can choose to either install emission controls or purchase allowances from sources with excess allowances. Over time, the overall cap would decrease, increasing the scarcity of emission allowances and increasing their market price. As the price for the emission allowances increases, more firms will choose to install emissions controls. In theory, such controls would lead to reductions in both ground level ozone and particulate matter, two pollutants for which many areas are out of attainment of the National Ambient Air Quality Standards (NAAQS) (U.S. Environmental Protection Agency 2008).

The rule was wholly vacated by the US Appeals Court for the District of Columbia for several fundamental reasons (D.C. Cir. 2008). In particular, CAIR sets uniform region-wide emission reduction targets and allocated state allowances based on

the Title IV program without regard to the contribution of a specific state's emissions to pollutant concentrations in downwind areas. Additionally, recent studies have shown large differences in the health effects of air pollution based upon the location of emissions (Mauzerall, Sultan et al. 2005). Since emissions sources could potentially purchase emission allowances through the trading program in lieu of installing controls, the Court ruled that CAIR does not adequately ensure that downwind areas will meet the Clean Air Act requirements for attainment of the NAAQS in all areas. In a later ruling, the Court granted a stay of its mandate allowing the EPA to apply CAIR, deciding that the rules were acceptable temporarily in lieu of having no regional air quality management policy at all, though it warned that the case may be reopened if the issues found in the original ruling are not addressed by a new policy (D.C. Cir. 2008).

Here, we propose a method using air quality modeling and sensitivity analysis to address the Court's concerns over the spatial distribution of emissions from a trading system. Spatial emission reductions are calculated using an iterative inverse method which to find the minimum change in precursor emissions needed to achieve a desired reduction in downwind air pollution. Applied on a multi-state scale, the method finds a region-wide emissions cap and further allocates adjustments to state level emissions. The method addresses some of the concerns of the Court by linking changes in emission source regions to specific downwind air pollution effects.

In addition to calculating how emissions must change based upon downwind effects, we propose an alternative scenario where emission reductions in each state are weighted by their costs. In effect, instead of finding the minimum amount of emissions

adjustments needed to reach a desired reduction in air pollutants, we find emissions adjustments which minimize overall control costs.

While the Court listed other problems with the implementation of CAIR in its ruling, a method such as ours allows the EPA to respond in part to the Court's decision by including the specific contributions of upwind sources in a future rule. Furthermore, as this method does not require an explicit listing or modeling of possible control strategies in each state, it is especially suited for a market-based approach where the exact methods for air pollution control are determined by methods other than regulators specifying controls.

4.2 Methods

As the name implies, the iterative inverse method iteratively calculates the concentrations and sensitivities using a forward model while adjusting emissions using a least squares inverse method. The method is described in detail in Chapter 2. A summary follows here.

4.2.1 Forward modeling

Simply, air quality models describe air quality concentrations as a function of meteorology and emissions. We assume that meteorology during the modeled episode is descriptive of conditions that typically lead to elevated air pollution. While an historical episode of elevated concentrations is presented here as a demonstration of the method, in practice care would be taken to ensure that the modeled episodes are representative of future climates and the range of conditions which lead to elevated air pollution concentrations. We approximate the relationship of ambient air pollution concentrations to changes in precursor emissions by:

$$\Delta C_{i,r} = P_{E_{j,p}}^{i,r} \cdot \chi_{j,p} \quad (4.1)$$

where:

$\Delta C_{i,r}$ *= concentration of species i at receptor r*

$P_{E_{j,p}}^{i,r} = \partial C_{i,r} / \partial E_{j,p} \cdot E_{j,p}$ *= total sensitivity of species i at receptor r to emissions from source species j from source parameter p*

$\chi_{j,p} = \Delta E_{j,p} / E_{j,p}$ *= percentage change in emissions of species j from source parameter p*

We use the Community Multiscale Air Quality Model extended with the Direct Decoupled Method in three dimensions (CMAQ/DDM-3D) (Cohan, Hakami et al. 2005; Byun and Schere 2006) to model air pollution concentrations and find their sensitivity to changes in emissions. This modeling suite has been shown to be efficient at calculating sensitivities for multiple species from source areas of varying size (Cohan, Hakami et al. 2005).

4.2.2 Inverse modeling

Inverse methods, as applied in air quality modeling, calculate adjustments in the input parameters (e.g. source emissions) of a forward model needed to produce a desired change in simulated air pollutant concentrations. Previous studies have defined the desired change in concentrations as the difference between modeled concentrations and measurements taken from air quality monitoring stations (Hartley and Prinn 1993; Chang, Hartley et al. 1996; Mendoza-Dominguez and Russell 2001; Gilliland, Dennis et al. 2003) or field campaigns (Mulholland and Seinfeld 1995). In these studies, inverse methods have been used to model adjustments to global and regional fluxes of

atmospheric components (Chang, Hartley et al. 1996; Mendoza-Dominguez and Russell 2000), source apportionment (Hartley and Prinn 1993; Gilliland, Dennis et al. 2003), and to correct model assumptions (Mulholland and Seinfeld 1995; Mendoza-Dominguez and Russell 2001). In the context of using inverse methods for air quality planning, the desired concentrations are used in the place of observed measurements.

By taking the inverse of the sensitivity matrix **P**, Equation 4.1 may be converted to find the equivalent change in emissions to offset a residual difference in concentrations (Equation 4.2).

$$\chi_{j,p} = \mathbf{G} \cdot (C_{i,r}^{Desired} - C_{i,r}^{Simulated}) \tag{4.2}$$

where:

G = *inverse gain matrix relating changes in concentrations to shifts in emissions*

$(C_{i,r}^{Desired} - C_{i,r}^{Simulated})$ = *the model residual of species i at receptor r – here defined as the difference between the desired and simulated air quality.*

The number of receptors included in the model is only limited by the description of the desired concentrations, yet the number of source parameters considered in the inverse model is limited by the calculation cost of finding sensitivities of air pollution to emissions. Since the number of residuals is more than the parameters to be adjusted, simply converting Equation 4.1 to find the gain matrix, $\mathbf{G} = (\mathbf{P}^{\mathbf{T}}\mathbf{P})^{-1}\mathbf{P}^{\mathbf{T}}$, cannot find an exact solution. A solution may be found using a weighted least squares objective function to minimize both the model residual and the percent change in emissions (Mendoza-Dominguez and Russell 2000):

$$J = \mathbf{x}^{\mathbf{T}}\mathbf{W}_{\mathbf{x}}\mathbf{x} + \mathbf{e}^{\mathbf{T}}\mathbf{W}_{\mathbf{e}}\mathbf{e} \quad (4.3)$$

where:

$\boldsymbol{x^T} = [\chi_1 \ldots \chi_p]$ = *vector of percent changes in emissions from each emission source parameter, p*

$\boldsymbol{W_x}$ = *(p x p) weighting matrix of the emission adjustment factors. In this application, the weighting matrix controls the amount a source parameter may change, preventing negative sources and increases in emissions.*

$\boldsymbol{e^T} = [\varepsilon_1 \ldots \varepsilon_r]$ = *model residual at every receptor r*

$\boldsymbol{W_e}$ = *(r x r) weighting matrix of the receptors. In this application, this represents the uncertainty surrounding the modeled concentration at a single receptor and the consensus over what change in pollutant concentrations is desired.*

Equation 4.3 is minimized when $\partial J/\partial \chi = 0,$ and the equation is solved to the form of Equation 4.2. The resulting gain matrix is found as:(Mendoza-Dominguez and Russell 2000)

$$\mathbf{G_k} = (\mathbf{P_k^T}\mathbf{W_x}\mathbf{P_k} + \mathbf{W_e})^{-1}\mathbf{P_k^T}\mathbf{W_x} \quad (4.4)$$

where:

$\mathbf{P_k}$ = *matrix of sensitivity values with rows relating the kth iteration of the modeled sensitivities of to emissions from each emission source 1 to p*

For each iteration, the concentrations and sensitivities are modeled by CMAQ/DDM and emissions are adjusted by the inverse method. The process iterates

until the change in emissions is less than ten percent of the original emissions. See Chapter 2 for a discussion for how the weighting matrices, $\mathbf{W_x}$ and $\mathbf{W_e}$, are determined.

4.2.3 Model Domain and Episode

The example application shown here reduces locally produced ozone concentrations (LPO_3) by adjusting emissions of NO_x from across the southeast United States. The other main precursor for ozone, volatile organic compounds was not considered as a part of the CAIR emissions trading system. LPO_3 concentrations are calculated by subtracting ozone concentrations by the sensitivity of ozone to ozone transported into the domain. The modeling period is Aug 3-8th, 1999, an historic episode that has been shown to be representative of elevated ozone concentrations in the Atlanta, GA area (Cohan, Tian et al. 2006). The domain covers Georgia and portions of neighboring states with a 12-km resolution (Figure 4.1). The emission inventories for this domain and meteorology modeling for this episode were originally developed for the Fall Line Air Quality Study (Chang 2004).

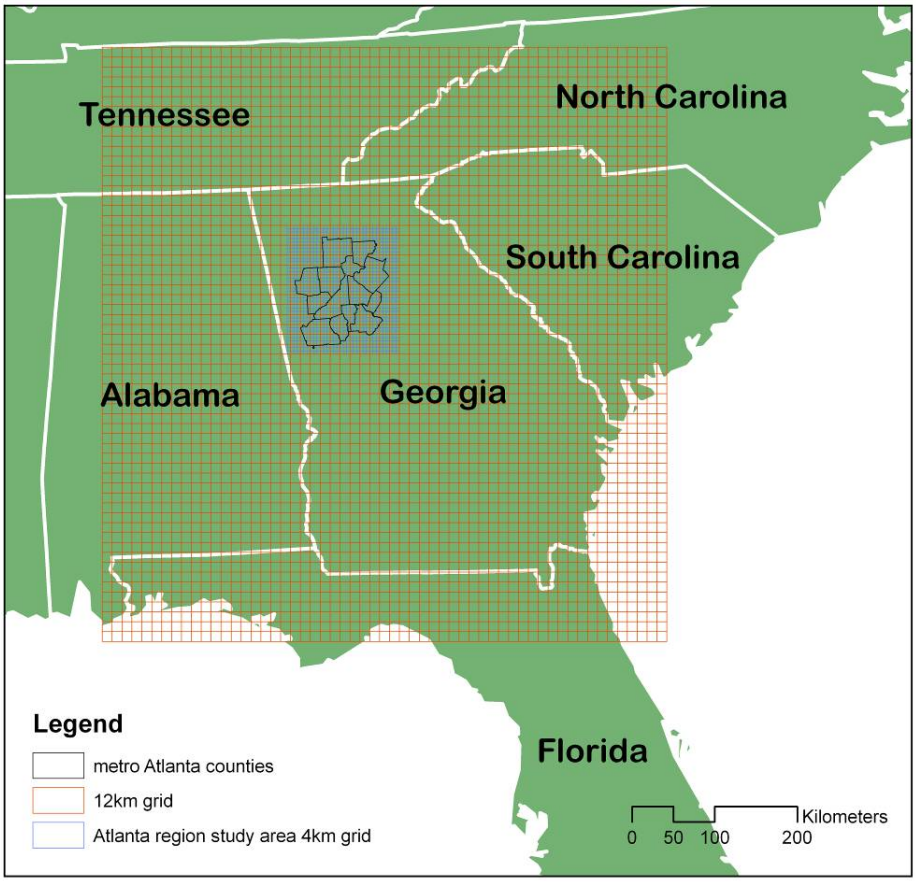

Figure 4.1: 12km Modeling Domain, Fall Line Air Quality Study (57x60). The Atlanta, GA region is highlighted in grey. Map courtesy of Ann Carpenter.

4.2.4 Cost-weighted Inversions

While the inverse method does not require prior knowledge of specific control options, estimates of the costs or availability of possible abatement solutions may be used in the method to develop more economically or politically viable emission adjustments. As an example of this, we weight the inverse model by the relative abatement costs between source regions to minimize the total cost for the emission adjustment scenario. In effect, the sensitivity values which relate concentration changes to emission changes

are converted to cost sensitivities which relate concentration changes to dollars spent on emission controls:

$$Q_{C_{j,p}}^{i,r}(\chi) = \frac{P_{E_{j,p}}^{i,r} / E_{j,p}^{CMAQ}}{C_{j,p}(\chi)} \tag{4.5}$$

where:

$Q_{C_{j,p,\chi}}^{i,r}$ *= Cost-weighted sensitivity of the concentrations of species i at receptor r based on dollars spent for a* χ% *reduction of emissions of species j at source p*

$E_{j,p}^{CMAQ}$ *= total mass of emissions of species j at source p in the CMAQ modeled episode*

$C_{j,p}(\chi)$ *= average cost per ton for reducing species j at source p by* χ%

The cost-weighted sensitivities are then substituted into Equation 4.4, creating a gain matrix which relates changes in concentrations to dollars spent on emissions reductions. Once the adjustments from the inverse calculation are within the acceptable range (see the discussion of the $\mathbf{W_e}$ matrix in Chapter 2 for a description of this range), the sensitivities are weighted by the costs. Because the average cost for emission abatement is dependent on the percentage of emissions reductions, the cost-weighted sensitivities are iteratively solved along with the reductions in emissions. If a source has high costs for reductions, Q is reduced relative to another source which has less impact on downwind concentrations. This iterative process captures the non-linearity of the cost assumptions.

Relative emissions abatement costs for each state were found using a database of emission controls, AirControlNET v4.1(E. H. Pechan & Associates 2005) which contains costs of specific emissions control measures along with their expected reduction

in air pollution emissions. Using the AirControlNET software, least cost reduction scenarios were found to reduce emissions by multiple levels for each source parameter. The controls included in these scenarios were then ranked in terms of cost per ton of emission reductions, and the percent reductions for each abatement option was found in reference to the total controllable emissions included in the AirControlNET database for the source. Emission abatement costs vary by state (Figure 4.2). The costs for reducing emissions up to 30% are similar in Alabama, South Carolina, North Carolina, and Tennessee. Beyond 30% emission reductions are primarily made in mobile sources and therefore vary between states based upon population. Due to the relatively larger quantity of emissions in Florida and Georgia, the percentage control costs are larger as reducing emissions by one percent requires a greater absolute amount of emission reduction. The control options included in these cost estimates may correspond to the same facility and do not directly correlate with sources included in the air quality modeling. However, on a relative basis, this is sufficient for our purposes to demonstrate the effect of a cost-weighting factor in the inverse method. Were cost-weighting to be applied to develop an emissions reduction strategy with specific recommendations on abatement options, least cost curves for each of the source regions similar to Cohan et al. (2006) could be developed.

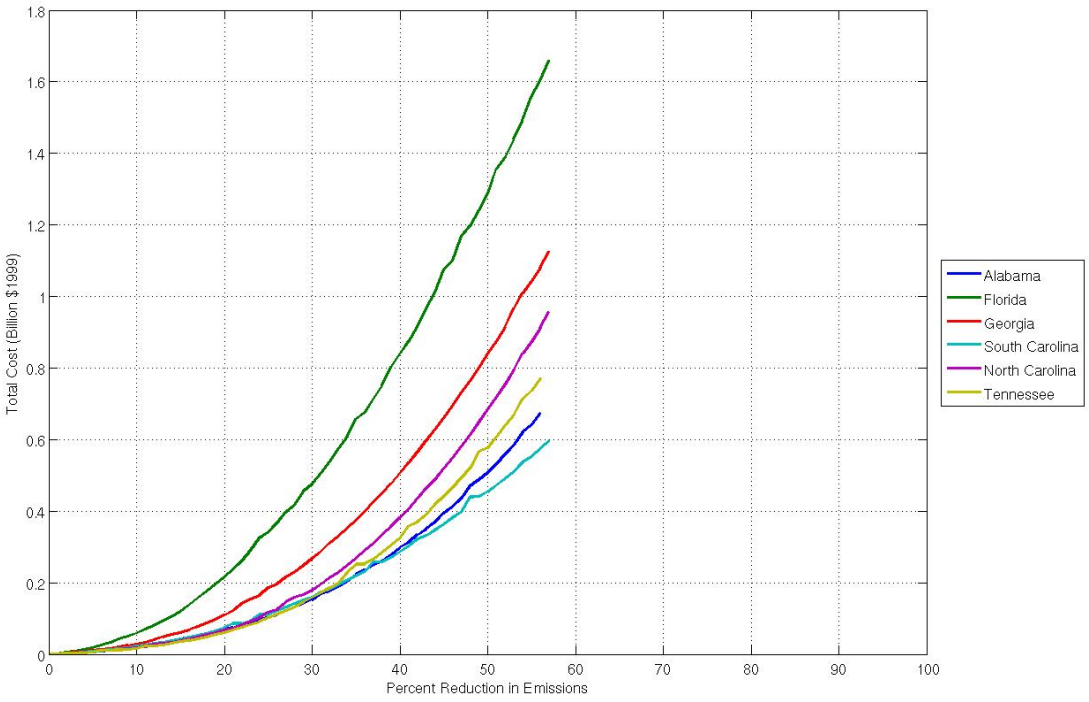

Figure 4.2: Theoretical east cost curves for each state. The abatement costs for a series of goal reductions in emissions are taken from the least cost module of the AirControlNET database (E. H. Pechan & Associates 2005). Theoretical total abatement costs were found using these values. While these values are originally tied with actual emission abatement solutions, the feasibility of applying these solutions in the domain are not accounted for in the total costs shown here. The costs are used here to demonstrate how the method may be weighted to include control costs, if known.

4.3 Results

For the results shown here, the receptor cells are defined as any cell-hour with locally produced 8-hour average ozone concentrations above 0.060ppm. It is possible to set a higher threshold value to control peak concentrations. However, since elevated concentrations are reached during peak hours in limited areas, they are highly dependent on the meteorological patterns during those hours. In tests where only concentrations within Atlanta are considered and the threshold value is increased to 0.08ppm, the state-by-state adjustments have high variability with some states being called to achieve significant reductions while others have little or no emissions adjustment. Such results are due to including only a relatively small number of hours in the inversion. By including areas with moderate concentrations in the inversion, the emission adjustments are distributed more evenly. Although current NAAQS focus solely on peak concentrations, alternative standard metrics including moderate values have been proposed to reduce chronic long-term human exposure (Lippmann 1993) and ozone effects on vegetation (Lefohn and Foley 1992). In addition, by structuring the CAIR replacement rule as a method to reduce regional baseline concentrations, the EPA may avoid some of the Court's criticism yet still allow many marginal regions to avoid reaching nonattainment status.

Desired concentrations are set here as a percentage shift in current concentrations, though explicit limits or reductions can be set as the air quality outcome goal. While it is possible to set specific reductions in each area, having a blanket reduction in all areas is

consistent with reducing chronic exposure throughout the region. The desired concentrations are set at ten percent less than the base case concentrations.

Sensitivity fields for the episode hour with the highest simulated ozone concentrations (19:00EST August 7, 1999; Figure 4.3) indicate very little sensitivity to interstate NO_x transport though a large fraction of ozone is transported into the area from the northern and southern boundaries. Sensitivities are dominated by emissions from the Atlanta region including a few areas with negative sensitivities to NO_x directly downwind of large sources. During this hour, ozone concentrations in Montgomery, AL, Birmingham, AL and Columbia, SC are most sensitive to NO_x emissions within their states. Ozone concentrations in Nashville, TN are negatively sensitive to local NO_x emissions due to large amounts of ozone being transported across the northern border of the domain and local scavenging by fresh NO_x emissions.

LPO_3 is above the threshold primarily in central Alabama, Georgia and South Carolina (Figure 4.4), though high total ozone concentrations are reported in Tennessee and North Carolina (Figure 4.5). The majority of this area also shows high sensitivity to NO_x emissions from Atlanta (Figure 4.3a). The highest LPO_3 concentrations occur over Atlanta, GA, Macon, GA and Birmingham, AL during this hour.

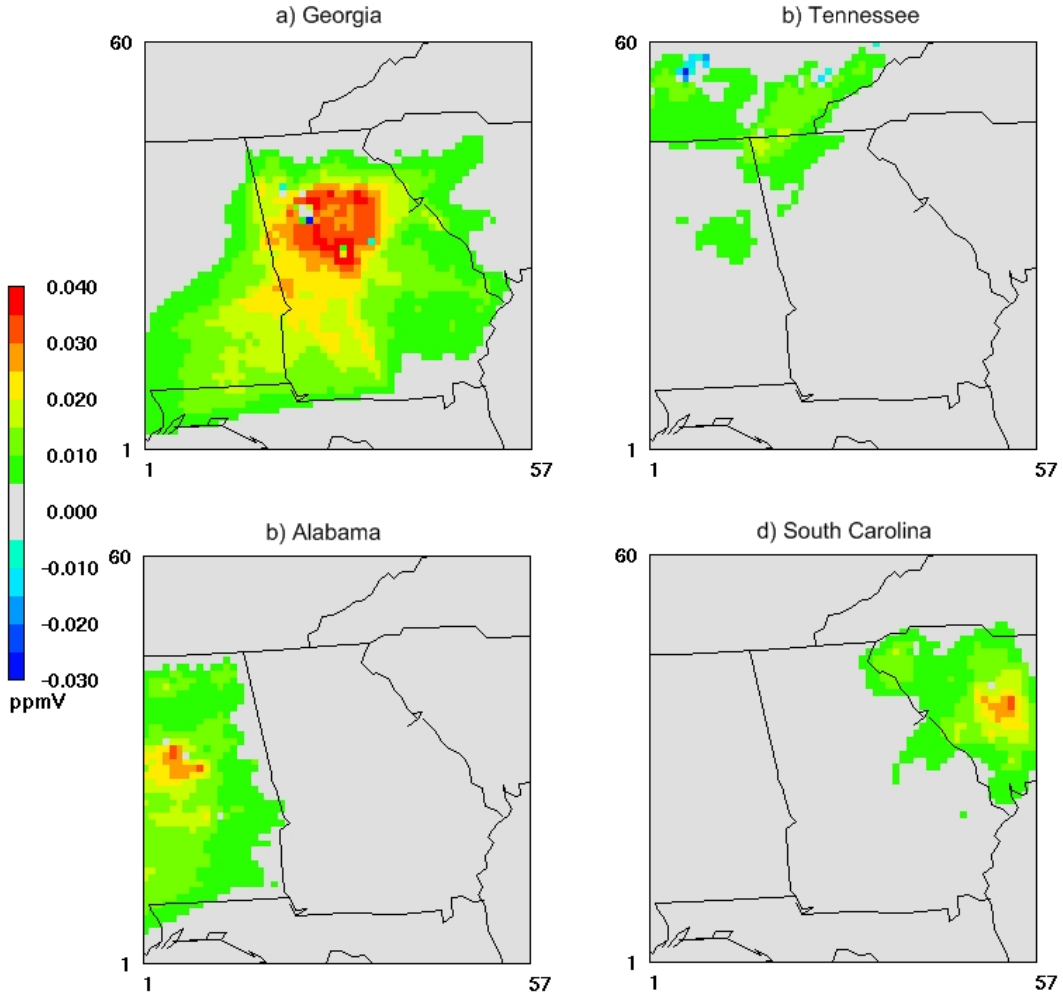

Figure 4.3: Peak hour (19:00EST August 7, 1999) ozone sensitivity to NO_x for each state (a-f) and ozone concentrations sensitive to ozone transport across the boundaries (g). Values shown are estimated from a 100% change in emissions from the state or boundary. The amount of interstate sensitivity is limited though NO_x emissions from Georgia have the greatest interstate effects during this hour, impacting ozone concentrations in south Alabama and western South Carolina. Ozone concentrations in three major cities, Atlanta, GA, Columbia, SC and Birmingham, AL have large sensitivities to NO_x emissions from within their respective states. Ozone transported from the boundaries dominates concentrations in Tennessee, North Carolina and Florida.

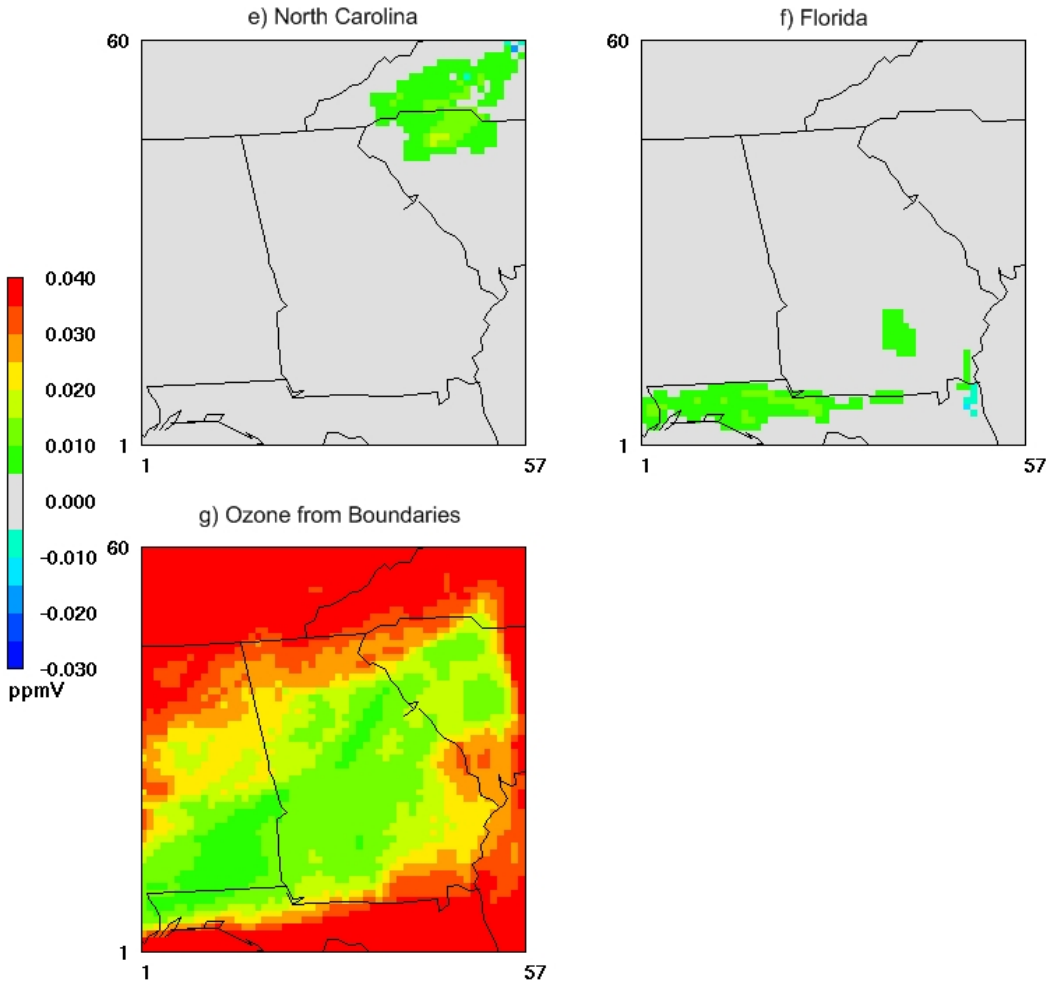

Figure 4.3 continued

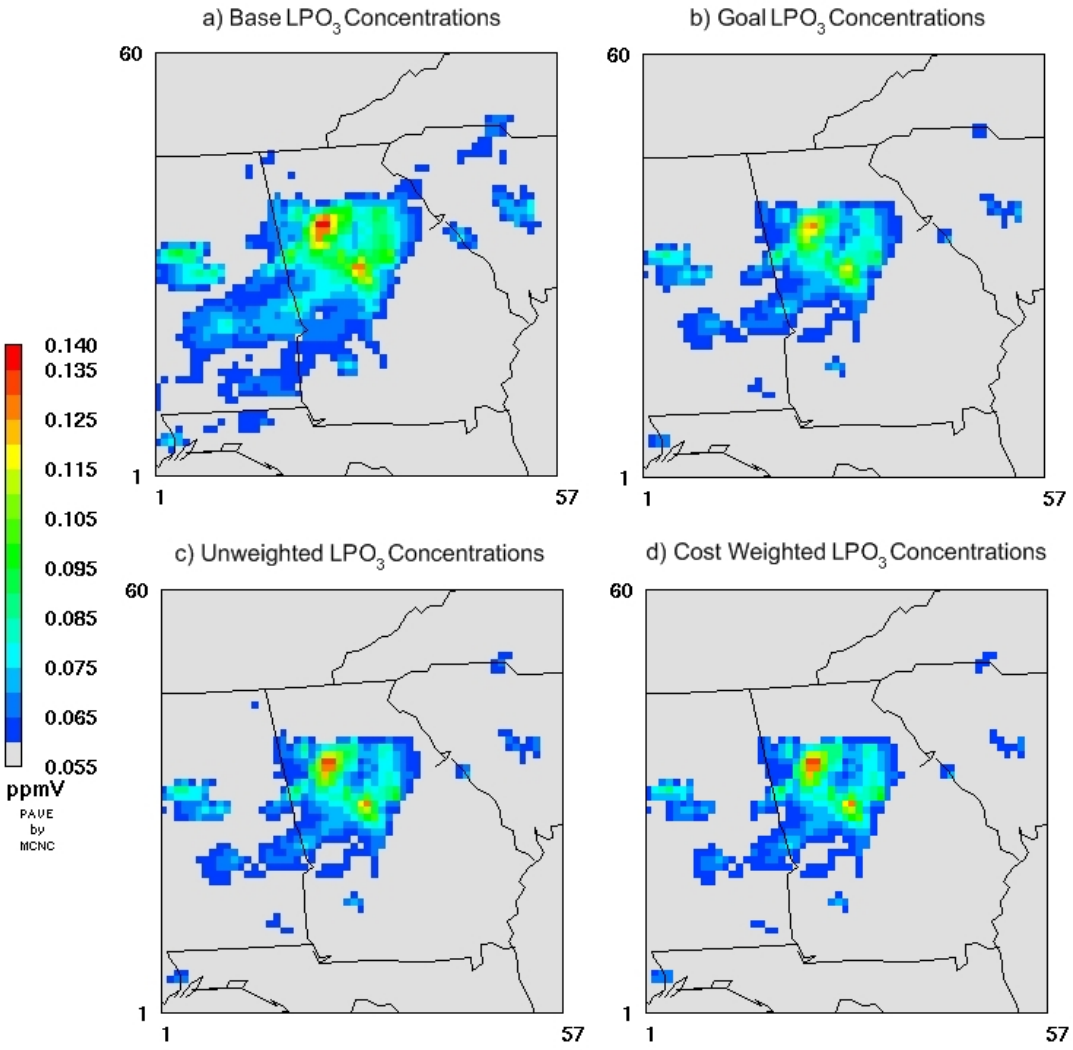

Figure 4.4: LPO_3 concentrations simulated at 19:00EST August 7, 1999. Atlanta and Macon, GA have the highest simulated LPO_3 concentrations (a). While the peak values in these areas are not reduced after adjustment (c – unweighted, d – cost-weighted) to the levels set in the goal (b), areas with lower concentrations (primarily in southeast Alabama and western Georgia) closely match the goal concentrations.

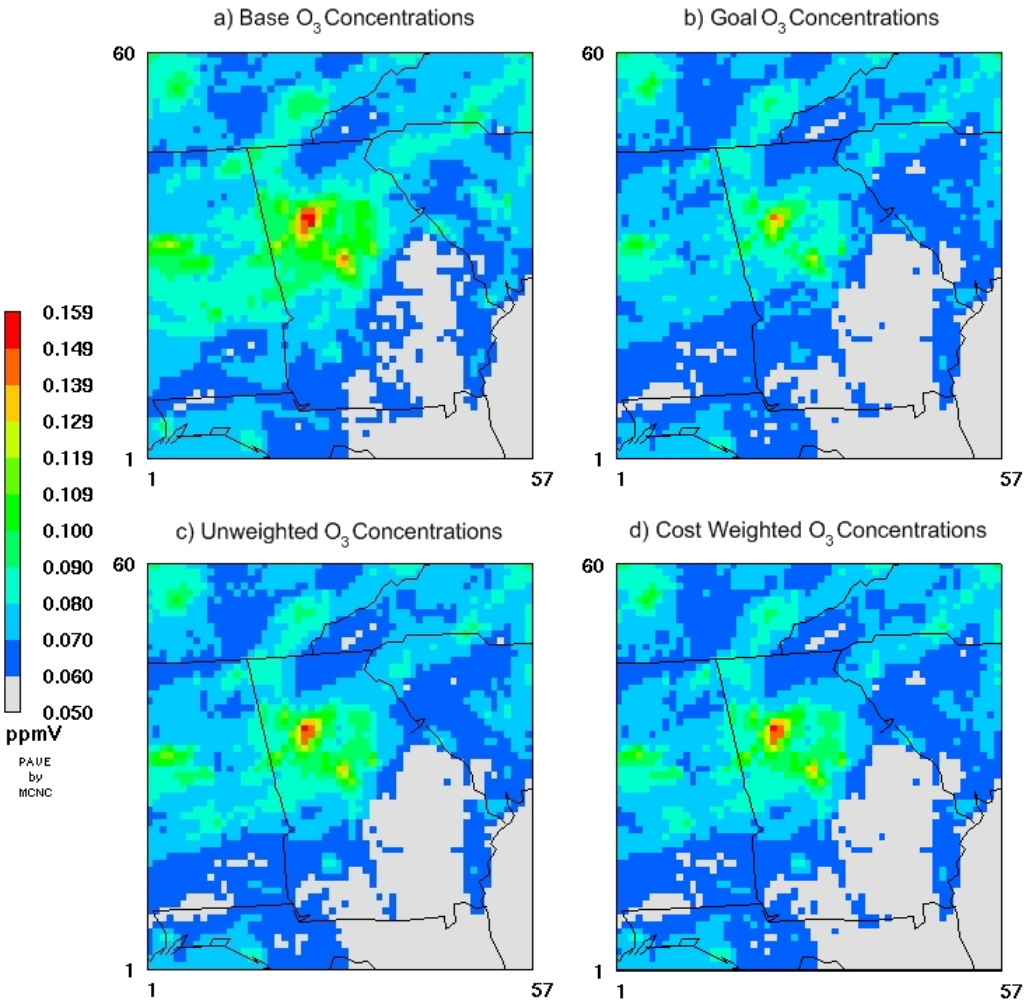

Figure 4.5: Total O_3 concentrations simulated at 19:00EST August 7, 1999. With the domain wide emission reductions, concentrations in Tennessee and North Carolina are reduced even though they were not included in the inversion model directly. Peak concentrations in Atlanta and Macon, GA are not reduced to the goal levels though areas outside these regions show lower concentrations after emissions adjustment.

In the case where cost-based weighting was not used, the inverse method calls for a 23.6% reduction in domain-wide NO_x emissions. The inverse results and final emission totals are listed in Table 4.1. The unweighted adjustments in state-by-state NO_x emissions fall into a narrow band with reductions of 20-24% with the exception of Florida (31.7%). On average, domain-wide NO_x emissions are reduced by 23.6%.

In the cost-weighted case, emissions are equitably reduced based on calculated abatement costs, averaging $150 million per year (1999$US) spent on emission abatement in each state. Since costs for controls in Florida are higher than other states (Figure 4.2), the higher level of emissions reductions in Florida called for in the unweighted case is reduced by half after cost-weighting is applied. To compensate for less emission abatement in Florida, the cost-weighted adjustments in other states increase on average by 6.9%. Emissions reductions in Georgia do not increase as further reductions will likely lead to ozone reductions beyond the 10% goal in moderate downwind areas. Overall, the cost-weighted regime calls for more total emissions reductions than the unweighted case, however at lower theoretical cost overall (Table 4.1).

Table 4.1: Adjustment factor results with total adjusted emissions rates and cost estimations

	Adjustment Factors		Total Emissions (tons/day)			Cost for Adjustment (millions 1999$)	
	Unweighted	*Cost-weighted*	*Base*	*Unweighted*	*Cost-weighted*	*Unweighted*	*Cost-weighted*
AL	-23.1%	-29.0%	236.7	182.0	168.0	$87.8	$141.1
FL	-31.7%	-16.5%	154.0	105.1	128.5	$528.2	$148.5
GA	-23.2%	-22.7%	429.1	329.5	331.9	$153.5	$152.5
SC	-20.7%	-29.4%	149.8	118.8	105.8	$75.7	$153.4
NC	-24.1%	-27.8%	154.1	117.0	111.3	$102.6	$150.0
TN	-20.4%	-29.7%	193.6	154.2	136.2	$63.2	$152.6
Total	**-23.6%**	**-25.5%**	**1317.3**	**1006.6**	**981.8**	**$1,011.0**	**$898.0**

After emissions are adjusted by the inverse procedure, average domain-wide hourly concentrations in grid cells with base case concentrations above 0.06 ppm closely match those of the desired concentrations in both the unweighted and cost-weighted cases (Figure 4.6). The root mean squared error, measuring the average residual between the desired and simulated LPO_3 concentrations at any one cell-hour, is reduced from 7.2×10^{-3} ppm initially to 2.4×10^{-3} ppm and 2.5×10^{-3} ppm in both the unweighted and cost-weighted cases, respectively. Since the goal concentrations are scaled from the base concentrations, the initial mean bias is equal to the root mean square error, 7.2×10^{-3} ppm. After the inverse method adjustments, the error is minimized and the mean bias is reduced to near zero (1.6×10^{-3} ppm in the unweighted case and 7.5×10^{-4} ppm in the cost-weighted case).

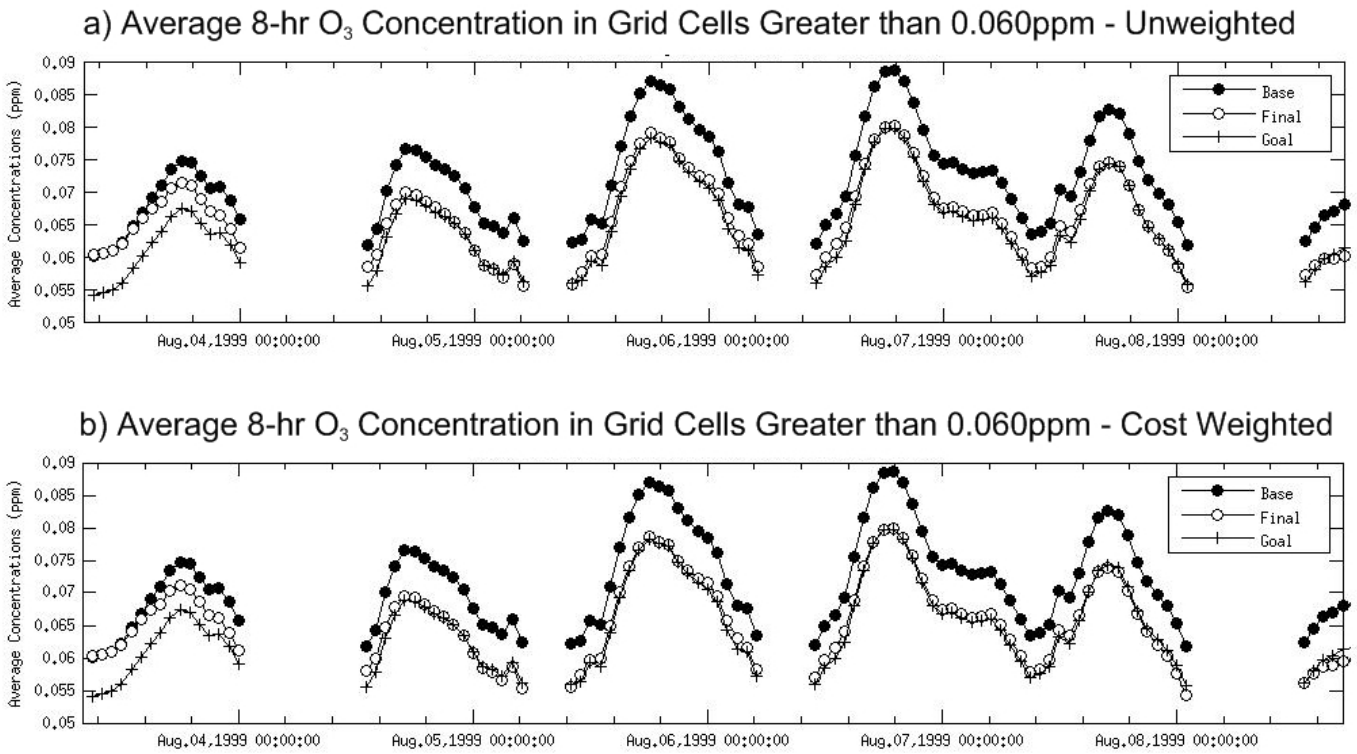

Figure 4.6: Hourly Average LPO_3 Concentrations. After adjustment, the average concentration in cells with initial LPO_3 concentrations over 0.06 ppm converges on the desired concentration

Considering peak hour concentrations, ozone over most of the domain is reduced by the goal amount in both the unweighted and cost-weighted cases. Exceptions include the peak concentrations in downtown Atlanta and Macon, GA which do not achieve a full 10% reduction from base levels. These downtown locations show negative ozone sensitivity to NO_x reductions in Georgia (Figure 4.3). At regions of extremely high ozone, NO_x emissions can destroy more ozone through NO scavenging than they produce. Further reductions in Georgia NO_x emissions will cause an increase in ozone concentrations at these locations. This indicates that VOC reductions will be needed to reduce the peak concentrations for this hour.

4.4 Discussion

The method outlined here shows the potential for inverse air quality modeling to address the concerns of the DC Circuit on the EPA's proposed CAIR. By using such an approach, it is possible to include the downwind impacts to develop an understanding of how each state's emissions should change to achieve reductions in air pollution in areas across the region. While a representative test case is shown here for a series of cities in central Georgia and neighboring states, regional modeling on an expanded domain can find optimal emission reductions for all of the CAIR states to reduce ozone and particulate matter below the ambient standard levels.

With specific emissions adjustments for each state, the EPA can regulate emission trades to prevent allowances from being transferred to areas where emissions have a worse impact on air quality, though such oversight of trades may lead to increased regulatory costs (Tietenberg 1995; Bryner 1999). Because the method does not specify how emissions can be controlled, emissions sources may be transferred between states, as long as these transfers occur to regions where emissions are below the caps established by the inverse method. If a broad regional approach is abandoned, the emissions adjustments may be used to set state specific caps in trading programs at the state level. In the past, several states have implemented such trading programs with success (Bryner 1999).

One of the benefits of this approach is that it does not require the *a priori* specification of emission abatement solutions. The method produces aggregate adjustments in emissions by state, leaving the identification and implementation of specific emission controls to local air quality managers. It is possible to achieve the suggested emission reductions by a traditional command and control method, where state and local governments mandate specific emission reductions based upon technical feasibility. However, more sophisticated market-based solutions may be adopted to allow firms to find the least costly abatement methods to reach the air quality improvement targets. In the place of the traditional command-and-control methods, effluent charging systems may be implemented where polluters or end users pay a fixed rate based on the amount of environmental impact. Such charges are theoretically most efficient when polluters (or end users) pay fees based on the social cost of their emissions. Regulators may use spatial emission reduction targets in optimally setting these fees (Stavins 2003).

With an understanding of how much emissions should change in a region, more unconventional methods for finding emission reductions may be proposed. Sales of emission permits or a taxation scheme may be used to raise funds from existing sources to incentivize firms to make initial emission reductions. If reductions from the taxation scheme are not sufficient to reach the reductions proposed by the inverse method, these funds may be disbursed to fund further emission reductions. Alternative emission sources in an area may place bids for this funding if they can verifiably reduce emission levels at cheaper rates than others. Alternatively, a bounty, similar to the X-prize seen in the aerospace industry, may be set for finding new solutions which reduce emissions by a certain amount. Such programs may include groups that are not traditionally a part of the CAIR system. For example, if members of a local community organization or neighborhood school are able to verifiably reduce their personal emissions, they may make a bid for tax funds or compete in the bounty competition.

As recent debate of the creation of a carbon trading program has shown, the allocations of emission permits and the effects of increasing abatement costs on specific industries is a highly political topic. With estimates of how emissions should change within each area, this legislative process may be better informed to prevent local political interests from creating emission hotspots. Moreover, the inverse results may be weighted to include costs as was shown in the cost-weighted case here preventing too much burden on a single state or region.

While in the cases modeled here, a blanket percentage reduction in ozone concentrations is set as the goal, it is possible to include variations in the goal air quality endpoints (e.g. reductions required to meet a set of standards). These can be linked with

integrated assessment modeling to calculate exposure and health effects from a spatial distribution of ozone concentrations (Mauzerall, Sultan et al. 2005; Tong, Muller et al. 2006). By linking these exposure models to the inverse method presented here, regional emission adjustments may be found to maximize positive health outcomes in the eventual replacement of CAIR.

4.5 References

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CHAPTER 5

MULTIPLE POLLUTANT IMPACTS FROM SEASONAL EMISSIONS CONTROLS

5.1 Introduction

The United States Congress set criteria under the Clean Air Act for limiting air pollution to protect human health and environmental wellbeing. Six air pollutants are regulated under these criteria by the United States Environmental Protection Agency (U.S. EPA): nitrogen dioxide (NO_2), sulfur dioxide (SO_2), carbon monoxide, lead, particulate matter, and ozone. The first four criteria air pollutants are directly emitted into the atmosphere. Managing these pollutants has been largely successful, as emission sources of these "primary" pollutants have been identified and reduced using available control technology (U.S. Environmental Protection Agency 2003). The last two, ozone and a portion of fine particulate matter (i.e., $PM_{2.5}$, particulate matter with aerodynamic diameters less than 2.5 microns), are considered "secondary" pollutants since they are not directly emitted and instead are formed in the atmosphere from emissions of other precursor species. Therefore, designing management strategies for ozone and secondary $PM_{2.5}$ relies on controlling precursor species emissions (U.S. Environmental Protection Agency 1997).

Since ozone and $PM_{2.5}$ have precursors in common, precursor controls should be evaluated for their effects on both pollutants. In their 2004 report on air quality management in the United States, the National Research Council recommended that the

U.S. EPA and states consider an integrated multipollutant approach to air pollution control using these common dependencies to reach reductions in both pollutants and to ensure that controls for one pollutant do not hamper efforts to reduce concentrations of other pollutants (National Research Council of the National Academies 2004). Studies have found that more cost effective solutions for air quality management may be developed by including ancillary benefits of emissions reductions (Chestnut, Mills et al. 2006).

Additionally, there is recent evidence that the health impacts from multiple air pollutants exceed those seen from an individual air pollutant (Tolbert, Klein et al. 2007; Mauderly and Samet 2009). A study by the NARSTO currently under review attempts to go beyond the typical emphasis on managing ambient air quality concentrations by linking the risk from air pollution mixtures directly to emissions of common precursors (Brook, Demerjian et al. 2009). To mitigate health damage from exposures of mixtures of pollutants, it will be necessary to first understand how precursor emissions impact multiple pollutants.

Air quality models (AQM) simulate how possible precursor controls will affect air pollution and are used by air quality managers to ensure that the proposed emission reductions will lead to the desired air quality outcomes (U.S. Environmental Protection Agency 1997; U.S. Environmental Protection Agency 1999). Cohan et al. (2007) demonstrates the use of AQM for calculating both the cost efficiency and health benefits from reducing the common precursors of ozone and $PM_{2.5}$. Liao et al. (2008) used air quality modeling to study how climate change and future emission controls will affect the production of secondary pollutants from emissions of precursor species.

Here, we calculate the sensitivity of ozone and particulate matter species to domain-wide emissions of several emission precursors: Anthropogenic Volatile Organic Compounds (AVOC), Nitrogen oxides (NO_x), and SO_2. Implications for emission controls on each of these species are compared in regards to how they affect pollutant concentrations in multiple seasons. An inverse modeling case is used to develop a multipollutant reduction strategy for an episode of elevated ozone and $PM_{2.5}$ concentrations. The effect from basing a strategy on this summertime episode on the remaining year is evaluated for the annual average $PM_{2.5}$ concentrations and the maximum ozone concentrations.

5.2 Methods

The Community Multiscale Air Quality Model version 4.5 (CMAQ) (Byun and Schere 2006) was applied to May 2007-April 2008 on a 12-km domain covering the southeastern United States centered on Atlanta, GA (Figure 5.1). Sensitivities were calculated using the Direct, Decoupled Method in three dimensions (DDM-3D) (Cohan, Hakami et al. 2005; Napelenok, Cohan et al. 2006).The meteorology and emission input files for the simulation were originally developed to forecast ozone and particulate matter to aid in the issuing of air quality advisories (Odman, Hu et al. 2007) and have been applied to model the impact of prescribed fires in the southeast (Hu, Odman et al. 2008). Meteorology inputs were calculated using the Weather Forecasting and Research model (WRF, version 2.2), with initial and boundary conditions taken from the 84 hour 00Z forecast from the North American Mesoscale (nomads.ncdc.noaa.gov) model. In addition, NAM analysis data was assimilated by WRF at 6 hour intervals. The Sparse Matrix Operator Kernel Emissions model version 2.3(Carolina Environmental Program 2003)

was used to produce the gridded emissions using a 2007 inventory projected from a 2002 "typical" year inventory

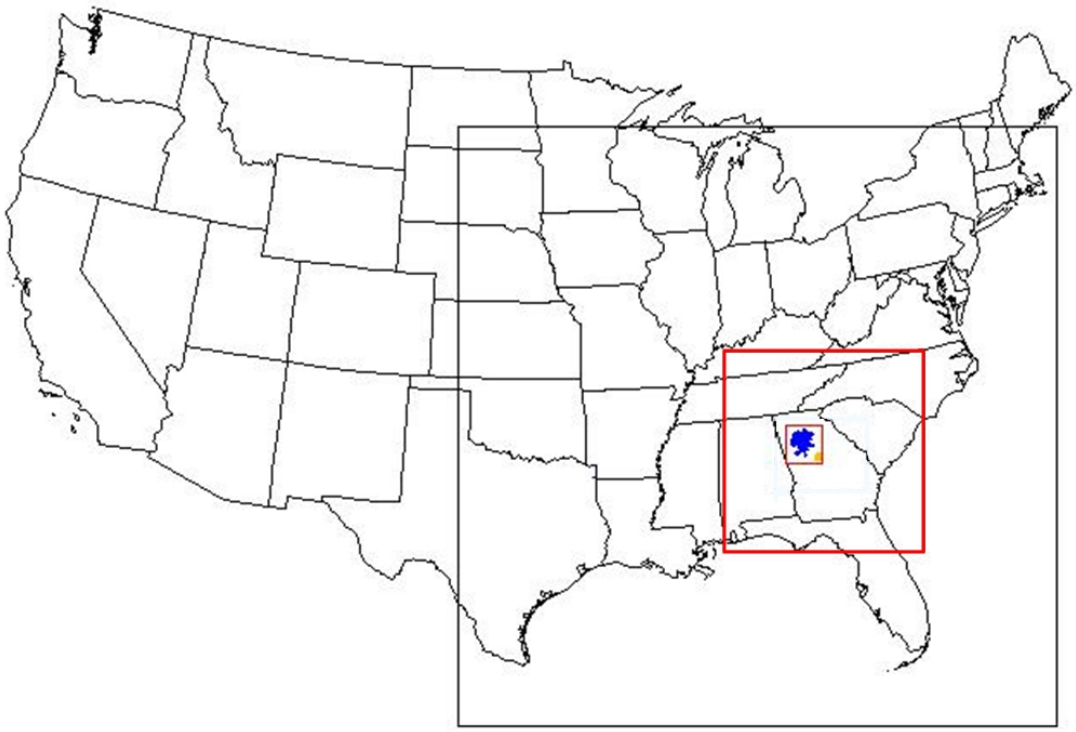

Figure 5.1: Model domain: The 36-km black box shows the 36 km mother domain. The 12 km domain is outlined in red. Atlanta, GA is shown within the inner red box. Map courtesy of Dr. Yongtao Hu,

(MACTEC 2005). To produce initial and boundary air quality concentrations for the 12-km domain, CMAQ was first run with clean boundaries for a 36-km mother domain covering the eastern United States with the meteorology and emissions inputs prepared using the same way as for the 12-km domain. CMAQ was updated for strict mass conversation (Hu, Odman et al. 2006) and included the SAPRC-99 chemical mechanism (Carter 2000).

5.2.1 Sensitivity Analysis

Sensitivities found by the DDM-3D model estimate the effects of precursor emissions on the modeled pollutant concentrations:

$$P_j^i = \frac{\Delta C_i}{\Delta \varepsilon_j} E_j \tag{5.1}$$

where:

P_j^i *= Total sensitivity of pollutant species i to emissions of precursor species j*

ΔC_i *= Concentration of pollutant species i*

$\Delta \varepsilon_j$ *= Perturbation in emissions of species j*

E_j*= Total emissions of precursor species j*

DDM-3D calculates these sensitivities concurrently with simulating the chemistry and transport of the atmosphere, and multiple sensitivities may be calculated for a variety of precursor species during a single simulation. Further details of the DDM-3D implementation in CMAQ may be found in Cohan et al. (2005) and Napelenok et al. (2006). As presented here, these sensitivities may be interpreted as the amount of pollution reduction that will occur from a total removal of emissions of a precursor species and, in effect, as the total contribution of a pollutant from a precursor species. Negative sensitivity values indicate that a reduction in precursor emissions will lead to an increase in pollutant concentrations. These sensitivity values estimating the contributions or reductions of air pollutants from precursor emission controls may then be compared to find which emission controls will be the most effective.

5.3 Model comparison with observed concentrations

The Georgia Environmental Protection Division measures ambient ozone and particulate matter at several locations around the Atlanta, GA metropolitan area (Georgia Environmental Protection Division http://www.gaepd.org/air/amp/). Observations from three of these monitor locations are compared with the simulated concentrations. Two urban monitors, South Dekalb and Confederate Avenue, are located in a single 12-km grid cell and were averaged together for comparison with the simulated concentrations. Additionally, simulated concentrations are compared with observations from a rural monitoring site, at Yorkville, approximately 70 km WNW of Atlanta.

Ozone concentrations reach a daily maximum during the summertime months due to increased photochemistry due to longer periods of sunlight and warmer temperatures. Two-month averages of the simulated maximum daily 8-hour average ozone concentrations for the grid cells containing the urban and rural monitors are shown in Table 5.1a-b. Ozone observations at the rural monitor are higher than those for the urban monitors on average, though the urban site observed more days with concentrations above 80 ppb. To describe concentrations across the Atlanta area, two month average values are given based on the daily maximum 8-hour average ozone concentration simulated in any grid cell over Atlanta, GA (Table 5.1c). The average maximum 8-hour ozone concentration simulated anywhere in Atlanta was 0.017 ppm higher than the average simulated values at either monitor site.

The composition of particulate matter changes between seasons. In the winter, lower mixing heights combined with higher levels of biomass burning and heating

combustion, particulate matter concentrations are higher than summertime levels (Tian, Hu et al. 2008). With relatively low photochemistry, the oxidation of SO_2 and organic compounds is reduced and primary aerosol becomes a larger fraction of the simulated $PM_{2.5}$ concentrations (Table 5.1), reaching up to 65.7% of total $PM_{2.5}$ mass for the maximum simulated values in Atlanta in January-February 2008. In the summer, with highly active photochemistry, secondary pollutants such as sulfate and secondary organic aerosol (SOA) become a greater fraction of the simulated $PM_{2.5}$. In the summer, the dominate secondary $PM_{2.5}$ species is sulfate, reaching up to 59.3% of secondary $PM_{2.5}$ in July-August 2007. Aerosol nitrate is a minor fraction in the summer, but they comprise a larger (25.5-26.6%) fraction in the winter due to lower temperatures. The urban site has larger simulated fractions of primary aerosols than the rural site during the year (47% at the urban monitor versus 39.4% at the rural monitor).

Comparisons between the simulated maximum daily 8-hour average ozone concentrations with the observations at the urban monitors show a positive bias in the modeled concentrations during periods of low ozone and negative bias during periods with the highest concentrations (Figure 5.2b, Table 5.2a) The overall model performance was similar for the rural monitor and urban monitors. The rural site monitor did not report ozone concentrations during the peak hours for several days in July-August 2007. These values skew the error and bias estimates (Table 5.2b). Ozone was not monitored during the winter months (November – February).

Table 5.1: Average Concentrations

Table 5.1a: South Dekalb and Confederate Ave

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	Primary PM2.5 *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	1.200	0.137	0.052	2.012	3.319	11.341	4.622	0.060	0.004	0.004	0.023
Jul-Aug 2007	1.402	0.071	0.043	1.863	4.199	12.403	4.826	0.065	0.004	0.005	0.029
Sept-Oct 2007	1.433	0.391	0.092	2.646	3.672	14.356	6.122	0.054	0.006	0.005	0.029
Nov-Dec 2007	1.720	2.116	0.165	1.698	3.076	17.935	9.159	0.038	0.004	0.008	0.048
Jan-Feb 2008	1.452	1.981	0.211	1.347	2.455	17.890	10.444	0.041	0.003	0.009	0.048
Mar-Apr 2008	1.369	1.162	0.136	1.673	2.804	14.372	7.228	0.052	0.004	0.006	0.033

Table 5.1b: Yorkville

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	Primary PM2.5 *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	1.264	0.165	0.053	2.599	3.630	11.662	3.950	0.061	0.004	0.008	0.014
Jul-Aug 2007	1.464	0.066	0.025	1.796	4.882	11.828	3.594	0.065	0.004	0.011	0.011
Sept-Oct 2007	1.517	0.428	0.109	2.990	4.036	14.316	5.237	0.057	0.005	0.006	0.017
Nov-Dec 2007	1.552	1.869	0.136	1.898	2.860	14.442	6.127	0.042	0.004	0.007	0.020
Jan-Feb 2008	1.230	1.703	0.172	1.421	2.142	13.921	7.253	0.044	0.002	0.009	0.020
Mar-Apr 2008	1.396	1.135	0.108	1.760	2.986	12.501	5.117	0.053	0.004	0.007	0.014

Table 5.3 Continued
Table 5.1c: Atlanta

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	Primary PM2.5 *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	1.777	0.507	0.130	3.792	5.250	23.940	12.485	0.074	0.025	0.020	0.059
Jul-Aug 2007	2.075	0.283	0.110	3.402	6.795	25.912	13.249	0.082	0.025	0.023	0.061
Sept-Oct 2007	2.037	0.946	0.192	4.476	5.409	27.486	14.427	0.067	0.030	0.019	0.065
Nov-Dec 2007	2.333	3.623	0.228	3.355	4.130	33.371	19.702	0.049	0.018	0.020	0.092
Jan-Feb 2008	2.019	3.174	0.274	2.516	3.541	33.587	22.062	0.050	0.011	0.023	0.097
Mar-Apr 2008	2.016	2.321	0.214	2.903	4.105	27.915	16.356	0.059	0.021	0.019	0.065

ANH4 = Aerosol Ammonium; ANO3 = Aerosol Nitrate; AORGA = Secondary Organic Aerosol from Anthropogenic Volatile Organic Compounds; AORGB = Secondary Organic Aerosol from Biogenic Volatile Organic Compounds; ASO4 = Aerosol Sulfate;

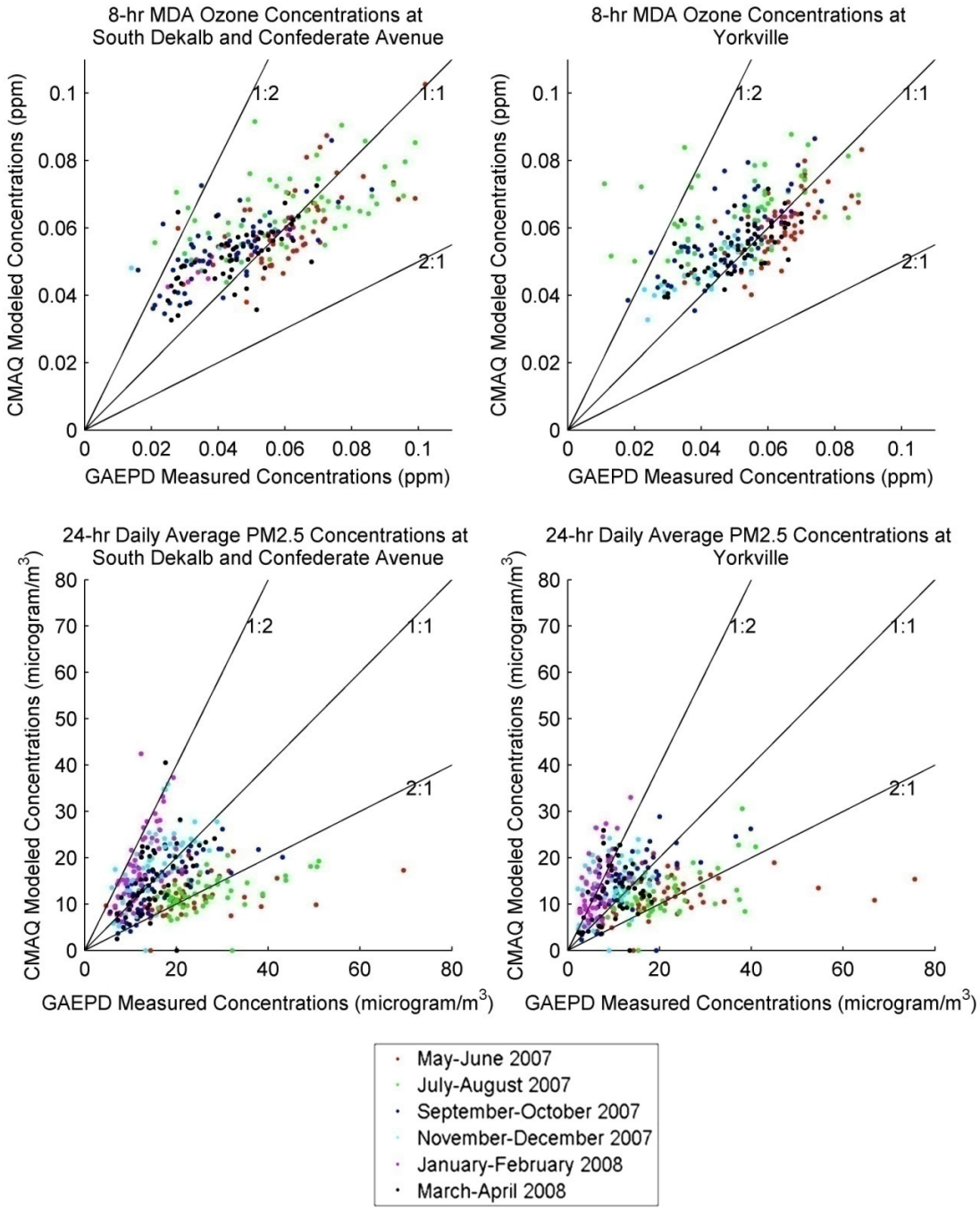

Figure 5.2: Comparison of observed concentrations and simulated concentrations.

Table 5.2:Performance Evaluation: Ozone

Table 5.2a: South Dekalb and Confederate Avenue

	N	RMSE *(ppm)*	ME *(ppm)*	MB *(ppm)*	MNE %	MNB %
May-June 2007	58	0.0114	0.0090	-0.0003	16.84	3.49
July-August 2007	61	0.0177	0.0141	0.0034	29.03	16.42
September-October 2007	60	0.0151	0.0125	0.0108	37.99	35.59
November-December 2007	2	0.0260	0.0239	0.0239	138.75	138.75
January-February 2008	4	0.0132	0.0128	0.0128	42.73	42.73
March-April 2008	57	0.0113	0.0088	0.0066	24.44	20.52

Table 5.2b: Yorkville

	N	RMSE *(ppm)*	ME *(ppm)*	MB *(ppm)*	MNE %	MNB %
May-June 2007	58	0.0084	0.0070	-0.0031	11.38	-3.66
July-August 2007	61	0.0206	0.0163	0.0136	50.05	46.43
September-October 2007	55	0.0131	0.0105	0.0096	26.48	24.99
November-December 2007	27	0.0085	0.0071	0.0055	20.86	17.89
January-February 2008	0	--	--	--	--	--
March-April 2008	57	0.0086	0.0064	0.0028	14.91	9.00

N = Number of days with observations, RMSE = Root Mean Square Error, ME = Mean Error, MB = Mean Bias, MNE = Mean Normalized Error, MNB = Mean Normalized Bias

Simulated daily average $PM_{2.5}$ concentrations at the monitoring sites have positive bias in the winter and negative bias in the summer months when compared with observations (Figure 5.2, Table 5.3). Several extremely high $PM_{2.5}$ concentrations observed in May-June 2007 are due to large wildfires on the Georgia-Florida border that were not included in the emissions inventory and are therefore severely underestimated by the simulations (Figure 2; Hu, Baek et al. 2008). The low simulated values in the summertime are likely due to underestimations of the SOA production from biogenic VOC (BVOC) within the CMAQ model (Hu, Baek et al. 2008; Kroll and Seinfeld 2008). The overestimated $PM_{2.5}$ concentrations in winter are likely due to errors in the emission inventory for primary organic aerosol from residential wood burning (Tian, Hu et al. 2008).

Table 5.3: Performance Evaluation: $PM_{2.5}$
Table 5.3a: South Dekalb and Confederate Avenue

	N	RMSE ($\mu g/m^3$)	ME ($\mu g/m^3$)	MB ($\mu g/m^3$)	MNE %	MNB %
May-June 2007	52	14.91	11.38	-10.99	47.34	-39.95
July-August 2007	60	15.53	13.38	-13.34	49.02	-48.71
September-October 2007	57	5.94	4.30	-2.27	25.40	-7.68
November-December 2007	58	6.58	4.97	3.22	39.17	25.81
January-February 2008	56	8.78	6.71	6.22	55.25	51.37
March-April 2008	55	6.02	4.33	-0.46	29.39	-1.84

Table 5.3b: Yorkville

	N	RMSE ($\mu g/m^3$)	ME ($\mu g/m^3$)	MB ($\mu g/m^3$)	MNE %	MNB %
May-June 2007	53	16.12	10.81	-10.06	43.55	-33.55
July-August 2007	53	11.07	8.52	-8.12	37.44	-33.58
September-October 2007	46	6.18	4.81	0.98	47.45	28.13
November-December 2007	56	7.90	6.12	5.07	100.16	91.25
January-February 2008	52	9.14	7.53	7.49	129.73	129.22
March-April 2008	52	6.65	5.26	2.29	58.29	34.77

N = Number of days with observations, RMSE = Root Mean Square Error, ME = Mean Error, MB = Mean Bias, MNE = Mean Normalized Error, MNB = Mean Normalized Bias

5.4 Pollutant sensitivities to precursor emissions

5.4.1 Sensitivities to NO_x emissions

Nitrogen oxide (NO) and NO_2 are grouped together for analysis as NO_x since they are rapidly interconverted in the atmosphere. NO_x is formed from the reaction of N_2 with O_2 at high temperatures during combustion of fossil fuels. Surface NO_x emissions are predominately from mobile sources in urban areas. Emissions of elevated NO_x is mostly due to point sources such as electrical generating units (Heinsohn and Kabel 1999). NO_x can be a respiratory irritant at high concentrations and contributes to acid deposition.

In the summertime, the photolysis of NO_2 by sunlight produces ozone. However, under certain conditions, NO_x emissions may scavenge ozone ($NO + O_3 \rightarrow NO_2 + O_2$). Tropospheric ozone build up in the summer is due to the conversion of NO back into NO_2 through alternative reactions with VOC and other radicals (Haagen-Smit 1952; Duncan and Chameides 1998). In July-August 2007, total NO_x contributed 21.0% of the ozone at the urban site and 20.4% at the rural site based on the sensitivity analysis. The sensitivity analysis indicates that NO_x controls are effective at reducing aerosol nitrate concentrations though nitrate is only a minor component of secondary $PM_{2.5}$ in summer (<1% in July-August 2007) (Figure 5.3, Table 5.4). Concentrations of organic and sulfate aerosols are sensitive to NO_x emissions since there will be less production of oxidants from NO_2 photolysis.

In the winter with shorter periods of sunlight for NO_2 photolysis, ozone concentrations show a negative sensitivity to NO_x as the NO scavenging reaction dominates (Figure 5.3, Table 5.4). At the urban site, based on the sensitivity analysis, total removal of NO_x emissions reductions would increase ozone by 19.0%. Though the concentrations remain below the NAAQS, studies have indicated that health risks from ozone exposure are present even at low concentrations (Bell, Peng et al. 2006). Aerosol nitrate is sensitive to NO_x emissions though it is more sensitive to ammonia (NH3) (see section 5.4.4). Due to its competition for oxidants, emissions of NO_x in winter decrease the available oxidants to react with VOC and SO_2 leading to less SOA and aerosol sulfate though these interactions are small (Napelenok, Cohan et al. 2006; Liao, Tagaris et al. 2008).

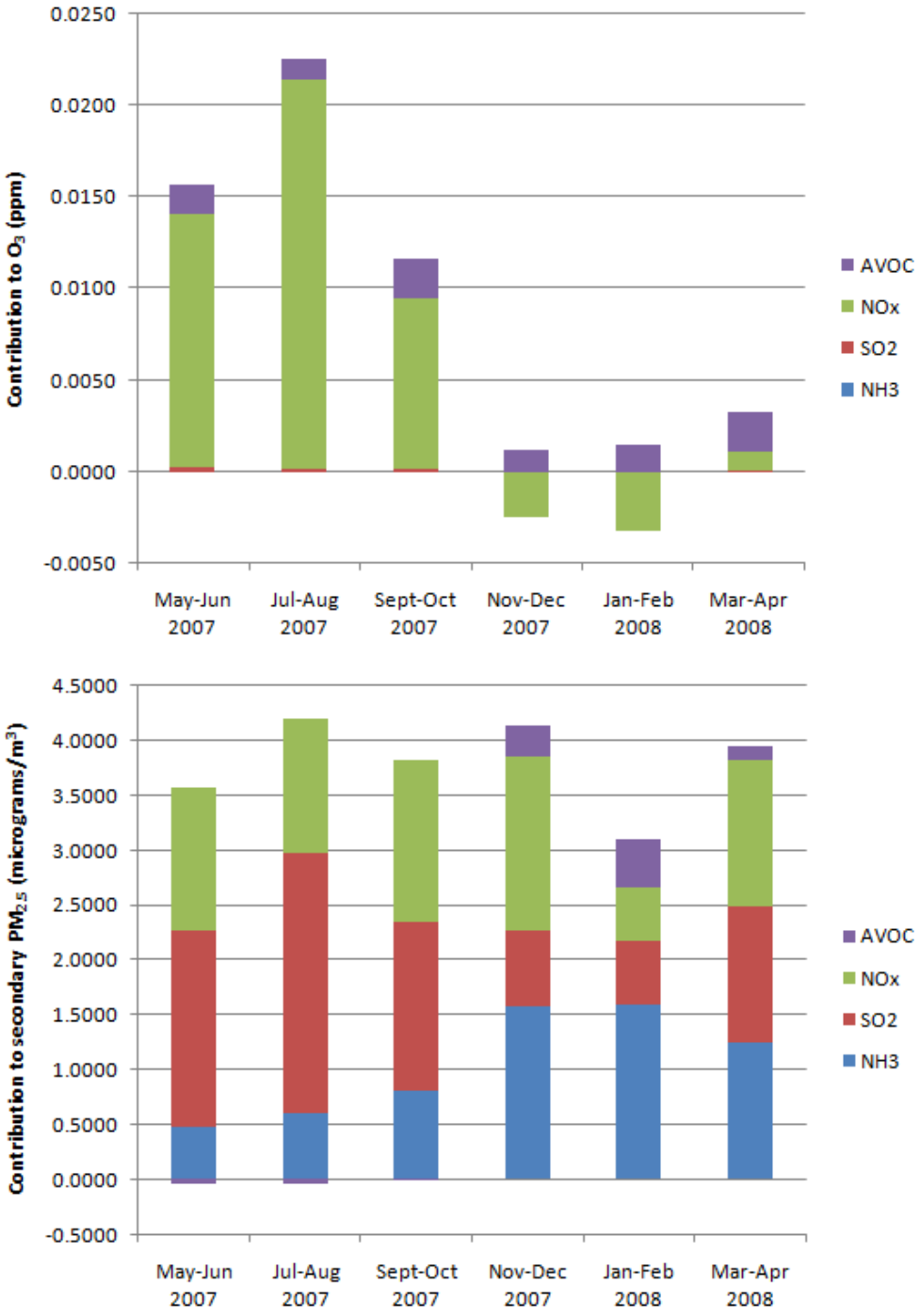

Figure 5.3: Total sensitivity of ozone and secondary $PM_{2.5}$ to anthropogenic volatile organic compounds, oxides of nitrogen, sulfur dioxide, and ammonia.

Table 5.4: Average sensitivity to NO_x emissions

Table 5.4a: South Dekalb and Confederate Ave

	ANH_4 *(μg/m³)*	ANO_3 *(μg/m³)*	AORGA *(μg/m³)*	AORGB *(μg/m³)*	ASO_4 *(μg/m³)*	$PM_{2.5}$ *(μg/m³)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	2.40	0.11	0.01	0.05	0.30	0.58	0.0087	-0.0001	-0.0001	0.0039
Jul-Aug 2007	0.10	0.06	0.01	0.07	0.35	0.59	0.0136	0.0000	-0.0001	0.0040
Sept-Oct 2007	0.16	0.31	0.01	0.03	0.21	0.73	0.0050	0.0000	0.0000	0.0045
Nov-Dec 2007	0.20	0.88	-0.04	-0.26	-0.14	0.64	-0.0095	-0.0001	0.0000	0.0125
Jan-Feb 2008	0.11	0.61	-0.08	-0.22	-0.22	0.20	-0.0093	0.0000	0.0000	0.0112
Mar-Apr 2008	0.13	0.50	-0.03	-0.18	-0.06	0.35	-0.0033	0.0000	0.0000	0.0065

Table 5.4b: Yorkville

	ANH_4 *(μg/m³)*	ANO_3 *(μg/m³)*	AORGA *(μg/m³)*	AORGB *(μg/m³)*	ASO_4 *(μg/m³)*	$PM_{2.5}$ *(μg/m³)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	0.13	0.15	0.01	0.25	0.27	0.81	0.0095	-0.0001	-0.0001	0.0027
Jul-Aug 2007	0.10	0.06	0.01	0.21	0.36	0.73	0.0131	0.0000	-0.0001	0.0032
Sept-Oct 2007	0.17	0.36	0.01	0.27	0.22	1.03	0.0067	-0.0001	-0.0001	0.0040
Nov-Dec 2007	0.15	0.67	-0.03	-0.13	-0.14	0.52	-0.0054	0.0000	0.0000	0.0073
Jan-Feb 2008	0.12	0.58	-0.05	-0.13	-0.16	0.37	-0.0057	0.0000	0.0000	0.0066
Mar-Apr 2008	0.19	0.68	0.00	0.04	-0.10	0.81	-0.0009	0.0000	0.0001	0.0044

Table 5.4c: Atlanta

	ANH_4 *(μg/m³)*	ANO_3 *(μg/m³)*	AORGA *(μg/m³)*	AORGB *(μg/m³)*	ASO_4 *(μg/m³)*	$PM_{2.5}$ *(μg/m³)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	0.20	0.33	0.01	0.35	0.42	1.30	0.0138	-0.0002	-0.0002	0.0120
Jul-Aug 2007	0.15	0.21	0.01	0.31	0.54	1.23	0.0212	-0.0002	-0.0003	0.0119
Sept-Oct 2007	0.22	0.57	0.01	0.43	0.24	1.47	0.0093	-0.0002	-0.0001	0.0178
Nov-Dec 2007	0.32	1.48	-0.05	0.03	-0.19	1.59	-0.0025	-0.0003	0.0000	0.0328
Jan-Feb 2008	0.13	0.75	-0.08	-0.11	-0.21	0.49	-0.0032	-0.0002	0.0001	0.0341
Mar-Apr 2008	0.24	1.22	-0.03	0.14	-0.23	1.35	0.0010	-0.0001	0.0001	0.0201

5.4.2 Pollutant sensitivities to anthropogenic volatile organic compound emissions

Volatile organic compounds (VOC) are non-methane hydrocarbons with boiling points below 100°C. Anthropogenic VOC (AVOC) emission are primarily from their use as solvents in many industrial applications (Heinsohn and Kabel 1999). Though bigenic sources have greater emission rates than anthropogenic sources in Atlanta, air quality management policies can only control the anthropogenic fraction easily (Chameides, Lindsay et al. 1988). As they are degraded by radicals in the atmosphere, VOC play an important role in both ozone and $PM_{2.5}$ production. In the case of ozone, VOC oxidation products convert NO to NO_2 without the destruction of ozone, creating more NO_2 to photolyze and net ozone production. In the absence of VOC, the destruction of ozone by NO would inhibit high ozone concentrations in urban areas. VOC oxidation products tend to be less volatile and can condense increasing particulate matter mass. The variety of organic species and the number of possible reactions makes characterizing the formation of SOA from VOC difficult in air quality models and they contribute to the uncertainty between simulated and observed concentrations of $PM_{2.5}$ (Kroll and Seinfeld 2008).

Ozone concentrations are positively sensitive to AVOC emission controls throughout the year (annually 2.2% for the urban site), though more so in the winter season (3.2%) (Figure 5.3, Table 5.5). For particulate matter in the summer, reductions in AVOC emissions reduce the fraction of SOA that is formed from these compounds. However, anthropogenic SOA comprises a small fraction of the total $PM_{2.5}$(< 1% by mass) in our simulation due to known problems the model's simulations of SOA formation in summer (Morris, Koo et al. 2006). In the results presented here, the net sensitivity of secondary $PM_{2.5}$ to AVOC is slightly negative in the summer through its

Table 5.5: Average sensitivity to Anthropogenic Volatile Organic Compounds (AVOC) emissions

Table 5.5a: South Dekalb and Confederate Ave

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	1.20	0.00	0.05	0.00	-0.06	-0.02	0.0007	0.0000	0.0000	-0.0001
Jul-Aug 2007	-0.01	0.00	0.04	0.00	-0.04	-0.02	0.0003	0.0000	0.0000	0.0000
Sept-Oct 2007	-0.02	0.00	0.07	-0.01	-0.06	-0.01	0.0005	0.0000	0.0000	-0.0001
Nov-Dec 2007	0.02	0.05	0.14	0.01	0.02	0.25	0.0016	0.0000	0.0000	-0.0003
Jan-Feb 2008	0.04	0.10	0.20	0.02	0.04	0.39	0.0020	0.0000	0.0000	-0.0004
Mar-Apr 2008	0.00	0.03	0.12	0.01	-0.02	0.14	0.0020	0.0000	0.0000	-0.0003

Table 5.5b: Yorkville

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	-0.02	0.00	0.05	-0.02	-0.06	-0.05	0.0008	0.0000	0.0000	-0.0001
Jul-Aug 2007	-0.01	0.00	0.02	-0.01	-0.05	-0.05	0.0005	0.0000	0.0000	0.0000
Sept-Oct 2007	-0.02	0.00	0.09	-0.03	-0.07	-0.04	0.0014	0.0000	0.0000	-0.0002
Nov-Dec 2007	0.02	0.05	0.11	0.00	0.02	0.20	0.0012	0.0000	0.0000	-0.0003
Jan-Feb 2008	0.03	0.06	0.14	-0.01	0.03	0.25	0.0014	0.0000	0.0000	-0.0003
Mar-Apr 2008	-0.01	0.00	0.09	-0.01	-0.03	0.03	0.0015	0.0000	0.0000	-0.0002

Table 5.5c: Atlanta

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	-0.02	0.00	0.05	-0.02	-0.06	-0.05	0.0008	0.0000	0.0000	-0.0001
Jul-Aug 2007	-0.01	0.00	0.02	-0.01	-0.05	-0.05	0.0005	0.0000	0.0000	0.0000
Sept-Oct 2007	-0.02	0.00	0.09	-0.03	-0.07	-0.04	0.0014	0.0000	0.0000	-0.0002
Nov-Dec 2007	0.02	0.05	0.11	0.00	0.02	0.20	0.0012	0.0000	0.0000	-0.0003
Jan-Feb 2008	0.03	0.06	0.14	-0.01	0.03	0.25	0.0014	0.0000	0.0000	-0.0003
Mar-Apr 2008	-0.01	0.00	0.09	-0.01	-0.03	0.03	0.0015	0.0000	0.0000	-0.0002

ANH4 = Aerosol Ammonium; ANO3 = Aerosol Nitrate; AORGA = Secondary Organic Aerosol from Anthropogenic Volatile Organic Compounds; AORGB = Secondary Organic Aerosol from Biogenic Volatile Organic Compounds; ASO4 = Aerosol Sulfate;

interactions with other species, particularly sulfate, though the effect is not significant (< 1% of secondary $PM_{2.5}$ mass). In the winter, secondary $PM_{2.5}$ is positively sensitive to AVOC, but again, the total sensitivity is low from 3.75% at the rural site to 5.23% at the urban site.

5.4.3 Pollutant sensitivities to Sulfur Dioxide Emissions

While there are significant natural sources of SO_2, the majority of SO_2 in urban areas comes from sulfur compound impurities released during coal combustion (Amar, Senior et al. 2009). SO_2 emissions are oxidized in the atmosphere either in the gas phase or after absorption into water droplets, forming aerosol sulfate. Aerosol Sulfate is the largest component of secondary particulate matter during summertime (55.4% at the urban site and 59.3% at the rural site). During times where the concentrations of oxidant species are reduced, a significant fraction of the SO_2 may be removed from the atmosphere through dry and wet deposition (Heinsohn and Kabel 1999).

At the rural site, nearly 25% of the secondary $PM_{2.5}$ is sensitive to SO_2 emissions in summer (Table 5.1) mostly due to its effect on aerosol sulfate. Aerosol nitrate is negatively sensitive to SO_2 emissions throughout the year, as less sulfate formation frees ammonia to form ammonium nitrate aerosol (Liao, Tagaris et al. 2008). In summer the increase in aerosol nitrate (0.05 $\mu g/m^3$ at the urban site) for a 100% reduction in SO_2 emissions is small in comparison with the amount of sulfate reduction (1.63 $\mu g/m^3$ for the same site and conditions). In winter, the negative sensitivity of nitrate to SO_2 emissions plays a larger relative role. At the urban site nitrate concentrations increase by 0.17 $\mu g/m^3$ at the urban site while sulfate is reduced by only 0.62 $\mu g/m^3$ for a 100% change in

Table 5.6: Average sensitivity to SO_2 emissions

Table 5.6a: South Dekalb and Confederate Ave

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	1.20	-0.05	0.00	0.00	1.06	1.28	-0.0001	-0.0002	0.0019	0.0000
Jul-Aug 2007	0.29	-0.05	0.00	0.00	1.38	1.63	0.0000	-0.0002	0.0018	0.0000
Sept-Oct 2007	0.28	-0.08	0.00	0.00	0.97	1.17	0.0000	-0.0002	0.0017	0.0000
Nov-Dec 2007	0.14	-0.20	0.00	0.00	0.65	0.59	0.0000	-0.0001	0.0029	0.0000
Jan-Feb 2008	0.10	-0.18	0.00	0.00	0.53	0.46	0.0000	-0.0001	0.0036	0.0000
Mar-Apr 2008	0.22	-0.15	0.00	0.00	0.80	0.86	0.0001	-0.0002	0.0025	0.0000

Table 5.6b: Yorkville

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	0.26	-0.04	0.00	0.00	1.21	1.38	0.0001	-0.0002	0.0060	0.0000
Jul-Aug 2007	0.28	-0.03	0.00	0.00	1.77	2.02	0.0002	-0.0002	0.0091	0.0000
Sept-Oct 2007	0.31	-0.09	0.00	0.00	1.25	1.48	0.0001	-0.0003	0.0048	0.0000
Nov-Dec 2007	0.13	-0.15	0.00	0.00	0.60	0.58	0.0000	-0.0001	0.0039	0.0000
Jan-Feb 2008	0.08	-0.10	0.00	0.00	0.39	0.36	0.0000	-0.0001	0.0048	0.0000
Mar-Apr 2008	0.22	-0.18	0.00	0.00	0.93	0.98	0.0001	-0.0003	0.0046	0.0000

Table 5.6c: Atlanta

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	0.40	-0.08	0.00	0.00	1.60	1.80	0.0003	-0.0005	0.0105	0.0000
Jul-Aug 2007	0.41	-0.07	0.00	0.00	2.04	2.38	0.0002	-0.0006	0.0125	0.0000
Sept-Oct 2007	0.35	-0.11	0.00	0.00	1.31	1.55	0.0002	-0.0004	0.0087	0.0000
Nov-Dec 2007	0.17	-0.20	0.00	0.00	0.73	0.70	0.0000	-0.0002	0.0093	0.0000
Jan-Feb 2008	0.13	-0.17	0.00	0.00	0.62	0.57	0.0000	-0.0001	0.0112	0.0000
Mar-Apr 2008	0.30	-0.23	0.00	0.00	1.16	1.24	0.0001	-0.0003	0.0097	0.0000

emissions. The sensitivity results show SO_2 controls will be effective at reducing secondary $PM_{2.5}$ throughout the year (Figure 5.3). Ozone concentrations show a very slight positive sensitivity to SO_2 emissions (<0.5% at all sites) in the summer and are insensitive to SO_2 emissions in the winter (Figure 5.3, Table 5.6).

5.4.4 Pollutant Sensitivities to Ammonia Emissions

NH_3 is emitted into the atmosphere mostly from biological decay though anthropogenic sources, primarily from agriculture, contribute to NH_3 emissions as well (Heinsohn and Kabel 1999; Gilliland, Dennis et al. 2003) . While NH_3 has no interaction with ozone chemistry, it plays a significant role in the production of aerosol sulfate and nitrate. Ammonia also reacts with nitric acid in the gas phase to form ammonium nitrate particulate (Seinfeld and Pandis 1998) though to the vapor pressure of ammonium nitrate, this process is only significant in winter (Liao, Tagaris et al. 2007). In the aqueous phase, NH_3 dissolves in water droplets as NH_4^+ where it reacts with SO_4^{2-} and NO_3^- to form particulate matter (NARSTO 2004).

According to the sensitivity analysis, reductions in NH_3 do not affect aerosol sulfate concentrations greatly (~1% decrease due to 100% NH_3 control). Aerosol nitrate is positively sensitive to NH_3 emissions throughout the year. In winter, $PM_{2.5}$ is most sensitive to NH_3 controls (23.5% decrease in secondary $PM_{2.5}$ due to 100% NH_3 control in January-February 2008) (Figure 5.3).

5.5 Multi-pollutant Inverse modeling

In previous chapters, inverse methods have been shown to be able to identify optimal adjustments to emissions of a single precursor species to reduce ambient

Table 5.7: Average Sensitivity to NH_3 emissions

Table 5.7a: South Dekalb and Confederate Ave

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	0.18	0.14	0.00	0.00	0.02	0.35	0.0000	0.0011	0.0000	0.0000
Jul-Aug 2007	0.31	0.12	0.00	0.00	0.02	0.45	0.0000	0.0009	0.0000	0.0000
Sept-Oct 2007	0.19	0.30	0.00	0.00	0.05	0.59	0.0000	0.0018	0.0000	0.0000
Nov-Dec 2007	0.41	1.10	0.00	0.00	0.01	1.51	0.0000	0.0012	0.0000	0.0000
Jan-Feb 2008	0.47	1.23	0.00	0.00	0.05	1.75	0.0000	0.0007	0.0000	0.0000
Mar-Apr 2008	0.27	0.68	0.00	0.00	0.06	1.01	0.0000	0.0012	0.0000	0.0000

Table 5.7b: Yorkville

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	0.25	0.14	0.00	0.00	0.01	0.41	0.0000	0.0009	0.0000	0.0000
Jul-Aug 2007	0.36	0.09	0.00	0.00	0.01	0.46	0.0000	0.0007	0.0000	0.0000
Sept-Oct 2007	0.20	0.32	0.00	0.00	0.03	0.63	0.0000	0.0019	0.0000	0.0000
Nov-Dec 2007	0.38	0.96	0.00	0.00	0.01	1.35	0.0000	0.0013	0.0000	0.0000
Jan-Feb 2008	0.36	0.92	0.00	0.00	0.01	1.29	0.0000	0.0006	0.0000	0.0000
Mar-Apr 2008	0.31	0.66	0.00	0.00	0.06	1.03	0.0000	0.0013	0.0000	0.0000

Table 5.7c: Atlanta

	ANH_4 *($\mu g/m^3$)*	ANO_3 *($\mu g/m^3$)*	AORGA *($\mu g/m^3$)*	AORGB *($\mu g/m^3$)*	ASO_4 *($\mu g/m^3$)*	$PM_{2.5}$ *($\mu g/m^3$)*	O_3 *(ppm)*	NH_3 *(ppm)*	SO_2 *(ppm)*	NO_x *(ppm)*
May-Jun 2007	0.22	0.22	0.00	0.00	0.02	0.47	0.0000	0.0062	0.0000	0.0000
Jul-Aug 2007	0.40	0.19	0.00	0.00	0.01	0.60	0.0000	0.0067	0.0000	0.0000
Sept-Oct 2007	0.28	0.45	0.00	0.00	0.08	0.80	0.0000	0.0102	0.0000	0.0000
Nov-Dec 2007	0.40	1.14	0.00	0.00	0.03	1.57	0.0000	0.0059	0.0000	0.0000
Jan-Feb 2008	0.43	1.14	0.00	0.00	0.03	1.60	0.0000	0.0032	0.0000	0.0001
Mar-Apr 2008	0.31	0.88	0.00	0.00	0.06	1.25	0.0000	0.0061	0.0000	0.0000

concentrations of a pollutant to a desired level. This approach may be extended to a multipollutant case to find adjustment factors for several precursor species which reduces multiple pollutant concentrations (here, ozone and secondary $PM_{2.5}$) by a desired amount. Mendoza-Dominguez et al. (2001) used inverse methods to adjust emission inventory estimates of both primary particulate matter and precursor species based on observed concentrations. The inverse method used here for development for the multipollutant case is identical to that presented in Chapter 2 except multiple pollutants are included in the residual error vector, **e**, and the corresponding sensitivity values for each pollutant-precursor emission parameter pair are listed in the total sensitivity matrix, **P**:

$$\mathbf{x_{k+1}} = (\mathbf{P_k^T W_x P_k} + \mathbf{W_e})^{-1}\mathbf{P_k^T W_x e_k} \tag{5.2}$$

where:

$\mathbf{x_{k+1}^T} = \left[\chi_1^{k+1} \ldots \chi_p^{k+1}\right]$ = *[1 x p] = vector of emission adjustment factors*

$\mathbf{e_k^T} = \left[\varepsilon_{1,1}^k \ldots \varepsilon_{i,r}^k\right]$ = *[1 x i · r] = vector of differences between modeled and desired concentrations for all species i at all receptors r*

$\mathbf{P_k} = \begin{bmatrix} P_{E_{1,1}}^{1,1,k} & \cdots & P_{E_{j,p}}^{1,1,k} \\ \vdots & \ddots & \vdots \\ P_{E_{1,1}}^{i,r,k} & \cdots & P_{E_{j,p}}^{i,r,k} \end{bmatrix}$ = *[i · r x j · p] = matrix of sensitivity for each pollutant at each receptor location to emissions of each precursor species from each parameter*

$\mathbf{W_x}$ = *weighting matrix of the scaling factors*

$\mathbf{W_e}$ = *weighting matrix of the modeled differences*

The algorithm for finding weighted least square solution from Equation 5.2 is identical to that presented in Chapter 2. Concentrations and sensitivities are modeled using CMAQ/DDM-3D. Equation 5.2 is then used to calculate the change in emissions

necessary to minimize the residual error between the desired and simulated $PM_{2.5}$ and ozone concentrations.

Due to the computational time required for running the sensitivity analysis, the inverse method is applied for a short episode (August 1-8, 2007) of elevated ozone and $PM_{2.5}$ concentrations. Pollutants transported across the boundaries are removed and only locally produced pollutant concentrations are included in the inverse calculation. Based on 2007 design values (U.S. Environmental Protection Agency 2009), peak ozone concentrations will need to be reduced by 21% to reach attainment of the new 8-hour ozone standard of 0.075 ppb, and secondary $PM_{2.5}$ concentrations will need to be reduced by 7.4% to be in attainment of the annual standard of $15\mu g/m^3$. Ozone concentrations above 0.06 ppm and all $PM_{2.5}$ concentrations are included in the model.

The domain-wide emissions of NO_x, SO_2, AVOC, and NH_3 were set as separate source parameters in the inverse model analysis. For the locations and times considered by the inverse analysis, ozone is positively sensitive to NO_x and AVOC emissions, and peak ozone concentrations are sensitive to NO_x reductions (Figure 5.4). Particulate matter is positively sensitive to NO_x, SO_2, and NH_3 emissions (Figure 5.5; Napelenok, Cohan et al. 2006). While it is not a contributor to ozone production, NH_3 controls may play a role in attaining the annual NAAQS for $PM_{2.5}$ given its positive sensitivity to secondary $PM_{2.5}$ throughout the year (Figure 5.3).

Most of the emissions adjustment in the proposed multipollutant reduction strategy for the summertime episode was in NO_x and AVOC emissions (reductions of 17.5% and 26.0%, respectively). Emission adjustments for SO_2 and NH_3 were smaller

(reductions of 8.51% and 8.13%, respectively) since the desired change in $PM_{2.5}$ concentrations can be mostly achieved by the adjustments in both NO_x and AVOC emissions (Figure 5.5).

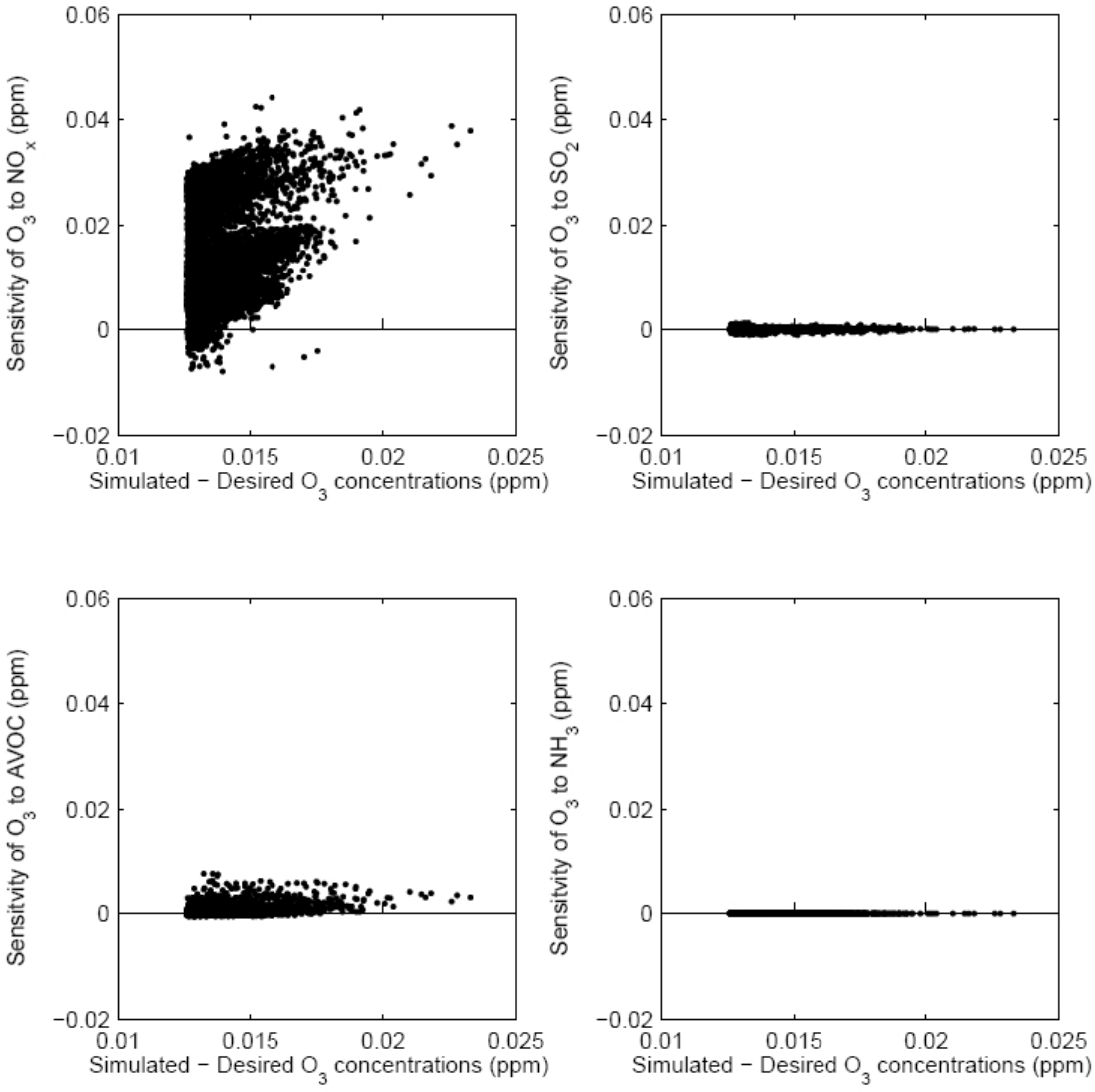

Figure 5.4: Sensitivities of secondary ozone to precursor emissions in cells with base concentrations greater than 0.060 ppm for Aug 1-8, 2007. Ozone concentrations are most sensitive to NO_x and AVOC emissions with only marginal sensitivities to changes in SO_2 and NH_3 emissions. Peak concentrations of ozone are sensitive to NO_x reductions.

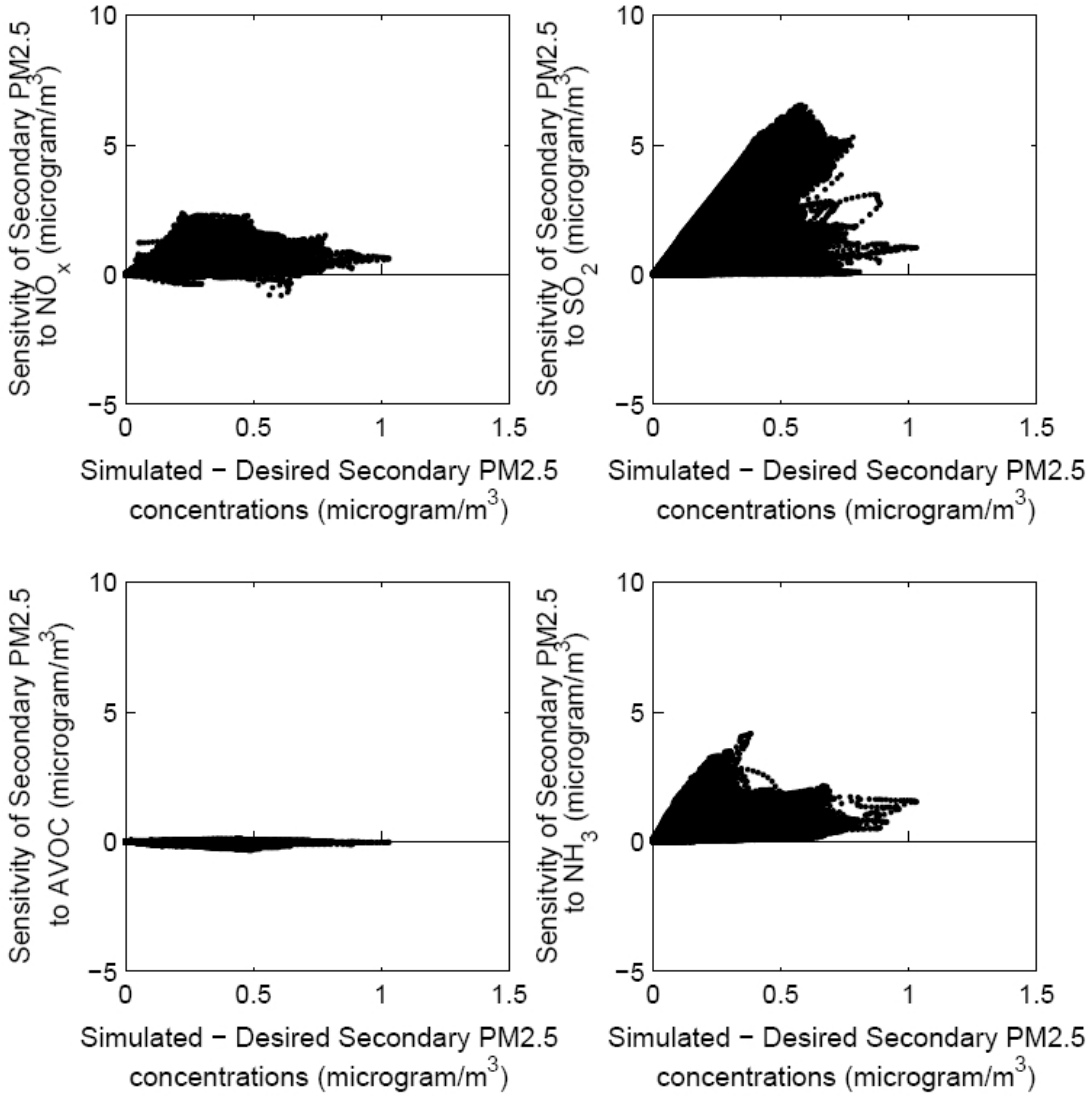

Figure 5.5: Sensitivities of Secondary PM to precursor emissions in all grid cells for Aug 1-8, 2007. Secondary $PM_{2.5}$ is sensitive to emissions of NO_x, SO_2 and NH_3.

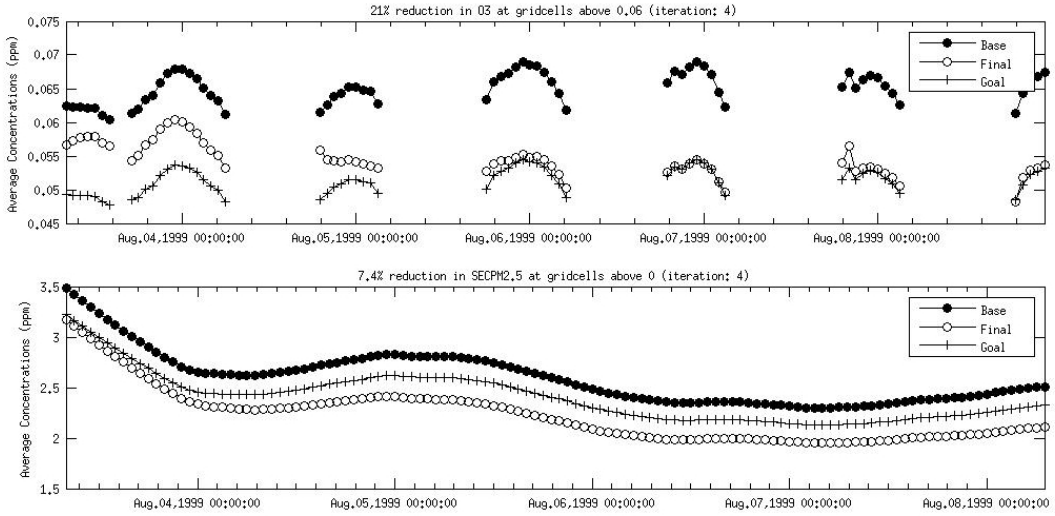

Figure 5.6: Average concentrations for base, goal and simulated cases: 8-hour average Ozone values in grid cells with base case concentrations above 0.06ppm (upper graph) and twenty-four hour average secondary $PM_{2.5}$ concentrations for the entire domain (lower graph). Concentrations after emissions adjustment (open circles) are closely match the desired concentrations (crossed lines) for ozone but are reduced beyond the goals for secondary $PM_{2.5}$.

Emission adjustments necessary to reduce a pollutant in one grid cell may lead to reductions beyond the desired levels in other cells and/or pollutants. The inverse method attempts to minimize this error, though it is unavoidable given the overdeterminedness of the inverse problem (Mendoza-Dominguez and Russell 2000). It may even be desirable if health or environmental benefits continue beyond the set goal amount. For the episode modeled here, to reach the ozone reduction goal, secondary $PM_{2.5}$ is reduced beyond the desired concentrations (Figure 5.6).

5.6 Multi-seasonal effects episode controls

Without running CMAQ for the entire year with the adjusted emissions, the effect of the emission adjustments obtained using the summer episode on $PM_{2.5}$ or ozone during

other seasons may be estimated by using the sensitivities from the rest of the year in a first order Taylor approximation:

$$C_i^{adjusted} = C_i^{base} + \sum_1^j S_{j,p} \cdot \chi_{j,p} \quad (5.3)$$

where:

$C_i^{adjusted}$ *=Adjusted species i concentration*

$C_i^{initial}$ *= Base species i concentration*

S_p *=Sensitivity of* $PM_{2.5}$ *to emissions of precursor species j from parameter p*

χ_p *=Adjustment factor from summertime episode for precursor species j from parameter p*

Although this approximation neglects possible nonlinear relationships of ozone and particulate matter concentrations to precursor emissions, previous studies show that, for ozone, the sensitivities are linear within the range of emission adjustments produced by the inverse run here (Cohan, Hakami et al. 2005), or, for $PM_{2.5}$, the nonlinear interactions tend to be small (Napelenok, Cohan et al. 2006).

When applied to the entire year, the emission adjustments based upon the summertime episode reduce secondary $PM_{2.5}$ concentrations by an average of 3.4% averaged across monitoring locations (Table 5.8). The reduction percentage of secondary $PM_{2.5}$ was constant across seasons. Similarly, ozone concentrations decrease from 3.1-3.8% between the monitor grid cells. Ozone concentrations are reduced in the summer though wintertime concentrations are not reduced significantly or show slight increases in some cases.

Table 5.8: Annual response of secondary PM2.5 and ozone to emission adjustments

Bi-monthly Mean Daily 24-hr Secondary $PM_{2.5}$ Concentration	**South Dekalb & Confederate Avenue**			**Yorkville**			**Atlanta Daily Highest Simulated Value**		
	Base ($\mu g/m^3$)	*Adjusted ($\mu g/m^3$)*	*Percent Change*	*Base ($\mu g/m^3$)*	*Adjusted ($\mu g/m^3$)*	*Percent Change*	*Base ($\mu g/m^3$)*	*Adjusted ($\mu g/m^3$)*	*Percent Change*
May-Jun 2007	6.86	6.63	-3.4%	8.02	7.68	-4.3%	11.91	11.32	-5.0%
Jul-Aug 2007	7.65	7.37	-3.6%	8.44	8.11	-3.9%	12.95	12.49	-3.5%
Sept-Oct 2007	9.26	8.97	-3.2%	10.20	9.83	-3.6%	14.77	14.29	-3.2%
Nov-Dec 2007	10.90	10.55	-3.2%	10.48	10.17	-2.9%	17.28	16.76	-3.0%
Jan-Feb 2008	9.50	9.19	-3.3%	8.73	8.46	-3.1%	14.85	14.47	-2.5%
Mar-Apr 2008	8.89	8.62	-3.0%	9.07	8.73	-3.8%	14.63	14.13	-3.4%
May 2007-Apr 2008	**8.84**	**8.56**	**-3.2%**	**9.16**	**8.83**	**-3.6%**	**14.40**	**13.91**	**-3.4%**

Bi-monthly Maximum Daily 8-hr Ozone Concentration	**South Dekalb & Confederate Avenue**			**Yorkville**			**Atlanta Daily Highest Simulated Value**		
	Base (ppm)	*Adjusted (ppm)*	*Percent Change*	*Base (ppm)*	*Adjusted (ppm)*	*Percent Change*	*Base (ppm)*	*Adjusted (ppm)*	*Percent Change*
May-Jun 2007	0.1026	0.0974	-5.1%	0.0833	0.0791	-5.0%	0.1083	0.1022	-5.6%
Jul-Aug 2007	0.0915	0.0858	-6.2%	0.1129	0.1086	-3.8%	0.114	0.1086	-4.7%
Sept-Oct 2007	0.0859	0.0805	-6.3%	0.0865	0.0822	-5.0%	0.0931	0.089	-4.4%
Nov-Dec 2007	0.0541	0.0539	-0.4%	0.0577	0.0573	-0.7%	0.0625	0.0613	-1.9%
Jan-Feb 2008	0.0537	0.0536	-0.2%	0.0555	0.0551	-0.7%	0.0578	0.059	2.1%
Mar-Apr 2008	0.0726	0.0718	-1.1%	0.0715	0.0701	-2.0%	0.0805	0.0799	-0.7%
May 2007-Apr 2008	**0.0767**	**0.0738**	**-3.8%**	**0.0779**	**0.0754**	**-3.2%**	**0.0860**	**0.0833**	**-3.1%**

5.7 Discussion

Annual measures of air pollution were not reduced to the goal values set in the inverse case for either pollutant. This discrepancy may be due to the choice of modeling period or how the concentration reduction goals were set. For the episode included in the inverse analysis, $PM_{2.5}$ concentrations were reduced more than the goal percentage. Since this was not the case for the entire year, additional modeling episodes are needed to find adjustment factors which achieve the desired reduction in annual mean secondary $PM_{2.5}$ concentrations during different conditions. The discrepancy can be expected in the case of ozone since the inverse model included all cells with ozone concentrations greater than 0.06 ppm and not the daily maximum simulated ozone concentrations averaged in Table 5.8.

Depending on the time of year, secondary pollutant concentrations are sensitive to different precursor emissions. For example, in the case of ozone, summertime ozone concentrations are most sensitive to NO_x emission controls. However, wintertime NO_x reductions increase ozone concentrations which, though still below the current ozone standard, may have an effect on public health if a safe threshold for ozone is below 40 ppb (Bell, Peng et al. 2006). On the other hand, NO_x emission reductions during January and February reduce secondary $PM_{2.5}$ concentrations which may be of greater importance to policy makers than the increase in ozone. The case for NO_x emission controls illustrates the need for a multi-seasonal analysis of emission control options. By using an inverse method on multiple seasons these balancing and competing influences may be incorporated in finding an emissions reduction plan which mutually reduces air pollutants.

The analysis presented here considers changes in precursor emission to be independent of one another. This is not the case in reality, as many sources emit multiple primary pollutants or precursor species (U.S. Environmental Protection Agency 2007). For example, coal fired electric generation produces SO_2, NO_x, primary $PM_{2.5}$, and carbon dioxide. While some controls, such as catalyst based controls, may selectively target specific species for capture and removal, other control strategies such as increasing home efficiency would decrease the electrical demand and reduce the amount of coal being burned. By reducing the use of coal power altogether, multiple pollutants are reduced (Amar, Senior et al. 2009). Similar proposals may be made for reducing and controlling other fossil fuel combustion sources though increases in efficiency or substitutions of alternative energy sources. These interactions will need to be included as control strategies are developed to achieve the emission adjustments identified by the inverse analysis. Correlations between the emissions of multiple pollutants may be directly included in the inverse method optimization through the use of the adjustment factor weighting matrix ($\mathbf{W_x}$ in Equation 5.2) or by defining multiple-species source parameters for specific industries or source categories.

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CHAPTER 6

CONCLUSIONS AND FUTURE WORK

6.1 Inverse modeling in air quality management

Air quality management in the United States has historically focused on reducing the ambient concentrations of six criteria pollutants: lead, sulfur dioxide, carbon monoxide, nitrogen dioxide, ozone and particulate matter. In areas where these pollutants are determined to be dangerous to public health and environmental well being, air quality managers have used modeling to develop emission abatement plans to reduce concentrations of these pollutants to safer levels. Since these plans take anywhere from years to decades fully implement, they are often based on uncertain predictions of future socioeconomic and technological conditions. Once the proposed emission strategy is simulated to achieve the National Ambient Air Quality Standard (NAAQS), it is implemented without a review of whether the underlying predictions used in the development of the plan occur. In its report evaluating air quality management in the United States, the National Research Council of the National Academies has suggested that the current air quality management process be replaced with an integrative, iterative one where emission strategies are continually reevaluated for their effectiveness (National Research Council of the National Academies 2004).

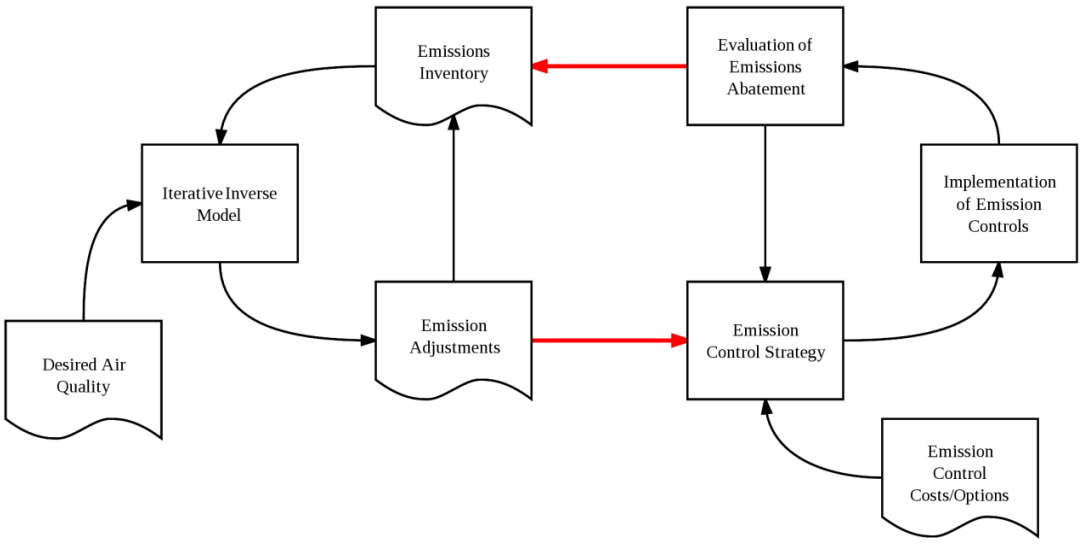

Figure 6.1 Proposed integrative air quality management system. The system is divided into two iterative processes. The first uses the iterative inverse model to find optimal emission adjustments. The second iterates to find the most effective emissions abatement strategy to reach the optimal emission adjustments.

As outlined in this thesis, inverse air quality modeling can play a significant role in creating such an integrative process. Emissions adjustments produced by the inverse method are not linked to specific control options, so choices on how to implement these options can be evaluated separately. Air quality management can then be split into two simultaneous processes, one calculating the optimal emissions adjustments based upon desired air quality, the other searching for a feasible emissions abatement strategy to reach the emission adjustment goal (Figure 6.1).

The emission adjustments depend on an estimate of the desired air quality in a region. As new information about the health effects of air pollution is uncovered and as

air pollution concentrations change, the desired (or known safe) level of air pollution may change. As our economic analysis in Chapter 3 shows, there are a number of ways to estimate how individuals value healthy air. Planners may use the inverse model approach described here to find the mathematically optimal change in total emissions for each of these levels.

The inverse air quality modeling approach here builds upon past proposals to use sensitivity analysis in such an air quality management system (e.g. Cohan, Boylan et al. 2007). The inverse air quality model distributes adjustments to emissions based upon their spatial and temporal impact on simulated pollutant concentrations. Additional information over the control costs and health effects of air pollution may be included in the inverse model, as was shown in Chapter 4 where theoretical costs for controls are included to minimize the total dollars spent for controls.

The applications presented in this thesis demonstrate the versatility of inverse modeling in air quality management. They have been applied on the urban scale to calculate emission reductions in specific source types and spatial regions. The adjustment factors produced by inverse modeling can be used to understand the necessary changes in long-term trends in air pollution – informing decisions over land use that are not typically a part of air quality management. At the regional scale, they can be used to mitigate the problem of interstate transport of pollution by addressing complications that arise when creating emissions trading programs, specifically, that the location of emissions is significant. In multi-pollutant abatement optimizations, inverse modeling may be used to ensure that the controls for one pollutant do not negatively impact concentrations of other pollutants.

The emission adjustments then provide the basis for planners to develop and evaluate a specific emissions abatement strategy. In each of the cases presented here, different issues will arise. In the case of applying emission adjustments as a part of a determination of attainment of the NAAQS process, careful limits must be placed on the amount current sources may change based on feasible short-term emission control options. In a long term framework, planners will have to adopt new approaches to alter long-term trends in land use and infrastructure management to achieve emissions reduction goals. In the case of a regional market based system, emission planners will need to develop emission trading plans which promote innovation within the marketplace to find cost effective solutions and while ensuring an equitable (and desireable) reduction in pollution exposure. By considering the total effect of a precursor species on air quality, air quality managers may find common solutions to address multiple pollutants. Designing such a system will require managers to account for how emission controls affect multiple precursors, and choose strategies that best fit the optimal emission adjustments.

After an emissions abatement strategy is chosen and implemented, a review process using ambient measurements, specific source monitors, or other evaluating data can be used to assess the effectiveness of the abatement strategy on reducing emissions to the aggregate adjustment amount. If the review process determines that the abatement strategy was not successful, air quality managers can revise the existing plan or develop a new plan based upon new information or technology. This emissions review process can be used to update the emissions inventory of the inverse air quality modeling system. With a better estimate of the existing emissions, the inverse modeling approach can

develop more accurate emission adjustments. The two iterative processes can continually evaluate and update air quality management plans based upon both changing desires in air pollution or changing conditions in emissions abatement technologies.

6.2 Future Work

6.2.1 Application of inverse methods in air quality management

Though they are based on a representative historical episode of elevated ozone concentrations and a recent accounting of emissions, the desired concentration reductions modeled in this thesis are used to demonstrate the applicability of the iterative, inverse method in air quality management. Applications of inverse methods to achieve specific air quality standards will require additional information:

1. *Well defined goal concentrations.* In Chapter 2, we defined goal reductions as series of relative changes in from currently simulated concentrations. Goals are similarly defined to demonstrate attainment of the NAAQS in modeling simulations (U.S. Environmental Protection Agency 1997; U.S. Environmental Protection Agency 1999). While statutory requirements will keep the NAAQS as the primary goal of air quality managers, multiple stakeholders, from business leaders to environmental groups to government leaders, can use the inverse air quality model to be better informed in the debate over emissions abatement.

2. *Expanded/Representative Modeling Episode.* Inseparable from defining the goal concentrations is determining a representative modeling episode. Because meteorology plays a large role in determining the relationship between precursor emissions and ambient concentrations of pollutants, it is essential to choose a modeling period which represents typical conditions leading to elevated air quality levels. It should be noted that a variety of conditions lead to elevated air pollution and multiple episodes may need to be modeled to ensure that emission adjustments are sufficient to reduce air quality under all conditions. Multiple episode concentrations and sensitivities may be included in a single inversion application to capture these effects.
3. *Accurate emissions inventory*. The inverse method relies on adjusting emissions as determined by the inputs into the air quality model. Without an accurate emissions inventory, adjustments produced by the inverse method would be meaningless. Additionally, while a benefit of the inverse method application is that it does not require *a priori* definition or forecasting of emissions growth, information of available control options is essential for designing control strategies based on the adjustment factors produced by the inverse analysis.

Outlined below are several specific possible applications of emission adjustments on air quality at differing scales.

6.2.1.1 Urban scale: Land use planning and air quality

Additional study is needed to relate and quantify how emissions may be changed based upon urban land use design. In Chapter 3, we show one way of quantifying this relationship. We compared the urban structure of two neighborhoods to find indicators of why households in two neighborhoods with similar demographic makeup and physical location have different driving habits. By understanding the relationship between hard infrastructure and emissions, air quality considerations may be included in decisions on long-term development of an area, lessening the need for retroactive control measures. For example, an urban design that introduces clean transportation alternatives to automobile use can prevent the need for finding new solutions for increasing automobile efficiency or producing alternative fuels.

6.2.1.2 Regional scale: Air quality management: Cap-and-trade market systems

The application of inverse models on regional emissions is demonstrated in Chapter 4. While our application included a limited number of states, an expansion of the modeling domain to include all Clean Air Interstate Rule states is necessary to understand how emissions must change under the proposed rule (or its successor) to achieve the air quality goals in multiple areas. Additional research is needed to develop a regional market-based system which maintains the spatial emission reduction goals produced by the inverse modeling.

6.2.1.3 National and international scale: Implications on climate change legislation

With the recent court ruling against the U.S. EPA's Clean Air Interstate Rule, the U.S. EPA is currently writing a new rule to address regional emissions of NO_x and SO_2.

Concurrently, Congress is debating new legislation to limit and reduce emissions of carbon dioxide. Both programs will likely establish cap-and-trade emissions reduction programs. Since both seek to adjust emissions from common sources, particularly in the energy sector, care should be taken that the design of one system does not impact the goals of the other. Properly applied, the two systems may work together to preferentially reduce common sources and find an overall economically optimal solution.

6.2.2 Possible methods for defining desired air quality

The application of this method raises the question of how to define a regionally appropriate measure of air quality and what level of air quality is acceptable to the public. Extensions of the method may be made to define desired air quality based on current regulatory requirements and new understanding of the dangers posed by air pollution

6.2.2.1 Understanding the regulatory effects of proposed national standards

The current process in the Clean Air Act stipulates specific criteria for setting the National Ambient Air Quality Standards (NAAQS) based upon protecting public health and the environment. The U.S. EPA is charged with reviewing whether the NAAQS satisfy these criteria every 5 years. The process of reviewing the standard is a contentious one with many stakeholders proposing different standards. Given that the inverse method can be applied to any of these proposed standards, future applications of inverse modeling may assess the regulatory impact of each proposed standard.

6.2.2.2 Addressing air quality in multiple areas

The regional application in Chapter 4 set a goal of a 10% reduction in ambient ozone concentrations from the entire domain. However, some areas have worse air quality than others, and this general goal may not define an air quality that is optimal for each area of the region. Therefore, future applications may define a desired air quality reduction for specific areas of the domain. For example, when the model is applied on a regional multi-state domain, a spatial distribution of desired concentrations can be created by averaging the reductions needed for reaching attainment of the NAAQS in multiple non-attainment areas in the domain.

6.2.2.3 Population weighting

In the results presented here, ambient air concentrations were weighted equally across the modeling domain. However, the actual exposure from ambient concentrations is highly dependent on the spatial distribution of the air pollutant and the population of the area. This may be addressed by scaling the desired reductions relative to the population, effectively making the desired scaling factor, λ, from Chapter 2 a function of population.

6.2.2.4 Exposure modeling

Population weighting of the desired air quality concentrations can be taken a step further with the application of an exposure model. Mauzerall et al. (2005) integrated an exposure analysis with a regional air quality model to understand the regional health outcomes of different spatial distributions of emissions. Using such a model, sensitivities for ambient concentrations may be converted to health outcomes, i.e. sensitivity values

which are currently in terms of the concentration change due to a change in emissions may be rewritten in terms of a change in health outcomes due to a change in emissions. Additionally, applying such sensitivities in the inverse method would require desired air quality to be restated in terms of health outcomes, potentially allowing for a more relatable indicator of future air quality than the ambient concentrations employed in this thesis.

6.2.2.5 Net-benefit weighting

In Chapter 4, the sensitivities used in inverse method were weighted based on the control costs of each source parameter. In future applications, the benefits of the change in concentrations may be included to offset these costs. As emission changes are calculated by the inverse model, the expected monetary benefits in avoided health effects from the resulting change in concentrations can be calculated. Therefore, instead of distributing the costs equally between source parameters, the net-benefits (or costs) can be distributed. Since health benefits of reducing ozone concentrations may be seen below the 0.06 ppm threshold used in the inverse modeling (Bell, Peng et al. 2006), such a net-benefit approach will include areas (mostly rural and nighttime urban) that are not addressed in the applications modeled here.

6.2.2.6 Marginal cost

The cost-weighted case shown in Chapter 4 equalizes the total emission control cost burden between the states. Under an emissions trading system, the total costs are not necessarily equalized. Instead, the marginal costs for reducing emissions are equalized across the states since trading occurs based upon the relative price of purchasing

additional emission allowances and the costs of additional emissions abatement. This constraint can be included in the inverse method by including marginal costs in the place of total costs in Equation 4.5.

6.2.3 Effects of emission uncertainty in the use of inverse modeling for air quality planning

A major limitation of inverse air quality models is the reliance on accurate representations of current emissions. Any error in current emissions inventories will be reflected in the adjustments produced by the inverse analysis. If these errors are large enough, the emissions adjustment results may not lead to the expected results. Since implementing and accounting for the effectiveness of emissions controls requires a thorough knowledge of the sources present in the area, work must continue to be done to ensure that estimates of the current state of emissions are as accurate as possible. Inverse air quality modeling can aid in this process. Observations of ambient pollutant concentrations can be used in an inverse air quality model to adjust emission inventories for possible deficiencies (e.g. Mendoza-Dominguez and Russell 2001). The adjusted emissions may then be used as a starting point for additional inverse model runs for air quality management planning.

As noted in Chapter 3, the weighting matrix of the emission adjustment factors can contain a priori information of the expected growth or change in a source. If future emissions from a source are generally well known (such as those from a power plant with limited control options) the emission adjustments from the inverse model can be constrained to the expected amount. If the future strength of a source has a high degree of

uncertainty, it can be relatively unconstrained by the weighting matrix, and the inverse method results may be used then to inform policies on how the emission source will change in the future.

Therefore, in future applications of the method, a thorough accounting of the uncertainty of both the current state and the future state of emission should be made to ensure that the results of the method are valid. Defining these uncertainties can be incorporated in the process of developing and applying an emissions control strategy as outlined in Figure 6.1.

6.2.4 Use of inverse modeling in air quality forecasting

With reduced computational times for simulating air pollution concentrations, forecasts of daily air pollution levels by air quality models have become a useful tool in advising the public of potential danger from air quality (Odman, Hu et al. 2007; Hu, Baek et al. 2008). In these model applications, meteorology inputs are adjusted and modeled on a daily basis based upon observations, yet emissions inventory data remains relatively static. Using observations of air pollution from the previous day, inverse modeling may be used to identify daily trends in the emission inventory to produce more accurate air quality forecasts. Additionally, if air pollution is forecasted to reach dangerous levels during the next day, inverse modeling can be used to identify the best measures to lower concentrations based on the forecasted meteorology. For example, currently, power plants alter their daily electrical generation based upon expected power load. With information over the day-to-day impact of their facilities, energy companies may choose to alter their activity based upon their downwind impacts.

6.3 References

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