UNITED STATES ENVIRONMENTAL PROTECTION AGENCY
Office of Air Quality Planning and Standards (OAQPS)
Research Triangle Park, North Carolina 27711

MEMORANDUM

SUBJECT: Comparison of air quality modeling with ambient NO_2 monitor concentrations in Atlanta, Georgia

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TO: NO_2 NAAQS Review Docket (EPA-HQ-OAR-2006-0922)

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Introduction

This memorandum documents the progress on evaluating modeled air concentrations used for part of the review of the primary National Ambient Air Quality Standard (NAAQS) for nitrogen dioxide (NO_2). Modeled NO_2 air concentrations generated using EPA's preferred dispersion model (AERMOD) were used as input to EPA's exposure model (APEX) to estimate population exposure in Philadelphia County. The methodology and results of the Philadelphia County exposure assessment were documented in the Risk and Exposure Assessment to Support the Review of the NO_2 Primary National Ambient Air Quality Standard: First Draft (hereafter, 1st draft NO_2 REA) and was reviewed by the Clean Air Scientific Advisory Committed (CASAC) in May 2008. As part of that review, CASAC recommended that EPA improve the comparison performed between the modeled air quality and monitored concentrations. Additional comparison of the modeled versus measured air quality in Philadelphia County is provided in Appendix B of the Risk and Exposure Assessment to Support the Review of the NO_2 Primary National Ambient Air Quality Standard: Second Draft (hereafter, 2nd draft NO_2 REA), submitted in August 2008.

A second case-study was selected for the exposure assessment to be included in the 2nd draft NO_2 REA. Atlanta, Ga. was chosen based on the availability of health effects data associated with ambient concentrations, the availability of personal exposure data for use in evaluating the exposure model estimates, and the analysis of the air quality data (i.e., an exceedance of a 200 ppb potential health effect benchmark level and containing an annual average NO_2 concentration above the 90th percentile considering all monitors in operation from years 1995-2006). A four-county area was set for the model domain (Cobb, DeKalb, Fulton, and Gwinnet Counties) that comprise the urban center of the Atlanta Metropolitan Statistical Area (MSA). Hourly NO_2 concentrations were estimated for each of 3 years (2001-2003) at each of the defined receptor locations (i.e., census blocks and on-roads) using hourly NO_x emission estimates and dispersion modeling. Three principal emission source categories were modeled and included on-road mobile sources, stationary sources, and emissions from Atlanta Hartsfield International Airport.

Following recommendations by CASAC and included as part of the Atlanta case-study, an improvement was made in the characterization of the source emissions. In the earlier Philadelphia County assessment, only major roads were included in estimating the mobile source emissions, likely contributing to the degree of upward adjustment needed when comparing the modeled versus measured air quality concentrations (see Appendix B of the 2nd draft REA for

details). In estimating the air quality for the Atlanta model domain, both major and minor roadway emissions (in addition to the stationary source and airport emissions) were estimated for use in the dispersion model. Following the estimation of air concentrations at receptors surrounding the three available ambient monitors (including the ambient monitor receptor locations themselves), a detailed evaluation of the predicted NO_2 air quality concentrations was performed.

Initial comparison of modeled versus measured air quality in Atlanta

As an initial comparison of modeled versus measured air quality, all modeled receptors within 4 km of each ambient monitor location, excluding those receptors on roadways or within 100 m of a major roadway, were used to generate a prediction envelope.[1] This envelope was constructed based on selected percentiles from the modeled concentration distribution at each receptor for comparison to the ambient monitor concentration distribution. The 2.5th and 97.5th percentiles from all monitor distribution percentiles[2] were selected to create the lower and upper bounds of the envelope, while the 50th percentile concentrations were combined to create a distribution representing the central tendency. As an example, Figure 1 presents this envelope of modeled air quality at receptors surrounding each of the three Atlanta NO_2 monitors. While much of the ambient concentration distribution falls within the prediction envelope and tracks the 50th percentile concentrations well, the modeled values exceed the measured concentrations at the upper end of the distribution. This trend in overestimating peak measured concentrations was of concern since the upper level concentrations were those of most interest in the exposure analysis. The next section provides background information related to AERMOD model performance, and the following sections summarize the results of further evaluations that have been conducted thus far to determine factors that may be contributing to this apparent overestimation.

Background on AERMOD model performance

AERMOD was promulgated in 2006 as EPA's preferred dispersion model for estimating ambient pollutant concentrations to support regulatory air permitting under the New Source Review (NSR) and Prevention of Significant Deterioration (PSD) programs, as documented in EPA's *Guideline on Air Quality Models*, published as Appendix W to 40 CFR Part 51. AERMOD incorporates advanced state-of-the-science algorithms for simulating dispersion from emission sources for transport distances of up to 50 kilometers. The AERMOD model performance was evaluated by comparing modeled vs. measured concentrations from a total of 17 field study data bases. The focus of these model evaluations was on the performance of AERMOD relative to its role to support regulatory permitting involving demonstrations of compliance with National Ambient Air Quality Standards (NAAQS) and PSD increments. As a result of this focus, the primary metric of model performance was on AERMOD's ability to predict the peak of the observed concentration distribution, unpaired in time and space. Applications such as this study, involving comparisons of modeled concentrations at individual monitor locations, place an added burden on model performance paired in time and space beyond

[1] 500 m to 4 km is the area of representation of a neighborhood-scale monitor, according to EPA guidance.

[2] As an example, suppose there are 1000 receptors surrounding a monitor, each receptor containing 8,760 hourly values used to create a concentration distribution. As an example, a 73rd percentile concentration prediction is calculated for each receptor. Then, the lower bound of the 73rd percentile would represented by the 2.5th percentile of all the calculated 73rd percentile concentration predictions, i.e., the 25th highest 73rd percentile concentration prediction across the 1000 73rd percentile values from all of the receptors. Thus, at any given percentile along either of the envelope bounds as well as the central tendency distribution (the receptor 50th %ile) the concentration from a different receptor could be used.

the routine regulatory applications of the model. The performance of AERMOD under these more rigorous requirements has not yet been fully assessed.

While the number and range of field study data bases used in AERMOD's evaluation is large relative to other model evaluations, these field studies are dominated by elevated buoyant releases from power plant stacks. In most cases, emission rates are known with a high degree of accuracy, often based on continuous emission monitors (CEMs) for operational facilities or based on controlled emissions in the case of tracer releases. Model performance for mobile source emissions across an urban area is not well documented, and evaluating model performance for such applications is complicated by a number of challenges and uncertainties. These include uncertainties regarding the temporal and spatial distribution of emissions; physical characteristics of the emission sources (such as release height and initial dilution parameters); the representativeness of the meteorological data input to AERMOD, including the influence of surface characteristics (primarily surface roughness); the ability of the model to account for NO_x chemistry in the estimation of NO_2 concentrations; and urban boundary layer and terrain influences on dispersion.

Model Input Parameter Evaluation

The potential impacts of some of the more significant factors identified in the previous section are discussed below.

Emission Estimates

Apportionment of the estimated concentrations at the monitors indicated that mobile sources were dominant, contributing to over 90% of the NO_2 concentrations predicted at each of the monitors (Figure 2). Given the fundamental importance of emission estimates to model performance, the first parameter evaluated was the diurnal profile for the mobile sources emissions. A step-function diurnal profile was used in the initial modeling to reflect the four time periods for which the travel demand modeling data specifies traffic counts since no information was provided from the regional planning agency about temporal variation within the four time periods. When a diurnal profile of the predicted concentrations was constructed (not shown) it became evident that, while an increase was expected during periods of increased traffic (morning and afternoon rush hour), the large concentration increases and decreases at certain hours were a direct result of the form of the step-function. Based on comparison with the diurnal profile of the measured concentrations, it was decided that smoothing the on-road emissions temporal profile by using a 5-hour moving average might provide a more realistic temporal distribution of emissions. While some hours of the day remained unchanged and others had small increases (about 5 to 10%) in estimated concentrations following adjustment of the mobile source emission profile, the peak concentrations for periods when predicted concentrations were well above the ambient monitor concentrations were reduced by up to a factor of two, improving the comparison of modeled versus measured concentrations.

The diurnal pattern of ambient monitored and modeled concentrations considering the adjusted emission temporal profile is presented in Figure 3 at each of the three Atlanta ambient monitor locations. These plots show generally good agreement between the modeled monitor and measured concentrations during the midday and overnight hours, with the overprediction occurring primarily during the early morning and late afternoon rush hour periods.

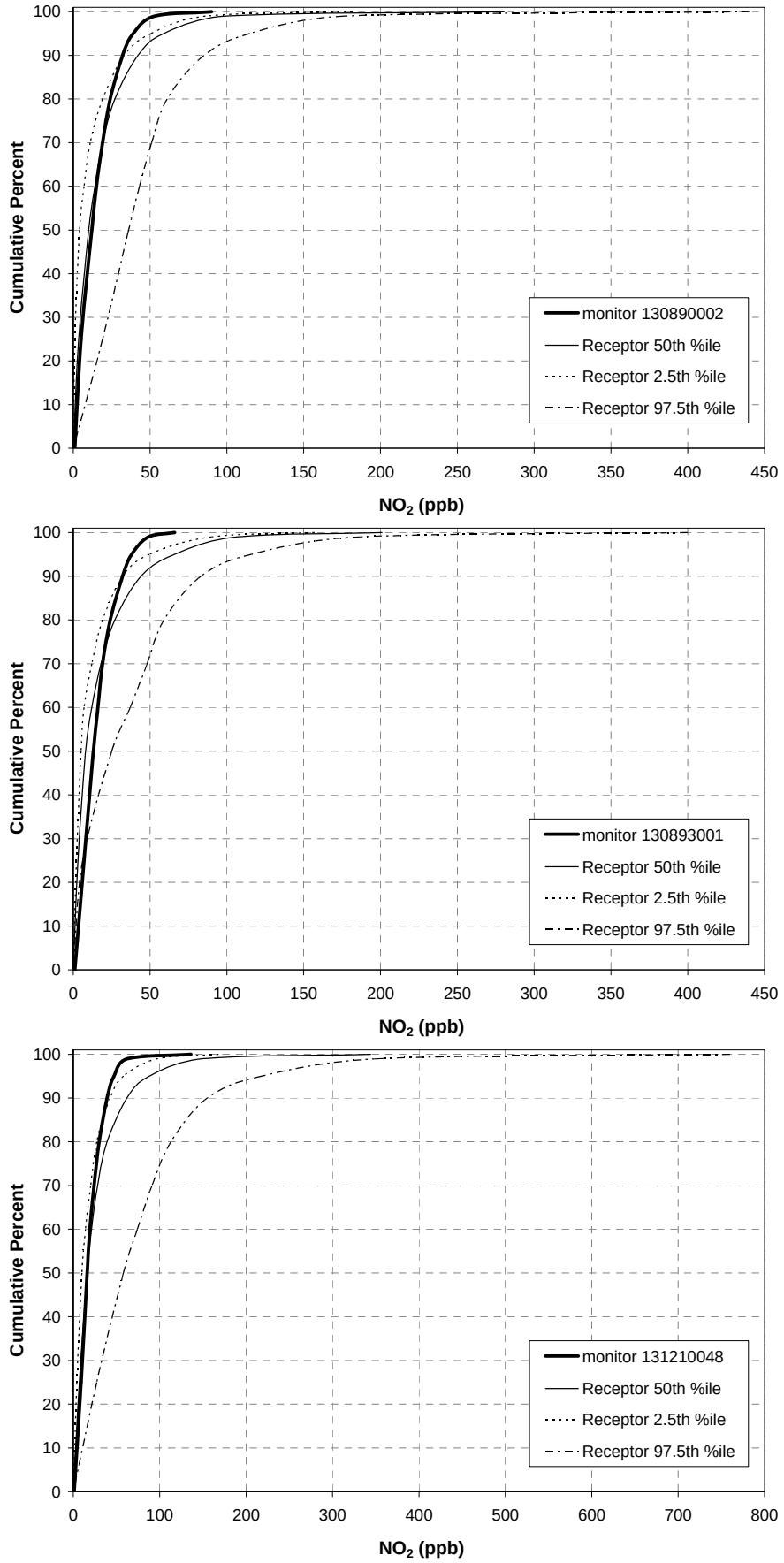
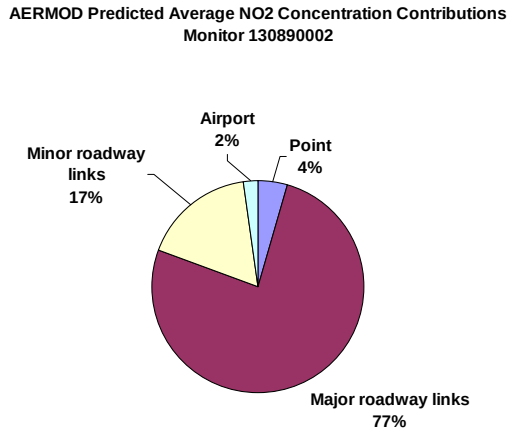
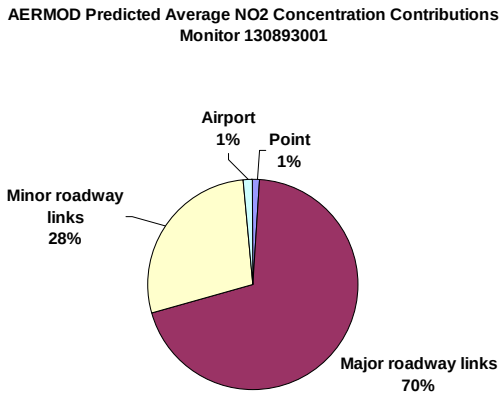


Figure 1. Comparison of measured and modeled receptor NO_2 concentration distributions within 4 km at three ambient monitor locations in Atlanta for Year 2002.





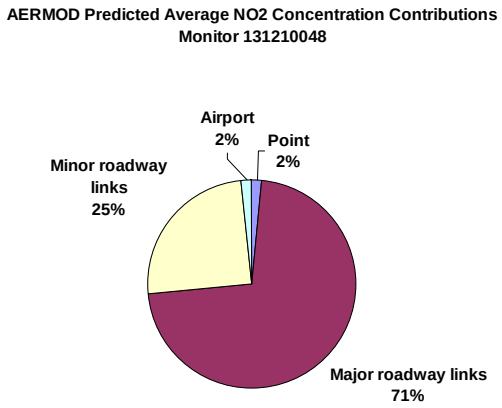


Figure 2. Estimated NO_2 concentration contributions from four emission sources to each of three monitoring locations in Atlanta for Year 2002.

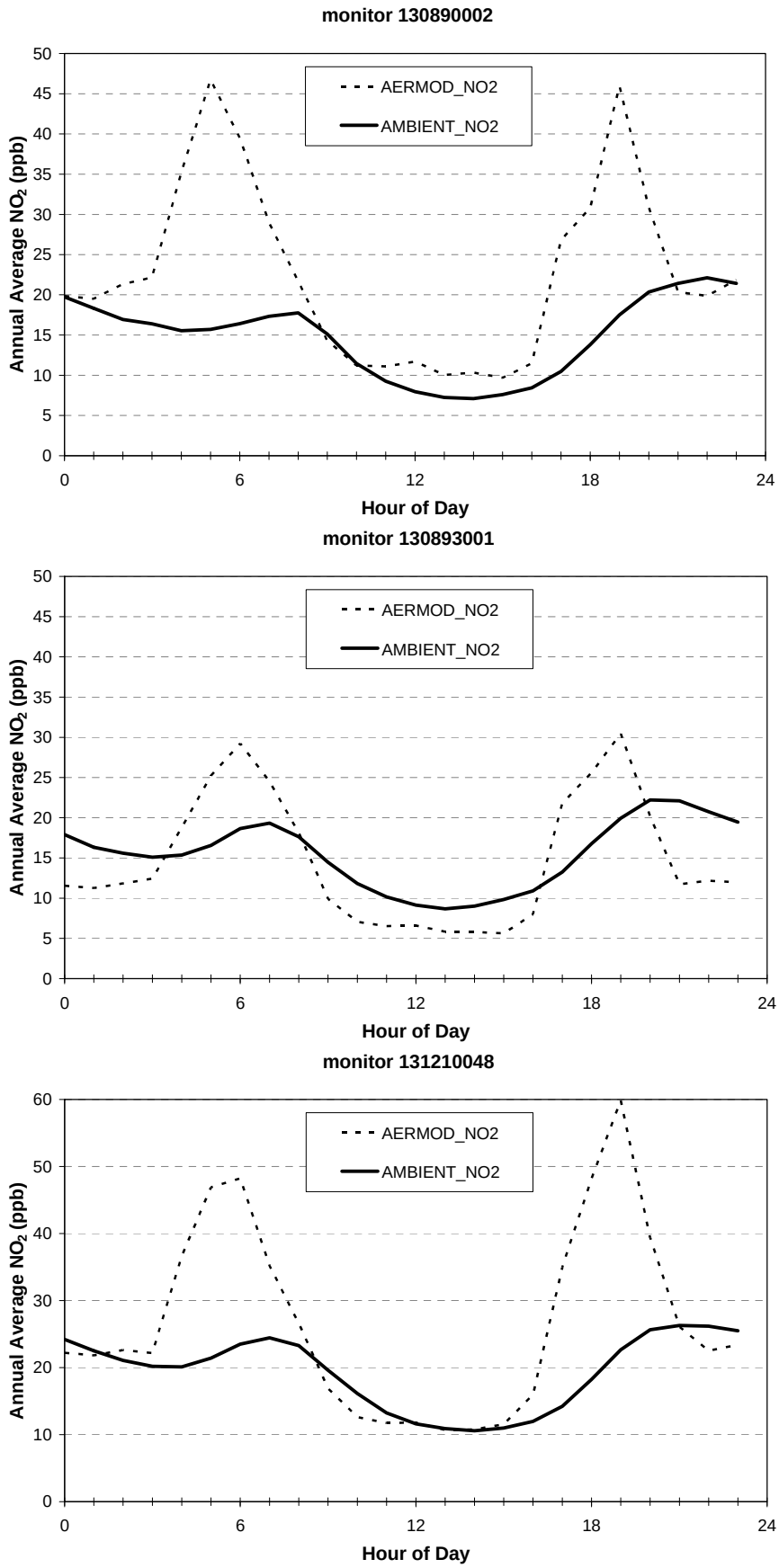


Figure 3. Comparison of measured and modeled receptor NO_2 diurnal concentration profiles at three Atlanta ambient monitors for Year 2002.

Source Characteristics

Unlike stationary stack emissions, which have well-defined source characteristics including stack height, stack diameter, and effluent temperature and velocity, determining appropriate source characteristics for mobile source emission involves additional uncertainties due to the fact that the emission "points", i.e., vehicle exhausts, are in motion to varying degrees, and vehicles vary significantly in terms of their aerodynamic influence on the atmosphere through which they move. The mobile source emissions have been spatially allocated to roadways using a link-based approach. Each road link is simulated as an elongated area source, with the area source width based on the width of the roadway. The other two characteristics of importance to modeling mobile source emissions in AERMOD are the effective release height and the initial vertical dilution of the plume associated with the vehicle wake. The approach proposed for this study is to specify emission-weighted averages of release height and initial dilution for each road link based on the emission mix of light duty and heavy duty vehicles. Release heights for light duty vehicles may be underestimated in the preliminary modeling, and initial dilution may also be underestimated for both vehicle categories.

Meteorological Data Representativeness

The representativeness of meteorological data is another key consideration for any dispersion modeling application. The meteorological data used for this study were based on National Weather Service (NWS) observations from the Atlanta airport, processed for input to AERMOD through the AERMET meteorological processor. One of the advances of the AERMOD model relative to its predecessor, ISCST3, is its ability to account for the influence of surface characteristics on dispersion. Of the three surface characteristics needed for input to AERMET, albedo, Bowen ratio, and surface roughness, the surface roughness is likely to have the most important impact for low level releases which are dominant in this study. Surface roughness pertains to the presence of buildings, trees, and other irregular land topography that is associated with its efficiency as a momentum sink for turbulent air flow, due to the generation of drag forces and increased vertical wind shear. It has been shown that increased surface roughness can affect the model predictions in several ways. The most important effect is the increase in mechanical turbulence, leading to greater vertical dispersion. For ground level emission releases (of which the mobile source emissions modeled here are) this increased vertical dispersion would result in lower ground level concentrations, all other factors being equal. As an example, Figure 4 presents the results of a sensitivity analysis illustrating the effect (from Brode, et al., 2008). As shown, doubling the surface roughness for a ground-level (0 meter) release in a rural setting resulted in about a 30% to 40% lower AERMOD annual average concentration prediction. The sensitivity to surface roughness was slightly less for an urban setting, which showed about a 20% to 30% lower annual average concentration.

EPA currently recommends processing meteorological data for input to AERMOD using the surface roughness derived from land cover data within about 1 kilometer of the meteorological tower (EPA, 2008), so that the meteorological data inputs are consistent with the physical conditions associated with them. EPA has also developed a tool called AERSURFACE that can be used to determine surface characteristics based on the USGS National Land Cover Data (NLCD). For the Atlanta airport, the average surface roughness is about 0.1 meters, which is typical of the generally open exposure found at most airport meteorological tower locations. However, the surface roughness is likely to be much higher around the emission sources in most cases for this study, due to the presence of buildings, trees, and other obstructions that typify an urban setting. A typical value of surface roughness associated with urban land cover is about 1

meter. Based on the sensitivity study cited above, a factor of 10 increase in surface roughness could result in about a factor of 2 decrease in annual average concentrations for ground-level releases. However, the increase in surface roughness would also tend to result in lower wind speeds, which would tend to offset some of the reduction due to increased turbulence.

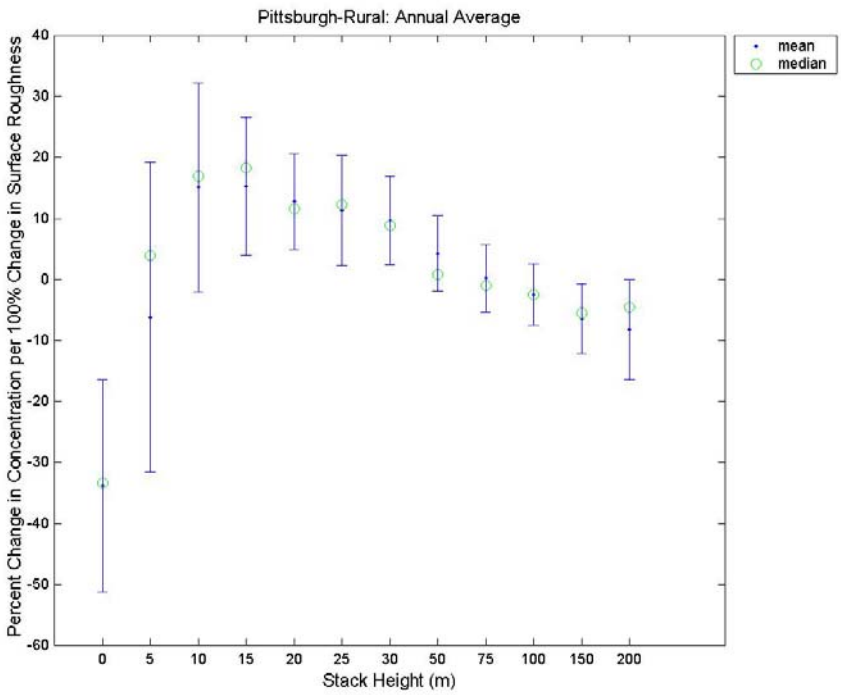


Figure 4. Sensitivity of AERMOD concentration predictions to surface roughness by stack height for non-buoyant releases (from Brode, et al., 2008).

While the NWS meteorological data are often the most readily available data source for dispersion modeling, alternative sources of meteorological data may be more representative for some applications. One such alternative data source that is currently being investigated is the SouthEastern Aerosol Research and Characterization Study experiment (SEARCH), which includes a meteorological monitoring station located on Jefferson Street in Atlanta, about 2 kilometers from one of the NO2 monitors. The surface characteristics around the SEARCH site appear to be more representative of typical emission source within the urban environment.

<u>NO_x Chemistry</u>

The AERMOD model regulatory options are designed primarily for simulating dispersion of inert pollutants, whereas NO_x emissions from most sources are primarily in the form of NO, rather than NO_2. While AERMOD does include two non-regulatory options for simulating NOx chemistry, the Ozone Limiting Method (OLM) (EPA, 2006) and the Plume Volume Molar Ratio Method (PVMRM) (Hanrahan, 1999a and b), these options have been developed and evaluated primarily for modeling stack emissions in rural settings. Application of OLM and/or PVMRM for mobile sources in an urban setting involves significant uncertainties.

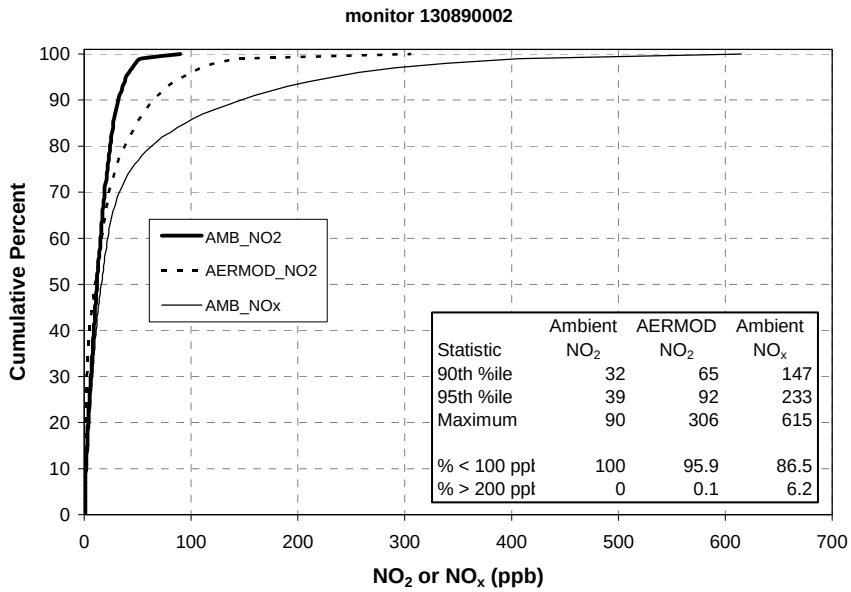
One indication of the potential significance of NO_x chemistry to these AERMOD model results for Atlanta is provided in Figure 5, which shows the cumulative distribution of concentrations of monitored NO_2 and NO_x at each of the three monitors, and AERMOD modeled concentrations of NO_2 at the monitor locations. While the AERMOD concentrations clearly

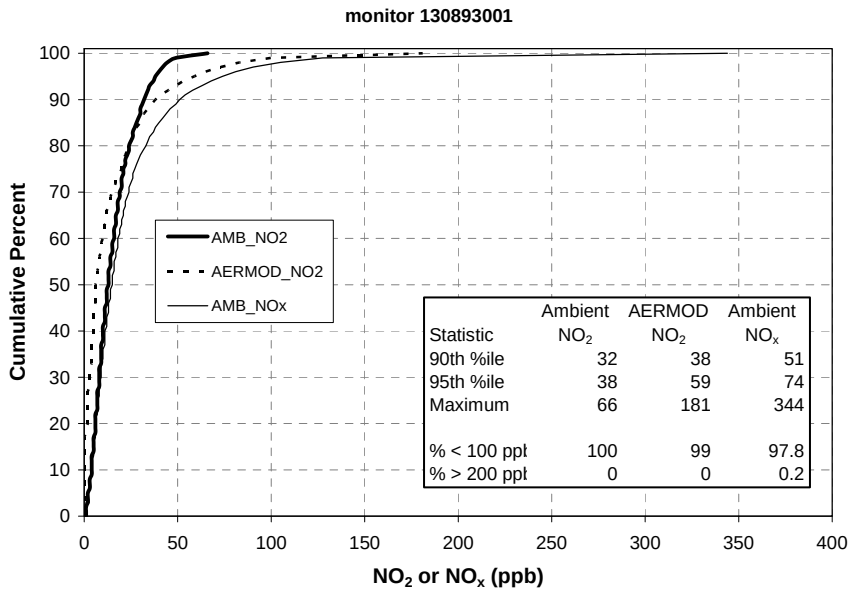
overestimate the monitored values of NO_2, there is better agreement with the monitored values of NO_x. This may be an indication that conversion of NO_x to NO_2 is being limited to a degree that is not properly accounted for by the AERMOD model options.

The preliminary modeling was based on applying the OLM option for each individual source, which means that all of the ambient ozone is available for conversion of NO to NO_2 for each plume. AERMOD also allows for merging plumes from nearby sources under the OLM option, which should introduce some ozone-limiting effects that would be more realistic of the emission distributions within an urban environment. The greatest potential reduction from this approach should occur for hours associated with the highest concentrations, especially during the early morning and late afternoon rush hour periods when ozone concentrations are likely to be relatively low.

Summary

Based on the assessments described above, a number of factors have been identified which could be contributing to an apparent overestimation of peak NO_2 concentrations for the Atlanta study. Many of these factors can be addressed through updates to the preliminary modeling analysis, which we expect would result in reasonable agreement between modeled and monitored NO_2 concentrations based on the few ambient monitors available within the Atlanta area. In summary, we feel that with these improvements to the model inputs, and given our current understanding of model performance, that the updated AERMOD modeling results should provide adequate estimates of hourly air concentrations for input to the risk and exposure assessment to support the review of the NO_2 primary NAAQS.





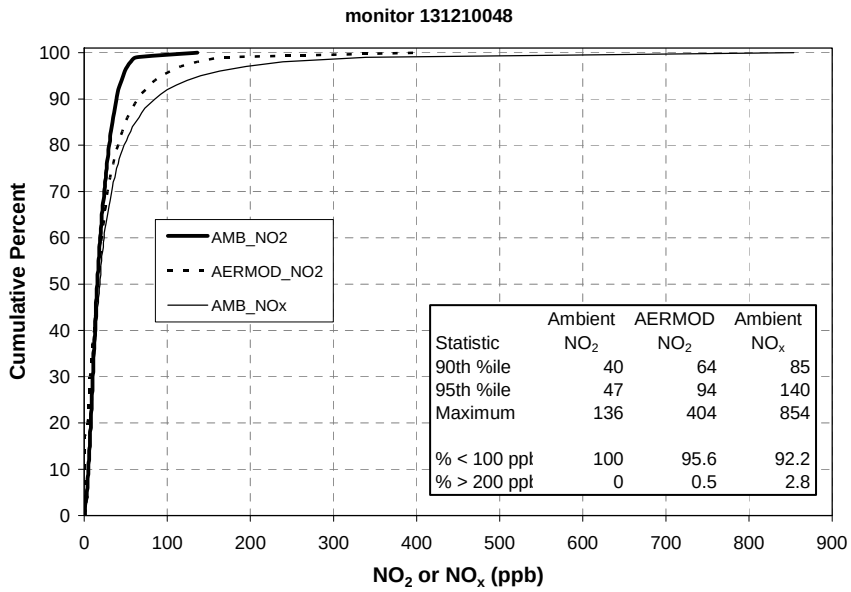


Figure 5. Cumulative concentration distributions of measured NO_2, measured NO_x, and modeled NO_2 at the three ambient monitor locations in Atlanta for Year 2002.

References

Brode, R., K. Wesson, J. Thurman, and C. Tillerson, 2008. AERMOD Sensitivity to the Choice of Surface Characteristics, Paper #811, Presented at the Air & Waste Management Association Annual Conference, Portland, OR, June 24, 2008.

EPA, 2006. User's Guide for the AMS/EPA Regulatory Model – AERMOD (EPA-454/B-03-001, September 2004), Addendum. U.S. Environmental Protection Agency, Research Triangle Park, North Carolina 27711.

EPA, 2008. AERMOD Implementation Guide. http://epa.gov/scram001/dispersion_prefrec.htm#aermod, U.S. Environmental Protection Agency, Research Triangle Park, North Carolina 27711.

Hanrahan, P.L., 1999a. "The plume volume molar ratio method for determining NO_2/NO_x ratios in modeling. Part I: Methodology," *J. Air & Waste Manage. Assoc.*, **49**, 1324-1331.

Hanrahan, P.L., 1999b. "The plume volume molar ratio method for determining NO_2/NO_x ratios in modeling. Part II: Evaluation Studies," *J. Air & Waste Manage. Assoc.*, **49**, 1332-1338.