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Evaluating the Design of Emissions Trading

Programs Using Air Quality Models

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Evaluating the Design of Emissions Trading Programs Using Air Quality Models

by:

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Dedication:

This dissertation is dedicated to my mom and dad.

Their love and support is what made this possible.

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Evaluating the Design of Emissions Trading Programs Using Air Quality Models

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In order to meet the US EPA's National Ambient Air Quality Standards as set under the provisions of the Clean Air Act, states and regions throughout the United States are designing cap and trade programs aimed at reducing the emissions of the two dominant precursors for ozone, nitrogen oxides (NOx) and Volatile Organic Compounds (VOCs). While emission cap and trade programs are becoming more common, relatively few analyses have examined the air quality implications of moving emissions from one location to another (due to trading of emissions between facilities), from one sector to another (due to the use of technologies such as Plug-in Electric Hybrid Vehicles - PHEVs), and changing the temporal distribution of emissions (through emissions trading among facilities with different temporal profiles). This thesis will examine, in detail, the air quality implications of two emission cap and trade programs. The first program is a

NOx trading program that covers Electricity Generating Units (EGUs) in the

Northeastern United States. Results show that refining the temporal limits on this cap

and trade program, by charging facilities more to emit NOx on days when ozone is most

likely to form, has the potential to significantly reduce NOx emissions and ozone

concentrations. Additionally, this research also shows that, for this region, the spatial

redistribution of NOx emissions due to trading leads to greater ozone reductions than

similar amounts of NOx emission reductions applied evenly across all facilities.

Analyses also indicate that displacing emissions from the on-road mobile sector

(vehicles) to the EGU sector through the use of PHEVs decreases ozone in most areas,

but some highly localized areas show increases in ozone concentration. The second

trading program examined in this thesis is limited to Houston, Texas, where a VOC

trading program is focused on a sub-set of four Highly Reactive Volatile Organic

Compounds (HRVOCs), which have been identified as having substantial ozone

formation potential. Work presented in this thesis examined whether this trading

program, in its current form or in an expanded form, could lead to air pollution hot spots,

due to spatial reallocation of emissions. Results show that the program as currently

designed is unlikely to lead to ozone hot spots, so no further spatial limitations are

required for this program. Expanding the trading to include Other VOCs, fugitive

emissions and chlorine emissions, based on reactivity weighted trading, is also unlikely to

lead to the formation of ozone hot spots, and could create more flexibility in a trading

market that is currently not very active. Based on these air quality modeling results,

policy suggestions are provided that may increase participation in the trading market. These case studies demonstrate that use of detailed air analyses can provide improved designs for increasingly popular emission cap and trade programs, with improved understanding of the impacts of modifying spatial and temporal distributions of emissions.

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Chapter 1 Introduction to Emissions Trading

Background

Beginning with the 1970 Clean Air Act Amendments, the United States (US) federal
government set National Ambient Air Quality Standards (NAAQS) for six common air
pollutants, limiting their concentration in the environment. (EPA 1990) The NAAQS
have been established for Carbon Monoxide, Lead, Nitrogen Dioxide, Particulate Matter,
Ozone and Sulfur Oxides. These six air pollutants are commonly referred to as criteria
air pollutants because the NAAQS established allowable concentrations (criteria) for
these pollutants in the atmosphere. Areas of the country with concentrations of these air
pollutants above the levels set by the NAAQS, concentrations determined to be
detrimental to human health, are called non-attainment areas. States in which non-
attainment areas are located must develop a plan describing how non-attainment areas
will meet the goal of reducing concentrations of these pollutants below acceptable levels.
These are called State Implementation Plans (SIPs).   (EPA 2008a)

Of the six criteria pollutants, ozone and particulate matter are the most problematic and,
given the widespread exposure to these pollutants, are most likely to negatively affect
human health. (EPA 2008). The focus of this thesis will be on programs that have the
objective of reducing ozone concentrations.

Ozone is a secondary pollutant formed by the reactions of Volative Organic Compounds
(VOCs) and nitrogen oxides (NOx) in the presence of sunlight. The chemistry of ozone
formation is non-linear and introduces time lags between emissions and ozone formation.
Both classes of ozone precursors (VOCs and NOx) have anthropogenic and biogenic
sources, and emissions of each precursor have varying degrees of impact on ozone
formation based on their relative ambient concentration levels. (Tong 2006) These

issues mean that the design of emissions control strategies for ozone precursors is not straightforward and typically requires the application of photochemical grid models in order to evaluate the potential effectiveness of emission reductions for air quality initiatives and State Implementation Plans (SIPs). (Martin 2007, Tong 2006, Mauzerall 2005)

Emissions Trading

Prior to 1990, regulation to control air pollution was primarily "command-and-control". Emission sources would be required to use current best available technology, often regardless of cost. In order to offer more flexibility in meeting emission reduction requirements, emissions cap-and-trade programs were introduced in 1990 as part of the Clean Air Act Amendments. As opposed to regulating all individual emission sources based on available technologies or facility emission limits, a cap and trade program establishes an emission budget for a region. Scientific modeling methods are used to determine the level of total emissions that can be allowed in an area while maintaining a certain air quality. This amount, the emissions "cap", is set on an annual or seasonal basis. The emissions cap is set at an initial level and then is typically decreased each year until a goal is met. The emissions associated with the regional cap are distributed to individual facilities as allocations. The allocation each facility receives can be based on historic emissions quantities, production volume, or historic fuel consumption. The facility is then able to use its allocation, sell excess allocations if it emits less than allowed, or buy additional allocations from other facilities if its emissions exceed its allocations. (Farrel 1999)

Emission cap and trade programs allow markets to determine which facilities can most economically achieve emission reductions. They also allow regions to continue to add new facilities, even if regional emissions are capped, since new facilities may buy existing credits from other sources before beginning operations.

This thesis will examine the design and operation of two emissions cap and trade programs designed to reduce emissions of NOx and VOCs (ozone precursors). The first trading program that will be examined is for NOx emissions from Electricity Generating Units (EGUs, power plants). Because the EGUs are located in primarily rural settings, which frequently have large amounts of local biogenic VOC emissions, ozone formation due to EGUs is more effectively reduced by lowering emissions of NOx. (EPA 2005) An ozone season NOx cap for EGUs has been implemented in the entire eastern half of the United States. The ozone season runs from April to September, and all emissions during this period are treated as equivalent. (Martin 2007) However, the time and location of emissions can have a large effect on the likelihood that NOx emissions will lead to ozone production. Depending on the meteorology, what is happening upwind, and the temperature, certain days during the ozone season may have conditions that make the formation of ozone from NOx more likely. This opens the door for a more focused NOx emissions control plan that will have a larger impact on the reduction of ozone.

The design of such a focused strategy will be examined in this thesis, for a case study region of Pennsylvania, New Jersey and Maryland (referred to as PJM). PJM is a four-state area that includes the three states for which it is named, as well as Delaware. PJM operates a regional electricity grid that allows for dispatching of power generation among EGUs in the four state area. A hypothesis to be examined in this thesis is that dispatching power generation away from areas and time periods that are conducive to ozone formation, and creating financial incentives for doing this dispatching, would reduce ozone concentrations. If successful and if implemented, this would be the first emission cap and trade program with daily variability in emission pricing. A second hypothesis to be examined is that shifting emissions to the EGU sector, from the motor vehicle sector, with temporal constraints, through the use of Plug-in Hybrid Electric Vehicles (PHEVs) will improve air quality.

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The second cap and trade program that will be examined in this thesis has been implemented in the Houston/Galveston ozone non-attainment area of Southeast Texas. In this case, the Texas Commission on Environmental Quality (TCEQ) has developed a cap and trade program to control emissions of a subset of VOCs that are emitted in large quantities in the region and that are very reactive in the atmosphere and therefore more likely to form ozone. This subset is termed Highly Reactive Volatile Organic Compounds (HRVOCs) and includes ethylene, propylene, 1,3 butadiene and isomers of butene. HRVOCs have been targeted for emission reductions in this area in addition to NOx emission reductions. In the Houston/Galveston area, air quality modeling showed that a reduction in VOC reactivity along with a reduction in NOx, instead of reducing NOx alone, is the more effective way to reduce ozone (TCEQ 2004). An annual cap has been placed on HRVOCs in Harris County. The cap and trade program was started at the beginning of 2007, but is still under review. This cap and trade program contains a number of provisions that are unique. It is the first program to separate a group of VOCs for emission trading based on their reactivity and it allows for a reactivity weighted trading scheme. This thesis will examine a number of issues related to this reactivity weighted trading, including whether the choice of reactivity index is appropriate, whether trading might introduce localized high concentrations of ozone (hot spots), and whether additional compounds could be added to the reactivity-weighted trading. Since the trading program is still evolving, these evaluations have the potential to influence program design.

In modeling both of these cap and trade programs, the approach will be to employ detailed regional air quality models with models to evaluate the trading program designs.

Chapter 2 of this thesis will review the literature on emission trading. Chapters 3 and 4 will examine NOx emission trading involving EGUs in the PJM region. Chapter 5 will examine the HRVOC emissions trading program in Houston, and Chapter 6 will synthesize the results of the thesis.

Chapter 2 Literature Review

Cap-and-Trade Programs

Regulation to control air pollution has traditionally been of a "command-and-control" form. Best available technologies are identified for controlling emissions from major sources, and these controls must be used regardless of cost. In order to offer more flexibility in meeting emission reduction requirements, market-based systems of pollution control have been developed, and one example of this type of emission management is a cap-and-trade program. (Burtraw 2005)

In cap and trade programs, the level of total emissions that can be allowed in an area are estimated, setting a target emissions "cap". At the start of a typical cap and trade program, the emissions cap is set close to the level of current emissions and then is decreased until the target emissions cap is met. Emissions totaling the capped amount are allocated as credits, and the credits are allocated to facilities in the regulated area. The number of credits each particular facility receives can be based on factors such as historic emissions quantities, production volume, or historic fuel consumption. (Mackenzie 2008) If a facility emits more than its allocation, it must purchase additional credits, or face financial penalties. If a facility emits lets than its allocation, it may sell its excess credits.

This review of cap and trade programs will examine three multi-state and three local or in-state cap and trade programs, identifying common issues that arise in the implementation of cap and trade programs.

Federal Programs: SO$_2$ Emission Trading, Northeast US NOx Cap-and-Trade, and the Clean Air Mercury Rule

The first emissions cap and trade program was developed and introduced by the US Environmental Protection Agency (EPA) as part of Title IV of the Clean Air Amendments of 1990. (EPA 1990) This program was designed to reduce SO_2 emissions from Electricity Generating Units (EGUs, or power plants) in the Northeastern US (NE US) and trading began in 1994. SO_2 emissions contribute to acid rain and fine particulate matter formation and because the NE area of the US contains, and is downwind of, a large number of EGUs, acid rain and elevated particulate matter concentrations are a significant concern in the region. EGUs are the source of approximately 68% of the nation's SO_2 emissions (EPA 2008c).

As a result of the US Acid Rain program, SO_2 emissions were cut in half, from 1990 emission rates, by 1999, four years after the start of the program. While original estimates predicted SO_2 emissions market prices of $1000/ton, actual prices market prices were around $130/ton the first few years and averaged about $75/ton by 1996. Actual prices for the costs of emissions reductions around that time were approximately $78 per ton of SO_2 reduced. (Conrad 1996). Costs of emissions credits have since steadily increased upwards to about $150 in 2003, then jumped to about $700 by 2004 due to increases in Natural Gas costs (which is used as an alternate fuel) and increased electricity demand (Burtraw et. al 2005).

It is estimated that the health benefits from the program, due to decreased particulate matter, were approximately $10 billion per year in 1997 and will be $40 billion per year in 2010 when the program is fully implemented. (Benkovic 2001) Additional recognized benefits of the program were a decrease in the acidity of rainfall, increased acid neutralizing capacity of northeastern lakes and streams as well as decreased damage to property. (Benkovic 2001) Initial costs of the program were much lower than expected for several reasons. Deregulation of railroads reduced the shipping costs of lower sulfur coal from remote areas of the western US where this type of coal is primary located. (Popp 2003). Natural gas was also utilized as another cheaper alternative to high sulfur

coal. However, as an additional benefit to the market based emissions control strategy, the industries that design and sell control equipment, with the goal of staying competitive, found ways to make a cheaper, more effective product. (Popp 2003)

While there have been reports of different regional benefits from trading of SO_2, for example, Burtraw (1999) reported greater levels of SO_2 deposition in some areas of the country, specifically states like Kentucky, Illinois and Indiana in the Midwest, it is generally agreed that the overall benefits of SO_2 trading outweighed the negatives. (Conrad 1996, Benkovic 2001, Burtraw 1999, Burtraw 2005).

Seeing a similar need for a collaborative effort among the states, the EPA first introduced a NOx trading program ten years after the start of the SO_2 trading program. (Burtraw 2005) EGUs account for approximately 22% of NOx emissions in the Northeastern US. (EPA 2003) While EGUs are not the largest source of NOx (mobile emissions release almost 60% of NOx in the NE US), (EPA 2003) they are a significant source. The NOx program was slightly different in that it was a summer seasonal trading program. (EPA 2008b) NOx contributes to acid rain, like SO_2, but in addition, NOx is a precursor for ozone. Ozone is especially problematic because of the complicated chemistry involved in its formation. NOx and VOC must be present in the right relative concentrations in presence of warm temperatures and sunlight in order to form ozone. This is most likely to occur between May and September, and this led to the focused seasonal cap.

Reducing ozone formation, due to NOx emissions, is a regional problem and requires that all the states with emissions sources in an airshed cooperate. The original NOx trading program included 11 states on the east coast. It was found that sources farther upwind were affecting ozone non-attainment areas. (Bergin 2007) Because of this, in 2003, the EPA expanded the program to include 29 states as shown in Figure 2-1, and required them to revise their State Implementation Plan (SIP) and show specifically their ozone attainment demonstration plan. In addition, the US EPA's Clean Air Interstate Rule

(CAIR) strengthened the program in 2005 by tightening caps on both NOx and SO_2. Most recently (2008), the CAIR rule has been overturned by the federal courts, throwing the future of the cap and trade program into doubt, but also offering the opportunity for changes to the program. (EPA 2008b)
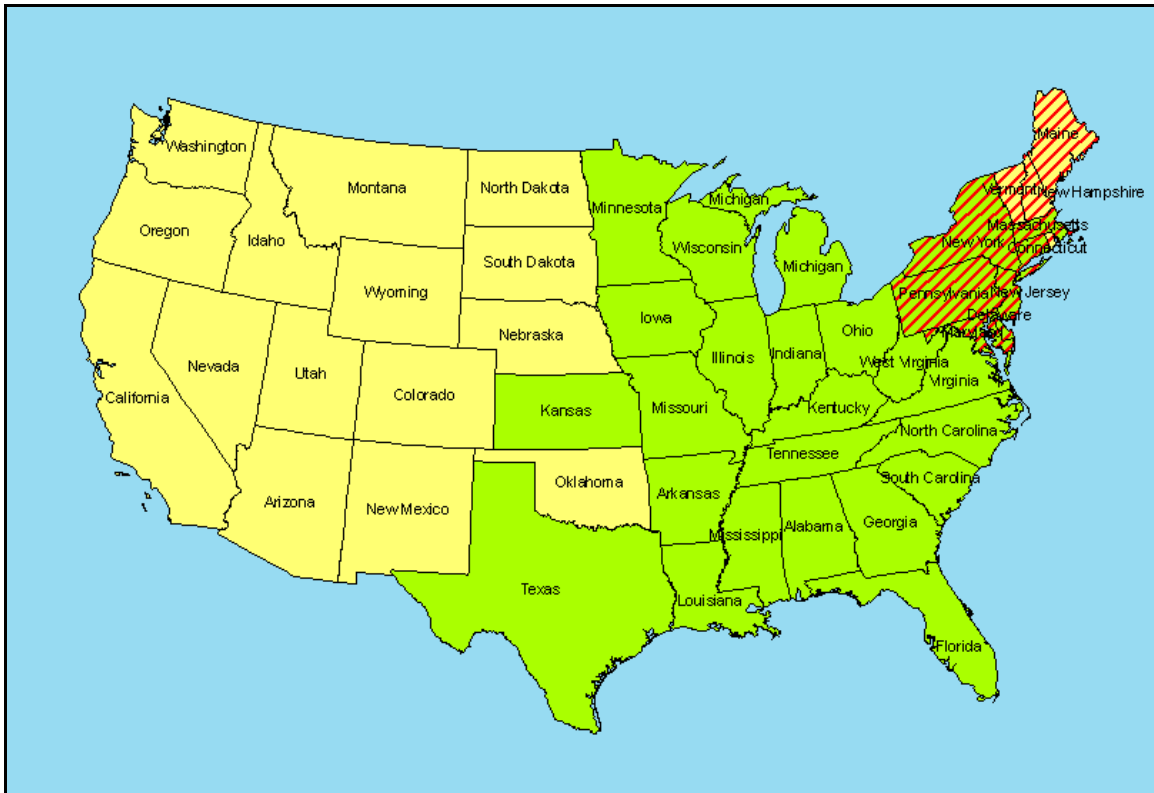
Figure 2-1. The 29 states included in the Clean Air Interstate Rule, as of 2003, are shown in green. The original 11 states of the OTC are shown with red stripes.

For the NOx program, regional caps were decided upon based on a desired air quality effect, in this case, the attainment of ozone standards. (EPA 2008b) Once the cap was determined, allowances were distributed to individual states based on historic production, and the total emissions that would occur in each state, if across the board reductions of emissions were made. (Burtraw et. al. 2005) From there, the states were allowed to allocate the credits to individual sources however they saw fit.   Thus far, no spatial

restraints on trading have been put into place for the NE NOx trading program. Little air quality modeling work has been done to determine whether ozone hot spots are occurring as a result of the program. Studies do indicate that the largest sources of NOx have shown the largest decreases of NOx emissions since implementation of the trading program indicating that areas that needed improvement the most, saw it. (Swift 2004) Studies have also shown that days with the highest levels of ozone, saw the largest decrease of NOx emissions (Swift 2004), while other studies show that average and peak NOx emission periods have been reduced equally (Farrell 2003). These results, collectively may ease fears of temporal hot spots resulting from the NOx program, but they also suggest that more focused strategies may improve air quality benefits. The work done for this thesis suggests that spatially focused trading rules designed to reduce emissions in a location predicted to have high ozone forming potential, resulting in emissions being traded out of that particular area into another area within the region with less ozone forming potential, could improve local air quality, but may also lead to hot spots down wind of the trading region.

Temporal trading is slightly restricted because of the seasonal nature of the program. Credits cannot be traded into the ozone season but EGUs are free to use credits at any point within the ozone season. Unfortunately, this can create a problem because of the episodic nature of ozone. Not all days within the ozone season have the same ozone formation potential. It has been found that EGUs, in order to ensure they meet program caps, and allow for more flexibility within the season, reduce NOx emissions more at the beginning of the ozone season, during the months of May and June when temperatures are relatively lower and it is cheaper to make cuts in emissions. (Martin et. al. 2007) When electricity needs are lower, EGUs require a smaller percentage of their units to be online. This gives them flexibility in which units they choose to use. For example, if Natural Gas prices are low, companies can reduce emissions by burning natural gas instead of using costly emissions control units. This leaves them with more credits at the end of the season, during July and August when temperatures are higher, and ozone

formation is more likely. This reduces the benefits of the seasonal ozone cap by leading to temporal hot spots of ozone.

Both cap and trade programs (NOx and SO$_2$) are considered to be successful in reducing emissions cost effectively. Initial problems with price fluctuations and unknowns related to control strategy performance worked themselves out within the first few years and now the programs are meeting reduction goals and have active trading markets. (Burtraw 2005) For the SO$_2$ program, costs associated with compliance under the cap and trade program are about half of what they would be for the same emission reductions under a command and control approach. (Carlson 2000, Ellerman, 2000). Data from the first year of the NOx trading program indicate a decrease of NOx emissions by about 64% from 1990 levels at costs lower than predicted. (Farrell 2001). As low S coal becomes more expensive and companies need to rely on emissions control technology to meet caps, the SO$_2$ trading market will be tested again. However, as will be shown in this thesis, developing programs that create incentives for greater reduction in emissions when those emissions are more likely to lead to the formation of the air pollutants of concern may allow the programs to become even more effective.

Another example of a regional cap and trade program is the Clean Air Mercury Rule (CAMR) developed by the EPA to create a trading market between EGUs for emissions of mercury. (EPA 2008d) It is estimated that 50 of the 165 tons of mercury released into the air in the US each year come from EGUs. (Stivers 2006) Once mercury is released into the air, it deposits on the ground and in water via dry and wet deposition, and from there can be methylated into a form of mercury that can bioaccumulate and is toxic to humans and animals. (Stivers 2006) The exact chemistry of movement of mercury between its various forms is complex and incompletely characterized. However, once methyl mercury is formed it is often consumed by small aquatic life, and accumulates in larger fish and mammals as it moves up the food chain. This has lead to fish consumption warnings in many areas of the country and world. (Stivers 2006)

Mercury is a hazardous air pollutant (HAP) and thus the Clean Air Act [CAA] requires application of Maximum Available Control Technology to reduce emissions. (EPA 1990) Trading of emissions of mercury allow EGUs to avoid MACT and the costs associated with these controls, however critics argue that this form of regulation doesn't guarantee the same level of reductions. Most of the problems arise with the possibility for formation of hot spots. If trading of mercury emissions is allowed, it is likely that at least one area of the US will see an increase in mercury emissions. The fact that mercury is a hazardous air pollutant has made the issue of hot spots a major barrier to the implementation of trading. (http://www.doj.state.wi.us/news/2006/nr052206_ENV.asp)

State and local trading programs: HRVOC trading in Houston, RECLAIM in southern California and EGU NOx emission trading in Texas

In addition to the multi-state regional cap and trade programs developed by the EPA, several smaller in-state programs have been started. In Houston and Southern California, cap and trade programs for HRVOC and NOx, respectively, have been developed for the reduction of ozone. Later chapters of this thesis (Chapter 5) will look in detail at the development of the HRVOC cap and trade program. Here we will briefly look at the NOx trading program developed in the eastern half of Texas as well as the NOx trading program in California.

In the eastern half of Texas, a NOx emissions trading program (Mass Emissions Cap and Trade, MECT, program) has been implemented as part of the state's ozone SIP. (TCEQ 2008b) This program reduces NOx emissions from EGUs. A bill was passed in 1999 that deregulated the electricity generating industry in Texas and forced a 50% reduction of NOx emissions from the 1997 levels. (Nobel et. al. 2001) A cap and trade program was developed to help ease the financial burden of that responsibility. NOx trading as part of

the Houston MECT program has been fairly active. Approximately 300 trades were made each of the first three years of the program with average price per ton steadily increasing from approximately $100 in 2002 to almost $500 in 2004. (TCEQ 2008b)

A study in Eastern Texas found that while ozone hot spot formation could occur as a result of NOx trading, emissions trading could also lead to greater air quality benefits than across the board reductions (Nobel et al. 2001). More refinement of the allowed spatial limitations on trading was suggested as a means for reducing the potential for hot spots and improving the effectiveness of the program.

Largely because of varying level of biogenic emissions of VOCs, Texas presents a wide variety of relative ozone precursor scenarios. In addition, Texas can be considered an extreme example of variable meteorological conditions leading to ozone production. These factors make Texas a particularly challenging area in which to design emission cap and trade programs.

Another, less successful example of this type of program is the one developed by the South Coast Air Quality Management District (SCAQMD) for the region surrounding Los Angeles, California, also called the South Coast Air Basin. At the time, this area had the worst air pollution in the country. The Basin was designated a severe non-attainment area in 1991 and the SCAQMD was required to develop a plan to reach attainment. RECLAIM (Regional Clean Air Incentive Market) was introduced in 1994 as part of the solution. (EPA 2002) Reclaim includes all stationary sources of emissions in the area emitting more than 4 tons of NOx and SOx per year in its market. Originally VOCs were included in the program, but they were withdrawn from the trading program for several reasons, including the difficulty associated with monitoring VOC emissions, the lack of information about VOC control technology as well as a vastly different ozone forming potential between different VOCs due to their different reactivities. (Zerlauth 1999)

The main source of NOx and SOx pollution is the combustion of fuel. Because of this, credits were given to companies based on the historic fuel consumption multiplied by an emission coefficient. Using this method to determine the distribution of credits more accurately represents relative emission reduction capabilities. If credits were instead given based on historic emissions it could benefit companies that have never had any emissions control systems.

Each credit unit, worth 1 US pound, is valid for only one year and credits cannot be banked. Banking was not permitted in order to prevent the formation of temporal hot spots that could occur if companies banked credits to allow for anticipated growth or process upsets. In order to avoid problems associated with end of the year market rushes and price hikes, the facilities that were participating in the trading program were split into two groups. The two groups had year long cycles in which the validity of the credits ended at two different times within the year. Companies were free to buy and sell credits between the two cycles. (EPA 2002)

The area under RECLAIM was divided into two regions, the coastal region and the inland region. Trades within each region were unrestricted, but trades between the regions were not allowed. This is because of the meteorology of this area. There is limited air mixing between the two regions at certain times of the day, creating a situation where hot spots are more likely to form. In order to avoid hot spots, the regulators reserve the right to limit trading at any time. If a certain area becomes problematic temporally or spatially, credit sales into that area can be restricted at any time. (EPA 2002)

Within two months of the end of a cycle, each company must send a report to the South Coast Air Quality Management District (SCAQMD) which documents the total emissions and the credits used to cover those emissions. Any inconsistencies or missing data is filled in with a worst case scenario dataset. Credits must be available to account for any

missing data or severe monetary fines can be imposed and the amount of credits in excess of the available credits will be deducted from the violators remaining credits for the next few years.

RECLAIM had many problems associated with it. A main problem with RECLAIM was the lack of transparency. Issues that arose (including overallocation of emissions, and lack of understanding of current and future emission reduction technology) created unknowns in the trading market, which caused emissions credit prices to change dramatically. This made companies hesitant to get involved with the trading market. Deregulation of the electric industry in 1998 also added uncertainty. (Burtraw et. al. 2005)

One of the few benefits of RECLAIM was the installation of measuring and monitoring equipment. This provided emissions data that had previously been unavailable. However, these benefits came with a price and many companies were unhappy with the expenses relating to purchasing and maintaining this equipment. Additionally, while NOx and SOx were covered by RECLAIM, all other regulated pollutants were still subject to the Command and Control system. This required companies to have two pollution control programs in place.

Electricity generators were pulled out of the program in 2001, before the market could stabilize itself. SCAQMD has proposed that they be added back in to the trading program (Burtraw, et al. 2005).

Summary

Previous attempts at air quality regulation through cap and trade programs have illustrated strengths and weaknesses of the approach. While these programs give emission sources the freedom to determine the cheapest way to meet air quality

regulations, if the emissions market is not well known for any reason, markets may fail. In addition, since the success of a trading program relies on a complete and accurate emissions inventory, emissions monitoring is critical. Improved emissions monitoring has the added benefit of helping improve results from air quality models, however, it can add considerable expense to programs.

Another critical feature of an emissions trading program is the method for allocation of credits. Allocation must be done in a way considered fair by all involved. Allocating credits based on historical emissions rewards high emitters, but it is not always straightforward to allocate based on some measure of benefit to society (ie: production). Once credits are allocated, studies need to be conducted to test the necessity of trading restrictions in time or space to limit the formation of hot spots.

Finally, once the program is designed and air quality benefits tested, a viable trading market must be created. This usually requires some knowledge of the costs and reliability of emissions control technology. It is also important to clearly set out the goals and future plan for the program so that facilities involved can plan ahead. If implemented correctly, a trading program can lead to emission reduction goals at a much lower price than historically utilized command and control emissions regulations.

Chapter 3 NOx Trading in the Northeastern United States

Introduction

Despite more than 30 years of regulation, some of the most densely populated regions in the United States are still in non-attainment of the ozone concentration standards set through the Clean Air Act (Figure 3-1). In these areas, ozone concentrations frequently exceed a threshold value established by EPA as necessary to protect human health. In responding to and reducing these ozone concentrations, one of the complicating factors is that ozone is not emitted directly, but rather is formed by complex reactions between oxides of nitrogen (NOx) and Volatile Organic Compounds (VOCs), two ozone precursors, in the presence of sunlight. (Tong 2006) The response of ozone concentrations to reductions in emissions of ozone precursors is typically non-linear, exhibits time lags, and is moderated by interactions with naturally occurring releases to the atmosphere. Further, the ozone production potential of each precursor can vary between different regions. For example, rural regions in the northeastern United States contain vegetation that releases very reactive hydrocarbons (isoprene and various mono-terpenes) in large quantities (NRC 1991), while other regions (the Los Angeles basin, for example) have very limited naturally occurring emissions from vegetation.
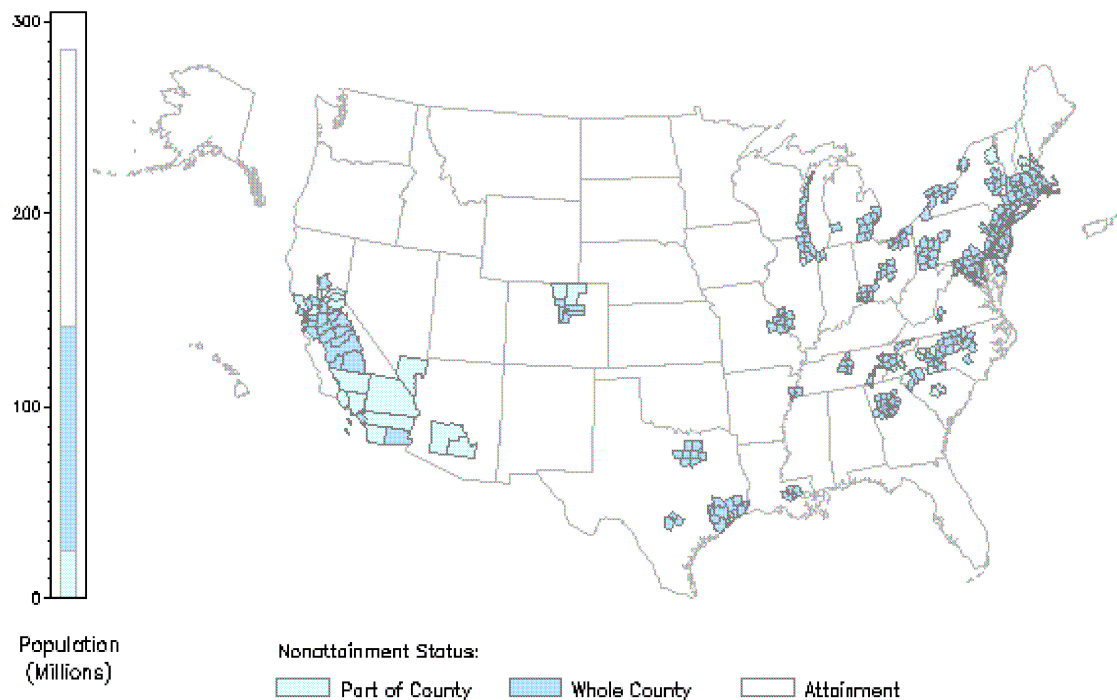
Figure 3-1. Nonattainment areas for ozone, with concentrations averaged over 8 hours; 347 counties, with combined populations of more than 140 million, exceed the standard as of February 2008.

Source: http://www.epa.gov/air/data/nonat.html?us~USA~United%20States

As shown in Figure 3-1, large regions in the northeastern United States (NE US) violate the National Ambient Air Quality Standard (NAAQS) for ozone. In March of 2008, the EPA proposed a new, stricter 8-hr ozone standard that, if adopted, would cause many more areas of the country to go into non-attainment. (EPA 2008c) In the urban areas of the NE US both VOC and NOx emission controls are used to reduce ozone concentrations, however, in the more rural areas of the NE US, reactive VOC emissions from vegetation are extensive, and controlling anthropogenic VOC emissions would have a very small impact on ozone formation. As a consequence, over large portions of the NE US, the focus in reducing ozone concentrations is on NOx emission controls. (Krupnick 2000)

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Approximately 60% of anthropogenic NOx in the NE is emitted by the transportation sector. The second largest NOx emitters are point sources. Approximately 22% of NOx emissions come from point sources and 97% of those are due to Electricity Generating units (EGUs), or power plants. (EPA 2003)

Emissions from power plants in the NE US are subject to an emission cap and trade program. In a cap and trade program, an individual EGU can precisely meet its cap, reduce NO_x emissions below its cap, or emit more than its cap. If a facility emits less than its allocated cap, it can sell its excess emission allowances (the difference between its allocated cap and its actual emissions) in an emissions trading market. If a facility emits more than its cap, it must purchase allocations on the market. Chapters 3 and 4 of this thesis will examine new approaches to cap and trade programs for EGUs using a four state case study region. The states are Pennsylvania, Maryland, New Jersey and Delaware (the PJM region). As shown in Figure 3-2, much of the 4 state region is designated as a non-attainment area for ozone according to the old standard set at 85ppb. It is likely that more of this area would be considered in non-attainment when the new standard has been promulgated.
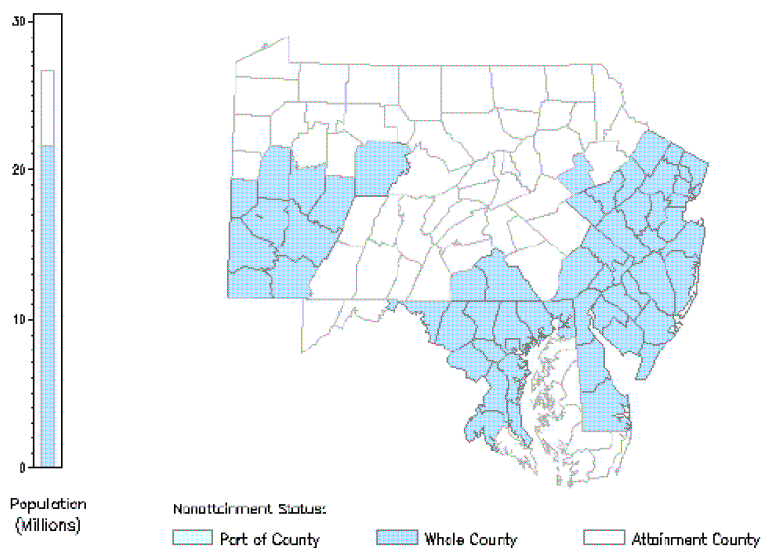
Figure 3-2. Non-attainment counties in the PMJ as of February 2008. (EPA 2008b)

Regulatory Framework for EGU NOx Emissions

In order to reduce NOx emissions from EGUs in the NE US, a seasonal NOx cap was placed over the area as part of the 2005 Clean Air Interstate Rule (CAIR) (EPA 2008b). A seasonal cap differs from a yearly cap by limiting the total emissions allowed over the course of an ozone season (which runs from April to September) as opposed to a limit on the yearly total.

Emissions during all days of the ozone season are treated as equivalent. EGUs, by deciding whether or not to enter the market, and by determining when in the season emissions occur, have flexibility in where and when they release NO_x during the ozone season, without regard for whether those times and locations are better or worse for ozone formation.

One of the challenges in reducing ozone concentrations is the mismatch between the existing incentives to reduce NO_X, in the form of a seasonal cap placed by CAIR, and the

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highly variant temporal and locational impact of NO_X precursor emissions on ozone formation in any given area during an ozone season. Ozone is an episodic problem and numerous conditions, including wind, sunlight, and concentrations of VOCs, determine whether reductions of NO_X at a given time and location will lead to reductions of ozone in a target area. Consequently, the literature has called for a more finely differentiated regulation of NO_X emissions to address the temporal and locational variation in the contribution of NO_X to ozone formation, but to date they have not been implemented because of the difficulty in adequately modeling the air quality impacts (Mauzerall, 2005; Tong, 2006). Advances in meteorological modeling and air quality modeling now allow high ozone days to be predicted, with the same degree of advance notice as predicted peak temperatures, which currently impact electricity dispatching decisions (see, for example, http://airnow.gov/).

This chapter examines the air quality impacts of emissions control that is more spatially and temporally detailed than the current seasonal cap and trade program. Instead of regulating the entire ozone season equally, the hypothesis to be examined in this thesis is that placing stronger regulation, in the form of more credits (higher cost) required per ton emitted, on days during the ozone season when NOx emissions are more likely to form ozone, will have a larger impact in reducing the formation of ozone. Additionally, this thesis will examine the hypothesis that spatially detailed regulation, charging more for emissions that are located in areas that at certain times would lead to higher ozone formation, would cost effectively decrease ozone formation. The result would be a more successful and cost-effective program.

Several factors now enable a more spatially and temporally resolved cap and trade program. The existence of real-time electricity markets make it possible for operators of EGUs to respond to varying NOx price signals up to a day or even hours ahead of time. Electric utilities make daily and hourly allocation decisions for generation capacity largely based on economic criteria such as the cost of operating the plant and the

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transmission losses that will occur in delivering power to the customer. (Martin 2007) Under the current seasonal and annual caps, operators have little incentive to incorporate environmental considerations in these daily allocation decisions. However, the potential exists to include these considerations. In addition, air quality modeling is now routinely done in forecast mode, enabling estimates of the ozone impacts of EGU NOx emissions, which can then be translated into daily cap and trade cost signals.

The success of this approach depends on the integration of air quality modeling and economic modeling of the electric utility dispatch. This research is a joint effort with collaborators at the Massachusetts Institute of Technology (MIT) to develop an integrated modeling framework that represents electricity generation, transmission, and dispatch decisions, resulting NOx emissions, meteorological conditions and transport, and photochemistry. This thesis will examine the air quality impacts of the dispatching decisions using photochemical modeling.

Methods

Grid dispatching model

Researchers at MIT (Martin et. al. 2007) developed a model of the electricity generation and transmission grid for the PJM region. The model contains data that accurately represents electricity generating capacity and emission rates at every location. The model also contains all the information about power line load constraints and supply and demand data, and network congestion data. EGU locations often have several different units that run on different fuels with varying emissions levels, and also may have the ability to turn on and off emissions controls. This flexibility makes it possible to vary emission levels even when electricity is at its peak demand. The model contains all this information and is able to not only provide the extent to which emissions can be reduced

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without threatening electricity supply, but also the approximate reduction of emissions that will result from varying the cost of NOx emissions.

Air quality model

The air quality model chosen for this study is the Comprehensive Air quality Model with extensions (CAMx). CAMx is a 3D Eulearian photochemical grid model that predicts the spatial and temporal movement, production and depletion of aerosol and gas-phase pollutants using data on emissions, meteorology, chemistry and deposition (www.camx.com). CAMx has been used in regulatory applications, evaluating the effectiveness of emission reduction strategies, in states throughout US including by the Ozone Transport Commission in development of the NE US NOx cap and trade program. (ENVIRON 2008)

Input data required by CAMx includes meteorological data, emissions data from all source categories, and ambient and boundary conditions. The current scope of this project employs a CAMx episode that was already created and used by the Central Regional Air Planning Association (CenRAP) for regional haze and visibility studies. The modeling period that was used is June - September 2002.

The model uses a nested grid, with horizontal resolution of 36 km and 12 km. The grid is shown in Figure 3-3. The finer scale, with a 12 km horizontal resolution, was used in the PJM area in the NE.
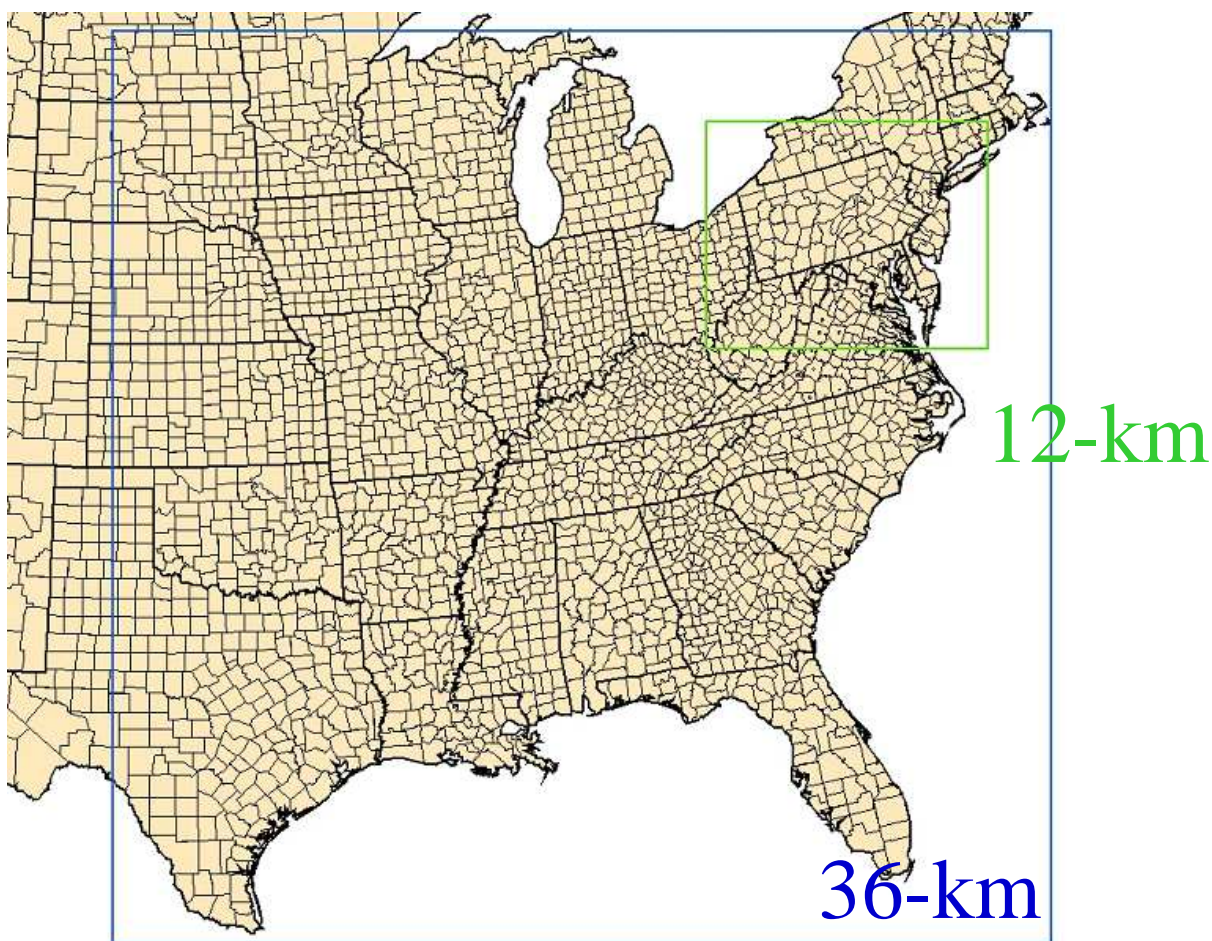
Figure 3-3. 36km grid over the entire central and eastern portions of the US, and the 12km flexi-nest grid over the area of interest in the NE.

Meteorological data was developed by the Iowa Department of Natural Resources (IDNR) using the NCAR/PSU Mesoscale Model (MM5) and was then formatted for CAMx using an MM5CAMx processor. MM5 uses mathematics and physics to include topography, boundary conditions, and all meteorological inputs to develop a detailed layered meteorological input to air quality models. (UCAR) IDNR completed a 36km resolution grid simulation for the continental US. (ENVIRON 2007) For this study, a flexi-nested 12km grid was added over the area of interest in the NE. While the point source emissions were distributed and modeled with the definition of the 12km grid, the

surface area emission and meteorology were defined only for the 36k grid and were interpolated to the 12km grid.

The emissions inventory for non-EGU sources were developed by CENRAP, based on the EPA's 2002 National Emissions Inventory with updates and corrections provided by individual states. The emissions inventories were processed using the SMOKE emissions processing system as preparations for EPS3. (ENVIRON 2007)

The biogenic emissions inventory was developed using the Global Biosphere Emissions and Interaction Systems (GloBeis) with temperatures estimated using MM5, cloud cover estimated using satellite data, and land cover/land use data developed by CENRAP for the 1999 emissions inventory. The base anthropogenic emissions inventory was developed using EPA's National Emissions Inventory. This includes emissions of all point sources, area sources, off shore sources, and on and off road mobile sources, and was adapted for use in CAMx for CENRAP (Yarwood et al 2006). Point source data were provided in AFS format with information on individual point sources including name of source, type of industry, specific locations, stack heights and diameters, and exit gas temperature and velocity. These data allow changes to be made in the emissions rates of individual sources, or groups of sources to test various EGU dispatching scenarios.

Proof of Concept Analyses

Economic and air quality analyses of a single multi-day ozone episode are performed to test the central hypothesis of this work, that placing stronger regulation, in the form of more credits required per ton emitted (more cost), on days during the ozone season when NOx emissions are more likely to form ozone, will have a large impact in reducing the formation of ozone.

This first step of the research aims to answer the following questions:

1. How much emissions reduction can be realized during periods of peak demand?
2. What corresponding amount of financial motivation is needed to see specific reductions?

Within the June through September 2002 time period, all high ozone episodes were examined to identify an appropriate short modeling episode for representative economic modeling and the proof of concept study. All of the episodes are examined in the seasonal modeling described later in this chapter. High ozone episodes were defined for this case as 2 or more days in a row with maximum 1 hr ozone concentrations above 84ppb at 5 of the 6 monitoring stations in the Philadelphia non-attainment area. Five episodes were identified (data used in the episode characterization taken from the EPA's Air Quality System Database (EPA 2007b)):

1. June 24-27: Max one-hour ozone (ppb): 110, 135, 111, 97
   During this episode weather conditions included clouds/rain and a nearly stationary front in the immediate Philadelphia area.
2. July 8-9: Max one-hour ozone (ppb): 144, 130
   Local ozone concentrations were likely impacted by magnitude and transport of smoke plumes from Quebec
3. July 17-19: Max one-hour ozone (ppb): 111, 110, 123
   Clouds and rain in the immediate Philadelphia area, high fine particulate matter concentrations. Episode is dominated by long-range transport from the west.
4. August 2-4: Max one-hour ozone (ppb): 140, 146, 135
   Stationary cold front and substantial change of wind direction with respect to height in NE US.

The fifth episode that occurred during the 2002 ozone season, August 10-14 had the following characteristics: Max one-hour ozone (ppb): 117, 126, 143,147,132

1. Episode was an exceptionally strong regional transport/stagnation event with high pressure centered over the mid-Atlantic and northeastern US states. The episode represents one of the most severe pollution events in the northeastern US during the previous decade. Extremely high fine particulate matter concentrations as well.
2. Long-range transport patterns indicated by 72-hour back-trajectories were northerly (8/10), southwesterly (8/11 and 8/14) and westerly from the Ohio River Valley (8/12 and 8/13).
3. Episode included the observation of a southwesterly nocturnal low-level jet on some days.
4. Episode was characterized by mostly clear skies with no precipitation.

This episode was chosen for economic modeling and proof of concept; its selection was primarily due to the range of long-range transport patterns that would allow potential evaluation of emissions sources throughout the NE US. In addition, the predicted ozone concentrations would not be highly sensitive to the modeled locations of clouds/rain or the location of any stationary fronts.

Back trajectories (paths taken by air parcels that arrive in Philadelphia on each day of the episode) from the five days of this episode are shown in Figures 3-4 a-e. The trajectories were calculated using the National Oceanic and Atmospheric Administration's HYbrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model (ARL 2008) and show the varying types of meteorology that lead to high ozone concentrations.
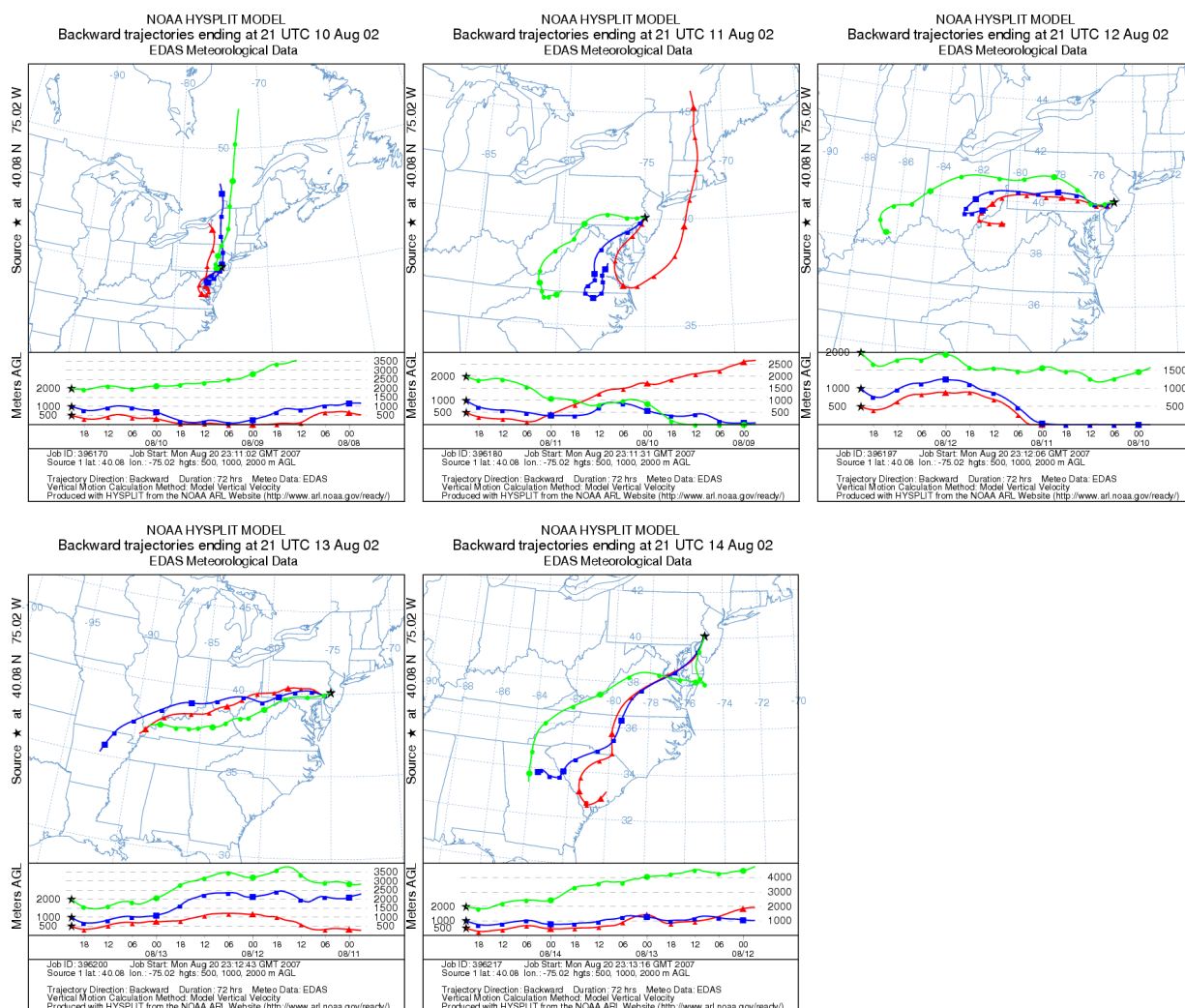
Figures 3-4. Back trajectories going back 72 hours (we are most interested in the last 36) of the individual days of the August 10-14th high ozone episode. Different colors represent different ending elevations for the air parcel.

As stated in Chapter 2, ozone is a regional problem and some of the ozone that is measured in the NE forms from precursors that are released in other areas of the country. For example, August 12th and 13th show back trajectories that indicate that air was brought in from the Ohio River Valley. August 11th and 14th show back trajectories that

indicate that air was brought in from the Carolinas and Virginia. On August 10th, air comes in from the north and becomes somewhat stagnant over the PJM area, collecting emissions and holding them over the area.

Economic Simulations

For the economic modeling of this study, the CENRAP basecase emissions inventory was altered to represent increased NOx emissions costs. In separate runs performed by collaborators at MIT, costs of $10,000, $30,000, $50,000, $100,000, and $125,000 were applied for each ton of emissions of NOx from EGUs in the NE on August 12th, a representative day. The economic model was run using area demand on that day, and the dispatch that would occur as a result of each of those emissions prices. Emissions resulting from the various dispatching strategies were then used as input to CAMx (at the University of Texas, UT) in order to model resulting air quality changes.

Since only August 12th was examined using the economic model, the spatial and temporal distribution of emissions from that day will be used to model every day of the episode. This is broadly consistent with modeling practice used in air quality planning. When annual point source emissions data are assigned to individual days in CAMx, the allocations are generally the same for all ozone-season weekdays. Therefore it is reasonable to use the August 12th emissions from economic model for other summer weekdays. Point sources receive lower emissions by CAMx allocation factors on Saturdays and Sundays. (August 10, 2002 was a Saturday and August 11, 2002 was a Sunday) Therefore, using a weekday emissions inventory input for a weekend day could be considered a worst case scenario. For this proof of concept demonstration, the distribution of emissions developed by the MIT economic model for August 12th will be used to model the entire episode, and later in the chapter, the entire season.

The overall reductions of emissions from EGUs that occurred in each cost scenario
(assuming emission costs of $10,000, $30,000, $50,000, $100,000, and $125,000 for each
ton of emissions of NOx from EGUs, compiled by collaborators at MIT) are shown in
Figure 3-5. The increase in slope of the cost versus percent emissions reduction curve at
$50,000 indicates an increase in the costs associated with making emissions reductions
while still meeting electricity demand. These results indicate that large changes in total
NOx emissions are possible, while meeting electricity demand on a hot summer day,
using dispatching strategies.
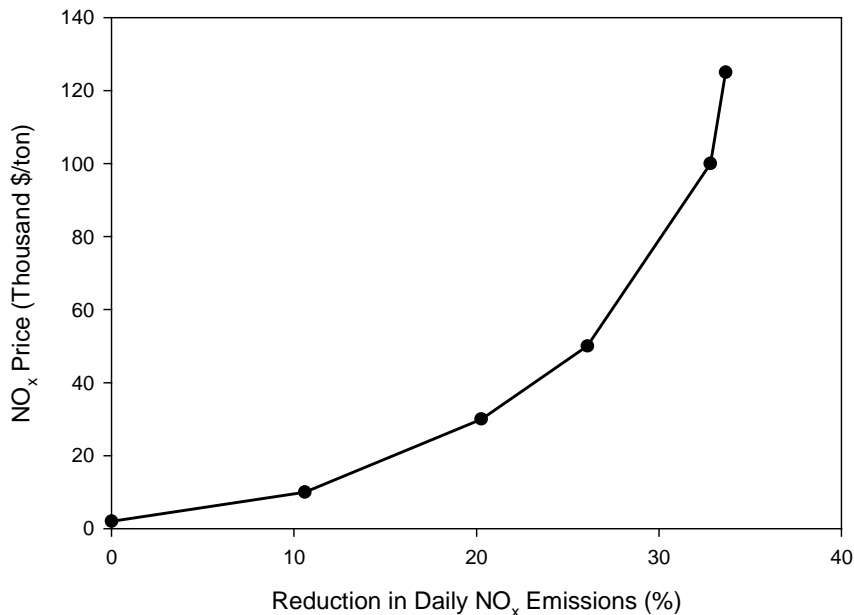
Figure 3-5. Percentage reduction in NOx emissions versus cost of NOx emissions per ton.

Figures 3-6 a through e show the reductions in 8 hr averaged ozone concentrations on
August 10th – 14th, 2002 that resulted from a charge of $125,000 for a ton of emissions of
NOx. These figures show that while ozone reductions are pervasive (up to 8.7 ppb for
the maximum 8-hour averaged concentration), there are small areas where increases do
occur. The areas of increase are mostly downwind and outside of the region and the
maximum increase is 2 ppb. Increases might occur when emissions costs increase
because electricity generation is often moved from high emissions units (coal fired

boilers without control technology) to lower emissions units (units with controls). While these moves are often in the same general area, they are not always and these changes in emission location can lead to increases in emissions in some regions. Additionally, the increases in ozone over Newark are likely associated with NOx reduction disbenefit (discussed in more detail in Chapter 4).

E-125k minus Basecase

E-125k minus Basecase

August 10,2002 0:00:00
Min= -5.208 at (39,12), Max= 1.773 at (52,37)

August 11,2002 0:00:00
Min= -7.843 at (39,11), Max= 2.013 at (52,38)

E-125k minus Basecase

E-125k minus Basecase

August 12,2002 0:00:00
Min= -8.747 at (41,12), Max= 2.013 at (52,36)

August 13,2002 0:00:00
Min= -7.964 at (39,10), Max= 1.187 at (52,37)

E-125k minus Basecase

mx.PJM_bc.20020814.o3.8hr.grd3, x=camx.PJM_episodes_125k.20020814.o:

August 14,2002 0:00:00
Min= -3.983 at (39,12), Max= 2.419 at (48,30)

Figure 3-6. a-e. Differences in daily maximum 8 hour ozone due to $125,000 emissions for August 10th through August 14th, 2002.

The results presented in Figures 3-6a-e show one measure of air quality – changes in maximum ozone concentrations. However, because ozone concentrations increase in some areas and decrease in others, this single measure of air quality changes is not sufficient to represent the net effect of the reduction and redistribution of emissions. Left unanswered are questions such as how the changes in emissions impact human exposures to ozone and whether the predicted increases in ozone concentrations occur in regions with low or high baseline ozone concentrations. In order to present results of this proof of concept study in a more robust manner, a set of air quality metrics, in addition to total emission reductions and ozone concentrations, are used. The metrics will quantify a variety of changes in ozone concentrations, and population exposure to ozone. The four metrics used are total area with eight hour averaged ozone concentrations above a threshold concentration, total population living in grid cells with eight hour averaged ozone concentrations above a threshold value, time integrated ozone area above the threshold, and time integrated ozone above the threshold multiplied by population. Metrics are calculated twice, first for threshold defined as the 75ppb standard and then for the threshold defined as the 84ppb standard. Days during which the maximum ozone

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concentration is below the standard are not included in the metrics calculations. The following equations describe how the metrics are calculated.

1. Total Area Above Threshold (km^2)

$$A_{\text{Area of exceedance}} = \sum_g a_g \max\{\delta_{g,h}\}$$

$$\delta_{g,h} = \begin{cases} 0 & c_{g,h} \leq threshold \\ 1 & c_{g,h} > threshold \end{cases}$$

Where a_g is the area of grid cell g, and $c_{g,h}$ is the ozone concentration in grid cell g in hour h. This metric is calculated by determining all ground level grid cell ozone concentrations in the PJM area for each day, calculating the maximum ozone concentration in each cell, and comparing the maximum concentration to the threshold. If the maximum concentration exceeded the threshold, then the area of that grid cell is added to the total.

2. Total Population Above Threshold (capita)

$$M_{\text{Total Population}} = \sum_g p_g \max\{\delta_{g,h}\}$$

$$\delta_{g,h} = \begin{cases} 0 & c_{g,h} \leq threshold \\ 1 & c_{g,h} > threshold \end{cases}$$

Where p_g is the population in grid cell g, and $c_{g,h}$ is the ozone concentration in grid cell g in hour h. This metric is calculated by determining all ground level grid cell ozone concentrations in the PJM area for each day, calculating the maximum ozone concentration in each cell, and comparing the maximum concentration to the threshold.

If the maximum concentration exceeded the threshold, then the population in that grid cell is added to the total.

3.   Time integrated area * excess (km^2 ppb)

$$M_{\text{Time Area}} = \sum_{h}\sum_{g} a_g e_{g,h}$$

$$e_{g,h} = \begin{cases} 0 & c_{g,h} \leq threshold \\ c_{g,h} - threshold & c_{g,h} > threshold \end{cases}$$

Where a_g is the area of grid cell g. This metric is calculated by determining the maximum ozone concentration in all ground level grid cells in the PJM area for each hour of each day. If that maximum is above the threshold, the excess is calculated by subtracting the threshold from the ozone concentration in the cell, and the excess is multiplied by the area. The sum is taken over the area and over the hours of the day.

4.   Time integrated population * excess. (ppb * capita)

$$M_{\text{Time Pop}} = \sum_{h}\sum_{g} p_g e_{g,h}$$

$$e_{g,h} = \begin{cases} 0 & c_{g,h} \leq threshold \\ c_{g,h} - threshold & c_{g,h} > threshold \end{cases}$$

This metric is calculated by determining the maximum ozone concentration in all ground level grid cells in the PJM area for each hour of each day. If that maximum is above the threshold, the excess is calculated by subtracting the threshold from the ozone concentration in the cell, and the excess is multiplied by the population density. The sum is taken over the area and over the hours of the day.

Proof of Concept Results

Table 3-1 shows the air quality improvements, in terms of the four metrics described above that result when there is a $125,000 charge per ton of NOx emissions. While both Table 3-1 and Figure 3-6 show air quality improvements, the goal of the proof of concept study is to show that, even on hot summer days when electricity demand is at its highest, it is possible to reduce emissions, and see a significant improvement in air quality, while still meeting electricity demand. It should also be noted that while much of the area of interest does see an improvement in air quality in the form of ozone concentration reductions, there are localized areas where ozone concentrations increase due to the scenario modeled.

Figure 3-7 shows the maps of values calculated for metric #4, Daily Population Exposure for August 10th through August 14th for the $125,000/ton NOx case for both the standard defined as 75 ppb (left column) and the standard defined as 85ppb (right column). In these maps, any grid cell colored yellow, orange or red is experiencing an increase in population exposure over the course of the day. This means that in these grid cells, ozone concentrations have increased relative to the basecase at some point in the day. Any grid cells colored in green-blue through dark blue are seeing decreases in population exposure relative to the basecase over the course of the day.

August 10th and 11th show decreases in exposure over much of the area surrounding Baltimore and Philadelphia with the largest decreases adjacent to Baltimore, but an increase in one grid cell north of Philadelphia. August 12th also shows decreases, with the largest decreases located in cells adjacent to and within both cities, and one cell showing an increase on the Jersey Shore directly east of Philadelphia. August 13th shows only decreases with the largest being closest to the two cities. August 14th shows mostly decreases around both cities with increases in four cells west of Philadelphia when the

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threshold is set at 75 ppb. Increases in exposure are likely caused by local increases in NOx emissions.

Table 3-1. Percent reduction calculated for each of the four metrics for the $125,000 case relative to the basecase. These values are averaged for the August 10th – 14th episode and metrics are calculated for both the 75 ppb and 85 ppb thresholds.

$125,000 / ton NOx	Threshold = 85 ppb	Threshold = 75 ppb
Area above Standard	-6%	-5%
Population above Standard	-7%	-5%
Daily Area Exposure	-11%	-8%
Daily Population Exposure	-8%	-7%

Daily Population Exposure

75 ppb Standard
Episodes-125k minus Basecase

August 11,2002 6:00:00
Min= -3992 at (40,18), Max= 207 at (48,29)

Daily Population Exposure

85 ppb Standard
Episodes-125k minus Basecase

August 11,2002 6:00:00
Min= -2508 at (40,18), Max= 119 at (48,29)

Daily Population Exposure

75 ppb Standard
Episodes-125k minus Basecase

August 12,2002 6:00:00
Min= -3881 at (48,27), Max= 85 at (54,29)

Daily Population Exposure

85 ppb Standard
Episodes-125k minus Basecase

August 12,2002 6:00:00
Min= -3445 at (48,27), Max= 52 at (54,29)

Daily Population Exposure

75 ppb Standard
Episodes-125k minus Basecase

August 13,2002 6:00:00
Min= -4335 at (40,18), Max= 0 at (1,1)

Daily Population Exposure

85 ppb Standard
Episodes-125k minus Basecase

August 13,2002 6:00:00
Min= -3461 at (40,18), Max= 0 at (1,1)

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Figure 3-7. Difference in exposure between the Episodes-$125,000 case and the Basecase for August 10th – 14th, 2002 for 75ppb standard and 85 ppb standard.

The August 10th through 14th ozone episode was one of the worst episodes in the Northeastern US in over a decade. Back trajectories showing air movement on those days (Figure 3-4) show patterns that could likely lead to high ozone formation. However, it is important to show that results occurring within this episode are applicable to other times. The next section of this chapter will examine meteorological patterns of high ozone days over a five-year span. This information will be used to ensure that the August 10-14 episode is representative. A final section of the chapter will examine modeling results performed for an entire ozone season.

Meteorological Study

A study of the weather patterns that have been present during ozone episodes over a 5-year period is conducted. High ozone data from 2002 through 2006 are collected from the EPA, identifying all days where a maximum 1-hour concentration above 80 ppb was measured at any monitor in the non-attainment areas in this study. (EPA 2007b) Back trajectories are made for all of the days that met these criteria. Back trajectories are made

using HYSPLIT, a meteorological program available on the National Oceanic and Atmospheric Administrations Air Resource Laboratory (ARL 2008) and they show the trajectory that the air had traveled to arrive at the set location and time.

A cluster analysis is done on the high ozone days. The cluster analysis feature is part of HYSPLIT. (ARL 2008) The cluster analysis takes a series of back trajectories provided by the user, and makes a number of passes through the series equal to the number of trajectories. During each pass, the program combines the two closest trajectories into a cluster and records a measure of how close those two trajectories were. The cluster then becomes counted as another single trajectory. As the measure of similarity gets larger the program is combining trajectories that are less similar. A decision is made on the final number of clusters by looking for large increases in that measure as clusters are added. In this case, the final number of clusters was five. Figure 3-7 shows the five back trajectory clusters extended back 36 hours. These clusters represent the common weather patterns leading to high ozone days. They are North, Northwest, West, Southwest and stagnation.

A further analysis was done on the high ozone days that occurred between 2002 and 2006 (Concentrations above 75 ppb). Once each of those days was assigned a cluster, the maximum 1-hour ozone concentration for each, the month, and the cluster number were used to try to find patterns within the high ozone occurrences. Figure 3-8 a and b show two different analyses that were done. Clusters 2 and 5, corresponding to a western back trajectory and stagnation are the most common air patterns leading to high ozone, especially during the months of June, July and August. However, no additional patterns stood out. It appears that the five major back trajectories identified by the cluster analysis are all as likely to lead to high ozone concentrations at any time during the ozone season. Additionally it should be noted that August 10th of the 2002 episode corresponds to the stagnation pattern represented by cluster 5 and August 12th shows a westerly back trajectory represented by cluster 2. August 13th and 14th show a southwesterly back

trajectory represented by cluster 1 and August 11th shows a southerly trajectory represented by cluster 3. Based on this analysis, the August 10-14 episode can be viewed as broadly representative of most high ozone days for the region.
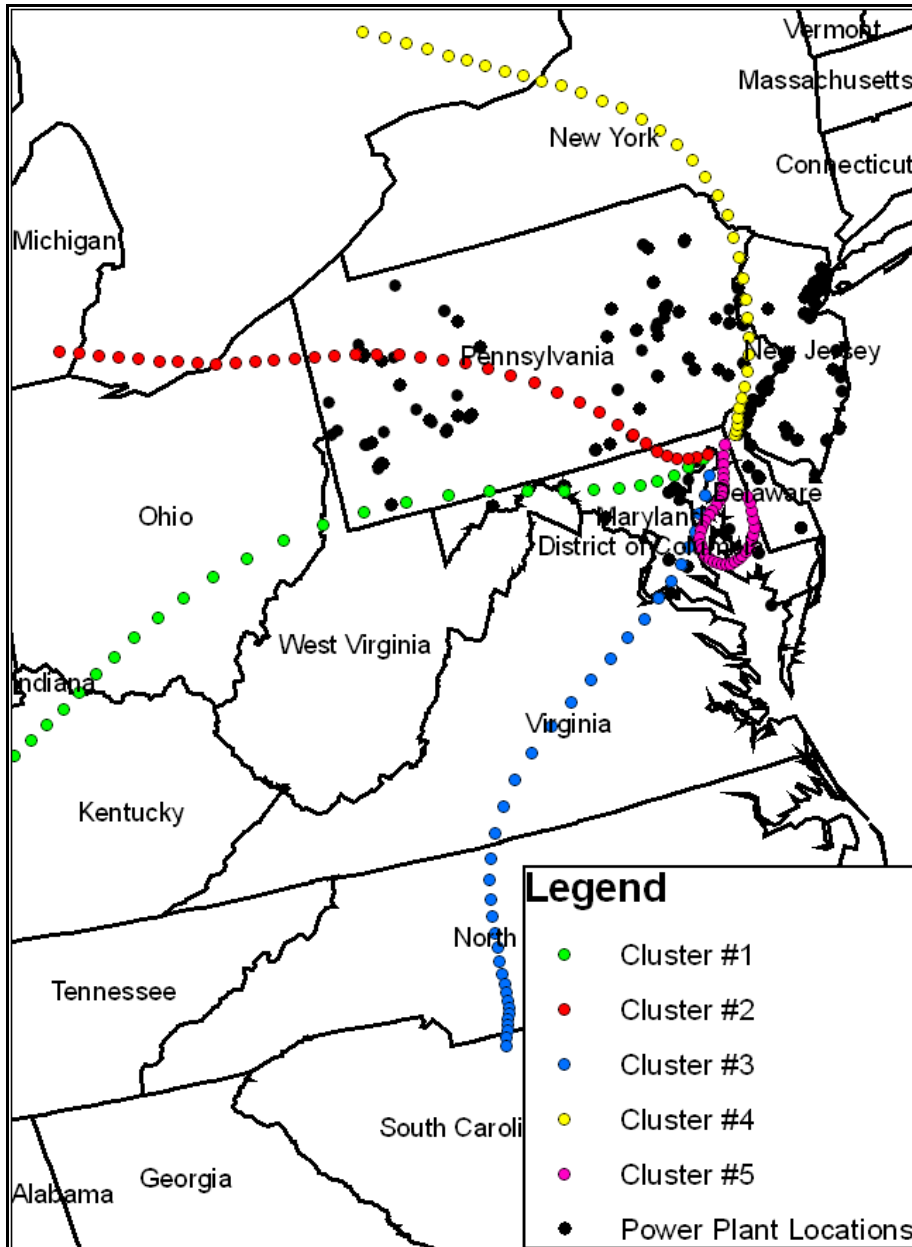
Figure 3-8. Five clusters determined by cluster analysis program.

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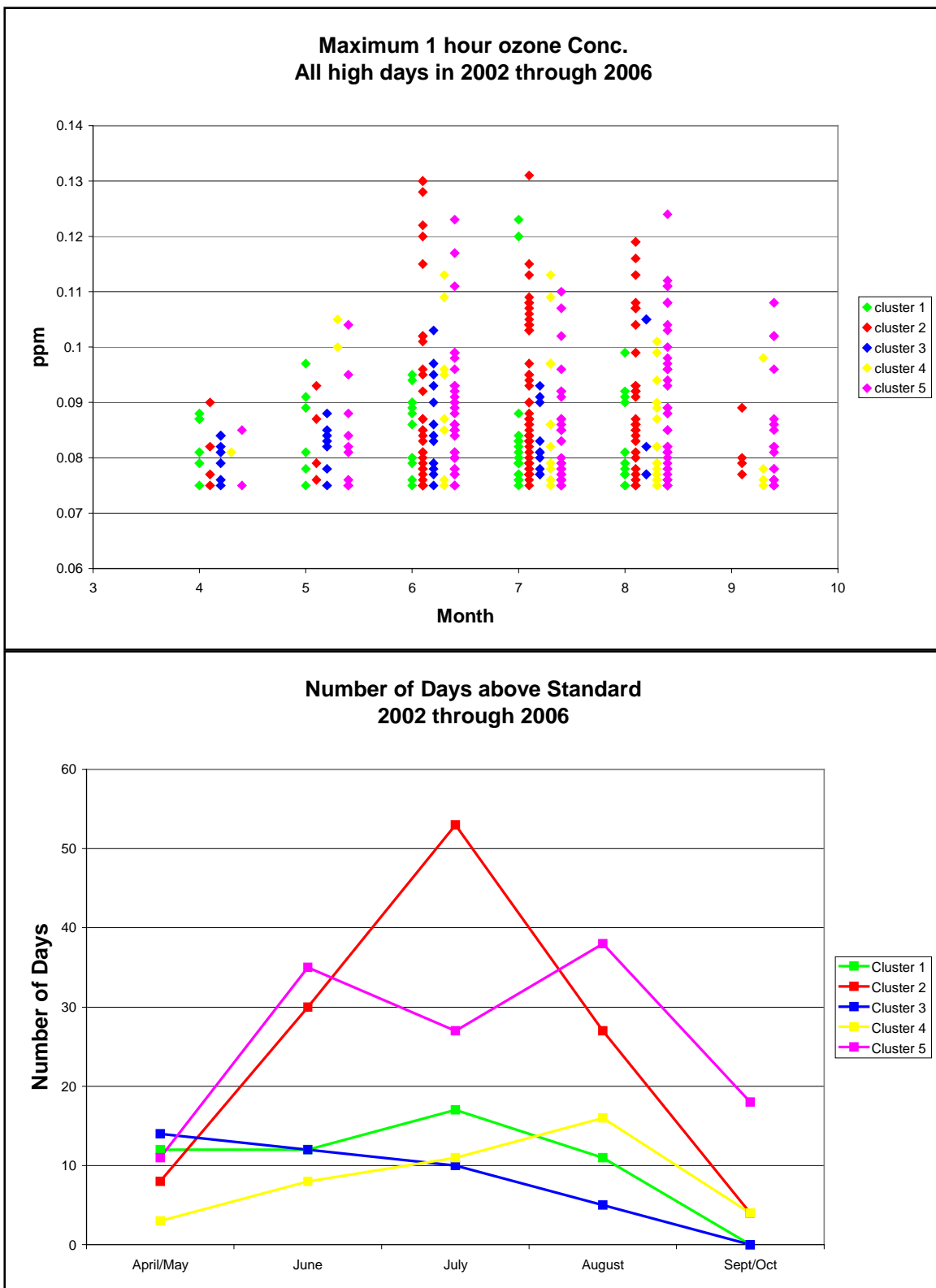
Figure 3-9. Analysis of the high ozone days in 2002 through 2006 and the cluster the

back trajectories leading up to those days are categorized with.
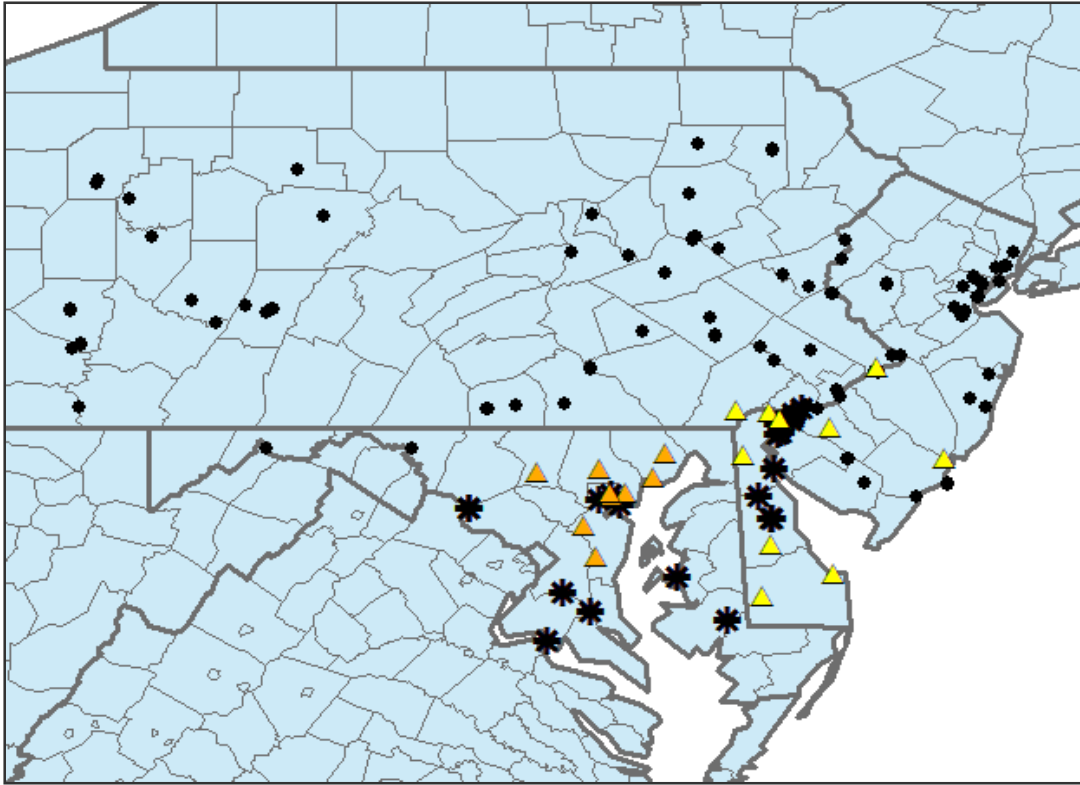
Figure 3-10. Location of EGUs with SW EGUs marked by black stars. EGUs located in the PJM grid, not controlled in the SW case are marked by black circles. Baltimore monitors are marked by orange triangles, and Philadelphia monitors are marked by yellow triangles.

Spatial Trading

In the proof of concept analysis described in the previous section, all power plants in the PJM grid were subject to higher pricing during the ozone episode. In this section, the question to be examined is whether increasing NOx emissions pricing along specific trajectories (as opposed to the entire PJM region as was done for the results shown in Figures 3-5 and 3-6) will be effective. Two case studies were run, a Southwesterly study on August 14th, a day with a southwesterly back-trajectory, and a Westerly study on

August 12th, a day with a westerly back-trajectory. Higher emissions pricing is implemented for power plants along each trajectory for each specific day, but not the rest of the region. The power plants along the southwestern trajectory are shown in Figure 3-10 and the trajectory is shown in Figure 3-11. A similar map of power plants located along the August 12th westerly trajectory (trajectory is shown in Figure 3-4) was created, and MIT was provided with a list of EGUs considered upwind for both cases. MIT estimated the emissions for both cases if these power plants, and only these plants, faced a NOx emissions price of $125,000 per ton.
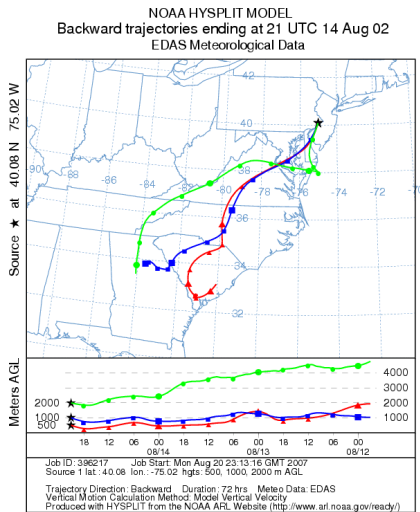
Figure 3-11. August 14th back-trajectory.

Those facilities along each trajectory are charged $125,000 for a ton of emissions of NOx while the remaining facilities in the modeling region are charged $2,000 per ton, the approximate value of current emissions in the trading program. Results from the spatial study, shown in Figure 3-11, indicate that area wide decreases are similar in scale if either a southwestern or a western trajectory is subjected to $125,000 per ton costs and that these emissions are only slightly reduced from the scenario where all facilities in the region face a $2,000 per ton cost. The overall reductions of NOx emissions were smaller in the spatial $125,000 studies than when all facilities in the region faced costs of $125,000 per ton.
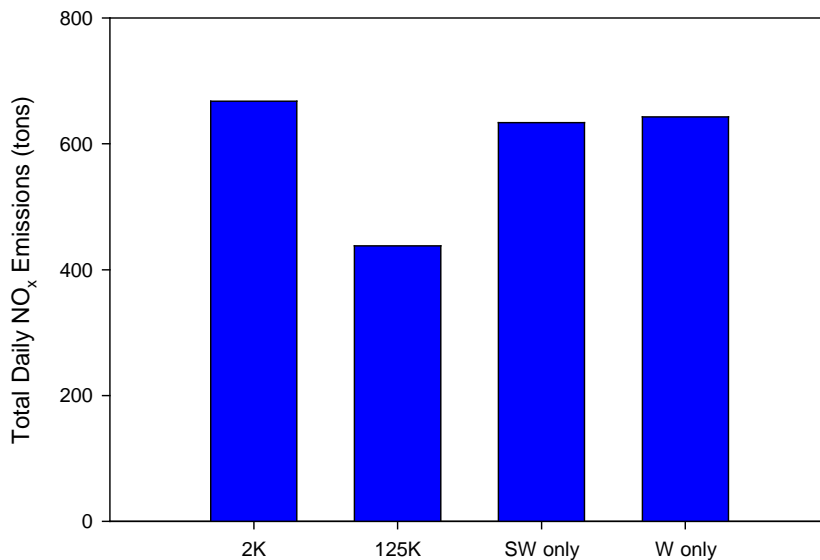
Figure 3-12. Total NOx emissions resulting from four different scenarios.

These results indicate that subdividing the region encourages, not overall reductions in emissions, but trading emissions out of the sub-region that has higher costs. The air quality impacts of both the $125,000 SW sub-domain and the $125,000 West sub-domain approaches are shown in Figure 3-13. The $125,000 W case showed ozone decreases in western Pennsylvania where the reductions were made, and increases in eastern Pennsylvania and New Jersey where the emissions were shifted to. Table 3-2 shows the metrics for both the $125,000 southwest scenario on August 14th and the $125,000 west scenario on August 12th and their corresponding $125,000 scenarios for comparison. All cases were compared to the Basecase. Only the $125,000 SW scenarios showed improvements relative to the corresponding $125,000 scenario. The $125,000 W scenario performed far worse because of the shift in emissions downwind.

This example of spatial regulation results in the shifting of emissions, not a reduction in emissions. The potential for downwind hot spot formation from this is large (as shown by the Western case) because emissions are being shifted instead of reduced. Because of

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the disbenefit to areas downwind of a spatially focused trading scheme, as well as the difficulty implementing this type of trading scheme, the focus for this work will be temporally focused trading.
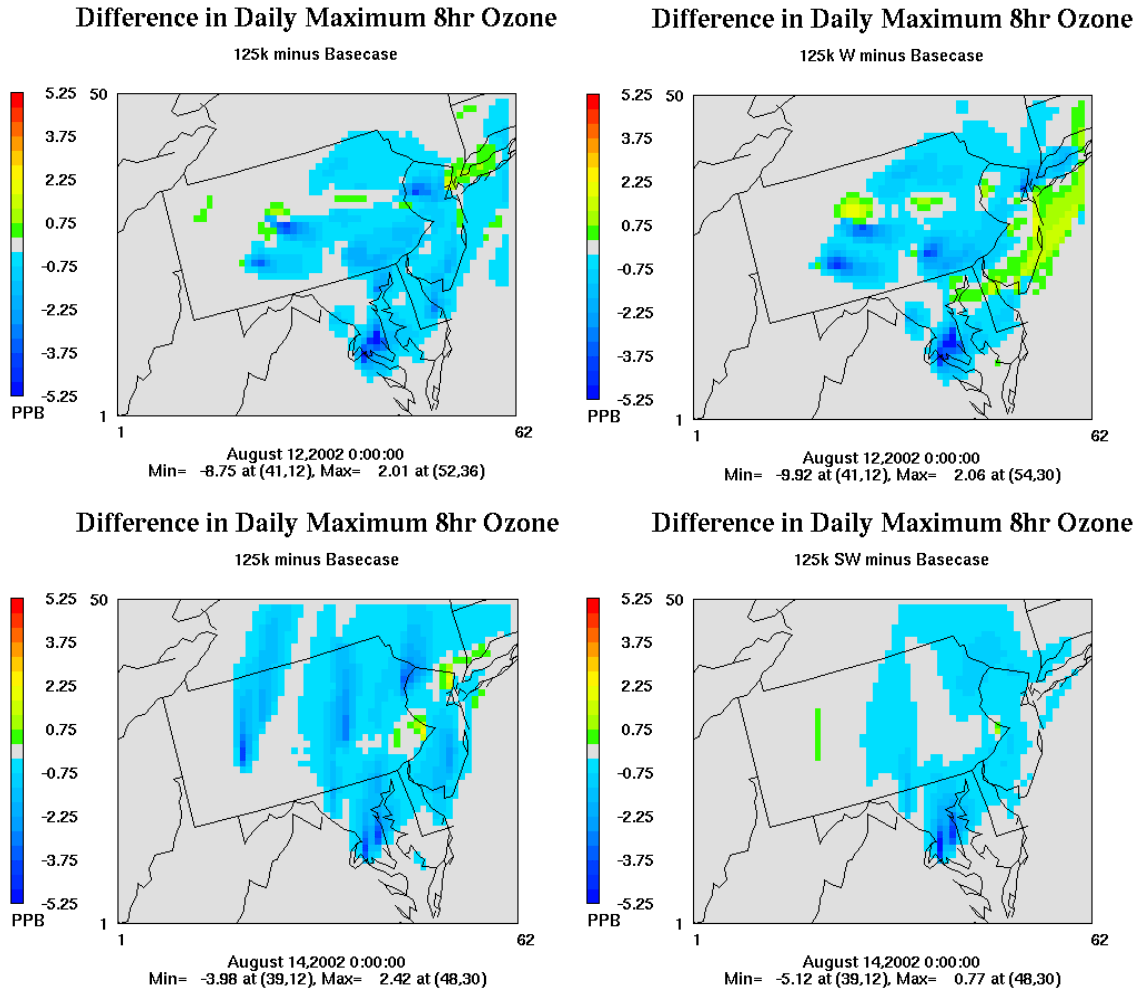
Figure 3-13. a thru d. Differences in Maximum 8 hour ozone on August 12th as a result of a. $125,000 scenario and b. $125,000-W scenario. Differences in Maximum 8 hour ozone on August 14th as a result of c. $125,000 scenario and d. $125,000-SW scenario.

Table 3-2. Percent reduction calculated for each of the four metrics for the $125,000 SW case, and the $125,000 case both relative to the basecase on August 14th. Then the $125,000 W case and the $125,000 case both relative to the basecase on August 12th. These values are calculated for both the 75 ppb and 85 ppb thresholds.

Threshold = 85 ppb	$125,000-SW vs Basecase August 14th	$125,000 vs Basecase August 14th	$125,000-W vs Basecase August 12th	$125,000 vs Basecase August 12th
Area above Standard	-14%	-10%	-1%	-4%
Population above Standard	-19%	-11%	0%	-1%
Daily Area Exposure	-18%	-19%	-6%	-10%
Daily Population Exposure	-36%	-33%	-6%	-7%
Threshold = 75 ppb	$125,000-SW vs Basecase August 14th	$125,000 vs Basecase August 14th	$125,000-W vs Basecase August 12th	$125,000 vs Basecase August 12th
Area above Standard	-3%	-9%	0%	0%
Population above Standard	-10%	-12%	0%	0%
Daily Area Exposure	-14%	-14%	-4%	-7%
Daily Population Exposure	-20%	-19%	-4%	-5%

Seasonal Modeling

The preceding sections have demonstrated that by increasing the cost of NOx emissions during an ozone episode period, there is a resulting reduction in ozone via NOx emission reductions while maintaining adequate power generation and distribution. This does not address the question of how air quality and exposure to ozone might change if emission reductions occur <u>only</u> during ozone episodes, as opposed to the entire ozone season. The question is whether potentially high cost emission reductions, implemented only during ozone episodes is better than or worse than across the board emission reductions (at an indeterminate cost) that occur throughout the ozone season.

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More specifically, the following questions are addressed in this section:

1. What are the relative benefits of targeting reductions on just high ozone days, vs. all days?
2. What are the changes in exposure and what are the changes in ozone exceedances as defined by a series of air quality metrics?
3. What are the implications of these findings for air quality policies in the Northeast US?

For this study, multiple air quality modeling scenarios were modeled using CAMx. The first scenario was a 2002 ozone season basecase, where the ozone season is defined as June through August. The basecase models actual emissions, and results are compared with concentrations measured at monitoring locations in the modeling domain. The other scenarios represent different control strategies and sensitivity analyzes. These scenarios are described in detail below.

The first two control strategy scenarios represent season long control strategies that would require all EGUs in the four-state PJM area to make across the board NOx emissions reductions for the entire ozone season (identical percentage emission reductions on all days at all facilities). Reduction amounts are chosen using the proof of concept results reported earlier in this chapter.

According to the model, on a summer day, charging $50,000 per ton of NOx emissions leads to approximately a 25% reduction in total NOx emissions from EGUs. Similarly, a reduction of 12.5% is roughly associated with a $10,000 per ton cost for emissions of NOx. Therefore, the preliminary results indicate that 12.5% and 25% NOx reductions are possible on high demand days. To compare these dispatching scenarios to across-the-board reductions, the across-the-board reductions were set at 25% and 12.5%; the across

the board reduction scenarios would, however, likely require some additional controls to be put in place.

Two scenarios, with blanket reductions of 25% and 12.5% respectively, are modeled in CAMx, over the entire 2002 ozone season. This is done by applying control factors of 0.75 and 0.875 to all NOx emissions from point sources with Standard Industrial Classification (SIC) codes 4911 or 4931, during CAMx preprocessing, and then running CAMx for the entire season. These two scenarios will be called Season-25%, and Season-12.5%. SIC codes are used by EPA to identify categories of industry. SIC codes 4911 and 4931 correspond to "Electrical Services" and "Electric and other Services Combined" respectively.

The other scenarios are more temporally focused. Instead of requiring emissions reductions every day of the ozone season, these control strategy scenarios apply emissions reductions to days within the high ozone episodes of the 2002 season. As stated earlier in this chapter, high ozone episodes are defined as 2 or more days in a row where 5 of the 6 monitoring stations in the Philadelphia area measured maximum one-hour ozone concentrations above the standard. The ozone episodes for the current 85 ppb standard are: June 24-27, July 8-9 and 17-19, and August 2-4 and 10-14. There are 17 days that fall within these ozone episodes. The 2002 ozone season was also examined for ozone episodes with a standard set at 75ppb. The following days are considered ozone episodes with the new lower 75ppb standard: June 22-27, July 1-3, 8-9 and 17-19, and August 2-4 and 10-14. There are 22 days that fall within the definition of an ozone episode if the standard is set at 75ppb. The sensitivity runs generated using data from the across-the-board control scenarios only on episode days will be called Episode(75 or 85)-25% and Episode(75 or 85)-12.5%.

In order to examine the effect of redistribution of emissions through increased pricing on episode days, compared to across the board reductions, days that fall within the two sets

of high ozone episodes are modeled in CAMx with the emissions adjusted using three sets of economic modeling emissions data that assume a NOx emission price of $10,000 per ton, $50,000 per ton, then $125,000 per ton. No changes (from the basecase) are assumed for the emissions for the rest of the ozone season.

It should be noted that two basecase scenarios were modeled. The first represented the emissions starting point for the blanket reduction scenarios. The second represented the emissions starting point for the scenarios modeled using the MIT economic model. Because the MIT model was not able to match 100% of the EGUs in the classic PJM grid, some facilities were left out of those scenarios. It is not uncommon for SIP attainment demonstrations to start with basecases that have slightly different values. Emissions inventories are constantly being changed and updated. This inconsistency with basecase emission inventories is one of the reasons results from studies such as this one are presented as changes from the basecase and not as absolute values.

Results

The results of the basecase scenarios are consistent with concentrations measured by monitor sites in the area during the August 10-14 ozone episode, as shown in Figure 3-14. The basecase CAMx simulation shows good agreement with concentrations measured by the monitor sites in both absolute values and hourly patterns. Even with good agreement with modeled and measured values, it is still good practice to present results as a relative change in ozone. All modeled scenarios are compared to the basecase to present a change in ozone metrics due to the regulatory scenario. In this case, results are presented in the form of percentage reduction for the four air quality metrics being used.
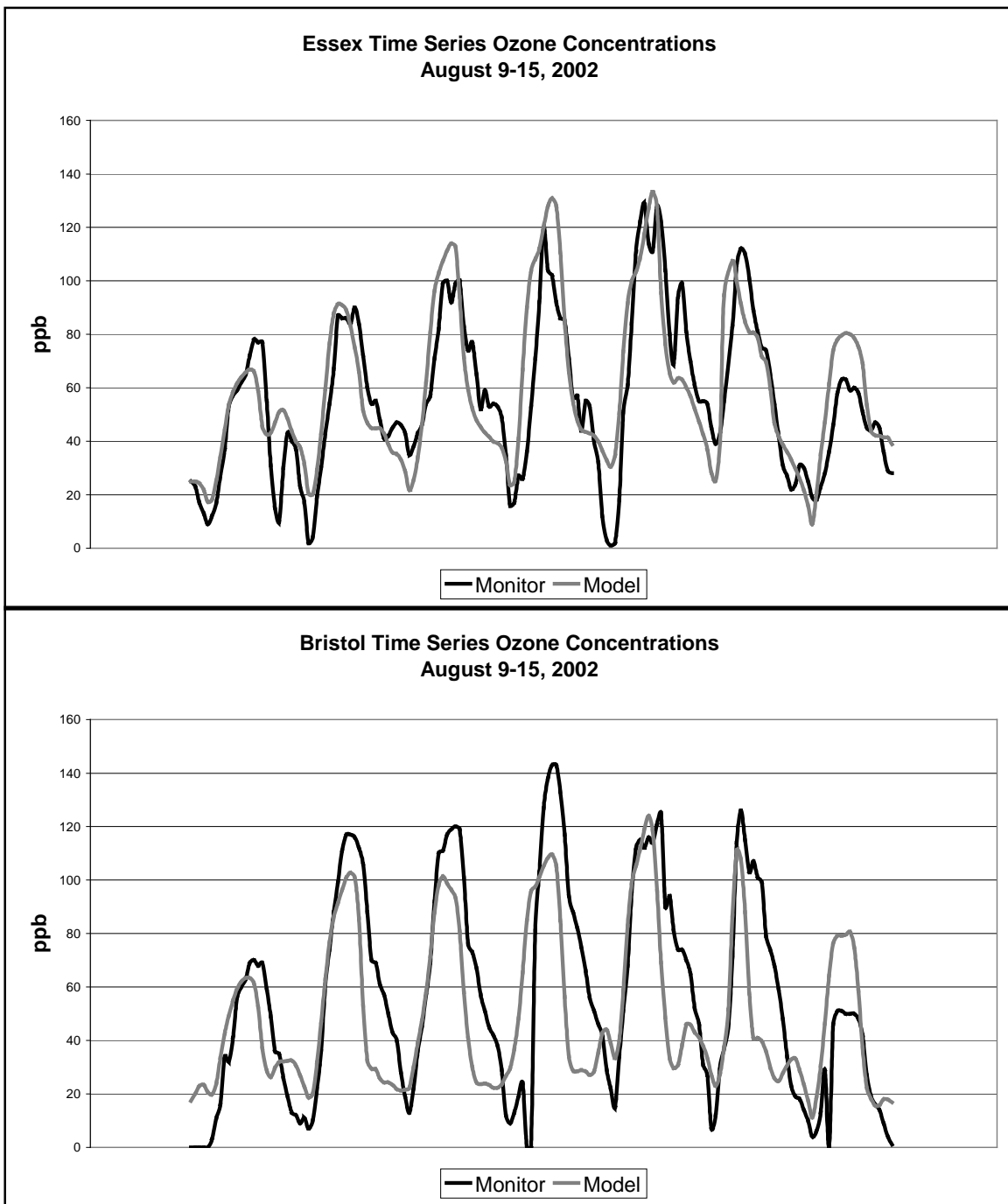
Figure 3-14. Comparison of modeled versus measured ozone values at two monitor locations in the PJM. Essex is located outside of Baltimore, and Bristol is located outside of Philadelphia.

Table 3-3. Summary of average NOx emission reductions, and total NOx emissions on a daily and seasonal basis, for all cases, for both threshold values.

NOx emissions reduction from Basecase (Tons)							
Daily	S - 12.5%	S - 25%	E - 12.5%	E - 25%	E - 10k	E - 50k	E - 125k
Avg Reductions	110	220	110	220	68	166	218
Avg Emissions	1,138	1,028	1,138	1,028	1,135	1,037	985
Threshold 85ppb							
Total Reductions	10,120	20,227	1,870	3,738	1,156	2,822	3,704
Total Emissions	104,709	94,602	112,959	111,092	109,533	107,867	106,986
Threshold 75ppb							
Total Reductions	10,120	20,227	2,420	4,837	1,496	3,652	4,793
Total Emissions	104,709	94,602	112,409	109,992	109,193	107,037	105,896

Table 3-3 shows a summary of the NOx emissions total and emissions reductions for the seven scenarios. The values in this table are the total tons of NOx emissions from all point sources that are used as input to CAMx. The table shows daily reductions for each control strategy as well as reductions that would occur over the course of a summer (June-August). Daily emission reductions for the seasonal 25% reduction (S-25%) and the episode focused $50,000 per ton reduction (E-50k) are similar, but the summer long reductions total is over five times larger in the seasonal case than in the episode focused case. While it will not be quantified exactly how much the cost difference would be between these two emission reduction scenarios, it may be considerably cheaper to have a temporally focused program. A similar comparison can be made between the S-12.5% case and the E-10k case. These cases show similar daily reductions, but again, the season long emissions reduction total is five times larger.

While emission reductions are important, ozone attainment is dependent on the ozone concentration reductions that result from NOx emission reductions. Therefore it is necessary to show the results of air quality modeling and the resulting changes in the

production of, and exposure to ozone. Table 3-4 shows the percent change from the basecase in each of the seven scenarios, for the four metrics defined earlier in this chapter.

Table 3-4. Percent reduction calculated for each of the four metrics, due to each of the seven control strategies for two threshold values.

Percent Change (from Basecase) Threshold = 85ppb							
Metric	S-12.5%	S-25%	E-12.5%	E-25%	E-10k	E-50k	E-125k
Area above Standard	-1.6%	-3.3%	-0.5%	-1.1%	-0.8%	-1.8%	-2.3%
Population above Standard	-1.1%	-2.0%	-0.3%	-0.6%	-0.7%	-1.5%	-1.8%
Daily Area Exposure	-2.9%	-5.8%	-1.4%	-2.8%	-1.2%	-3.1%	-4.1%
Daily Population Exposure	-2.2%	-4.3%	-1.1%	-2.2%	-1.1%	-2.8%	-3.7%
Percent Change (from Basecase) Threshold = 75ppb							
Metric	S-12.5%	S-25%	E-12.5%	E-25%	E-10k	E-50k	E-125k
Area above Standard	-0.7%	-1.4%	-0.3%	-0.5%	-0.6%	-1.0%	-1.1%
Population above Standard	-0.2%	-0.6%	-0.1%	-0.4%	-0.4%	-0.7%	-1.0%
Daily Area Exposure	-2.2%	-4.4%	-1.1%	-2.2%	-1.0%	-2.6%	-3.5%
Daily Population Exposure	-1.6%	-3.3%	-0.9%	-1.8%	-0.9%	-2.3%	-3.1%

*85 ppb metrics assume that reductions for episode focused scenarios (E) are made on the following days only: June 24-27, July 8-9, 17-19, and August 2-4, 10-14. 75 ppb metrics assume reductions on: June 22-27, July 1-3, 8-9, 17-19, and August 2-4, 10-14.

The ozone metrics in Table 3-4 show that the season long, blanket reduction scenarios result in larger air quality improvements than the episode focused scenarios with similar emission reductions. However, the sensitivity runs show that episode focused trading scenarios result in larger air quality improvements and lower exposure than episode focused blanket reduction scenarios with similar total reductions. The difference is in the location of the reductions. Table 3-5 shows a sample of the relative emission reductions by state. While the total NOx emissions reductions are similar, the locations where reductions are made are different. In the case of the market-driven scenario, the emissions decrease in Pennsylvania is relatively smaller than it is in the across the board

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reduction scenario while the decrease in New Jersey, Delaware and Maryland are all relatively larger. This result supports the idea that, while hard to control, the location of emissions is important in whether those emissions will form ozone.

Table 3-5. Total Basecase emissions and percent change in NOx emissions from corresponding Basecase, by state for two scenarios.

NOx Emission	E-Basecase	E-50k	S-Basecase	S-25%
	tons/day	% Change	tons/day	% Change
Delaware	68	-21%	45	-14%
Maryland	215	-23%	268	-19%
New Jersey	177	-30%	138	-16%
Pennsylvania	749	-6%	826	-18%
Total	1209	-14%	1275	-18%

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Daily Population Exposure

75 ppb Standard
Episodes-10k minus Basecase

August 12,2002 6:00:00
Min= -2250 at (40,18), Max=   426 at (49,29)

Daily Population Exposure

85 ppb Standard
Episodes-10k minus Basecase

August 12,2002 6:00:00
Min= -1777 at (40,18), Max=   375 at (49,29)

Daily Population Exposure

75 ppb Standard
S-25% Blanket Reductions minus Basecase

August 12,2002 6:00:00
Min= -3864 at (48,27), Max= 5394 at (40,18)

Daily Population Exposure

85 ppb Standard
S-25% Blanket Reduction minus Basecase

August 12,2002 6:00:00
Min= -3172 at (48,27), Max= 4681 at (40,18)

Daily Population Exposure

75 ppb Standard
Episodes-50k minus Basecase

August 12,2002 6:00:00
Min= -3658 at (40,18), Max=   210 at (49,29)

Daily Population Exposure

85 ppb Standard
Episodes-50k minus Basecase

August 12,2002 6:00:00
Min= -2833 at (40,18), Max=   180 at (49,29)

Figure 3-15 a-h. Difference from Basecase in Daily Population Exposure (Metric #4) on

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August 12, 2002 for a. and b.S-12.5%, c. and d.E-10k, e. and f.S-25%, and g. and h.E-50k for two standards. E-125k exposure maps can be seen in figure 3-7.

Figure 3-15 shows maps of the Daily Population exposure on August 12th for scenarios S-12.5%, E-10k, S-25%, E-50k for both a 75ppb standard (left column) and an 85 ppb standard (right column). As opposed to the metrics presented in Table 3-4 that average presents average changes in metrics across the entire season, Figure 3-15 shows only one representative day.

The top two rows of maps show scenarios S-12.5%, a blanket NOx reduction of 12.5% from EGUs within the classic PJM grid, and E-10k, reductions modeled by the economic trading model assuming a charge of $10,000 per ton of NOx, respectively. These two scenarios have similar daily NOx reductions. The grid cells showing exposure decrease (represented by green-blue to dark blue shading) in these two scenarios are located in the regions around Baltimore and Philadelphia. The main difference between S-12.5% and E-10k is the location and magnitude of exposure increases. In the blanket scenario S-12.5%, a large increase in exposure is seen in a grid cell located in Baltimore city. In E-10k, the market trading scenario, Baltimore is seeing large decreases but there is a small increase in exposure just north of Philadelphia. Increases in exposure are usually caused by very localized increases in NOx emissions, which is likely the case in the economic trading scenario E-10k. However, in the blanket reduction scenario, there is no increase in NOx and therefore, the exposure increase in Baltimore is likely caused by a NOx disbenefit. NOx disbenefit occurs when excess NOx that was reacting with and removing ozone is decreased. This is likely to occur in urban centers where there are extensive NOx emissions from vehicles.

The third and fourth row of maps show scenarios S-25%, a blanket NOx reduction of 25% from EGUs within the classic PJM grid, and E-50k, reductions modeled by the market trading model assuming a charge of $50,000 per ton of NOx, respectively. These

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two scenarios also have similar daily NOx reductions. These two scenarios show results that are similar to the previous two scenarios. The areas around Baltimore and Philadelphia show exposure reductions with the exception of one grid cell over Baltimore showing a large increase in the 25% blanket reduction scenario, and one(85ppb standard) or two(75 ppb standard) grid cells north of Philadelphia showing small increases in the economic trading E-50k scenario. These maps show that location of emissions has an effect on resulting ozone concentrations.

Conclusions

This chapter set out to answer the following five questions:

1. How much emissions reductions can be realized during periods of peak demand?
2. What corresponding amount of financial motivation is needed to see specific reductions?
3. What are the relative benefits of targeting reductions on just high ozone days, vs. all days?
4. What are the changes in exposure and what are the changes in ozone exceedances as defined by a series of air quality metrics?
5. How do the conclusions from this research apply to policy in the Northeast?

The proof of concept analysis showed that even on very high demand days, the classic PJM electricity grid has enough flexibility in generation and dispatch to reduce NOx emissions by up to approximately 30%. The cost for ton of NOx emissions corresponding with that level of emissions, according to the economic model developed by MIT, was $125,000. A full economic analysis of a temporally focused control strategy has not been done, but it is likely that actual emission reductions would cost significantly less if companies were given the options to install additional controls. Modeling scenarios showed that temporally focused control strategies are not as effective

as season long control strategies, but may be more cost effective because they would require only approximately 20% of the reductions. While metrics show a larger reduction in ozone exceedances for the season long control strategy, the temporally focused control scenarios show similar improvements for significantly fewer reductions. Additionally, allowing market-based strategies to determine the location of emission reductions can be more cost effective than requiring across the board reductions at all facilities. In order to apply this type of strategy to the Northeast, it would have to fit well with the existing control strategies. While the economic model uses cost per ton of NOx emissions, current regulation is based on an emissions credit system. In order for this work to be applicable, a connection needs to be made that will link cost of emissions with emissions credits. Instead of charging a fixed amount for a ton of NOx emissions, EGUs could be charged multiple emissions credits per ton on days with high ozone forming potential.

Chapter 4 Air Quality Effects of PHEVs

Most of the work reported in this chapter represents the contributions of the author of this thesis to a paper that is under review for publication in the journal Environmental Research Letters. (Thompson 2008)

Introduction

Chapter 3 of this thesis examined ways to improve cap and trade programs by focusing on NOx emissions from point sources in the northeastern United States (NE US). However, point sources only account for 22% of NOx emissions in the NE US. The transportation sector is the largest source of NOx emissions, releasing approximately 60% of anthropogenic NOx in the NE US. (EPA 2003) In order to achieve national ambient air quality standards for ozone in the NE US and in other regions of the US, it is necessary to address both transportation and point source emissions.

The regulation of point sources and transportation sources of emissions has been done separately. The regulations addressing point source NOx emissions, broadly over the NE US, started with the Ozone Transport Committee Budget Program in 1999, progressed to the NOx State Implementation Plan (SIP) Program in 2003, and finally reached the Clean Air Interstate Rule (CAIR, currently being challenged in the courts). (EPA 2008c) All three of these programs are market based cap and trade programs and regulate point sources only. In parallel, a series of emission control programs, largely focused on emission limits per mile traveled for new vehicles, has evolved since the mid-1960's. (for a review, see, NRC, 2002) These transportation (mobile source) emission controls have dramatically reduced new vehicle emissions, yet, in aggregate, transportation sources still comprise the majority of the NOx emissions in the NE US.

A new generation of vehicle designs will force the integration of transportation and point source emission controls. As vehicles, such as battery powered (electric), and plug-in hybrid electric vehicles begin to rely on stored electrical energy for a large fraction of their power, direct emissions from the transportation sector can be reduced, but at the expense of placing more demand on electric power generation. This Chapter will examine the air quality implications of widespread use of plug-in hybrid electric vehicles (PHEVs).

PHEVs

Since PHEVs are designed to run primarily on batteries, they are given a rating based on battery size that defines the distance the car can run on batteries alone. While running on batteries, PHEVs have no tailpipe emissions. Once battery power is exhausted, the car can then run on a regular gasoline engine. When the gasoline engine is started, tailpipe emissions are equal to gasoline vehicles. A typical PHEV battery has a range of 33 miles. Approximately 50% of daily drivers drive less than 40 miles on an average day (King 2008) making PHEVs particularly useful for most urban commutes.

Potential for PHEV Use in the NE

Electricity Generating Capacity in the US is developed to meet the needs of the very highest demand times. There is a very high demand for electricity during daytime periods, and the capacity of the network is designed to meet that demand. In the middle of the night, while most of the population is asleep and no longer running electrical equipment, and the temperature has gone down decreasing the load on air conditioners, the total electricity demand on the grid is much lower. These large differences in demand are handled using capacity that is a mix of baseload units and peak units. Peak capacity units are only turned on when electricity demand increases beyond what baseload facilities can provide. These peak load units are typically natural gas units that can be

turned on and off easily. Baseload facilities run throughout the day. Nuclear and Coal facilities are considered baseload. It is much more difficult to turn off nuclear facilities and so they are the bottom tier of baseload. Coal units are difficult to turn off completely, but production from coal can be decreased. Therefore, at nighttime or other times of lower electricity demand, peak load is turned off and where they can, baseload EGUs dial back their production levels.

The question to be addressed in this Chapter is: What would the effect to ambient ozone concentrations be if excess nighttime coal-fired electricity generating capacity is used to charge plug-in hybrid electric vehicles that would then be used for urban commuting the next day? It is expected that nighttime NOx, VOC and carbon monoxide (CO) emissions would increase around EGUs, but daytime traffic related NOx, VOC and CO emissions would decrease in urban areas. The PHEVs are assumed to be operated in urban areas within the PJM region, specifically the urban areas of Baltimore, Pittsburgh, Philadelphia, Newark and surrounding areas. This assumption is reasonable because PHEVs are targeted for short-distance commutes. The effects on ozone levels resulting from the shift of precursor emissions are not straightforward because of the complicated chemistry involved. Temporal and spatial details are important and so assessing the impacts of moving NOx, VOC and CO emissions from daytime in urban areas to nighttime in rural and urban areas requires regional photochemical modeling. This question will be addressed by modeling the emissions changes associated with PHEV utilization in the PJM region.

While several studies have looked generally at the feasibility and air quality effects of hybrid vehicles versus gasoline vehicles, all point to the importance of expanding this research. A study by the Pacific Northwest National Laboratory found that the existing electrical infrastructure and capacity could support a switch to PHEV by 84% of US cars, pickup trucks and sports utility vehicles assuming night-time charging. (Kitner-Meyer 2007) Another study was conducted in California only and concluded that the existing

capacity has the capability of supporting PHEV nighttime charging. (Lemoine 2008)
Both studies agree that there already exists a nationwide infrastructure that is capable of
supporting PHEVs. However, it is assumed in both studies that PHEVs would charge
only at night. Policy or market effects should be designed to limit PHEV charging to
nighttime hours when excess capacity exists. This can be done by reducing nighttime
electricity costs and designing chargers that would only allow charging during nighttime
hours. Economic studies of PHEVs have found that their introduction to the market
would reduce electricity costs due to increased and leveled-out electricity demand. (Scott
2007) Bradley (2009) evaluated the effects of switching emissions between sectors and
found that switching from conventional vehicles to PHEVs charged using coal-fired
electricity would lead to emission reductions of NOx, VOC, CO and CO_2.

The studies mentioned above look only at the ability of the electrical infrastructure to
support the excess nighttime demand. The effect on air quality is not addressed beyond
overall estimated emission impacts. The Electric Power Research Institute performed the
one study that has examined the air quality impacts of PHEV use, beyond total emission
changes.

The Electrical Power Research Institute (Knipping 2007b) predicted the air quality
effects of PHEV penetration into the market assuming PHEVs would become available in
2010, account for 15% of the new cars sales immediately, growing to 50% of all new
automobile sales by 2030 when they would account for 40% of the total vehicle fleet.
While the resulting higher electricity demand could be met using excess nighttime
capacity, this will lead to higher emissions from EGUs. However, EPRI assumed that
current regulations would remain unchanged. This would mean the NE NOx cap and
trade program would continue to decrease the cap as planned every year regardless of the
increased load to the units. This introduces an important policy issue. Since PHEVs
would be removing emissions from the road and increasing emissions from EGUs, it is
likely that existing cap and trade programs for NOx would need to incorporate this shift

by introducing more emissions credits to the existing NOx cap and trade program. The NOx emissions cap can still step down in 2010 and 2015 as proposed in CAIR (EPA 2008b), but it is likely that the cap would need to be raised to incorporate the addition of mobile sources to the point source load. And the cap reduction goals of 2010 and 2015 would need to be adjusted to reflect the additional generation.

Finally, studies have found that PHEVs in general would decrease GHG emissions to the atmosphere. (Stephan 2008) Many studies have reported that a switch to PHEVs from conventional vehicles will lead to reductions in GHG emissions. (Lokey 2007, Romm 2006) EPRI examined 9 scenarios spanning 3 levels of PHEV penetration and 3 levels of electrical sector CO_2 intensity and found that even in the worst-case scenario, CO_2 emissions were reduced. (Knipping 2007) Stephan (2008) found PHEVs would reduce CO_2 emissions by 25% in the short term, and up to 50% in the long term using existing spare nighttime capacity. Samaras (2008) looked at the entire life cycle of PHEVs and found that the worst-case scenario would lead to CO_2 emissions that are no greater than conventional vehicles. In addition to examining the impact of shifts in emissions of ozone and its precursors between on-road vehicles and EGUs, this Chapter will also briefly examine the effect of the shifts on greenhouse gas (GHG) emissions and Particulate Matter (PM) emissions.

Methods

The air quality impacts of shifting emissions from vehicles to EGUs will be examined using the Comprehensive Air quality Model with Extensions (CAMx), introduced in Chapter 3. The model predicts the spatial and temporal movement, production and depletion of air pollutants using data on emissions, meteorology, chemistry and deposition. CAMx was chosen for this work because of the availability of meteorological, land cover, boundary condition, initial condition and emission inputs for an air pollution episode from August, 2002, which will be used as a representative case

study in this work. The modeling inputs for this episode were developed by the Central Regional Air Planning Association (CenRAP) for regional haze and visibility studies. A performance evaluation for the 2002 episode was conducted by ENVIRON. (ENVIRON 2007) This is the same air quality modeling episode that was used in Chapter 3.

The air quality modeling domain is shown in Figure 3-3. The modeling domain has a grid with 12 km horizontal resolution nested within a grid with 36 km horizontal resolution. The 12 km grid covers the Pennsylvania, New Jersey, Maryland (PJM) region that will be the focus of this work. The classic PJM grid includes the three states for which it is named, as well as Delaware. The model inputs include meteorological data and emissions inventories. Wind fields were estimated by the Iowa Department of Natural Resources using MM5, cloud cover was estimated using satellite data, and land cover/land use data was developed by CENRAP. (ENVIRON 2007) Emissions inventory data, including point source, area source, mobile emissions on and off road, and biogenic emissions were based on the EPA's 2002 National Emissions Inventory with updates and corrections provided by individual states. The emissions inventories were processed using the SMOKE emissions processing system as preparations for EPS3, a CAMx preprocessing tool (ENVIRON 2007). The biogenic emissions inventory was developed using the Global Biosphere Emissions and Interaction Systems (GlobeBeis). (ENVIRON 2007)

The EGU emissions are of particular interest in this work and therefore will be described in detail. Locations of power plants within the PJM region are shown in Figure 4-1. The power plants for this analysis consist of a group of base load plants, which are largely coal-fired, and peaking units, which are primarily gas-fired. Table 4-1 shows the electricity generating capacities of the EGUs in the region and the utilization factors. The coal fired plants, which collectively have 26 GW of power generating capacity, are run primarily as base-load units. Nevertheless, they have a diurnal pattern of capacity utilization and emissions, shown in Figure 4-2, which is due to decreased electricity

demand at night. (Martin et. al. 2007) In this work, it is assumed that these plants are operated at constant capacity utilization, equal to their daytime maximum, and that the excess power generation at night is used for PHEV charging. The modified diurnal profile is shown in Figure 4-2. The excess generation available to PHEVs if coal plants run at 85% capacity factor is 107 GWh. It is assumed that this 107 GWh is 90% utilized making 96 GWh for charging PHEVs. (EIA 2002) The additional electricity is used to charge PHEVs, which will then displace emissions that occur during the day. The diurnal profile for weekday vehicular emissions is shown in Figure 4-3.

Of the traditional fuel sources used for electricity, coal-fired power plants without controls release the most CO_2, NOx, and SO_2 throughout the lifecycle (Jaramillo 2007) and so using coal generated electricity to charge PHEVs would represent a worst-case scenario for EGU emissions, assuming only existing capacity is utilized, and only at night. These additional emissions would be added to the grid, and once on the grid it is not possible to know that the additional capacity is used directly for PHEV charging. Nevertheless, it is assumed in this case study the additional generation is required because of the PHEV charging. The allocation patterns of additional nighttime demand would be decided using a traditional utility bidding system. (Martin 2007) The assumptions that charging would occur only at night is dependent on the development of policy or technology that would limit charging to nighttime hours only.

Table 4-1. Electricity utilization factors and generation capacity by fuel type and state. (EIA 2002)

Electricity Average Utilization 2002	Coal	NG[1]	Nuclear	Petro
Penn	71%	12%	95%	9%
Maryland	67%	17%	82%	9%
New Jersey	52%	24%	91%	3%
Delaware	38%	13%	0%	15%
Total	67%	18%	93%	8%

Electricity Capacity 2002 (MW)	Coal	NG	Nuclear	Petro
Pennsylvania	18,384	6,223	9,127	3,372
Maryland	4,897	1,490	1,685	2,922
New Jersey	2,124	9,237	3,875	2,533
Delaware	1,050	1,293	0	745
Total	26,455	18,243	14,687	9,572

Daily Total (MWh) Potentially available from Coal:[2]	539,670
Potential MWh available for PHEVs:	107,934

1: NG = Natural Gas

2: Assumes plants are running 85% of the time

64
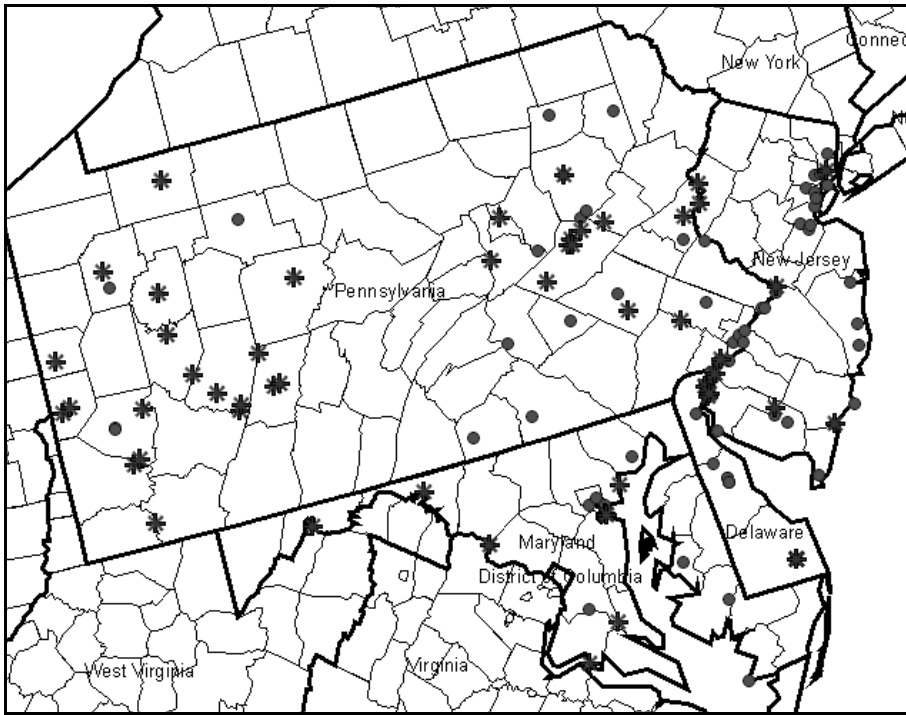
Figure 4-1. PJM region electric generating unit locations. Coal-fired power plants are represented with stars, all other EGU locations are represented by circles.
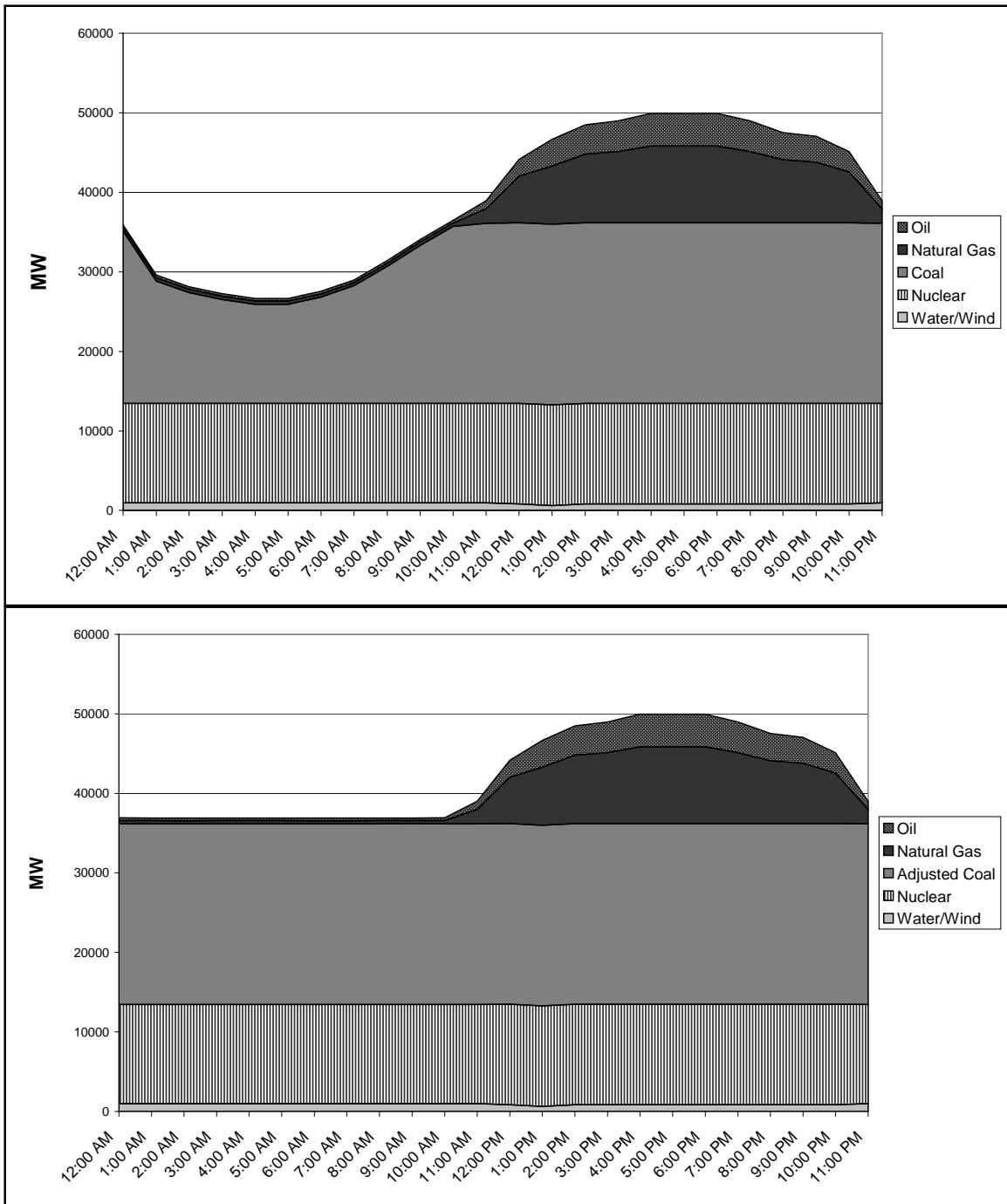
Figure 4-2 a and b. (a.) Hourly Electricity Generation in the PJM classic grid region on
August 12, 2002 (upper). (b.) Hourly Electricity Generation, with nighttime PHEV
charging using coal at 100% capacity factor (lower). (Martin et. al. 2007)

The additional electricity available for nighttime charging of PHEVs is 96 GWh (approximately 20% of Coal Plant Capacity). The additional emissions associated with this increased capacity utilization are calculated in two ways. First, an EPA AP-42 emissions factor is used to calculate the approximate NOx emissions associated with the addition of 96 GWh nighttime electricity generation. (EPA 1998) The EPA factor is 0.003 lb of NOx emitted per kWh generated. (EPA 2004) Using this factor, there would be approximately 144 tons of NOx emissions associated with 96 GWh. The second method for calculating emissions is to assume that the 20% increase in capacity utilization, represented by the 96 GWh of additional generation, would increase emissions by 20%. The total NOx added to the point source emissions inventory in CAMx, assuming a 20% increase in NOx emissions due to additional nighttime generation at coal-fired plants, is 168 tons. Since these two approaches to estimating emissions lead to similar results, a 20% increase in emissions to the coal fired power plants is applied. The temporal emissions profile is adjusted so that emissions assigned to coal fired plants are constant throughout the day. This same 20% increase, with the same temporal allocation procedure, is applied to VOC and CO emissions from coal fired EGUs.

To estimate the emissions reductions in the vehicle fleet associated with the use of PHEVs, the GWh available to PHEVs are converted to a total Vehicles Miles Traveled (VMT) by the PHEVs. The resulting VMT available to PHEVs are distributed to three categories of light duty vehicles according to the percentages of those vehicles in the existing fleet, as listed in Table 4-2. Table 4-2 also lists average energy economy factors for these three categories of light duty PHEVs. These estimates of energy use by PHEVs were obtained from an EPRI study (Knipping 2007) and assume less efficient use of electrical energy by PHEVs, compared to other studies. (Kinter-Meyer 2007, Stephan 2008) For example, the PHEV economy factors used by the Pacific Northwest National Laboratory (Stephan 2008) include transmission and distribution losses, as well as battery charging and use losses. The PNNL economy factors for a mid-size sedan are 300

Wh/mile, as compared to the 318 Wh/mile reported by EPRI, and used in this study. NOx, CO and VOC emission factors for light duty gasoline vehicles were obtained from EPA average emissions and fuel consumption data as reported in MOBILE6. MOBILE6 is EPA's Mobile Vehicle Emissions Modeling software that is used to model the grams per mile of emissions from most types and ages of on-road mobile vehicles under various operating conditions. (EPA 2007b) These data assume an average, properly maintained vehicle on the road in July of 2000 and the average fuel economy for each vehicle class. (EPA 2000) Percentages of each category of vehicle in service in 2002 are also listed and were obtained from Federal Highway Statistics data for 2002.(DOT 2002) Each of the energy economy factors (318 – 493 Wh/mile) are multiplied by the percentage of vehicles and the total excess nighttime MWh to calculate a daily total VMT available for PHEVs of approximately 245 million VMT.

Table 4-2. Emissions factors for light duty mobile vehicles by vehicle category.

Individual Vehicle Type	Gross Vehicle Weight (lb)	Percentage Of Light-Duty Passenger Fleet	MOBILE6 Adjusted AC Electricity Consumption (Wh/mi)	Grams NOx Emissions per mile	Grams CO Emissions per mile	Grams VOC Emissions per mile
Passenger Cars	-	65.04%	318.2	1.39	20.9	2.8
Gas Truck (SUV)	0-6000	13.50%	394.2	1.81	27.7	3.51
Gas Truck	6001-8500	21.46%	493.2	1.81	27.7	3.51

Using the average light duty vehicle emission factors obtained from EPA data (Table 2) and the percentage of each category of light duty vehicles on the road, the NOx emissions total from 245 million gasoline VMT is calculated to be 15% of the daily non-point source NOx emissions according to the EPA's National Emissions Inventory (NEI) emissions total for the 4 states. Non-point source emissions include on-road mobile, off-road mobile, and area emissions, but in the case of NOx, are dominated by on-road mobile emissions. For NOx, 15% of the non-point emissions inventory corresponded to

20% of the mobile emissions inventory. In the model, the mobile vehicle source NOx, VOC and CO emissions were reduced by 20% (300 t/d NOx, 180 t/d VOC and 2420 t/d CO) and these emission reductions were applied in the urban areas of the PJM region. Figure 4 shows a map of the PJM region, with the grid cells used in the modeling overlain. The urban areas in which PHEVs are assumed to operate are outlined in blue. The emission reductions are applied to daytime hours. Figure 4-3 shows a time series of the non-point source NOx emissions on August 12, 2002 with and without the emission reductions due to the use of PHEVs.

Non-Point Source Nox emissions by Hour as a Percentage of Daily Total
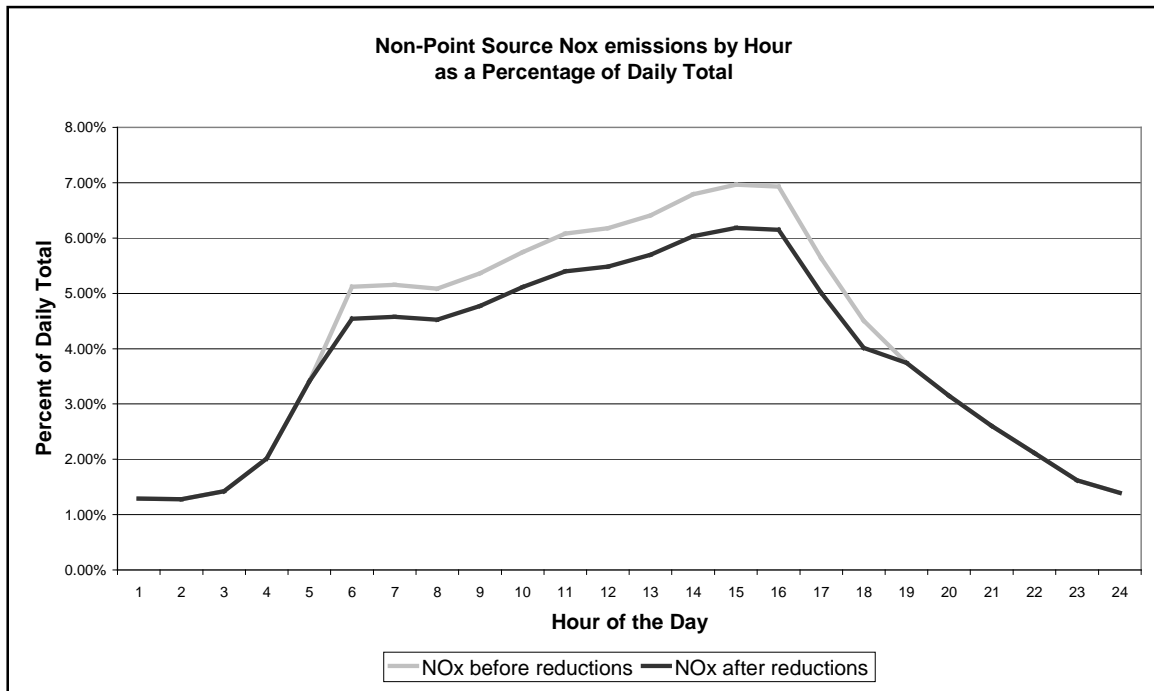
Figure 4-3. August 12th Hourly non-point source NOx emissions as a percentage of total daily non-point source hourly NOx, shown before and after reductions due to PHEVs are realized.
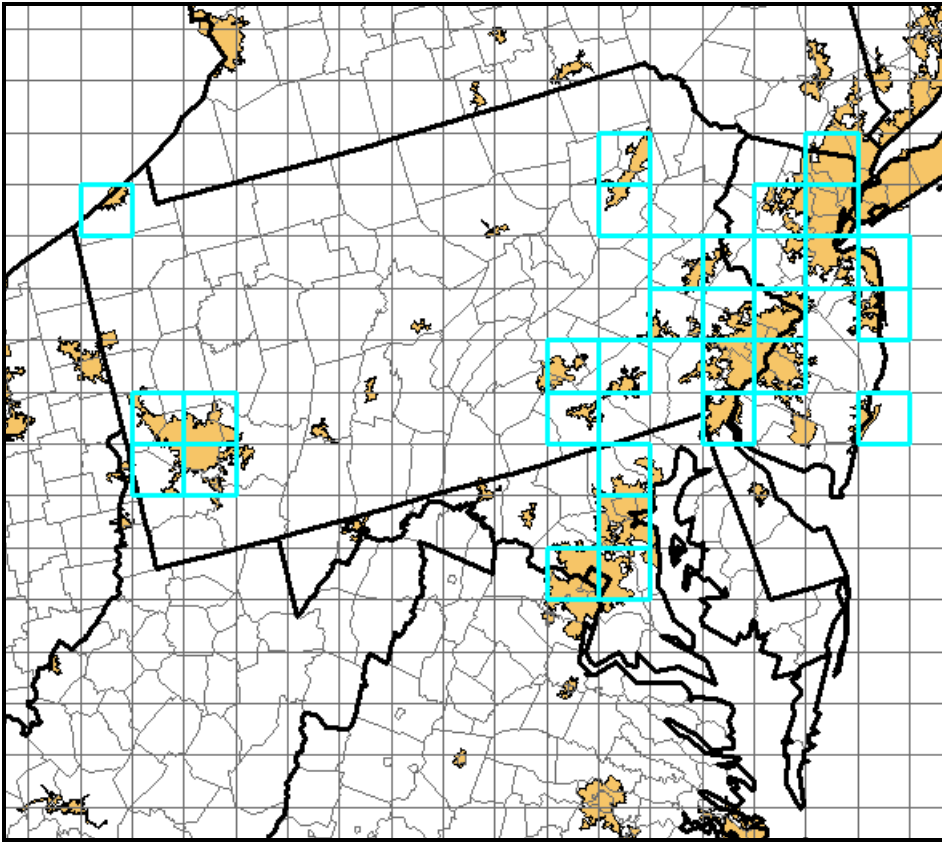
Figure 4-4. Map of the PJM area showing the urban areas in orange. Grid cells that received daytime mobile emissions reductions are outlined in blue.

To quantitatively evaluate the air quality impacts of PHEV use, four air quality metrics, in addition to total emissions and ozone concentrations, are used. These metrics are introduced in detail in Chapter 3. The four metrics used are total area with eight hour averaged ozone concentrations above a threshold concentration, total population living in grid cells with eight hour averaged ozone concentrations above a threshold value, time integrated ozone area above the threshold, and time integrated ozone above the threshold multiplied by population. Metrics are calculated twice, first for threshold defined as the 75ppb standard and then for the threshold defined as the 84ppb standard. Days during which the maximum ozone concentration is below the standard are not included in the metrics calculations

Modeling Scenarios

Photochemical modeling simulations were performed for the period of August 5th through 16th, 2002. This episode was chosen because it contains one of the most severe photochemical events in the past decade in the northeast US, with PJM area monitoring stations on August 10th through the 14th measuring maximum 1 hr average ozone concentrations of 117, 126, 143, 147 and 132 ppb, respectively. In addition to being a severe episode, this episode presents a variety of meteorological conditions. Figure 4-5 shows 36-hour back trajectories, calculated using the National Oceanic and Atmospheric Administration's HYbrid Single Particle Lagrangian Integrated Trajectory (HYSPLIT) model (ARL 2008), for air parcels arriving at a point in NJ at 5pm on each day for the period August 10th - 14th. The specific location in NJ represents the average latitude and longitude of the air quality monitoring stations located around the Philadelphia/Baltimore/Southern New Jersey non-attainment area. This map shows the path air travels during the 36 hours prior to arriving in this area. During the period, the prevailing winds shift from southerly to westerly, leading to very different mixes of ozone precursors encountered by the air parcels arriving in the area as the episode develops.
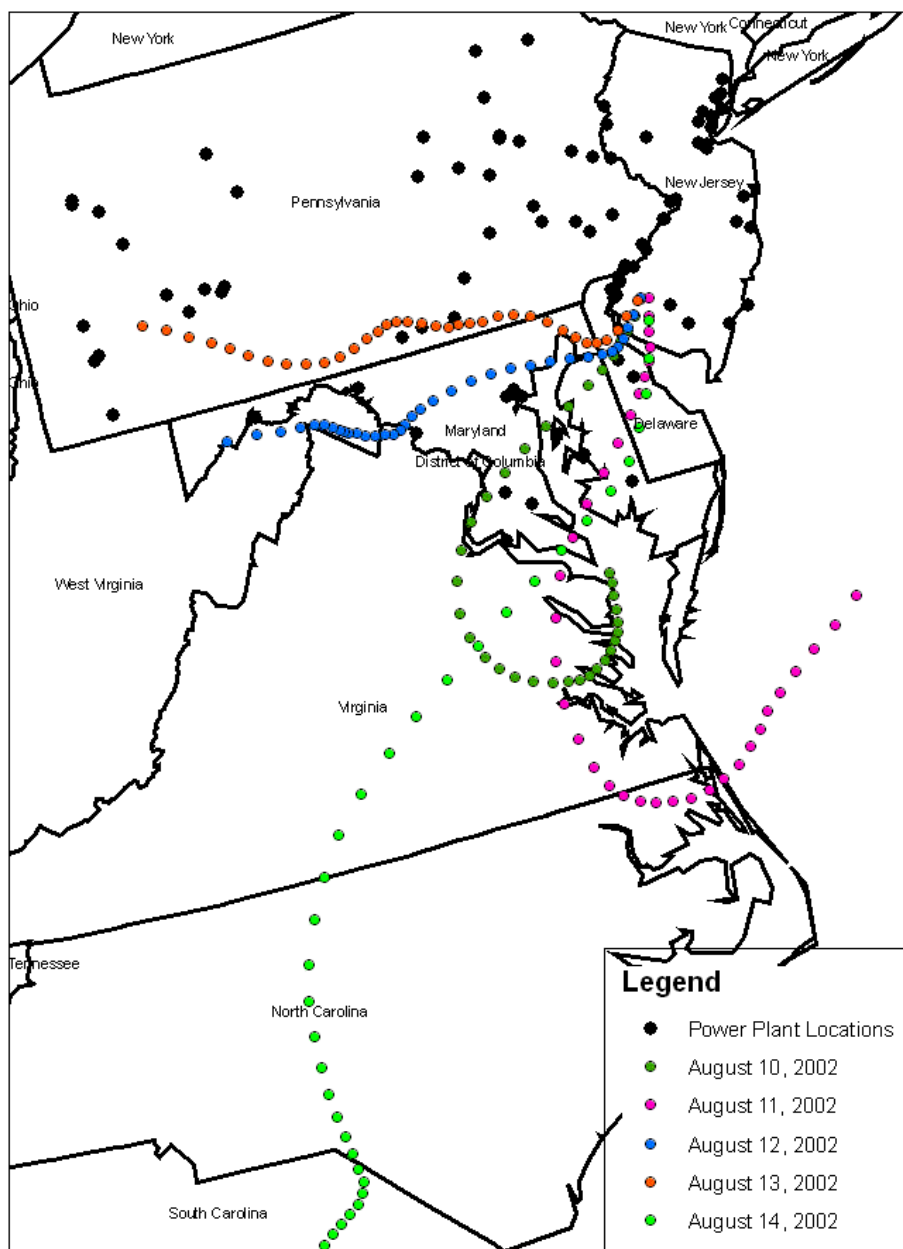
Figure 4-5. Map shows the back trajectories for the five days of an August 10th – 14th ozone episode as modeled by HYSPLIT. The back trajectories show that prevailing winds rotated from southerly to westerly over the episode. The small black circles show locations of EGUs.

Four air quality modeling simulations were conducted using CAMx. The first is a basecase with unchanged emission inventories representing the emissions as they occurred during the modeling period. The second simulation represented the changes to the emissions inventory that would occur due to the full utilization of PHEVs during the day, charged at night using electricity from coal-fired EGUs, as calculated above and is called PHEV-300. In this PHEV case, NOx emissions are increased by 168 tons during nighttime hours for EGUs in the four state PJM area because of increased nighttime electricity generation used to charge PHEVs. VOC and CO emissions are increased by 1.2 and 11.9 tons respectively. NOx emissions are decreased by 300 tons during daytime hours in urban areas (hence PHEV-300) from the substitution of gasoline vehicles by PHEVs. CO emissions are reduced by 2420 tons and VOC emissions are reduced by 180 tons.

For the third simulation, PHEV-150, emission reductions associated with PHEV use are halved. This notional scenario might arise due to lower charging and use efficiency, or the availability of a lower emitting base case fleet of vehicles. The additional nighttime electricity generation and associated emissions remain the same. For this third case, the nighttime emissions are increased by 168 tons, 1.2 tons and 11.9 tons, for NOx, VOCs and CO respectively as with the second case, but the daytime NOx, VOC and CO emissions are decreased by only half the amount from the PHEV-300 simulation. NOx emissions are reduced by 150 tons, CO by 1210 tons and VOCs by 90 tons. For the fourth simulation, changes are made to the mobile emissions only. No increases are made to nighttime emissions from EGUs. NOx, VOC and CO are decreased during daytime hours, in urban areas by 300 tons, 180 tons, and 2420 tons respectively, as with the PHEV-300 run. This simulation serves as a sensitivity analysis as well as a best case scenario, since it assumes that electricity used to charge PHEVs resulted in no increases in EGU emissions (due to the existence of an emissions cap or the use of electricity from a non-emitting source like wind or solar).

Results and Discussion

Figure 4-6 shows the maximum ozone concentrations in the PJM area for the basecase simulations on August 11th through 14th, the days with the highest maximum ozone concentrations for the episode. These results are consistent with concentrations measured in the area on those days by monitor sites; data from two representative sites are shown in Figure 3-12 in Chapter 3. The basecase CAMx simulation shows good agreement with concentrations measured by the monitor sites in both absolute values and hourly patterns.
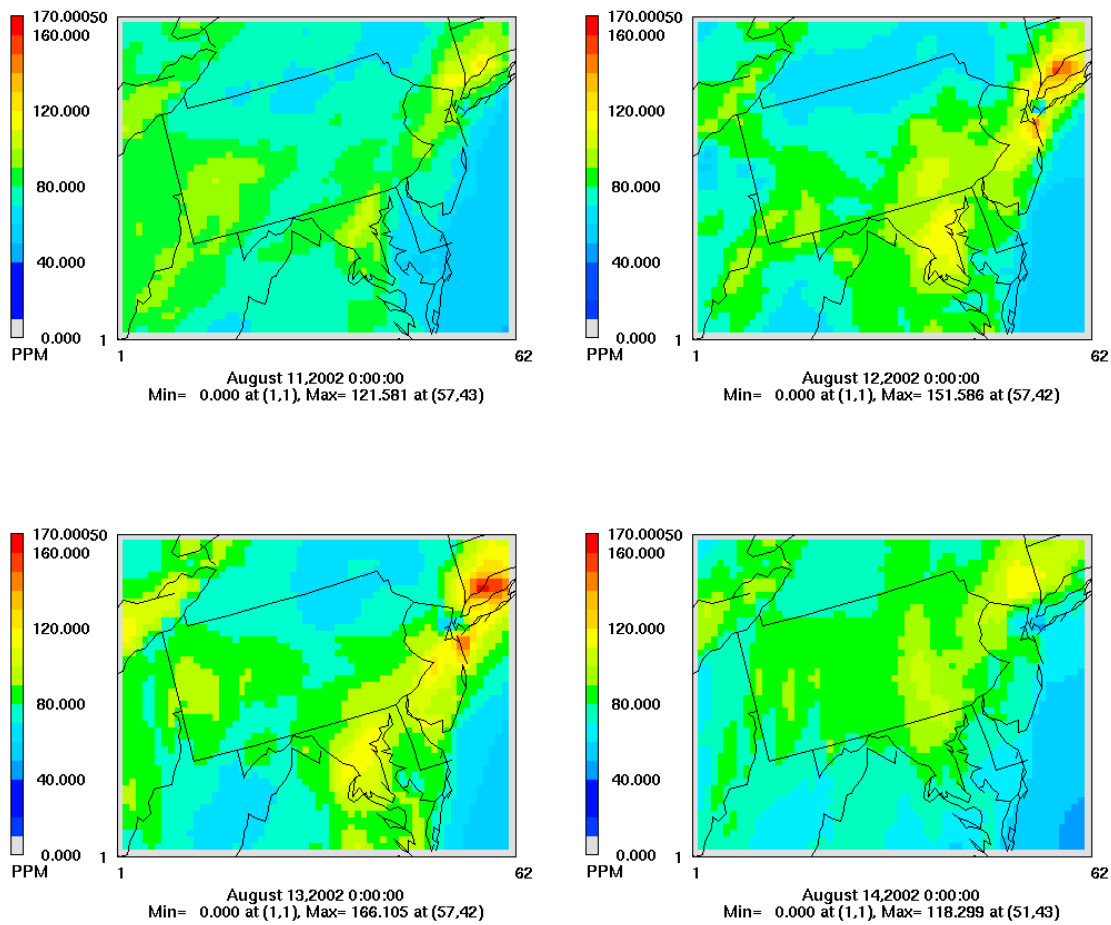
Figure 4-6. Maximum eight hour averaged ozone concentrations (maximum concentration achieved over the course of the day, regardless of time) for the basecase on August 11th – 14th 2002 as modeled by CAMx.

In order to show the effects of PHEV utilization, the maximum daily 8-hr average ozone concentrations are calculated for each case, in each grid cell for the modeling period. The differences between the maximum values for the basecase and for the PHEV-300 case are shown in Figure 4-7. Negative values represent ozone reductions in the PHEV-300 case.
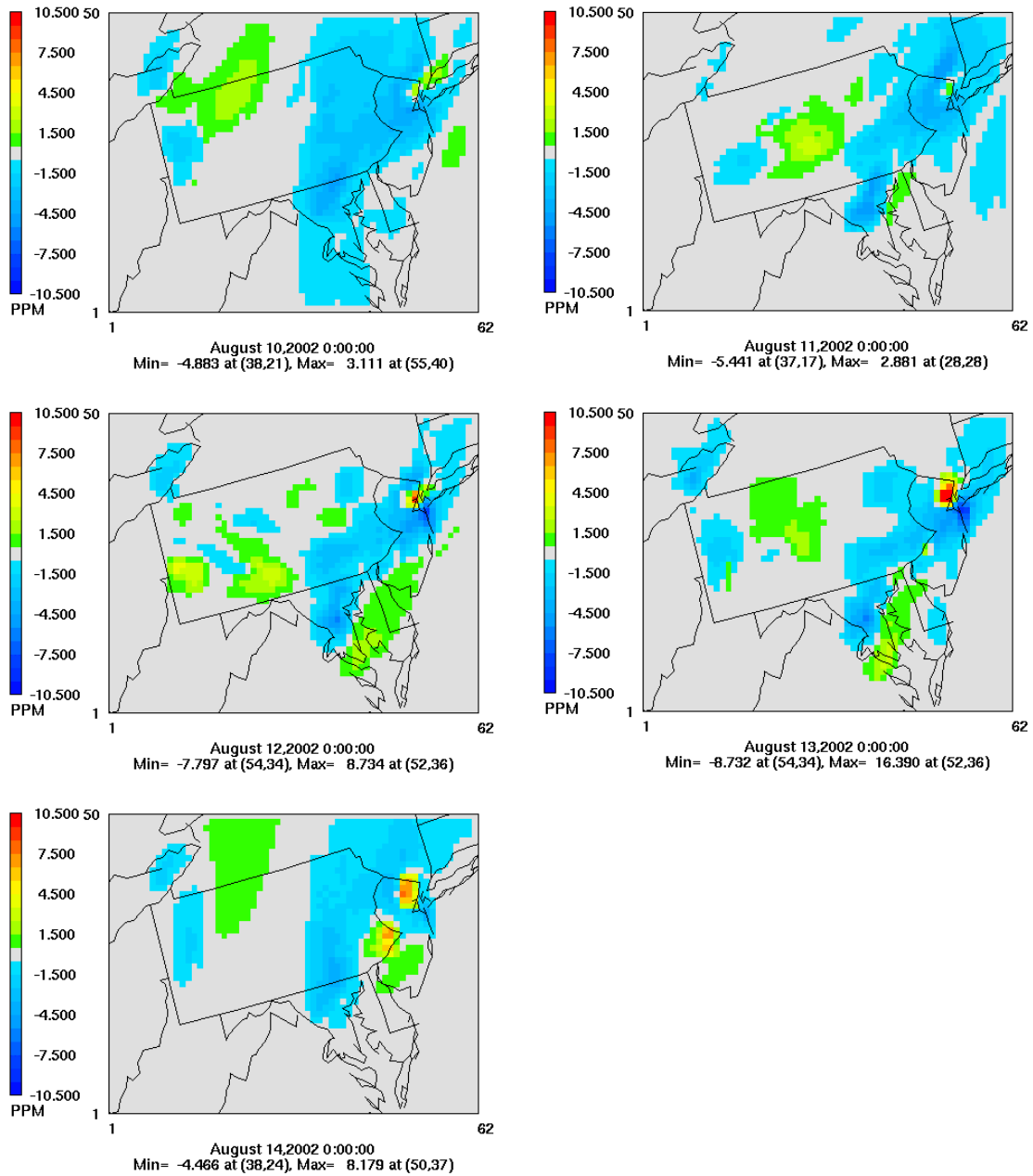
Figure 4-7. Eight Hour Maximum ozone, difference between the basecase and the PHEV-300 case for August 10th – 14th. (PHEV-300 case - Basecase)

The air quality modeling results show air quality improvement over the urban areas in Pennsylvania as well as Baltimore and most of northern New Jersey. The changes in emissions due to the substitution of PHEVs, in the PHEV-300 case, lead to a 2 to 8 ppb decrease in maximum 8-hour averaged ozone concentrations over these major urban areas on all days of the episode. The areas showing this ozone reduction have the highest basecase concentrations of ozone as well as the largest populations, meaning that PHEVs have the potential to significantly reduce ozone exposure in the northeastern US.

However, the August 12th – 14th results also show a NOx disbenefit (ozone concentrations increasing as NOx emissions decrease) occurring in the cells above Newark, NJ. On the 14th, there is also a NOx disbenefit occurring over Philadelphia. Under basecase conditions, the NOx emissions in these areas are relatively high and the NOx reacts with ozone, reducing the ozone concentrations. These NOx disbenefit conditions also caused Newark and Philadelphia to have lower ozone concentrations, in the basecase, than the surrounding areas, between 50 and 70 ppb, while surrounding areas were as high as 120 ppb. When NOx was decreased across the area, the titration effect was reduced and the ozone concentrations in these high NOx areas increased to the mid-70s while the surrounding cells, not affected by the NOx disbenefit, decreased by a greater amount.
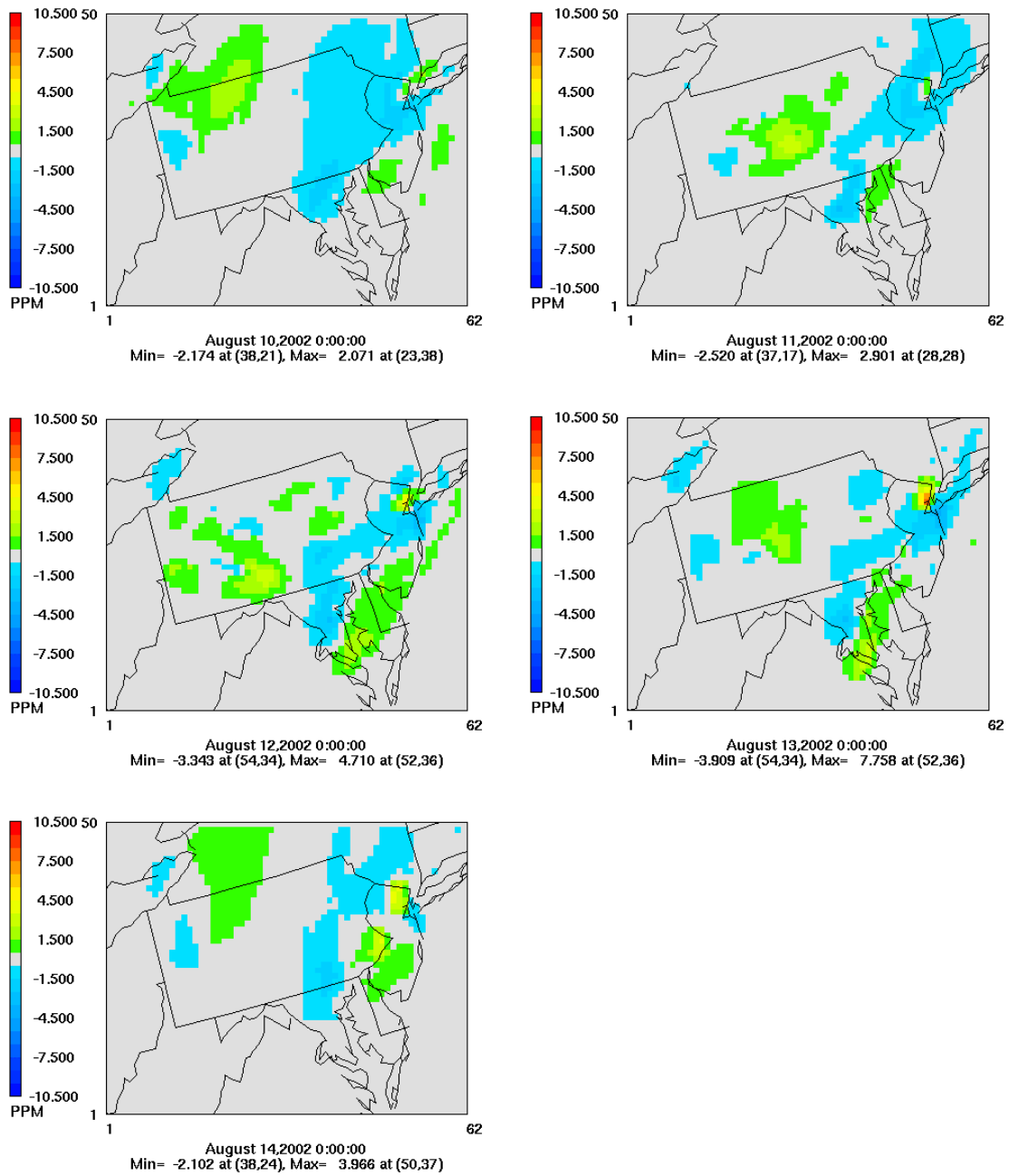
Figure 4-8. Eight Hour Maximum ozone, difference between the basecase and the PHEV-150 case for August 10th – 14th. (PHEV-150 case - Basecase)

The results from the PHEV-150 case show a smaller air quality benefit. The maximum reduction in 8-hr averaged ozone concentrations is only 3.9 ppb in this case as opposed to 8.7 in the PHEV-300 case. The PHEV-150 case shows the same NOx disbenefit, but to a lesser degree, above the cities of Newark and Philadelphia.

The data in Table 4-3, which show the air quality metrics defined in Chapter 3, more completely describe the results from the simulations. Metrics were calculated for two different ozone thresholds; the current ozone standard of 85ppb (8-hr average concentration), and the newly proposed standard of 75ppb (8-hour average). When the threshold is defined as 75ppb, both the PHEV-300 and PHEV-150 cases show both an increase in the total area and total population above standard (metrics 1 and 2), but the area and population exposures (a function of time and ozone concentrations) decreased, summed over all the hours of the day (metrics 3 and 4). Reduction of NOx emissions in urban areas is causing ozone concentrations in some very localized areas to increase above 75ppb. The areas surrounding the urban centers have decreases in ozone concentration that are larger than the localized increases, but concentrations are still above 75ppb. This effect can cause the total area and population exposed to concentrations above 75ppb to increase, while decreasing both the time-integrated population above 75ppb, and time integrated area above 75ppb.

When the ozone threshold is set at 85ppb (8-hour average) all metrics show air quality improvements, including both the area and population above the standard. Area and population exposure, time-integrated, show decreases of 11% and 7% respectively. These metrics also show that, in areas where reduction of the NOx disbenefit is causing an increase in ozone concentrations, the resulting concentrations are below 85ppb. At night, when EGU emissions increase, PHEV-300 nighttime 1-hr ozone concentrations show increases of 2 to 4 ppb in rural areas with decreases of 3 to 5 ppb in urban areas.

Due to the complexity of ozone chemistry and its sensitivity to temporal and spatial changes in emissions of ozone precursors, the results are not straightforward. There are scenarios where PHEV use worsens air quality in localized areas, depending on how air quality is measured.   However, these results highlight that PHEV scenarios, in general, reduce ozone concentrations and exposure. This reduction is especially true for the scenario where PHEVs are charged at night with non-emitting sources.

Table 4-3. Changes in ozone concentrations (using multiple metrics, equations 1-4) due to use of PHEVs.

Percent Change (from Basecase) Threshold = 75ppb			
Metric	PHEV-300	PHEV-150	PHEV_mobile_only
Area above Standard	0%	2%	-1%
Population above Standard	1%	2%	0%
Daily Area Exposure	-6%	-1%	-9%
Daily Population Exposure	-4%	0%	-7%
Percent Change (from Basecase) Threshold = 85ppb			
Metric	PHEV-300	PHEV-150	PHEV_mobile_only
Area above Standard	-3%	-1%	-5%
Population above Standard	-5%	-5%	-6%
Daily Area Exposure	-11%	-3%	-15%
Daily Population Exposure	-7%	-1%	-11%

Using the assumptions outlined in this paper concerning increased nighttime electricity generation at coal-fired power plants and decreased daytime utilization of gasoline vehicles in favor of PHEVs, the resulting change in total quantities of carbon dioxide (CO_2) released to the atmosphere was calculated. The additional capacity utilization of the coal-fired EGUs would lead to an increase of approximately 99,610 tons of CO_2 emissions. This emissions estimate was calculated assuming a 35% efficiency of heat to electricity at coal plants and an average heat density for coal for the year 2002 obtained from the Energy Information Administration (EIA) (EIA 2006). The calculated decrease

of CO_2 emissions from replacing gasoline vehicles with available PHEVs would be 122,670 tons. This value was calculated using average fuel economy standards (Table 4-2). Therefore, assuming that PHEVs are able to substitute for gasoline vehicles for at least 80% of the expected VMT calculated using an energy efficiency of 318 Wh/mi, the scenario considered in this work would not lead to increases in CO_2 emissions during fuel combustion. There are also likely differences between the greenhouse gas emissions due to producing, refining and delivering gasoline and mining and delivering coal. In general these emissions are substantially less that the greenhouse gas emissions associated with combustion, so a detailed estimate of these emissions was not prepared here.

The effect of PHEVs on emissions of Particulate Matter is complex, but some preliminary calculations indicate the general nature of the impact of PHEVs. A 20% increase in capacity utilization of the coal-fired power plants would lead to an increase of 790 tons per day of SO_2 emissions. Studies have measured the fractional conversion of SO_2 to sulfate, in the atmosphere, to be approximately 7%, which would lead to an increase of 55 tons per day in PM formation. (Nopmongcol 2006) Using the same method used to calculate CO and VOC emission reductions caused by the substitution of PHEVs for gasoline vehicles, average daily decreases of PM would be only 1-2 tons. (EPA 2005b) PM emissions from road dust and brake wear would add to this total.

Conclusions

Air Quality Modeling of the four-state classic PJM area show that substitution of PHEVs for just 20% of the mobile vehicle fleet VMT would reduce ozone by up to 8 ppb in the most densely populated areas in the PJM. The benefits would increase if cleaner sources are used to charge the PHEVs or if, subject to the availability of additional excess generation, PHEVs are substituted for a larger percentage of the mobile fleet. This work indicates that while there is the potential for improvements in ozone concentrations, there is also the potential for localized worsening of ozone concentrations as the spatial and

temporal patterns of emissions change. However, while the PHEV use scenarios
modeled in this research do not appear likely to help with ozone attainment
demonstrations, they do appear to reduce ozone exposure levels. Further, the air quality
impacts of PHEV use are not limited to ozone. If, for example, coal fired power plants
are used to generate electricity to power PHEVs, and local SO_2 emissions increased, then
more particulate sulfate would be formed. On the other hand, reduced emissions from
vehicle exhaust would lower particulate matter concentrations.

Chapter 5 HRVOC Trading in Houston, Texas

Most of the work reported in this chapter represents the contributions of the author of this thesis to two papers that were published and have appeared in the journal Environmental Science and Technology. (Wang, L, Thompson, T, Webb, A, McDonald-Buller, E, Allen, D. 2007 and Wang, L, Thompson, T, McDonald-Buller, E, Allen, D. 2007b)

The eight-county Houston/Galveston/Brazoria (HGB) area (shown in Figure 5-1) is currently classified as a severe non-attainment area under the NAAQS for ozone, with concentrations averaged over both 1-hour and 8-hours. Because emissions that lead to the formation of ozone have distinctive spatial and temporal patterns and the chemistry of ozone formation is non-linear and introduces time lags between emissions and ozone formation, design of emissions control strategies for ozone precursors is not straightforward and typically requires the application of photochemical grid models in order to evaluate the potential effectiveness of emission reductions for air quality initiatives and State Implementation Plans (SIPs). Houston is especially problematic because of the unique meteorology and the large number of sources in the area.
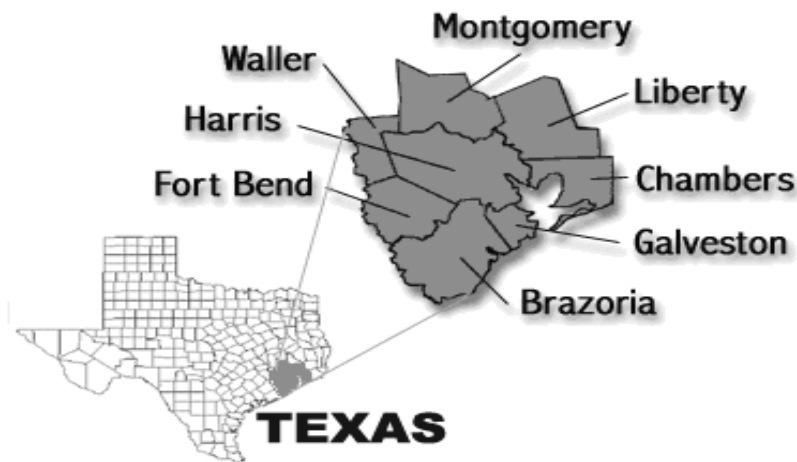
Figure 5-1. The 8-county Houston/Galveston/Brazoria ozone nonattainment area.

Photochemical modeling, performed by the Texas Commission on Environmental Quality (TCEQ) and others as part of TexAQS 2000, described below, indicates that in order to attain the NAAQS for ozone (with concentrations averaged over 1 hour and 8 hours), the HGB non-attainment area must reduce both NOx and VOC emissions (TCEQ 2004).

Texas Air Quality Study 2000 (TexAQS 2000)

During the summer of 2000, a group of researchers from across the nation conducted the largest air quality study ever done in the state of Texas. For six weeks beginning on August 14, 2000, extensive sampling was done at both ground level and in aircraft, throughout southeast Texas, to study the formation, accumulation, and transport of ozone and particulate matter. The results from this study indicated that there is a subset of Volatile Organic Compounds that accounts for a majority of the production of ozone. This subset has been termed Highly Reactive Volatile Organic Compounds (HRVOCs) and is made up of ethylene, propylene, 1,3 butadiene and butenes. Because of this study, regulation for the control of ozone in the state of Texas has been focused on reducing emissions of these four HRVOCs. (TCEQ 2008)

Cap-and-Trade Program in the HGB region

In December 2004, the TCEQ adopted rules 30 TAC §101.390-101.394, 101.396, 101.399-101.401, and 101.403, which established an emission banking and trading program for HRVOCs. The program is currently limited to Harris County, which contains most of the emission sources in the HGB area, but could be extended to other counties within the ozone non-attainment area with public notice. Approximately 80-90 facilities are covered by the rules and these facilities are primarily refineries, ethylene and propylene (olefin) manufacturing facilities and polymer manufacturing facilities. Only a subset of emission points at these facilities are currently in the trading program: vent gas streams, flares, and cooling tower heat exchange systems that collectively have the

potential to emit more than ten tons per year of HRVOC. Fugitive emissions are not currently part of the trading program. In the adopted rules, the TCEQ allowed some trading of emission reductions of other less-reactive VOCs (OVOCs) for emission reductions of HRVOCs, on a reactivity weighted basis. HRVOC allowances received from the conversion of OVOC emission reduction credits currently cannot exceed more than 5% of the site's initial HRVOC allocation. (TCEQ 2004)

Modeling studies done on the data collected during TexAQS 2000 have found that approximately a 90% reduction in HRVOC emissions (in connection with NOx reductions) is needed to meet attainment of the NAAQS for 1-hr averaged ozone concentrations. (TCEQ SIP Revisions 2004) Therefore the area wide emissions cap for the HRVOC Emissions Cap and Trade (HECT) program for the analyses described in this chapter will be set to represent the following HRVOC emissions reductions from the 2000 emissions levels:

1. 90% reduction to HRVOC non-fugitive sources (point and stack) that are part of the cap and trade program
2. 64% reduction to HRVOC and all Other Volatile Organic Compounds (OVOC) fugitive sources that are not currently in the trading program due to difficulties in measuring and documenting the emissions

(The non-fugitive emissions reductions will be applied to Harris county only, while the fugitive emissions reductions will be applied to the entire 8 county area.)

Emissions credits are distributed to sources based on average capped emissions of any previous three-year period. At this point, no spatial or temporal trading limits have been set. (TCEQ 2004)

The cap for the HECT program was determined based on modeling done for the 1 hour attainment demonstration. The reductions required to meet the cap, without trading, will

bring the area into attainment for 1 hour ozone averages.   This chapter examines the potential impacts of trading on the spatial and temporal distribution of ozone concentrations. Finally, in order for this program to work, there must be a viable trading market. So far in Harris County, companies have hesitated to enter the trading market. (TCEQ 2008b) The reasons for this hesitation and possible solutions will be examined in this thesis. Specifically, the following questions will be addressed:

1. Will the Trading Program in its current form lead to ozone hot spots?

There are currently no spatial limits on trading. Credits can be sold to and from any location in Harris County. Is there the possibility of increased levels of ozone if VOC emissions are concentrated in one area due to trading?   What are the factors that influence the ability of HRVOC emissions to affect ozone?

2. Can program modifications improve cost and air quality performance?

It has been proposed that VOC emissions trading or substitution based on reactivity weighted trading amounts is a viable option for a HRVOC/VOC cap and trade program. Is the reactivity scale that is used in the program appropriate? Can the trading also be expanded to include chlorine, another source of ozone production? Because of difficulty monitoring emissions of fugitive sources, they are not currently included in the trading program. Can fugitives be included in the trading?

3. What will the Supply / Demand for Allocations with the current program be?

Based on the required emissions reductions that go along with the trading program, what sources are going to be able to make reductions and sell excess emissions credits? What companies are going to depend on buying credits? Using emissions data collected by the

EPA and the TCEQ and information about allocations of emissions credits, the emissions credit trading that will be necessary to meet the caps will be quantified

Based on results and findings, recommendations for policy modifications will be suggested.

Results

Will the Trading Program, in its current form, lead to ozone hot spots?

Analyses have been performed assessing the likelihood of ozone hot spot formation as a result of unlimited spatial trading. The analysis was done using extreme trading scenarios. Four regions in Houston were identified based on locations of industrial sources involved with trading and each region was defined by NOx and VOC availability. The regions were characterized as high or low availability for each precursor, based on historic emissions of local industry. Figure 5-2a shows a map of Southeastern Texas with VOC emission rates from low (near ground) level man-made and natural emissions and elevated (stack) industrial sources.   The black box outlined within the top figure is expanded in Figure 5-2b to show the four trading regions and NOx availability. These four regions contain the top 25 out of 86 sources of HRVOC and VOC emissions in Harris County, which account for 90% of emissions of both by mass.
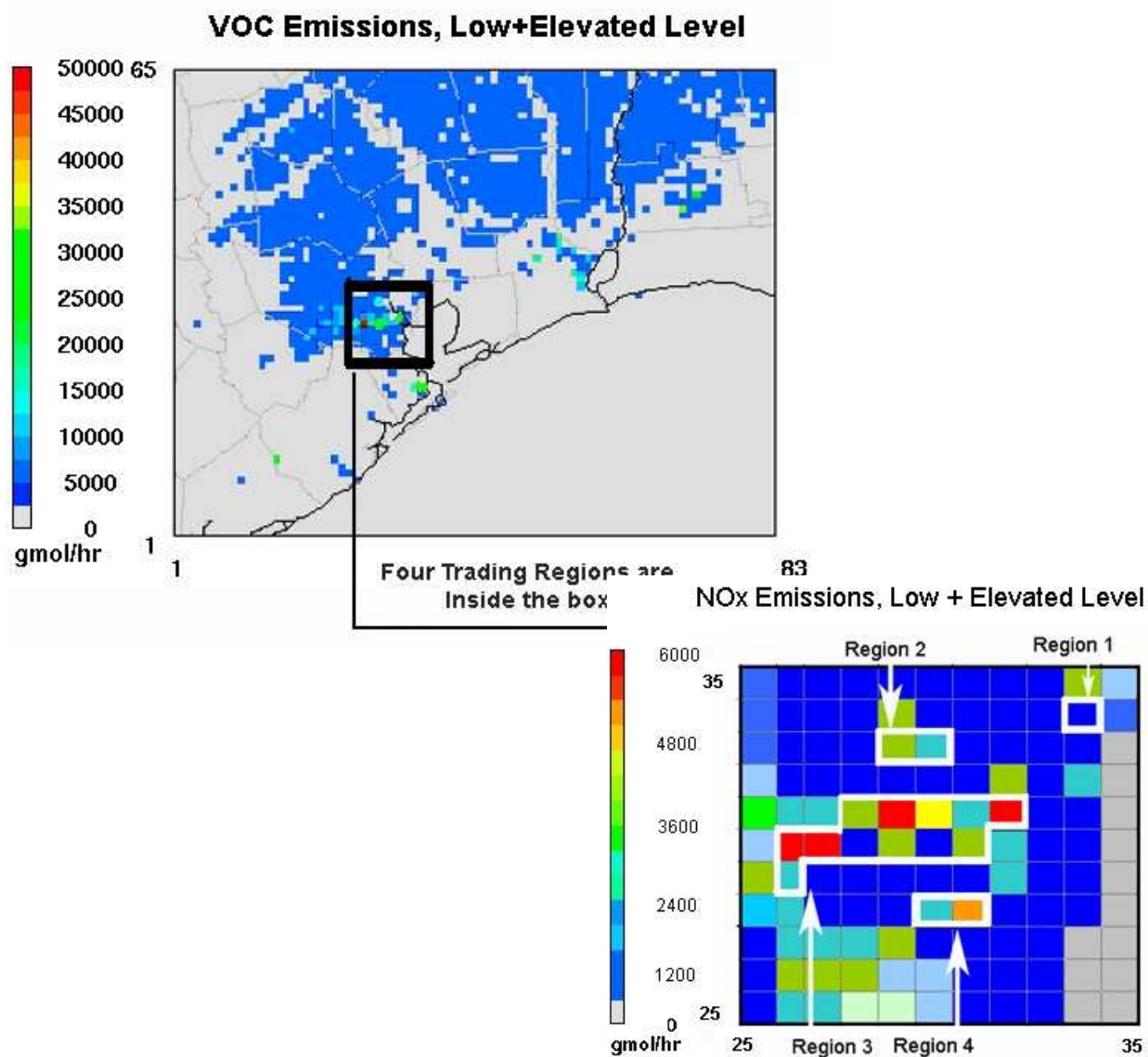
Figure 5-2 a and b. VOC (a) and NOx (b, shows the box outlined in the figure a. on a larger scale) emissions availability within the four regions of this study, near Houston, Texas.

The four trading zones are characterized as:

1. Region 1: Low, localized NOx (1.72 tons/day in one grid cell) and high, localized HRVOCs (13.3% of the total HRVOC emissions of the four regions) within one 4km x 4km grid cell and including 2 of the 25 accounts (8.2% of the total HRVOC of the 25 accounts).

2. Region 2: High, localized, NOx (8.69 tons/day in two grid cells) and high, localized, VOCs (10.3% of the total HRVOC emissions of the four regions) within two 4km x 4km grid cells and including 2 of the 25 accounts (25.4% of the total HRVOC of the 25 accounts).

3. Region 3: High and distributed NOx (37.25 tons/day in 12 grid cells) and high and distributed VOCs (68.9% of the total HRVOC emissions of the four regions) within twelve 4km x 4km grid cells and including 18 of the 25 accounts (61.1% of the total HRVOC of the 25 accounts).

4. Region 4: Low NOx (1.56 tons/day in two grid cells) and moderate VOCs (7.5% of the total HRVOC emissions of the four regions within two 4km x 4km grid cells and including 3 of the 25 accounts (5.3% of the total HRVOC of the 25 accounts).

To present the results of the modeling, the relative reduction factor for ozone (RRF) will be calculated for each monitor shown in Figure 5-3. RRFs are used in this study because of the role that they play in demonstrating attainment with the National Ambient Air Quality Standard (NAAQS) for ozone, with concentrations averaged over 8-hours. In contrast to the approach to attaining the NAAQS for one hour averaged concentrations, which was based on the absolute values of ozone concentrations predicted by a photochemical model, the newer approach to demonstrating attainment with the NAAQS for eight hour averaged ozone concentrations is based on the relative response of the photochemical grid model at multiple locations.

The first step in the new attainment demonstration process is to define an ozone "design value" for each monitor in the region. The design value is the fourth highest daily

maximum 8-hour averaged ozone concentration for each year, averaged over three years. If the ozone design value is greater than the standard (set at 85ppb when this research was conducted, recently lowered to 75ppb), the monitor is in non-attainment. To determine if emission reductions will lead to attainment at the monitor, a relative reduction factor (RRF) in ozone concentration is estimated using photochemical models. Base case and control scenarios are modeled. The maximum daily eight hour ozone concentration is found within a 7x7 block of grid cells centered around each monitor (7x7 required when using 4k horizontal resolution) for each scenario. The RRF is the ratio of the control case maximum to the basecase maximum. Attainment with the 8-hour ozone NAAQS is demonstrated when the model-predicted RRF, at each monitor, multiplied by the monitor design value, is lower than the standard. For example, if a monitor has a design value of 100 ppb and the photochemical modeling predicts a RRF at that site of 0.75 or less, the site will be in attainment (according to the new standard). RRFs are used to examine whether emissions trading scenarios that concentrate emissions in regions near monitors will have a significant effect on attainment demonstrations.
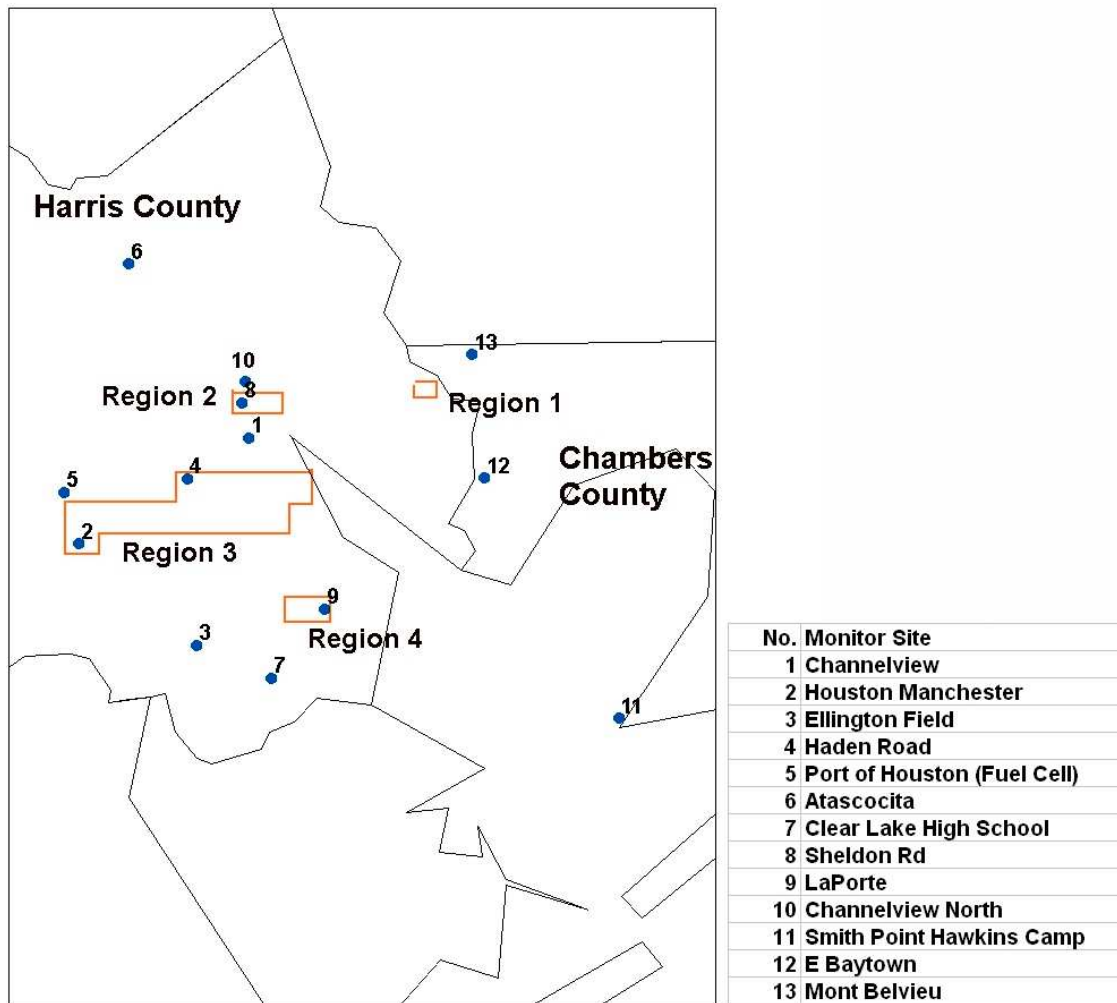
Figure 5-3. The monitors located near the four regions of the modeling scenarios.
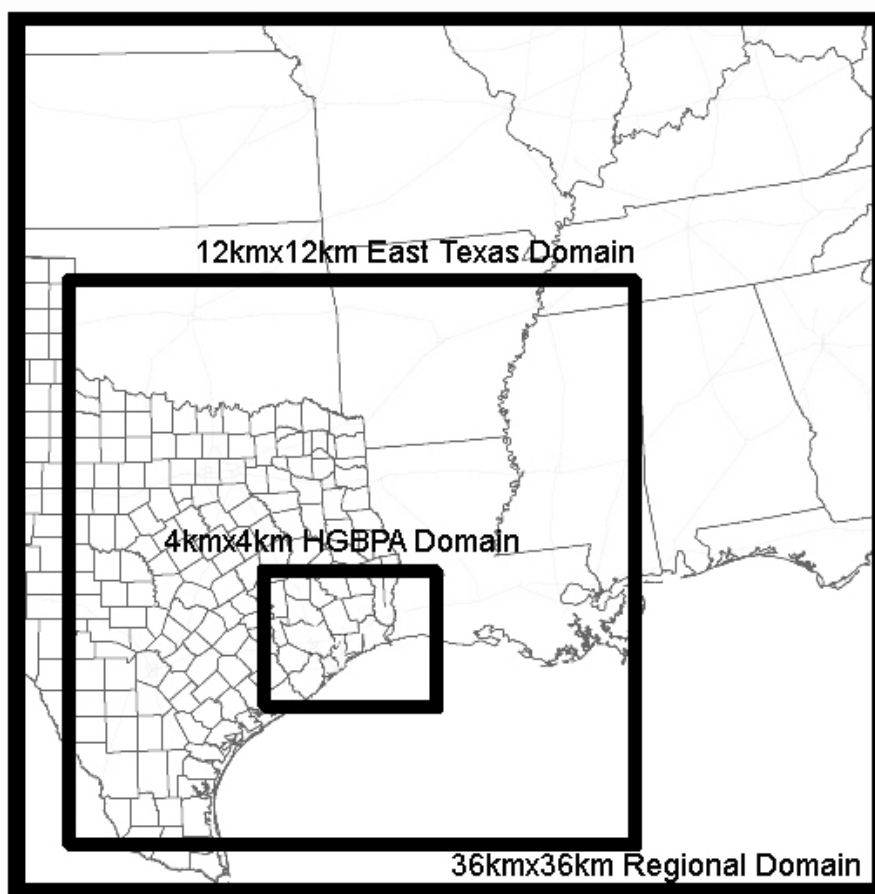
Figure 5-4. Modeling Domain of the HRVOC study. Three boxes outline the 36k horizontal resolution grid, the 12k horizontal resolution grid, and a 4k horizon resolution grid.

HRVOC trading

For this study, five air quality scenarios were modeled using CAMx. CAMx is a 3-D photochemical model which is introduced in detail in chapter 3. The modeling domain and grid resolution for the modeling are shown in Figure 5-4. The first modeling scenario is a basecase which represents the attainment demonstration (based on estimated 2009 emissions) modeled using meterological conditions based on an August 22-September 6, 2000 episode that has been used by the state of Texas in developing air

quality plans for Southeastern Texas. The remaining four modeling scenarios represent worst case scenarios. In each of four scenarios, all HRVOC emissions from three of the four regions are traded into each region in turn to test the effect of the various levels of precursor availability on the formation of hot spots when high levels of HRVOCs were present. Fugitive emissions were not changed in these scenarios. Results from these scenarios are shown in Table 5-1.

Table 5-1. Average RRF values for each trading scenario at each monitor; trading scenarios involve trading all HRVOC emissions in three of the trading regions into the fourth region.

Monitor (*)	Case 1	Case 2	Case 3	Case 4
Atascocita	0.999	1.001	1	1
Mont Belvieu (1)	1	1.003	1	1
Channelview North (2)	0.997	1.005	1	0.998
Sheldon Rd (2)	0.995	1.002	1.001	0.997
E Baytown (3)	0.997	1.001	1	0.999
Channelview (3)	0.995	1.002	1.001	0.999
Haden Road (3)	0.995	0.999	1.001	0.999
Port of Houston	0.997	0.999	1.001	0.998
Houston Manchester (3)	0.997	0.998	1.001	0.999
LaPorte (4)	0.995	0.998	1.001	1
Ellington Field	0.995	0.997	1.001	0.999
Smith Point Hawkins Camp	0.997	1	1	1
Clear Lake High School	0.996	0.998	1.001	1.001

*Number in parentheses represents the trading region the monitor is located in or directly adjacent to; monitors with no number indicated are close to trading regions.

Trading of all of the HRVOCs into a single region caused at most a 0.5% increase in the eight-hour average ozone concentration with only five RRF values above 1.001. Four of

these values were calculated for the case in which all HRVOCs were released in a region with high localized NOx concentrations (region 2) with the ozone measurements made at monitors in close proximity to the release. A majority of the monitors showed either no change or a decrease in the eight-hour ozone concentrations. These results led to the conclusion that the trading program, as currently designed, will not lead to ozone hot spots.

Can program modifications improve cost and air quality performance?

Reactivity Trading

The Texas SIP developed to meet the ozone NAAQS requires a 90% reduction in HRVOC emissions. Trading is allowed between facilities, but reductions in the emissions of other volatile organic compounds (OVOCs) can be traded, on a reactivity weighted basis, for only 5% of HRVOC allowances.

Reactivity based trading of VOC emissions is generally based on the concept of incremental reactivity (IR). Incremental reactivity is defined as the amount of additional ozone formation that results from the addition of a small amount of the VOC to the system in which ozone is formed, divided by the amount of compound added. (Carter 1994) Maximum Incremental Reactivities (MIRs), the measure of reactivity used in the HRVOC trading program, are incremental reactivities under conditions when NOx availability is not limited, i.e., when VOCs have the greatest ozone formation per unit of VOC added. Other measures of reactivity are also available. Maximum Ozone Incremental Reactivities (MOIR) are the incremental reactivities observed when NOx levels are adjusted to give the highest peak ozone concentration. Equal Benefit Incremental Reactivities are the incremental reactivity values observed when NOx concentrations are adjusted so that changes in VOCs have the same effect on ozone formation as equal changes in NOx. (Carter 1994) The values of these indices can be

quite different. For example, the MIR, MOIR, and EBIR for propene are 11.57, 4.57 and 3.18 respectively. Absolute differences between the incremental reactivity indices for a single compound are not the critical issue in the trading program, however. The more important issue is the ratio of indices between compounds that will be traded. For example the ratios of propene to propane reactivity are 0.46, 0.32, and 0.23 for MIR, MOIR and EBIR, respectively. So, if trading were based on MIR, MOIR and EBIR, different amounts of propane would need to be traded for propene.

The OVOC/HRVOC trading program developed for southeast Texas uses MIR as a measure of reactivity, but no evaluation of alternative measures was performed. This thesis has examined the use of the three reactivity weighting factors introduced above, for the HRVOC/OVOC trading program in southeast Texas and has evaluated whether the choice of reactivity index leads to the creation of ozone hot spots.

Reactivity weighted emissions were calculated for each of the 25 emission accounts considered in this work, for each of the three IR metrics, plus hydroxyl radical reactivity (MIR, MOIR, EBIR). These results are provided in Appendix A. HRVOC and OVOC emissions are reported separately. For the OVOC emissions, after the reactivity weighted emissions were determined, they were converted into equivalent masses of ethylene or propylene, since these two compounds account for ~75% of the mass of HRVOC emissions. Equivalent masses of ethylene and propylene were calculated by dividing the weighted emissions by the weighting factor (either MIR, EBIR, or MOIR) of ethylene or propylene. For example, the MIR weighted OVOC emissions for the 25 facilities were 84.5 tons * (g O3/ g VOC). Since the MIRs for ethylene and propylene are 9.07 and 11.57 (g O3/ g VOC), the OVOC emissions could be traded for 9.32 and 7.31 tons of ethylene and propylene emissions, respectively. Because the majority (~75%) of HRVOC emissions are ethylene and propylene, the reactivity values for these two species will be used to bound the resulting HRVOC equivalent mass.

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The original, tradable HRVOC emissions in the 25 accounts, after the HRVOC emissions cap has been put in place, expressed as a MIR reactivity weighted equivalent of ethylene emissions is 5.42 tons/d. If the HRVOC emissions are expressed as propylene equivalents, the emissions are 4.25 tons/d. If all the OVOC emissions are traded for HRVOC allocations, the MIR weighted OVOC emissions can be converted into an additional 9.32 and 7.31 tons/d of ethylene and propylene emissions, respectively. This results in total possible emissions of 14.74 and 11.56 tons/d of ethylene and propylene emissions, using an MIR based trading system.

Table 5-2 reports the ethylene and propylene equivalent masses that could be emitted at all facilities, using trading schemes based on MIR, EBIR and MOIR reactivity weighted emissions. As shown in the Table, if all of the OVOC emissions are converted into ethylene equivalents and are added to the HRVOC emissions, expressed as ethylene equivalents, trading schemes based on MIR, MOIR and EBIR lead to very similar results. Emissions vary from a low of 13.7 tpd to a high of 14.7 tpd, a difference of 7%.

Table 5-2. HRVOC equivalent mass summary for all three IR metrics.

	Emissions as equivalent ethylene mass (t/d)	Emissions as equivalent propylene mass (t/d)
Total **MIR** based emissions	14.74	11.56
HRVOC emissions	5.42	4.25
OVOC emissions	9.32	7.31
Total **MOIR** based emissions	14.42	11.29
HRVOC emissions	5.47	4.26
OVOC emissions	8.95	6.97

Total **EBIR** based emissions	13.74	10.97
HRVOC emissions	5.35	4.27
OVOC emissions	8.39	6.7

Table 5-2 demonstrates that the choice of reactivity index, from among time integrated measures of reactivity (MIR, MOIR, EBIR) would lead to small differences in overall emissions. Converting OVOC emissions into ethylene equivalent masses however, results in roughly 25% higher emissions than converting the OVOC emissions into propylene equivalent masses. Because the differences due to using alternative incremental reactivities (MIR, MOIR, EBIR) are small relative to the manner in which OVOC emission reductions are converted into HRVOC credits, the OVOC trading scenarios examined in this thesis will use MIR based reactivities.

As part of the answer to the second question introduced in the first section of this Chapter, a study was done to look at the air quality effects of unlimited OVOC trading. In this study, the same four trading regions shown in Figure 5-2 were used. Within each region, OVOC emissions reductions were made equal to the reactivity of the HRVOC reductions required by the SIP using MIR metrics. No HRVOC reductions are made.

OVOC Trading

Once OVOC emissions reductions are made, a serious of worst-case trading scenarios are modeled using CAMx. All emissions credits are traded into each of the four regions in turn and released as HRVOCs. Those four scenarios are then compared to the basecase to calculate an RRF for each scenario at each of the monitor sites. Table 5-3 shows the results of the OVOC modeling scenarios.

Table 5-3. Average RRF values for each trading scenario at each monitor; trading scenarios involve converting all OVOC emissions in three of the trading regions into HRVOC allocations, and trading those HRVOC emissions into the fourth region.

Monitor (*)	Case 1	Case 2	Case 3	Case 4
Atascocita	0.999	1.002	1.001	1
Mont Belvieu (1)	1.001	1.006	1	1
Channelview North (2)	0.995	1.01	1.001	0.997
Sheldon Rd (2)	0.993	1.006	1.004	0.997
E Baytown (3)	0.995	1.002	1.002	0.999
Channelview (3)	0.992	1.004	1.003	1
Haden Road (3)	0.993	1.001	1.004	1.002
Port of Houston	0.996	1	1.003	0.998
Houston Manchester (3)	0.995	0.997	1.002	0.999
LaPorte (4)	0.992	0.998	1.003	1.002
Ellington Field	0.993	0.996	1.005	1.002
Smith Point Hawkins Camp	0.996	1	1.002	1.001
Clear Lake High School	0.994	0.998	1.003	1.004

* Number in parentheses represents the trading region the monitor is located in or directly adjacent to; monitors with no number indicated are close to trading regions.

The results indicate that in all cases, increases in ozone concentration are 1% or less (RRF<1.01). Trading into regions 1 and 2 generally results in decreases in ozone concentrations, while trading into regions 3 and 4 generally results in increases in ozone concentrations. These results lead to the conclusion ozone hot spots will not be created, even if extensive OVOC for HRVOC trading is allowed.

Fugitive Trading

The final two parts of the second question ask about the air quality effects of including fugitive emissions and chlorine emissions in the HRVOC trading program. Fugitives were tested in the same way that OVOC emissions trading was tested. OVOC emissions, from both fugitive and non-fugitive sources, were reduced in each of the four regions and traded for HRVOC emission credits. Including fugitive emissions more than doubles the amount of material traded. The credits were traded into each of the four regions one at a time and the RRF values for the local monitors were calculated. The results are shown in Table 5-4.

The results reported in Table 5-4 indicate that if the amount of HRVOC emissions traded increases significantly, through the inclusion of fugitive emissions in the trading program RRFs are much more likely to be 1 or less (air quality improvements). The more extensive trading results in air quality improvements because, as the amount of emissions traded is increased, the amount of additional ozone formed in the region accepting the trades (which now have very high VOC to NOx ratios, with little sensitivity to added hydrocarbon reactivity) is more than offset by the lowering of ozone production in the regions from which the emissions are traded (which are generally NOx rich after the trades). The only RRFs greater than 1 tend to be associated with the locations nearest the regions that the emissions are traded into.

Table 5-4. Average RRF values for each trading scenario at each monitor; trading scenarios involve converting all OVOC emissions from both fugitive and non-fugitive sources in three of the trading regions into HRVOC allocations, and trading those allocations into the fourth region where they are released as HRVOC emissions.

Monitor (*)	Case 1	Case 2	Case 3	Case 4
Atascocita	0.998	1.001	1	0.999
Mont Belvieu (1)	0.999	1.004	0.998	0.998
Channelview North (2)	0.991	1.007	0.998	0.994
Sheldon Rd (2)	0.986	1	1	0.991
E Baytown (3)	0.992	0.998	1	0.996
Channelview (3)	0.987	0.999	1	0.995
Haden Road (3)	0.987	0.996	1	0.998
Port of Houston	0.993	0.997	1.001	0.995
Houston Manchester (3)	0.992	0.994	1.001	0.996
LaPorte (4)	0.988	0.994	1.001	0.999
Ellington Field	0.988	0.991	1.002	0.999
Smith Point Hawkins Camp	0.993	0.997	1	1
Clear Lake High School	0.99	0.994	1.001	1.002

* Number in parentheses represents the trading region the monitor is located in or directly adjacent to; monitors with no number indicated are close to trading regions.

Chlorine Trading

It has been found that Chlorine emissions from chlor-alkaline facilities, cooling towers, swimming pools and salt water are estimated to be up to 10 tons/day (Wang et. al. 2007b). These emissions can lead to increases in 1 hour ozone concentrations of up to 40 ppb in highly localized areas in the morning and up to 5-10 ppb at time of the day when peak ozone is occurring. Adding chlorine emissions to the HRVOC trading market would increase the flexibility of the market. Similar to HRVOC and OVOC trading,

before the addition of chlorine to the HRVOC trading market can be recommended, air quality modeling is done to test for hot spot formation.

The same four regions (Figure 5-2) are used in the chlorine study. In this case, Cl emissions must be added to the basecase. Then all Cl emissions in three of the four trading regions are eliminated and traded for HRVOC emission reductions based on MIR reactivity. Then they are traded into the fourth region and released as HRVOC emissions. RRF values are calculated for each of the four scenarios for the monitors located near the regions. These values are presented in Table 5-5.

Table 5-5. Average RRF values for each trading scenario at each monitor; trading scenarios involve converting all chlorine emissions in three of the trading regions into HRVOC allocations, and trading those HRVOC emissions into the fourth region.

Monitor (*)	Case 1	Case 2	Case 3	Case 4
Atascocita	0.995	0.997	0.997	0.997
Mont Belvieu (1)	0.981	0.982	0.98	0.98
Channelview North (2)	0.976	0.983	0.979	0.978
Sheldon Rd (2)	0.975	0.98	0.98	0.977
E Baytown (3)	0.983	0.985	0.986	0.984
Channelview (3)	0.976	0.983	0.979	0.978
Haden Road (3)	0.982	0.985	0.987	0.986
Port of Houston	0.981	0.983	0.985	0.983
Houston Manchester (3)	0.986	0.988	0.99	0.989
LaPorte (4)	0.984	0.986	0.988	0.989
Ellington Field	0.995	0.996	1	0.999
Smith Point Hawkins Camp	0.979	0.981	0.981	0.981
Clear Lake High School	0.996	0.998	1	1.001

* Number in parentheses represents the trading region the monitor is located in or directly adjacent to; monitors with no number indicated are close to trading regions.

Not only did hot spots not form when simulations were run with HRVOCs, but hot spots also did not form when OVOC, fugitive or chlorine emission reductions were traded for HRVOC emission reductions. The largest increase in 8hr ozone concentration was less than 1%. This clearly shows that the trading program, as currently designed, will not lead to the formation of hot spots, and there exists the potential to increase the participation of OVOC, fugitive and chlorine emission reductions on a reactivity weighted scale.

What will the Supply / Demand for Allocations with the current program be?

To answer the third question, emissions data have been compared to credit allocations. Emissions data is from a Special Inventory collected by TCEQ. TCEQ sent a survey to the companies that are involved in the HECT program requesting special emissions inventory information. (TCEQ 2007) Table 5-6 shows the results of that survey. Emissions totals include baseline emissions and event emissions. Allowances are current as of 2006.

Table 5-6. Allowances versus 2006 reported emissions (Allowances and emissions in tons)

SITE NAME	ORGANIZATION NAME	Allowances	2006 Actual Reported (excluding fugitives)	% of Allowances
LA PORTE PLANT	SUNOCO INC	40.2	43	106%
CHEVRON CHEMICAL CO	CHEVRON PHILLIPS CHEMICAL CO	242.7	170	70%
LA PORTE COMPLEX	EQUISTAR CHEMICALS LP	100.2	106	105%
EXXONMOBIL REF & SUPPLY	EXXONMOBIL CORP	423.5	61	14%
DEER PARK PLANT	SHELL OIL CO	345.8	312	90%
SUNOCO R&M BAYPORT	SUNOCO INC R&M	17.8	46	259%
LA PORTE PLANT	TOTAL PETROCHEMICALS USA INC	116.2	171	147%
BAYTOWN CHEMICAL PLANT	EXXONMOBIL CHEMICAL CO	191.5	124	65%
HOUSTON CHEMICAL COMPLEX	PHILLIPS CHEMICAL COMPANY	89.6	103	115%
POLYPROPYLENE PLANT	INEOS POLYMERS INC	39.2	49	126%
BASELL U.S.A., INC.	BASELL U.S.A., INC.	74.1	74	99%
BAYPORT HDPE PLANT	TOTAL PETROCHEMICALS USA INC	29	13	45%
POLYETHYLENE PLANT	BP SOLVAY POLYETHYLENE N AMERICA	64.4	47	74%
CHANNELVIEW COMPLEX	EQUISTAR CHEMICALS LP	435.5	206	47%
CHANNELVIEW PLANT	LYONDELL CHEMICAL CO	115.5	32	28%
KURARAY COMPANY INC	EVAL COMPANY OF AMERICA		171	
LA PORTE PLANT	MILLENNIUM PETROCHEMICALS INC	10.4	7	69%
BAYTOWN OLEFINS PLANT	EXXONMOBIL CHEMICAL CO	285.7	70	25%
PASADENA PLANT	PASADENA REFINING SYSTEM	0	69	
LA PORTE PLANT	EI DUPONT DE NEMOURS & CO INC		18	
ALBEMARLE CORP	ALBEMARLE CORP	5	99	1986%
NOLTEX LLC	NOLTEX LLC		13	
HOUSTON REFINERY	VALERO REFINING TEXAS LP	117.7	2	2%
PASADENA PLANT	BASF CORPORATION	8.5	5	55%
BARGE CLEANING FACILITY	KIRBY INLAND MARINE LP		24	
TX PETROCHEMICALS LP	TEXAS PETROCHEMICALS LP	190.5	31	16%
BARGE CLEANING AND REPAIR	SOUTHWEST SHIPYARD LP		47	
DEER PARK PLANT	ROHM & HAAS TEXAS		31	
LYONDELL CHEMICAL BAYPORT	LYONDELL CHEMICAL WORLDWIDE INC	39	28	71%
Total		2982	2172	73%

Yellow highlighted boxes indicate missing information. Table 5-6 clearly shows a need for a viable emissions trading market. Some facilities are significantly below their cap

while some facilities are significantly above. The total emissions in the area are 800 tons below the cap.

Also available are data on event emissions during the years 2003 to 2006. (TCEQ 2007) Emission events are periods during which emissions exceed permitted values, often due to unpredicted process upsets. Emission events, if they are large relative to the caps, present a challenge to emission cap and trade programs because they are unpredictable and facilities may choose to withhold tradable allocations in anticipation of events that may or may not occur. Table 5-7 shows allowances and emission events as a percentage of the total allowance for each facility. These data highlight specifically the uncertainties event emissions introduce to the trading market.

Table 5-7. Percentage of allowances used up by Emission events only (Allowances in tons)

ORGANIZATION NAME	Allowances	2003 Events	2004 Events	2005 Events	2006 Events
EQUISTAR CHEMICALS LP	435.5	20%	5%	3%	0%
EXXONMOBIL CORP	423.5	4%	4%	3%	0%
SHELL OIL CO	345.8	2%	31%	27%	0%
EXXONMOBIL CHEMICAL CO	285.7	3%	17%	73%	0%
CHEVRON PHILLIPS CHEMICAL CO	242.7	11%	22%	16%	5%
EXXONMOBIL CHEMICAL CO	191.5	3%	4%	1%	0%
TEXAS PETROCHEMICALS LP	190.5	0%	2%	1%	2%
VALERO REFINING TEXAS LP	117.7	11%	0%	13%	14%
TOTAL PETROCHEMICALS USA INC	116.2	10%	12%	2%	1%
LYONDELL CHEMICAL CO	115.5	36%	2%	1%	34%
EQUISTAR CHEMICALS LP	100.2	64%	57%	37%	0%
PHILLIPS CHEMICAL COMPANY	89.6	0%	1%	1%	103%
BASELL U.S.A., INC.	74.1	13%	14%	6%	0%
BP SOLVAY POLYETHYLENE N AMERICA	64.4	18%	0%	0%	0%
SUNOCO INC	40.2	2%	4%	13%	0%
INEOS POLYMERS INC	39.2	12%	6%	5%	3%
LYONDELL CHEMICAL WORLDWIDE INC	39	4%	3%	8%	1%
TOTAL PETROCHEMICALS USA INC	29	1%	0%	0%	1%
SUNOCO INC R&M	17.8	231%	95%	16%	1%
MILLENNIUM PETROCHEMICALS INC	10.4	14%	10%	0%	16%
BASF CORPORATION	8.5	30%	3%	3%	86%
ALBEMARLE CORP	5	0%	0%	0%	157%

Table 5-7 shows that it is possible for a facility to use a large percentage of their emissions credits with event emissions one year, and then a small percentage the next and vice versa. Because companies often cannot predict events, they may not trade excess emissions credits. This keeps companies who are able to reduce their baseline emissions below their cap from selling off excess credits to companies who cannot do so, and limits the trading market.

Recommendations and Conclusions

There are several ways to provide companies more flexibility in meeting their HRVOC emissions cap. Conversion of Other VOCs (OVOCs) emission reductions into HRVOC credits using an MIR reactivity scale is currently limited to 5% of the HRVOC cap at each facility. Work done for this thesis has shown that expanding the ability for companies to trade OVOC emissions reductions for HRVOC credits will not create ozone hot spots. The same is true for fugitive emissions. Allowing companies to trade fugitive emission reductions for HRVOC emissions credits will not create ozone hot spots.

Additionally, it has been shown in previous work that Chlorine emissions participate in the formation of ground level ozone in the HGB area. (Chang 2006) Chlorine emissions are not well documented and may be playing a large role in the formation of ozone. This work has shown that Chlorine reductions can also be traded for HRVOC emissions credits, weighted by reactivity, without causing ozone hot spots to occur.

As a result of these studies, it is proposed that the HECT expand or eliminate the limit on OVOC trading for HRVOCs. Additionally, if fugitive emissions monitoring and reporting is improved, fugitive emissions can be included in the trading program. It is also proposed that the HECT should include industrial releases of Chlorine in the HRVOC trading scheme and encourage better documentation of chlorine releases.

Companies should be encouraged to reduce baseline emissions and planned events below allowances. However, it has been shown that a safety net needs to be established for unplanned, major events. One method for accomplishing this would be to encourage improved monitoring of fugitive emissions and allow reductions in fugitive emissions with good documentation to be traded for event emissions above the cap. Allowing for unplanned, major emission events to be covered using a means other than existing emission credits will encourage more companies to get involved in the trading market.

And if baseline fugitive emissions are reduced in response to an unplanned event, the total emissions in the area will be decreased long term.

Chapter 6 Conclusions and Recommendations

This thesis has demonstrated how the use of air quality modeling can improve the design of emission trading programs, by allowing for rigorous analyses of spatial and temporal limits on trading. Three case studies are used to demonstrate this contribution and are presented in Chapters 3, 4 and 5.

Chapter 3 Main Points and Conclusions

1. How much NOx emissions reduction can be realized during periods of peak demand?

Even at times of peak demand, NOx emissions from EGUs located in the classic PJM grid in the Northeast United States can be reduced up to 30% while still meeting the electricity demand. These emission reductions lead to wide spread ozone concentration reductions of 4 to 8 ppb, and very localized increases of ozone concentrations around 2 ppb during periods of high ozone.

2. What corresponding amount of financial motivation is needed to see specific reductions?

An economic model developed by MIT showed overall NOx emissions reductions from EGUs to be approximately 12.5% when NOx emission cost $10,000 per ton, 25% when NOx emission cost $50,000 per ton, and close to 30% when NOx emission cost $125,000 per ton. The current NE trading program uses emissions credits worth approximately $2,000 per ton. As a result, it fits better with the current policy to charge some multiple of emissions credits instead of a specific amount. For example, on a day that is forecast to have high ozone concentrations in the NE, EGUs in the NE can be charged 5 or 10 credits per ton of NOx in order to reduce NOx and therefore ozone on that day.

3. Can ozone concentrations be reduced in the Baltimore/Philadelphia non-
   attainment areas by charging more for emissions from EGUs located downwind
   of the two areas on high ozone days?

Charging more for NOx emissions only in certain areas results in emissions being shifted
to other locations instead of being reduced. Shifting emissions is likely to lead to hot
spot formation downwind of the new location of the emissions.

4. What are the relative benefits of targeting reductions on just high ozone days, vs.
   all days?

While exact cost analysis was not performed in this thesis, it would cost significantly
more to target all days. In 2002, there were 17 days that fell within the definition of
ozone episodes when the standard is set at 85ppb. There are 22 when the standard is set
at 75ppb. There are 92 total days in the ozone season. Controlling just a fraction of the
total days could be significantly more cost effective.

5. What are the changes in exposure and what are the changes in ozone exceedances
   as defined by a series of air quality metrics?

Modeling scenarios have shown that while targeting reductions on all days of the ozone
season (in this case June though August) results in slightly larger seasonal average
decreases in exposure and area of exceedance than when targeting just high ozone days
(episode focused scenarios). Additionally, depending on the scenario, there were
different locations to areas of disbenefit. Blanket scenarios showed NOx disbenefit on
August 12th in the city of Baltimore, meaning that although NOx emissions were reduced,
ozone concentrations increased. The scenarios with NOx reductions modeled using
economic trading showed ozone increases in grid cells north of Philadelphia. This is
likely due to a slight shifting of emissions that occurred when low NOx units were
utilized in place of units with high NOx emissions. No scenarios lead to an increase in
ozone exceedances.

6. What are the implications of these findings for air quality policies in the Northeast US?

This thesis has shown that episode focused reductions can have similar benefits to season long reductions. Additionally, reductions that occur due to economic trading lead to larger exposure and area of exceedance decreases than blanket reduction scenarios. However, in implementing these policies it would be important to keep in mind that EGUs have not dealt with time varying NOx emissions prices. It will be difficult to predict what choices they will make when faced with a varying and largely unknown price for emissions.

Chapter 4 PHEV Main Points and Conclusions

7. What would the effect to ambient ozone concentrations be if excess nighttime coal-fired electricity generating capacity is used to charge plug-in hybrid electric vehicles that would then be used for urban commuting the next day?

Air Quality Modeling of the four-state classic PJM area show that substitution of PHEVs for just 20% of the mobile vehicle fleet VMT would reduce ozone by up to 8 ppb in the most densely populated areas in the PJM. The benefits would increase if cleaner sources are used to charge the PHEVs or if, subject to the availability of additional excess generation, PHEVs are substituted for a larger percentage of the mobile fleet. However, this work also indicates that while there is the potential for improvements in ozone concentrations, there is also the potential for localized worsening of ozone concentrations as the spatial and temporal patterns of emissions change. Further, the air quality impacts of PHEV use are not limited to ozone. If, for example, coal fired power plants are used to generate electricity to power PHEVs, and local SO_2 emissions increased, then more particulate sulfate would be formed. On the other hand, reduced emissions from vehicle exhaust would lower particulate matter concentrations.

Chapter 5 HRVOC Main Points and Conclusions

8. Will the HRVOC Trading Program in Harris County, Texas in its current form lead to ozone hot spots?

Modeling scenarios were designed that represented worst-case scenario trading of HRVOCs and it was found that unconstrained HRVOC trading would at most lead to a 0.5% increase in eight hour ozone concentrations and only at monitors located in close proximity to the point of emissions. This leads to the conclusion that the trading program as currently designed will not lead to ozone hot spot formation.

9. Can program modifications improve cost and air quality performance?

Currently OVOC reductions can be substituted for 5% of HRVOC emissions reductions weighted by MIR reactivity metrics. Worst case scenario modeling found that even when all HRVOC required reductions are substituted by OVOC reductions weighted by reactivity, at most would lead to a 1% increase in 8 hour ozone concentrations. Therefore it is concluded that the current program should be expanded to allow more OVOC trading. The same is true for fugitive emissions and chlorine emissions. Including both emissions in the HRVOC trading program will expand the flexibility of the program and will not lead to ozone hot spot formation.

10. What will the Supply / Demand for Allocations with the current program be?

Several reasons have been identified for why the market may be slow to emerge and developed policy recommendations have been based on these results. By examining emissions data obtained from the TCEQ website, it is clear that some companies will emit more than their allocations and some companies will emit less. It is also clear that unplanned events can be a major component of the yearly emissions and can cause companies to unexpectedly surpass their allowance. While much of the HRVOC work has been completed, a viable trading market still has not formed. This supports the need for increased flexibility in the trading market to act as a safety net. Recommendations to

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increase flexibility have been made in point #9. However, much is still unknown about costs associated with HRVOC emissions reduction. The HRVOC trading market could benefit from increased transparency in the costs associated with the market.

This thesis has shown that air quality modeling is an important part of the development of emissions cap and trade programs. This will become especially important as the new ozone standard is adopted and many areas throughout the country must reevaluate their state's State Implementation Plan for ozone. Several recommendations can be made based on the work presented here. In the Northeast United States, the NOx cap and trade program can improve air quality cost effectively by charging EGUs multiple credits per ton of NOx emissions on days when ozone is more likely to form. Additionally, the use of PHEVs in the northeast can expand the NOx cap and trade program by shifting emissions from the on-road mobile sector to the EGU sector. While much of the area will see benefits from use of PHEVs, there are localized areas that see a disbenefit from the reduction of NOx.

Finally, the HRVOC cap and trade program in Harris County, Texas has not been active thus far. More flexibility is needed to encourage facilities to participate in trading. The incorporation of OVOCs, fugitives, and chlorine emissions on a reactivity-weighted scale are ways to increase flexibility without the potential for hot spot formation. An analysis of the costs associated with the recommended programs was not included in this thesis but would be a beneficial addition to this study.

Appendix

Photochemical Modeling of Emissions Trading of Highly Reactive Volatile Organic Compounds in Houston, Texas. 1. Reactivity Based Trading and Potential for Ozone Hot Spot Formation

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As part of the State Implementation Plan for attaining the National Ambient Air Quality Standard for ozone, the Texas Commission of Environmental Quality has created a Highly Reactive Volatile Organic Compounds (HRVOC) Emissions Cap and Trade Program for industrial point sources in the Houston/Galveston/Brazoria area. This program has a number of unique features, including its focus on a limited group of ozone precursors and its provisions for trading emissions based on atmospheric reactivity. This series of papers examines the potential air quality impacts of this new emission trading program through photochemical modeling of potential trading scenarios; this first paper in the series describes the air quality modeling methods used to assess potential trades, the potential for localized increases in ozone concentrations (ozone "hot spots") due to HRVOC emission trading, and the use of reactivity scales in the trading. When HRVOC emissions are traded on a mass basis, the simulations indicate that trading of HRVOC allowances between facilities resulted in less than 0.15 ppb (<0.13%) and 0.06 ppb (<0.06%) increases in predicted maximum, area-wide 1-h averaged and 8-h averaged ozone concentrations, respectively. Maximum decreases in ozone concentrations associated with trading, as opposed to across-the-board reductions, were larger than the increases. All of these changes are small compared to the maximum changes in ozone concentrations due to the VOC emissions from these sources (up to 5–10 ppb for 8 h averages; up to 30 ppb for 1-h averages). When emissions of HRVOCs are traded for other, less reactive emissions, on a reactivity weighted basis, air quality simulations indicate that daily maximum ozone concentrations increased by less than 0.3%. Because these relatively small changes (<1%) are for unlikely trading scenarios designed to produce a maximum change in ozone concentrations (all emissions traded into localized regions), the simulations indicate that the implementation of the trading program, as currently configured and possibly expanded, is unlikely to cause localized increases in ozone concentrations ("hot spots").

Introduction

Emission trading is a market-based approach to air quality management designed to improve the efficiency and economic viability of emission control programs. Two general forms of air pollutant emission trading systems predominate in the United States: (1) offsets and (2) multisource cap and trade programs or allowance trading. Offset programs are used in areas that are designated as being in nonattainment of National Ambient Air Quality Standards (NAAQSs). In an offset program, new or expanding sources of emissions must be offset by additional emission reductions from existing sources. The primary objective of offsets is to allow continued economic growth and activity in a nonattainment area without increasing emissions that could negatively affect air quality. In emission cap and trade programs, facilities are allocated emission allowances and are able to sell, buy, and bank allowances in accordance with program guidelines. Total emissions in the area (the cap) are reduced over time by lowering the number of allowances. Emission cap and trade programs such as the U.S. Acid Rain Program, California's Regional Clean Air Incentives Market (RECLAIM), and the Northeast's NOx Budget Program have demonstrated that market-based programs can be implemented across different geographic scales and can encourage facilities to seek flexible and economically efficient alternatives for achieving air quality objectives (1–4).

Building on the foundation provided by these programs, the State of Texas has recently developed a new type of emission cap and trade program, which is designed to reduce emissions of a class of ozone precursors, highly reactive volatile organic compounds (HRVOCs), from industrial point sources in Houston. This cap and trade program is novel due to its focus on a subclass of volatile organic compounds and due to its provisions allowing for trading based on the atmospheric reactivity of volatile organic compounds (VOCs). This series of papers will examine the potential air quality impacts of this new emission trading program. This paper will describe the motivation for creating an HRVOC emission trading program, the form of the program, and air quality analyses that focus on the potential for localized increases in ozone concentrations (ozone "hot spots") due to currently planned, and possibly expanded, emission trading. The second paper in the series will examine issues associated with including additional types of emissions (chlorine) in the program.

Air Quality in Houston, TX. The eight-county Houston/Galveston/Brazoria (HGB) area (shown in Figure 1) is currently classified as a severe nonattainment area under the NAAQS for ozone, with concentrations averaged over 1 h. The region has a required attainment date of November 15, 2007. Photochemical modeling, performed by the Texas Commission on Environmental Quality (TCEQ) and others (5), indicates that in order to attain the NAAQS for ozone (with concentrations averaged over 1 h), the HGB nonattainment area must reduce both NOx and VOC emissions. Results from a large air quality field study indicated that, among the VOC emission reductions, controls on the releases of HRVOCs are particularly important (6, 7). HRVOCs have been defined as ethylene (ethene), propylene (propene), 1,3-butadiene, and butylenes. Aircraft measurements indicated

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FIGURE 1. The 8-county Houston/Galveston/Brazoria ozone non-attainment area.

that these compounds were emitted in significant quantities from refining and petrochemical facilities (classified as nonelectric generating units or NEGUs) (5) in the HGB area. Total estimated emissions of HRVOCs from industrial facilities in the HGB nonattainment area was in excess of 170 tons d^{-1} in the year 2000, prior to the implementation of the HRVOC cap and trade program (8). On a mass basis, the HRVOC emissions were roughly 20% of the total daily VOC emissions from all anthropogenic sources in the region in the year 2000 (789 tons d^{-1}) (8), but because of the reactivity of the emissions and the localized nature of the releases, these emissions play a significant role in ozone formation in Houston (6, 7).

In December 2004, the TCEQ adopted rules 30 TAC §101.390−101.394, 101.396, 101.399−101.401, and 101.403, which established an emission banking and trading program for HRVOCs (5). The program is currently limited to Harris County, which contains most of the emission sources in the HGB area, but could be extended to other counties within the ozone nonattainment area with public notice. Approximately 80−90 emission accounts are covered by the rules. Emission accounts are generally associated with a specific facility, and in the case of HRVOCs, the facilities are primarily refineries, ethylene and propylene (olefin) manufacturing facilities, and polymer manufacturing facilities. However, some facilities have multiple emission accounts. The focus in this work will be on separate accounts with tradable emissions. In addition only a subset of emission points at these facilities is currently in the trading program: vent gas streams, flares, and cooling tower heat exchange systems that collectively have the potential to emit more than 10 tons yr^{-1} of HRVOC. Fugitive emissions are not currently part of the trading program. In the adopted rules, the TCEQ allowed some trading of emission reductions of other less-reactive VOCs for emission reductions of HRVOCs, on a reactivity weighted basis (These are referred to as OVOCs in the TCEQ documentation; they will be referred to as other-VOCs in this paper.). Additional HRVOC allowances received from the conversion of other-VOC emission reduction credits currently cannot exceed more than 5% of the site's initial HRVOC allocation.

The first goal of the modeling simulations presented in this work will be to assess the extent to which the current, limited trading program might cause the generation of localized regions of high ozone concentrations (ozone "hot spots"). A second goal of the analyses will be to assess whether significant expansions of the trading programs might lead to ozone "hot spots".

Modeling Methodology

Photochemical modeling was used to assess the potential air quality impacts of emission trading scenarios. Although any comparable photochemical grid model could be used, the Comprehensive Air quality Model with extensions (CAMx)
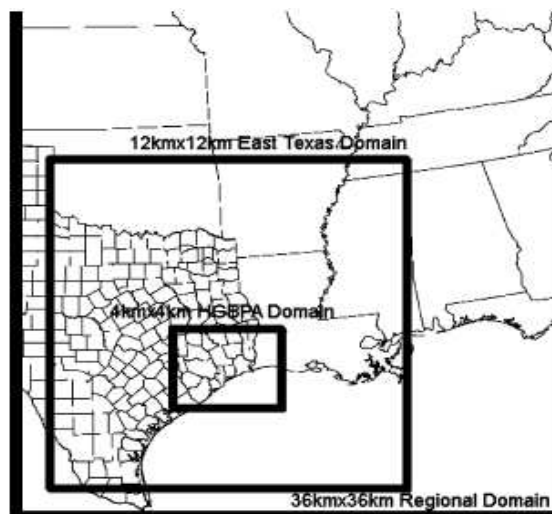

FIGURE 2. Nested modeling domain for the August 22−September 6 episode; the trading occurs in the Houston−Galveston−Bravoria−Beaumont−Port Arthur (HGPBA) domain.

(9) was selected for this study because it is currently being used by the State of Texas for attainment demonstrations in areas that have violated the National Ambient Air Quality Standards for ozone. The meteorological conditions used in the model were based on an August 22−September 6, 2000 episode that has been used by the State of Texas in developing air quality plans for southeastern Texas. The modeling domain was a nested regional/urban scale 36-km/12-km/4-km grid shown in Figure 2. Meteorological inputs required by the model were based on results from the Mesoscale Meteorological Model, version 5 (10, 5, 11). The Carbon Bond mechanism (version IV, CB-IV) was selected to model atmospheric chemistry in this work, in order to be consistent with the modeling done for regulatory analyses by the TCEQ. EPA default values for boundary conditions were used for most species, but concentrations of some important ozone precursors including isoprene and NO were modified based on monitoring data. Additional details on all of the modeling inputs may be found in the TCEQ documentation for the Houston air quality plan (5). The overall performance of the model in predicting ozone concentrations during the episode period has been evaluated by the TCEQ (8). A summary of the performance is provided in the Supporting Information.

The volatile organic compound (VOC) and nitrogen oxides (NOx) emission inventories used as input for the year 2000 modeling episode have been described by the TCEQ (8, 10). In this work, the focus is on trading of emissions once the HRVOC cap and trade program is put in place, and therefore the emissions "base case" that is of interest is the set of emissions with controls in place (including but not limited to the HRVOC cap and trade program). This "base case" is the scenario used by the TCEQ to demonstrate attainment with the National Ambient Air Quality Standard for ozone, with concentrations averaged over 1 h (5, 8). In this scenario, which will be referred to as the base case attainment demonstration, it is assumed that no HRVOC emission trading occurs. All accounts with HRVOC caps are assumed to emit at their capped rate.

The VOC emissions for the base case attainment demonstration have been developed by TCEQ (8, 10) and are presented here and in the Supporting Information. Information regarding NOx emission inventories in the base case attainment demonstration is also presented because of the
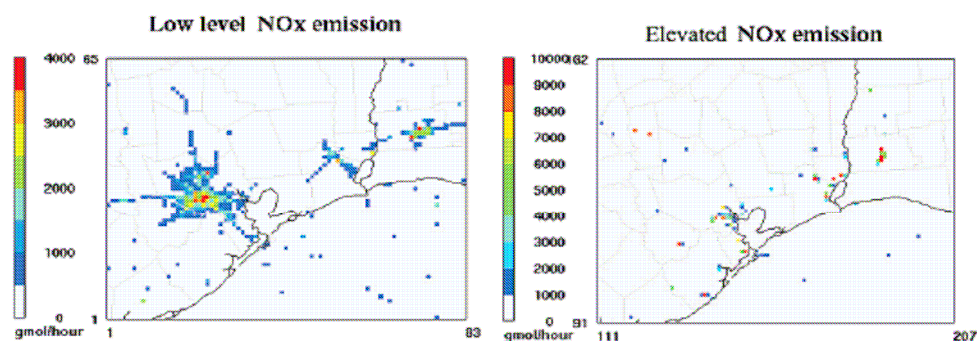
FIGURE 3. NOx emission rates from low-level and elevated anthropogenic and biogenic sources within the Houston area (HGBPA domain from Figure 2).
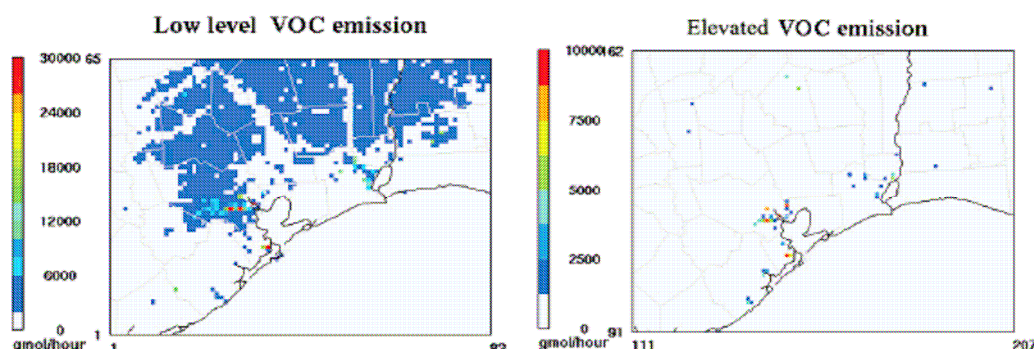

FIGURE 4. VOC emission rates from low-level and elevated anthropogenic and biogenic sources within the Houston area (HGBPA domain from Figure 2).

role of NOx emissions in establishing the trading zones described in this work.

Figure 3 shows the spatial distributions of elevated and low level NOx emission rates from anthropogenic and biogenic sources within the Houston portion of the modeling domain for the base case attainment demonstration. Figure 4 shows the spatial distributions of elevated and low level VOC emission rates, for the base case attainment demonstration, from anthropogenic and biogenic sources within the modeling domain. Typical of many metropolitan areas, low-level NOx emissions are concentrated in the downtown urban area due to mobile source emissions. Elevated NOx emissions as well as elevated and low-level VOC emissions are concentrated in the Houston industrial area (Ship Channel), located on the northwest portion of Galveston Bay, near the center of the maps.

The existing HRVOC cap and trade program is currently limited to Harris County, in which a total of 86 facilities (accounts) are currently subject to the HRVOC cap. Each of the industrial accounts has a number of emission points, associated with specific process units. Of the total of 13 033 industrial process units that emit more than one pound per day of VOC within the HGB area, 5167 of the units (40%) are in HRVOC service, and 4586 (89%) of these have other-VOC species in their emission streams, i.e., only 581 of the units emit only HRVOCs (11). Ethylene and propylene are the HRVOC species with the highest emissions. Some streams contain all ethylene; some contain all propylene; most streams are mixtures. Variability in composition within accounts is significant. Other VOCs that contribute to the total reactivity of emissions include light alkanes ($\leq$C7) and aromatics, most notably isomers of xylene and toluene (11, 12).

Twenty-five accounts, which contribute 90% of the mass of both VOC and HRVOC emissions, were selected for analysis in the current study. Tables in the Supporting Information, that accompanies this paper, show daily VOC emission rates for the 25 accounts and the speciation of those emissions. The tables report both the projected 2007 emissions, before controls, and the anticipated account allocations, after the cap and trade program and other controls are imposed (base case attainment demonstration). Prior to the cap and trade program, these accounts emitted a total of 172 tons d^{-1} of VOCs, including 107 tons d^{-1} of HRVOCs. After the cap and trade program and a leak detection and repair program for all VOCs are implemented, these 25 accounts emit 74 tons d^{-1} of VOCs and 26 tons d^{-1} of HRVOCs. Tables in the Supporting Information show HRVOC emission rates and NOx emission rates for each of the 25 accounts. Collectively, these emissions contribute significantly to ozone formation in the HGB area. Maximum differences in 1-h averaged ozone concentrations between the base case attainment demonstration and a simulation with all point source VOC emissions removed is up to 30 ppb (5−10 ppb for 8-h averaged concentrations, see the Supporting Information).

VOC and HRVOC sources are classified as nonfugitive and fugitive, as described in the Supporting Information. Nonfugitive sources are included in the current trading program, while fugitive sources are not. Fugitive and non-fugitive sources account for approximately equal portions of the total VOC mass.
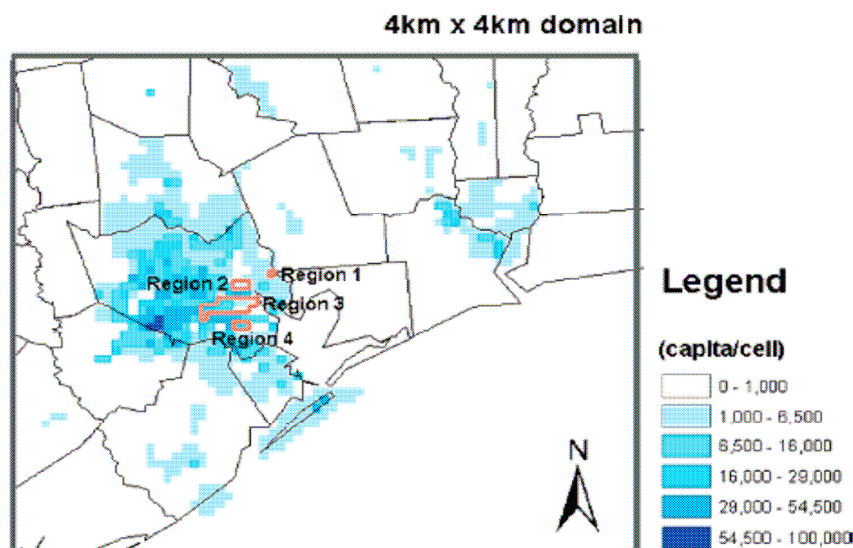
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4km x 4km domain

FIGURE 5. Population density (2000 Census) and trading regions in 4 km × 4 km modeling domain.

The 25 dominant HRVOC emission sources are located in four trading regions. The four regions, superimposed on a map of population density within the photochemical modeling domain, are shown in Figure 5. The four trading zones have different levels of HRVOC and NOx emissions, as summarized below: 1. Region 1: Low, localized NOx (1.72 tons/day in one grid cell) and high, localized HRVOCs (13.3% of the total HRVOC emissions of the four regions) within one 4 km × 4 km grid cell and including 2 of the 25 accounts (8.2% of the total HRVOC of the 25 accounts). 2. Region 2: High, localized, NOx (8.69 tons/day in two grid cells) and high, localized, VOCs (10.3% of the total HRVOC emissions of the four regions) within two 4 km × 4 km grid cells and including 2 of the 25 accounts (25.4% of the total HRVOC of the 25 accounts). 3. Region 3: High and distributed NOx (37.25 tons/day in 12 grid cells) and high and distributed VOCs (68.9% of the total HRVOC emissions of the four regions) within 12 4 km × 4 km grid cells and including 18 of the 25 accounts (61.1% of the total HRVOC of the 25 accounts). 4. Region 4: Low NOx (1.56 tons/day in two grid cells) and moderate VOCs (7.5% of the total HRVOC emissions of the four regions within two 4 km × 4 km grid cells and including 3 of the 25 accounts (5.3% of the total HRVOC of the 25 accounts). The emission percentages reported above are based on the base case attainment demonstration. Note that within the four regions, there are some sources, other than the 25 accounts, that also emit HRVOCs and NOx.

To address the air quality impacts of the trading, five air quality impact metrics were considered. Metrics were based on both 1-h averaged and 8-h averaged ozone concentrations, as predicted by CAMx and, as appropriate, a threshold concentration of 125 ppb (1-h average) or 85 ppbv (8-h average). Four of the five metrics selected to evaluate ozone impacts in this research were based on the work of Durrenberger et al. (13). These four metrics included maximum 1-h or 8-h averaged ozone concentration in the eight-county Houston area, total geographic area exceeding a threshold 1-h or 8-h average ozone concentration, time-integrated geographic area of exceedance above a threshold 1-h or 8-h average ozone concentration, and total daily population exposure of ozone concentrations above a threshold level.

The equations below demonstrate how the metrics were calculated (14).

1. Maximum 1-h average ozone concentration (ppb)

$$M_{max} = \max_{g,h}\{c_{g,h}\}$$

where $c_{g,h}$ = modeled ozone concentration (in ppb) in grid cell g at hour h.

This metric was calculated by examining all ground-level grid cells in the Houston area during each episode day and selecting the maximum ozone concentration.

2. Total geographic area exceeding a threshold ozone concentration (km²)

$$M_{total\ area} = \sum_g a_g \max\{\delta_{g,h}\}$$

where a_g = area of grid cell g (in km²)

$$\delta_{g,h} = \begin{cases} 0, c_{g,h} \leq \text{threshold} \\ 1, c_{g,h} > \text{threshold} \end{cases}$$

$$\delta_{g,h} = \{\delta_{g,1}, \delta_{g,2}, \delta_{g,3} \ldots \delta_{g,24}\}$$

This metric was calculated by examining each ground level grid cell in the Houston area and determining if, at any time of day, the ozone concentration exceeded the threshold concentration. If the threshold was exceeded, at any time of day, the area of the grid cell was added to the area of exceedance.

3. Time integrated geographic area of exceedance above a threshold ozone concentration (km²)

$$M_{time\ area} = \sum_h \sum_g a_g \delta_{g,h}$$

$$\delta_{g,h} = \begin{cases} 0, c_{g,h} \leq \text{threshold} \\ 1, c_{g,h} > \text{threshold} \end{cases}$$

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This metric was calculated by examining ozone concentrations in each ground level grid cell in the Houston area for each hour of each episode day and determining if the cells exceeded the threshold ozone concentration. The areas of all cells exceeding the threshold were then summed for each hour. The areas for each hour were then summed over the day.

4. Total daily population exposure of concentrations above a threshold. (ppb-capita)

$$M_{pop} = \sum_h \sum_g p_g s_{g,h}$$

where

$$s_{g,h} = \begin{cases} 0, c_{g,h} \leq \text{threshold,} \\ c_{g,h} - \text{threshold}, c_{g,h} > \text{threshold} \end{cases}$$

and p_g = population density in each grid cell. This metric is calculated, for each grid cell, by multiplying the population density by the ozone concentration over the threshold. The sum is taken over the total area of the eight counties and then summed over hours. M_{pop} is an overall measure of total daily ozone exposure over the threshold within the area of interest. It is responsive to the temporal and spatial extent of ozone exceedances as well as the exposure level. Figure 5 shows the population density in the 4 km × 4 km modeling domain with the 4 trading regions identified.

The fifth air quality impact metric considered in this work was the relative reduction factor for ozone (RRF). RRFs are important to consider because of the role that they play in demonstrating attainment with the National Ambient Air Quality Standard (NAAQS) for ozone, with concentrations averaged over 8 h. NAAQS attainment demonstrations for ozone, with concentrations averaged over 1 h, have required that model predicted ozone concentrations be reduced to below a maximum concentration. A region was considered to be in attainment when photochemical modeling indicated that the maximum absolute value of 1-h averaged ozone concentrations in the region was reduced below 125 ppb. In contrast to the approach to attaining the NAAQS for 1-h averaged concentrations, which was based on the absolute values of ozone concentrations predicted by the photochemical model, the new approach to demonstrating attainment with the NAAQS for 8-h averaged ozone concentrations is based on the relative response of the photochemical grid model at multiple locations (15, 16). To determine the extent to which emission changes will change ozone concentrations at various locations, a relative reduction factor (RRF) in ozone concentration is estimated. Photochemical models are used to determine the RRFs that emission reductions will achieve in the vicinity of monitors. This work will consider the RRFs associated with trading scenarios. The ozone concentrations in the trading scenario, relative to the base case attainment demonstration, predicted by the model at monitor locations, are used to estimate the RRF.

RRF = (ozone concentration$_{trading\ scenario}$)/
(ozone concentration$_{base\ case}$)

Relative reduction factors for ozone are calculated for each site in a nonattainment area that exceeds the NAAQS. In Houston, there are more than 25 such sites. This work will focus on results for 25 sites that are broadly representative of the entire nonattainment area. The procedure used for estimating the RRFs follows EPA guidance (15, 16). Details are provided in the Supporting Information.

Emission Trading Methodology

In considering trading of HRVOC emissions, based on mass, the focus is on trading among the four regions identified in

Figure 5. HRVOC emissions are traded from one region to another, without regard to whether the emissions are of ethylene, propylene, butylenes, or butadiene. However, as noted in the introduction, the trading program has provisions that allow trading of other-VOCs for HRVOCs, on a reactivity weighted basis. Reactivity based trading of VOC emissions is generally based on the concept of incremental reactivity (IR). Incremental reactivity is defined as the amount of additional ozone formation that results from the addition of a small amount of the VOC to the system in which ozone is formed, divided by the amount of compound added. NOx availability is a key factor in VOC reactivity (17–19). A variety of NOx scenarios have been adopted to test VOC reactivity. Maximum Incremental Reactivities (MIRs), which are employed in Texas and California rules (20, 21), are incremental reactivities under conditions when NOx availability is not limited, i.e., when VOCs have the greatest ozone formation per unit of VOC added (17). Maximum Ozone Incremental Reactivities (MOIR) are the incremental reactivities observed when NOx levels are adjusted to give the highest peak ozone concentration. Equal Benefit Incremental Reactivities are the incremental reactivity values observed when NOx concentrations are adjusted so that changes in VOCs have the same effect on ozone formation as equal changes in NOx (17). Incremental reactivities are defined as the mass of ozone formed per mass of VOC added and are often reported as a dimensionless quantity. Differences in incremental reactivity between different compounds can be large. For example, propylene, a highly reactive volatile organic compound has an MIR value of 11.57. n-Octane has an MIR value of 1.09 and therefore is considered to be almost 11 times less reactive than propylene. The absolute values of incremental reactivity are sensitive to the choice of reactivity index. For example, propylene has an MOIR value of 4.57 and an EBIR value of 3.18. n-Octane has an MOIR value of 0.37 and an EBIR value of 0.207. On a relative basis, however, incremental reactivities are relatively consistent. The ratio of the reactivity of propylene to the reactivity of octane is 11 for MIR, 12 for MOIR, and 15 for EBIR (17, 19).

A variety of analyses have been performed to examine the use of reactivity scales in regulatory applications (22, 23). The reports of the Reactivity Research Working Group are adding to these findings (24–27) but generally indicate that the choice of an appropriate reactivity scale will depend on the atmospheric chemistry of the region developing the controls. Therefore, in this work, a preliminary evaluation was performed of three reactivity scales for the tradable emissions.

Reactivity weighted emission rates were determined for each of the 25 emission accounts considered in this work. Emissions of each compound in each account were multiplied by a reactivity measure (MIR, EBIR, MOIR) and were then summed to provide a reactivity weighted emission rate for each account. The reactivity weighted emission rates have units of tons * (g O₃/g VOC) for MIR, EBIR, and MOIR weighted emissions and are reported in the Supporting Information.

MIR, EBIR, and MOIR values were obtained from studies done by Carter (17, 19). MIR, EBIR, and MOIR values were reported for hundreds of compounds (19), including most of the species emitted by the accounts examined in this work. For species whose reactivity ratios are missing, the following values were used: 1.5 for MIR, 0.5 for MOIR, and 0.4 for EBIR. These values are the average of the incremental reactivities for all other-VOC species represented in the emissions inventory. No HRVOC species were missing values. If all of the other-VOC emissions in the accounts are converted into HRVOC equivalents, trading schemes based on MIR, MOIR, and EBIR lead to emission scenarios that differ by less than 10%. This approximate equivalency of MIR, EBIR, and MOIR weighted emission ratios for these accounts may not

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be valid for other case studies involving other types of facilities or emission sources, particularly if aromatics concentrations are high. However, for these accounts, the results for the various reactivity metrics are similar, and consequently, only MIR reactivity weightings were used in the air quality simulations. The details of the MIR/MOIR/EBIR comparisons are reported in the Supporting Information.

Results and Discussion

Mass-Based HRVOC Emission Trading. The simulations reported in this section examined whether trading of HRVOC allocations between regions of high and low NOx availability, as allowed under the current trading program, would change the air quality impact metrics. Four trading scenarios will be reported. The scenarios examined the impacts of trading all of the HRVOC allowances into a single trading region. Thus, in each of the four scenarios, HRVOC emissions have been concentrated in one of the 4 regions, while accounts in the other three regions no longer have tradable HRVOC emissions (i.e., allowances have been traded). Overall the 25 accounts in the four regions still achieve the required emissions cap. The total amount of HRVOC emissions traded under these scenarios is relatively small. Only approximately 5 tons d⁻¹ are available for trading among the 25 accounts, out of a total of 26 tons d⁻¹ of HRVOC emissions and 74 tons d⁻¹ of total VOC emissions from these accounts in the base case attainment demonstration. The HRVOCs not available for trading are fugitive emissions, and the total VOCs are half from fugitive and half from nonfugitive sources. Even though the HRVOC emission being traded are roughly an order of magnitude more reactive (on an MIR scale) than the alkane-dominated VOCs, the emissions traded represent less than 20% of the total reactivity of the emissions from these 25 accounts. It is therefore not surprising that the trading of all of the HRVOCs into a single region caused less than 0.15 ppb (>0.13%) and 0.06 ppb (>0.06%) increases in predicted maximum, area-wide 1-h averaged and 8-h averaged ozone concentrations, respectively (see the Supporting Information for complete results). Compared to the total ozone formation that is attributed to these sources (up to 30 ppb based on 1-h averages and 5−10 ppb based on 8-h averages, see the Supporting Information), these impacts are small. Other indicators of air quality showed somewhat larger changes, as described in the Supporting Information. The area exceeding a threshold ozone concentration increased by up to 0.5%, the concentrations near monitoring locations (RRFs) increased by up to 0.5%, and a measure of population based exposure increased by up to 1%. Decreases in these metrics due to trading were at times greater than 1%, especially when emissions were traded into regions 1 and 2. The highest percentage changes, both positive and negative, were associated with the population exposure metric. The details of the changes in the air quality metrics are reported in the Supporting Information.

Collectively, these analyses indicate that spatial limits on HRVOC trading are not likely to be a concern when dealing with ozone attainment demonstration for the limited amount of trading allowed in the current program. However, the current program could be expanded to include more sources and trading of emission reductions of other-VOCs for HRVOC allocations. These scenarios are described in the next sections.

Reactivity Based Emission Trading. *Intra-Account Reactivity Based Trading.* One way in which the current trading program could be expanded would be to allow much more extensive trading of other VOC emissions for HRVOC allocations within individual accounts. The current limit on these trades is 5% of the HRVOC allocations or approximately 0.2 tons d⁻¹ of HRVOC allocations. The 25 accounts have a total of 74 tons d⁻¹ of VOC emissions, some of which could be converted to HRVOC allocations. To examine the air quality impacts of allowing intra-account trading of other-VOC emissions for HRVOC emissions, three intra-account trading (i.e., trading within the same account) scenarios were performed. All three scenarios are based on MIR reactivity. In these scenarios, a 100% reduction in the mass of other-VOC nonfugitive emissions (a total of 40 tons d⁻¹) was converted (traded) for HRVOC emissions in the same account. The total MIR equivalent mass emitted by the account remained constant, before and after the trade, but the other-VOC emissions were converted to HRVOC emissions. When the conversion to HRVOC emissions was performed, three methods were used. In the first method, the distribution of HRVOC emissions in each account was used to convert the other-VOC emission reductions into HRVOC allocations. So, for example, if propylene and ethylene both accounted for 50% of the MIR equivalent mass of HRVOC emissions before the conversion of other-VOC credits, they would also constitute 50% of the MIR equivalent mass of HRVOC emissions after the conversion. Other-VOC emissions in each account would be converted into HRVOC allocations based on the mass weighted average HRVOC reactivity in each account. This approach seems reasonable; however, recall that any single account may have hundreds of individual emission points. As described in the methodology section, the region has more than 5000 HRVOC emission points but only approximately 100 major accounts. The composition of each of the dozens of emission points in each account is highly variable. Since it is likely that the HRVOC emission credits will be applied at a subset of the emission points, rather than uniformly across the account, it is likely that the actual HRVOC emissions resulting from the conversion of other-VOC emission reductions would not equal the account average. Further, it is likely that account owners will want maximum flexibility in deciding which emission points to reduce. So, two scenarios were run to bound what might happen if account owners were given maximum flexibility in using HRVOC allocations. In one scenario, other-VOC emissions in each account were converted into HRVOC mass allocations based on the MIR of ethylene. In another scenario, other-VOC emissions in each account were converted into HRVOC allocations based on the MIR of propylene. Since the MIR of ethylene and propylene differ by about 25%, this leads to an uncertainty range of about ±10% in the conversion of other-VOCs into HRVOCs.

Clearly, the first scenario (account specific conversion of other-VOC emission reductions into HRVOC allocations) would appear to be the most reasonable approach. However, because most accounts have multiple HRVOC emission points, with varying compositions, a trading program which accurately tracks exactly which HRVOCs an account emits could be difficult to administer and might limit an account's ability to transfer HRVOC allocations from emission point to emission point. It might also complicate an account's ability to trade HRVOC allocations between accounts.

The details of the changes in air quality associated with the three intra-account trading scenarios are reported in the Supporting Information. None of the trading scenarios leads to large increases in ozone concentrations. Maximum 1-h averaged and 8-h averaged ozone concentrations increase by less than 0.1% when all other-VOC emissions are traded for HRVOC allocations, as compared to a scenario with no trading. Decreases of up to 0.23% in maximum ozone concentrations occur when other-VOC emission reductions are traded for HRVOC allocations based on the MIR of propylene. Increases in other air quality metrics were 2% or less; Increases in Relative Reduction Factors in areas surrounding monitors were smallest when other-VOC emission reductions were traded for HRVOC allocations based on the MIR of propylene (<0.1%) and were less than 0.3% in all of the simulations. All of these changes are small compared to

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the maximum changes in ozone concentrations due to all of the VOC emissions from these sources (up to 30 ppb for 1 h averages, see the Supporting Information)

In all cases, converting other-VOC emission reductions into HRVOC allocations, using the MIR of propylene, leads to smaller increases, or greater decreases, in ozone concentrations, compared to scenarios using other approaches for converting other-VOC emission reductions into HRVOC allocations. This is expected, since the MIR of propylene is greater than for ethylene and results in less overall emissions. The differences, however, especially for maximum ozone concentrations, are relatively small.

These small changes are more surprising than the small changes encountered in the trading of trading of 5 tons d^{-1} of HRVOC emissions between regions. Converting approximately 40 tons d^{-1} of other-VOC emissions into HRVOC allocations might be expected to lead to more significant changes. The results suggest that intra-account trading of other-VOC emission reductions for HRVOC does not lead to large localized increases in ozone concentrations when emissions are traded on an MIR basis.

Interaccount Reactivity Based Trading. Inter-regional trading of emissions, based on MIR reactivity, was examined through four trading scenarios. The scenarios examined the impacts of converting all of the other-VOC emissions in three trading regions into HRVOC allocations and trading those HRVOC allowances into a fourth region. Only nonfugitive emissions were considered (40 tons d^{-1} of other-VOCs). The regions have differing NOx availability, as described in the Methodology section. In these trading scenarios, the other-VOC emissions were converted into HRVOC allocations in each account using account specific average reactivity of HRVOC emissions. In addition, the fractional distributions of MIR equivalent HRVOC emissions were kept the same before and after trading. So, for example, if a particular account in the region accepting the traded emission accounted for 10% of the MIR equivalent mass of HRVOC emissions before the trading of other-VOC credits, it would also constitute 10% of the MIR equivalent mass of HRVOC emissions after the trade. Similarly, in any given account, if a compound such as propylene accounted for half of the MIR equivalent mass of HRVOC emissions before the trading of other-VOC credits, it would also constitute 50% of the MIR equivalent mass of HRVOC emissions after the trade. The results (reported in detail in the Supporting Information) show that trading all other-VOC emission reductions for HRVOC allocations in a single region results in a maximum increase in peak 1-h averaged and 8-h averaged ozone concentrations of less than 0.35 ppb (<0.3%) and 0.15 ppb (<0.15%), respectively. Some of the scenarios (trading HRVOC allocations into regions 1 and 2) lead to decreases in peak ozone concentrations. The area of exceedance metrics follow similar patterns; however, the percentage changes in the population exposure metric are larger in magnitude (both positive and negative) than the percentage changes in the other metrics. The maximum increases in the population exposure metrics, on a percentage basis, due to trading, occurs when trades are made into regions 3 and 4, which are located in regions with higher population densities than regions 1 and 2. The changes in RRFs at multiple monitoring sites indicate that in all cases increases in ozone concentration are 1% or less (RRF<1.01). Trading into regions 1 and 2 generally results in decreases in ozone concentrations, while trading into regions 3 and 4 generally results in increases in ozone concentrations.

To summarize, the simulations described in this work have examined the air quality impacts of the emerging HRVOC trading program in Houston. The analyses indicate that the relatively limited current program (5 tons d^{-1} of HRVOC emissions available for trading and limited reactivity

based trading) will have small impacts on maximum ozone concentrations and other air quality impacts. Possible expansions of the program were also examined, specifically, expanding the allowable trading of MIR equivalent other-VOC mass to HRVOC allowances.

Air quality simulations trading other-VOC emissions for HRVOC allocations at the same facilities (intra-account trading) showed little impact on air quality. When 100% of the nonfugitive other-VOC emissions (about 40 tons d^{-1}) were converted to HRVOC allocations based on MIR (only 5% is allowed in the current trading program), daily maximum 1-h averaged and 8-h averaged ozone concentrations increased by a maximum of 0.1% and decreased by a maximum of 0.2%, depending on the precise methodology used in performing the conversion.

Simulations of trading between regions of high and low NOx availability led to larger increases and decreases in ozone concentration than for intra-account trading. When 100% of the other-VOC emissions (nonfugitive) were converted to HRVOC allocations and these allocations were all traded into one region, daily maximum 1-h averaged and 8-h averaged ozone concentrations increased by a maximum of 0.3% and decreased by a maximum of 1%, depending on the region into which emissions were traded. Other indicators of air quality showed somewhat larger changes, up to an increase of 3%.

Supporting Information Available

Summary of performance of modeling configuration in predicting ozone concentrations in an historical episode, emission inventories for 25 key accounts for base case attainment demonstration, method for calculating relative reduction factors (RRFs), reactivity weighted emission inventories for 25 key accounts, impacts of industrial point source VOC emissions on ozone concentrations in base case attainment demonstration, and air quality metrics for HRVOC trading between regions and for trading of other-VOCs for HRVOCs. This material is available free of charge via the Internet at http://pubs.acs.org.

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Photochemical Modeling of Emissions Trading of Highly Reactive Volatile Organic Compounds in Houston, Texas. 2. Incorporation of Chlorine Emissions

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As part of the State Implementation Plan for attaining the National Ambient Air Quality Standard for ozone, the Texas Commission of Environmental Quality has created a Highly Reactive Volatile Organic Compounds (HRVOC) Emissions Cap and Trade Program for industrial point sources in the Houston/Galveston/Brazoria area. This series of papers examines the potential air quality impacts of this new emission trading program through photochemical modeling of potential trading scenarios; this paper examines the air quality impact of allowing facilities to trade chlorine emission reductions for HRVOC allocations on a reactivity weighted basis. The simulations indicate that trading of anthropogenic chlorine emission reductions for HRVOC allowances at a single facility or between facilities, in general, resulted in improvements in air quality. Decreases in peak 1-h averaged and 8-h averaged ozone concentrations associated with trading chlorine emissions for HRVOC allocations on a Maximum Incremental Reactivity (MIR) basis were up to 0.74 ppb (0.63%) and 0.56 ppb (0.61%), respectively. Air quality metrics based on population exposure decreased by up to 3.3% and 4.1% for 1-h and 8-h averaged concentrations. These changes are small compared to the maximum changes in ozone concentrations due to the VOC emissions from these sources (5–10 ppb for 8-h averages; up to 30 ppb for 1-h averages) and the chlorine emissions from the sources (5–10 ppb for maximum concentrations over wide areas and up to 70 ppb in localized areas). The simulations indicate that the inclusion of chlorine emissions in the trading program is likely to be beneficial to air quality and is unlikely to cause localized increases in ozone concentrations ("hot spots").

Introduction

The previous paper in this series (*1*) examined the air quality implications of an emissions cap and trade program that is due to be launched in 2007 in Houston, TX. The trading program caps industrial point source emissions of Highly Reactive Volatile Organic Compounds (HRVOCs), which are defined as ethylene (ethene), propylene (propene), butylenes, and 1,3-butadiene. Trading is allowed between facilities, and

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reductions in the emissions of other volatile organic compounds (other-VOCs) can be traded for HRVOC allowances, on a reactivity weighted basis.

The air quality simulations described in part 1 of this series of papers indicated that trading of HRVOC allowances between facilities, as currently allowed in the program, resulted in less than 0.13% increases in maximum predicted 1-h averaged and 8-h averaged ozone concentrations, and increases in other air quality metrics were less than 1%, for emission trading scenarios designed to create high localized concentrations of ozone. Expansion of the trading program to allow extensive trading of other-VOC emissions for HRVOC allowances, on a reactivity weighted basis, resulted in less than 0.3% increases in maximum predicted 1-h averaged and 8-h averaged ozone concentrations.

HRVOCs, other-VOCs, and oxides of nitrogen are not the only industrial point source emissions in the Houston/Galveston/Brazoria area that contribute to ozone formation, however. Point source emissions of molecular chlorine, from chlor-alkali facilities and from facilities that use chlorine as a biocide in cooling water, are estimated to be up to 5–10 tons d^{-1} (*2–4*). This emission rate is similar to the total emission rate of HRVOCs included in the trading program discussed in part 1 of this series of papers. These emissions participate in ozone formation when the chlorine photolyzes, producing Cl radical. These Cl radicals then react with hydrocarbons and other species in a manner similar but not identical to hydroxyl radical (OH•) (*5*).

The first direct evidence of chlorine radical (Cl•) chemistry in the Houston urban troposphere was based on the quantification of two products unique to the Cl• + isoprene reaction: 1-chloro-3-methyl-3-butene-2-one (CMBO) and chloromethylbutenal (CMBA) (*5–8*). Recent analyses suggest that the observed concentrations of these marker species, and other Cl reaction products, are consistent with a total anthropogenic emission rate of approximately 10 tons d^{-1} (*3*). The magnitude and reactivity of these emissions have the potential to enhance 1-h averaged ozone mixing ratios by 70 ppb, in very localized areas, during morning hours. Over wider areas, and at times of day when peak ozone concentrations are observed, the impacts of chlorine emissions on ozone concentrations are typically 5–10 ppb (*3*). Because the impacts of these emissions on ozone formation are equal to or greater than the impacts of HRVOC and other-VOCs emission allocations from point sources in the trading program being evaluated, this paper will examine the air quality impacts of including chlorine emissions in the trading program.

Allowing trading of chlorine emissions, which act as a free radical source, for HRVOC emissions, which propogate the free radical reactions, has the potential to cause changes in the magnitude and distributions of ozone concentrations and to cause qualitative changes in the atmospheric chemistry. It is the changes in the magnitude and distributions of ozone concentrations that are the focus of this paper. If chlorine emissions are included in the trading program at a future date, a more detailed analysis should focus on the changes in chemistry that result.

Methods

The model domain and air quality impact metrics that will be used in this work have been described in part 1 of this series of papers (*1*). This section will describe the emission inventory for chlorine and the changes in the chemical mechanism that accounted for the reactions of these emissions in the photochemical model. Both the emission

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TABLE 1. Chlorine Emissions for 25 Capped Accounts in Harris County

no.	cooling tower (tons/day)	point source (tons/day)	chlorine MIR equivalent mass tons/day * (g O3/g VOC)	HRVOC allocations (MIR equivalent mass) tons/day * (g O3/g VOC)
1	0.22	0.000	5.07	5.03
2	0.29	0.006	6.78	3.09
3	0.03	0.000	0.74	3.90
4	0.03	0.000	0.62	4.91
5	0.04	0.000	0.99	3.27
6	0.00	0.000	1.42	2.82
7	0.05	0.000	1.10	2.41
8	0.03	0.003	0.68	2.35
9	0.06	0.000	1.40	6.26
10	0.16	0.000	3.64	0.53
11	0.01	0.007	0.35	1.68
12	0.02	0.000	0.40	0.87
13	0.01	0.000	0.15	1.48
14	0.02	0.000	0.54	1.29
15	0.00	0.000	0.07	2.10
16	0.06	0.000	1.45	1.11
17	0.30	0.001	6.88	0.86
18	0.05	0.000	1.12	0.72
19	0.01	0.000	0.28	0.16
20	0.07	0.000	1.69	1.35
21	0.01	0.000	0.14	1.74
22	0.05	0.000	1.14	0.67
23	0.01	0.001	0.35	0.74
24	0.04	0.126	3.73	0.36
25	0.00	0.003	0.36	0.45
	1.58	0.15	41.08	50.18

inventory and the mechanism have been described in detail elsewhere and so are only summarized here.

Emission Inventory. The chlorine emission inventory developed by Chang et al. (2, 3) was used in this study. The chlorine emission inventory included four source types: (1) industrial stack sources, (2) volatilization from cooling towers where chlorine is used as a biocide, (3) volatilization from swimming pools where chlorine is used as a biocide, and (4) reactive chlorine released due to the reactions of chloride in sea salt. Other types of emissions (e.g., volatilization from water and wastewater treatment) were evaluated but were estimated to be less significant than the four primary sources.

In this work, the focus will be on the stack and cooling tower emissions, which together are estimated to account for 7 tons d^{-1} of chlorine emissions in the Houston–Galveston–Brazoria (HGB) area. Chlorine emissions from sea salt and swimming pools are included in the simulations but are considered to be unavailable for trading. Table 1 shows the chlorine emissions from point sources and cooling towers for each of the 25 capped accounts that are being considered in the trading program evaluation presented in this series of papers (1). These facilities do not dominate chlorine emissions in the same way that they dominate HRVOC emissions. Chlorine emissions at the facilities that dominate HRVOC emissions are only 1.7 t/d, which is approximately 25% of the estimated industrial chlorine releases. This discrepancy in the distribution of chlorine and HRVOC emissions is due to the wide distribution of cooling towers among industrial facilities, as opposed to the relatively focused use of HRVOCs. Even though the mass of the chlorine emissions is not as large as the mass of the HRVOC emissions, the relatively high maximum incremental reactivity (MIR) of chlorine (23.78 g O_3/g chlorine (9) as compared to 9.07 g O_3/g VOC for ethylene and 11.57 g O_3/g VOC for propylene (10)) causes the MIR equivalent mass of chlorine emissions and HRVOC emissions at the 25 facilities to be comparable, as shown in Table 1.

Chlorine Chemistry. As noted in part 1 of this series (1), the Carbon Bond mechanism (version IV, CB-IV) was used in the modeling done for this work. Chlorine chemistry was accounted for by adding to the CB-IV mechanism, using the reactions outlined by Tanaka et al. (5). Tanaka et al. (5) incorporated a 13-step mechanism for chlorine chemistry into the Carbon Bond IV chemical mechanism (11) in order to examine the regional impacts of Cl• chemistry in southeastern Texas. In this mechanism, chlorine radical is produced by photodissociation of Cl_2 and HOCl by visible and ultraviolet light. Atomic chlorine then reacts with ozone and hydrocarbons (RH). Under typical urban conditions, concentrations of hydrocarbons are sufficiently high so that the rate of reaction of atomic chlorine with RH is much faster than the rate of reaction with ozone (5). Hydrogen abstraction by the chlorine radical from hydrocarbons produces alkyl radicals and hydrogen chloride. The hydrocarbon radical then produces alkyl peroxy radicals, leading to ozone formation. Reaction of chlorine radical with olefinic species can result in chlorine addition, leading to the formation of unique molecular markers.

Modeling Scenarios. One base case (Cl2.Basecase), including chlorine emissions and chemistry, and five trading scenarios were used to examine the impacts of trading of HRVOCs with chlorine. The base case, with chlorine chemistry, included the NOx and VOC emission reductions used in the Houston-Galveston area to meet the National Ambient Air Quality Standard for ozone, with concentrations averaged over 1 h (base case attainment demonstration) (1). Note that the addition of chlorine emissions and chemical reactions resulted in different predictions of the magnitude and spatial distribution of ozone concentrations than the base case without chlorine chemistry reported in part 1 of this series (1). Figure 1a shows the difference in predicted 1-h averaged ozone concentrations between Cl2.Basecase and the Basecase without chlorine chemistry at 1400 on August 25, while Figure 1b shows the differences in predicted 8-h averaged ozone concentration, for the period beginning at 1000. Chlorine enhances ozone formation, and the difference in predicted maximum daily 1-h and 8-h averaged ozone concentration is as much as 8 ppb and 9 ppb, respectively. The maximum difference in ozone concentrations, due to adding the chlorine emissions and chemistry, occurs in the morning and, as shown in Figure 1c, is much larger (48 ppb for a 1-h averaged ozone concentration) than the difference in the daily maximum value. These differences due to chlorine chemistry differ very slightly from the results reported by Chang and Allen (3) due to small revisions to the point source VOC inventories used.

Five trading scenarios were examined. The first scenario examines intra-account trading (i.e., trading within the same account, where an account is generally the same as a regulated facility, as described in part 1 (1)). In this scenario, some of the required HRVOC reductions are offset by a 100% reduction of the MIR equivalent mass of chlorine emissions. The second through fifth scenarios represent inter-regional trading for which one trading region purchases HRVOC allowances in its region through reductions of 100% of the chlorine MIR equivalent mass from the other three trading regions.

Results and Discussion

Table 2 reports changes in the four air quality metrics, (a) daily maximum ozone, (b) area of exceedance, (c) integrated area of exceedance, and (d) population exposure, between the attainment demonstration and the various trading scenarios, averaged over all days of the episode. These air quality metrics are defined in part 1 (1). Table 2 indicates that, when all of the chlorine emissions are converted into HRVOC allocations, all trading scenarios lead to no change
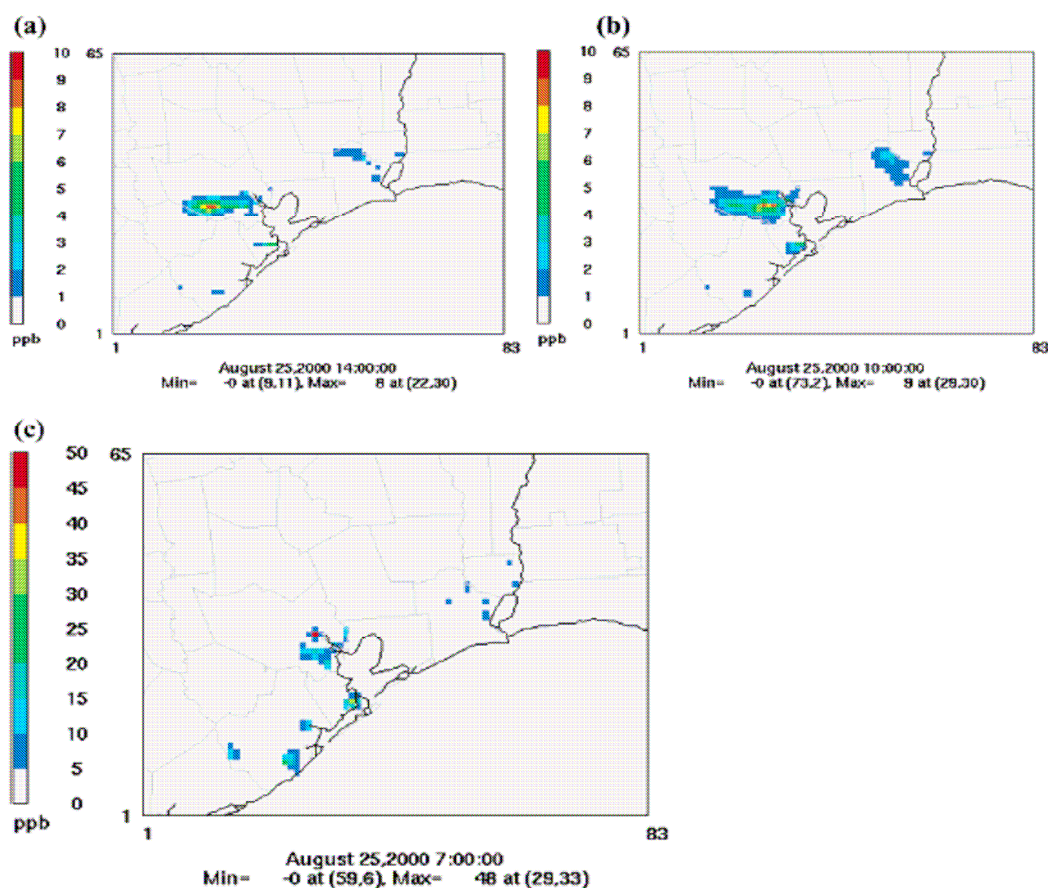
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FIGURE 1. Differences in predicted (a) 1-h and (b) 8-h averaged ozone concentrations between the base case with chlorine chemistry (Cl2.Basecase) and the base case without chlorine chemistry, at the times of day when the maximum ozone concentration occurs and (c) maximum difference in predicted 1-h average ozone concentration on August 25. Differences are expressed as $[O_3(Cl_2.Basecase) - O_3(base\ case\ without\ chlorine\ chemistry)]$. The complete model domain is described in part 1 of this series (1).

or improvements in the air quality metrics. Decreases in peak 1-h averaged and 8-h averaged ozone concentrations are up to 0.74 ppb (0.63%) and 0.56 ppb (0.61%), respectively. Decreases in the air quality metric based on population exposure (3.3% and 4.1% for 1-h and 8-h averaged concentrations) are, in general, larger than for the other metrics. For the maximum ozone concentration and area of exceedance metrics, these values are of the same magnitude as the results reported in part 1 of this series for inter-regional trading of HRVOCs. The changes in the time integrated area of exceedance metric and, to a lesser extent, the population based metric are larger for the chlorine trading than for the HRVOC trading, but the differences are still only a few percent.

Table 3 presents changes in another set of air quality metrics, relative reduction factors at Houston area monitors. These Relative Reduction Factors (RRFs) are defined as the ratio of the model predicted 8-h averaged ozone concentration in the trading case to the model predicted ozone concentration in the base case, in the area near an ambient monitor (1). RRFs are calculated for each day of the modeling episode and are averaged, for each monitor, over days when the model predicts 8-h averaged ozone concentrations greater than 85 near the monitor. Thus, a value of 1 for an RRF indicates, on average, no change in ozone concentrations

due to the emission trading. A value less than 1 indicates a decrease in ozone concentration associated with trading, and a value greater than 1 indicates an increase in ozone concentration. RRFs provide an indication of whether localized hot spots in ozone concentrations should be expected near monitors. The monitors for which RRFs are listed in Table 3 are distributed throughout the Houston area. The locations of the monitors are provided in the Supporting Information for part 1 of this series of papers (1).

The RRFs are consistent with the results reported in Table 2. The RRFs are almost exclusively less than or equal to 1, indicating a decrease in ozone concentrations associated with converting chlorine emissions to HRVOC emissions, based on the MIR reported by Carter (10). The few RRFs that are greater than 1 tend to be associated with the locations nearest the regions that the emissions are traded into.

A possible reason for the consistent improvements in air quality when chlorine emissions are traded for HRVOC emissions, based on MIR, is that the MIR value for chlorine under Houston conditions is underestimated. To test this hypothesis, changes in air quality metrics were evaluated under two scenarios. In the first scenario, all chlorine emissions were removed from the 25 accounts, and in the second scenario, all HRVOC emissions were removed from the 25 accounts. The ratio of the changes in air quality metrics,

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TABLE 2. Changes (Trading Case − Base Case) in Air Quality Metrics Based on 1-h and 8-h Averaged Ozone Concentrations, between Base Case and Cases Trading a 100% Reduction in Chlorine Emissions for an Equivalent MIR Weighted Mass of HRVOC Emissions[a]

	1-h averaged ozone concn			8-h averaged ozone concn		
	average SD		(diff./base case value) (%)	average SD		(diff./base case value) (%)
Maximum Daily Ozone (ppb)						
intra-account Cl_2 trading	−0.16 ± 0.51		−0.14	−0.33 ± 0.61		−0.37
inter-regional Cl_2 trading into region 1	−0.74 ± 0.73		−0.63	−0.56 ± 0.72		−0.61
inter-regional Cl_2 trading into region 2	−0.32 ± 0.62		−0.28	−0.40 ± 0.67		−0.44
inter-regional Cl_2 trading into region 3	−3.4E−02 ± 0.44E−01		−0.03	−0.34 ± 0.58		−0.37
inter-regional Cl_2 trading into region 4	−9.2E−02 ± 7.7E−01		−0.08	−0.38 ± 0.70		−0.42
Area of Exceedance (km²)						
intra-account Cl_2 trading	0.0 ± 5.8		0.00	−26 ± 38		−1.46
inter-regional Cl_2 trading into region 1	−8.0 ± 15		−1.99	−29 ± 36		−1.63
inter-regional Cl_2 trading into region 2	0.0 ± 8.3		0.00	−28 ± 36		−1.58
inter-regional Cl_2 trading into region 3	0.0 ± 10		0.00	−25 ± 44		−1.41
inter-regional Cl_2 trading into region 4	−2.0 ± 9.9		−0.50	−27 ± 45		−1.52
Integrated Area of Exceedance (km²)						
intra-account Cl_2 trading	−7.0 ± 26		−0.89	−1.3E+02 ± 1.6E+02		−2.27
inter-regional Cl_2 trading into region 1	−22 ± 35		−2.80	−1.8E+02 ± 1.8E+02		−2.99
inter-regional Cl_2 trading into region 2	−8.0 ± 23		−1.02	−1.4E+02 ± 1.5E+02		−2.36
inter-regional Cl_2 trading into region 3	−7.0 ± 30		−0.89	−1.3E+02 ± 1.6E+02		−2.21
inter-regional Cl_2 trading into region 4	−10 ± 33		−1.27	−1.3E+02 ± 1.6E+02		−2.29
Population Exposure (ppb*capita)						
intra-account Cl_2 trading	−8.5E+04 ± 3.3E+05		−0.74	−6.7E+05 ± 1.5E+06		−2.40
inter-regional Cl_2 trading into region 1	−3.8E+05 ± 1.4E+06		−3.30	−1.1E+06 ± 2.7E+06		−4.06
inter-regional Cl_2 trading into region 2	−8.2E+03 ± 3.4E+04		−0.07	−6.9E+05 ± 1.4E+06		−2.48
inter-regional Cl_2 trading into region 3	−9.4E+04 ± 3.8E+05		−0.81	−6.6E+05 ± 1.5E+06		−2.37
inter-regional Cl_2 trading into region 4	−2.2E+05 ± 8.9E+05		−1.90	−7.6E+05 ± 1.8E+06		−2.73

[a] Changes are also shown as percentage of the base case value.

TABLE 3. Average RRF Values for Each Trading Scenario at Each Monitor

	intra-account HRVOC/Cl_2 trading	inter-regional HRVOC/Cl_2 trading into region			
		1	2	3	4
Manvel	0.998	0.997	0.998	0.998	0.997
Jackson	1.000	1.000	1.000	1.000	1.000
Mustang	1.000	1.000	1.000	1.000	1.000
TC	0.999	0.997	0.997	0.999	1.001
Bayland	1.000	0.999	1.000	1.000	1.000
Aldine	1.000	0.986	0.987	0.987	0.987
Conroe	1.000	1.000	1.000	1.000	1.000
Seabrook	0.995	1.000	1.001	1.003	1.003
Lynchburg	0.988	0.981	0.984	0.986	0.985
Clinton	0.989	0.983	0.985	0.987	0.985
Galveston	1.000	1.000	1.000	1.000	1.000
Dancinger	1.000	1.000	1.000	1.000	1.000
Croquet	1.000	0.995	0.995	0.996	0.995
DeerPark	0.991	0.986	0.988	0.991	0.991
Channelview	0.986	0.980	0.983	0.985	0.983
Houston Manchester	0.992	0.986	0.988	0.990	0.989
Ellington Field	0.990	0.995	0.996	1.000	0.999
Haden Road	0.988	0.982	0.985	0.987	0.986
Port of Houston	0.991	0.981	0.983	0.985	0.983
Atascocita	1.000	0.995	0.997	0.997	0.997
Clear Lake High School	0.992	0.996	0.998	1.000	1.001
Sheldon Rd	0.986	0.975	0.980	0.980	0.977
LaPorte	0.986	0.984	0.986	0.988	0.989
Channelview North	0.989	0.976	0.983	0.979	0.978
Smith Point	0.996	0.979	0.981	0.981	0.981
E Baytown	0.994	0.983	0.985	0.986	0.984
Mont Belvieu	0.995	0.981	0.982	0.980	0.980

relative to the base case, for these two scenarios, can be used to evaluate the relative value of the incremental reactivities

TABLE 4. Interpollutant Trading Ratios for HRVOC and Chlorine, Averaged over the Modeling Episode

metrics	1-h averaged O_3 concn (ratio/0.45; see text)	8-h averaged O_3 concn (ratio/0.45; see text)
daily maximum ozone concn	0.58 ± 0.31 (1.3)	0.51 ± 0.41 (1.1)
area of exceedance	0.43 ± 0.48 (0.96)	0.33 ± 0.34 (0.73)
integrated area of exceedance	0.41 ± 0.48 (0.91)	0.38 ± 0.45 (0.84)
population exposure	0.39 ± 0.13 (0.87)	0.30 ± 0.26 (0.67)

of chlorine and HRVOCs, under Houston conditions. Specifically, the ratio

$$[\text{change in air quality metric due to eliminating HRVOCs}/\text{tons of HRVOC emissions reduced}]/[\text{change in air quality metric due to eliminating chlorine}/\text{tons of chlorine emissions reduced}]$$

was calculated for each of the air quality metrics. The results, averaged over the days of the modeling episode, are shown in Table 4.

The overall ratios listed in Table 4 can be compared to the ratio based on MIR. The ratio of the mass weighted MIR value for HRVOC emissions ($\sum MIR(i)*(massfraction)i(i)$, $i =$ HRVOC species) in the 25 accounts (10.67 g O_3/g VOC) to the MIR value of chlorine (23.78 g O_3/g chlorine) is 0.45. Thus, for ratios in Table 4 less than 0.45 (ratio/0.45 less than 1), more air quality improvement is expected from chlorine emission reductions than would be expected based on the MIR. This underestimate of the effectiveness of chlorine emission reductions, when using MIR to describe reactivity, accounts for the behavior of three of the air quality metrics

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(area of exceedance, time-integrated area of exceedance, and population exposure). The daily maximum ozone concentrations have a ratio higher than 0.45 because of anomalously high values on September 5 (1.30 for 1-h averaged concentration and 1.21 for 8-h averaged concentration). September 5th is unique relative to the other episode days in that ozone exceedances occur relatively early in the morning in locations close to the industrial source region, where chlorine reactivity has its greatest impact. This effect is not observed for the other air quality metrics because the impacts are restricted to a very small number of grid cells.

To summarize, the simulations presented in this work indicate that trading of chlorine emission reductions for HRVOC allowances at a single account or between facilities, in general resulting in improvements in air quality. Decreases in peak 1-h averaged and 8-h averaged ozone concentrations associated with trading chlorine emissions for HRVOC allocations on a Maximum Incremental Reactivity (MIR) basis were up to 0.74 ppb (0.63%) and 0.56 ppb (0.61%), respectively. Decreases in the air quality metrics based on population exposure decreased by 3.3% and 4.1% for 1-h and 8-h averaged concentrations. The simulations indicate that the inclusion of chlorine emissions in the trading program, using the MIR value of Carter (10), is likely to be beneficial to air quality and is unlikely to cause localized increases in ozone concentrations ("hot spots").

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