2005 – 2009 Monitored Ozone Data
Comparison of Model Predictions

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Background

The 1-hour nitrogen dioxide (NO_2) National Ambient Air Quality Standard (NAAQS) became effective on April 12, 2010. Compliance with the 1-hour NO_2 NAAQS is based on the multiyear average of the 98th-percentile of the annual distribution of daily maximum 1-hour values not exceeding 100 ppb. The highest 8th high (H8H) of the daily maximum 1-hour values across a year is an unbiased surrogate for the 98th-percentile.

The EPA provides a tiered approach for the conversion of NO to NO_2. Tier 1 assumes a full conversion of NO to NO_2. Tier 2, the Ambient Ratio Method (ARM), applies a national default ratio of 0.75 to the Tier 1 result; however, the EPA recommends the use of 0.80 as a default ambient ratio for the 1-hour NO_2 standard. Tier 3 employs detailed screening methods on a case-by-case basis such as the Ozone Limiting Method (OLM) or the Plume Volume Molar Ratio Method (PVMRM). These methods are non-regulatory default options within the AERMOD dispersion model. The two key model inputs for both the OLM and PVMRM options in the context of the 1-hour NO_2 standard is the in-stack ratio of NO_2/NO, emissions and background ozone concentrations. This report focuses on the latter of these key inputs, the background ozone concentrations as collected from ozone monitors throughout the state of Iowa.

Analysis

The latest version of AERMOD available at the time of this study (12060) was used to conduct a sensitivity analysis using monitored ozone data from twelve ozone monitors throughout the state of Iowa. The goal of this analysis was to determine the expected change in model result due to the change in ozone monitor location, and the change associated with hourly background data files and a single background concentration. This document summarizes the results from this sensitivity analysis.

A series of point sources were modeled with varying release heights between zero and 65 meters above ground, spaced every 15 meters. Two types of each source were modeled at each release height, one with more plume dispersion, and one with less. The sources with less plume dispersion were modeled with an ambient exhaust temperature and horizontally-oriented release, whereas the sources with more plume dispersion were modeled with a buoyant exhaust temperature and vertically-oriented release. This variety of sources were modeled for the 1-hour averaging period using each of the 19 preprocessed 2005-2009 meteorological data sets throughout the state of Iowa. The sources were modeled at the H8H to represent the 98th percentile as described above as well as at the highest 1st high (H1H).

The variety of sources listed above and the meteorological data sets were modeled in conjunction with monitored ozone concentrations from 12 sites throughout the state. Three of the 12 sites; Cedar Rapids, Des Moines, and Pisgah, represent data from two different monitors. Cedar Rapids and Pisgah employ data from one of the two monitors for the first four years, 2005-2008. For 2009, a second monitor was added in the respective region and the data from that monitor is used only at hours in which the data from the first monitor is missing. For the Des Moines site, one monitor is applied for the first two years, 2005 & 2006, upon which it was then decommissioned, and data from a second newly located monitor is used for 2007-2009. The monitored ozone concentrations were modeled in three different forms: filled, unfilled, and as a single background concentration for both OLM and PVMRM. The monitored data used in the modeling analysis coincides with the years represented by the meteorological data, 2005-2009.

- The filled ozone background files employ data from the Moline, IL ozone monitor, a year-round monitor. The data from the Moline monitor is used to fill missing ozone concentration data during the non-ozone months (November through March). Moline was solely used to fill non-ozone season data at all ozone monitors throughout Iowa as it is the closest monitor with available year-round data. Random missing 1-hour gaps within
the ozone months (April through October) were filled based on the average of the data before and after the missing hour. Missing 2-hour gaps were filled via linear interpolation and longer gaps were filled using the maximum 1-hour concentration from that site by hour of day and month.

- The unfilled ozone background files represent the data collected at each monitor without the filling of data from the Moline monitor for the non-ozone months. The unfilled files also exclude the filling of random missing days within the ozone months by the methods described above. A default value of “999” is applied to the hours in which there is no recorded data. Values of ozone concentrations that are less than zero or greater than or equal to 900 are regarded as missing by AERMOD. Full conversion of NO entrained by the plume to NO₂ through the availability of ambient ozone is assumed by the model for hours with missing ozone data.

- The single background concentration reflects one default value for the entire year based on the maximum 1-hour average of the ozone data collected for each monitoring site. The single concentration (ppb) modeled for each monitor is as follows:
  
  - Cedar Rapids (CR) – 88
  - Clinton (CL) – 97
  - Coggon (CO) – 96
  - Des Moines (DM) – 83
  - Emmetsburg (EM) – 80
  - Lake Aquabi (LA) – 84
  - Lake Sugema (LS) – 90
  - Pisgah (PI) – 95
  - Scott County Park (SC) – 93
  - Slater (SL) – 91
  - Viking Lake (VL) – 86
  - Waverly (WA) – 90

The OLM and PVMRM modules also require the input of an in-stack ratio and an equilibrium ratio. The in-stack ratio is the percentage of the stack gases that are already in the form of NO₂ before the gas leaves the stack. This ratio can vary from 0.1 to 1.0 but the current EPA default value of 0.5 was used in this analysis. As mentioned previously, the ARM uses a default equilibrium ratio of 75% (annual) and 80% (1-hour). The default 90% equilibrium ratio has been established by the EPA in AERMOD as the default ratio for both PVMRM and OLM. The equilibrium ratio as applied in AERMOD essentially sets a cap of no more than 90% conversion of NO to NO₂ for those hours that would typically see 100% or full conversion.

A few key observations were noted in the review of the results. Those observations entailed the affect of the data from the different ozone monitors on the results, and the differences between the filled, non-filled, and single ozone background values.

**Ozone Monitor Affect**

The sensitivity analysis included twelve ozone monitors from throughout the state of Iowa. Data from 2005 through 2009 was incorporated into the model for use with the Tier 3 ambient ratio methods of OLM and PVMRM. As shown in Figure 1, there is significant variability in the predicted concentrations between the 19 meteorological stations, however the difference in ozone monitor location has little variability in the modeling results. This chart reflects the average of all maximum concentrations from the combined H1H and H8H results for both OLM and PVMRM, at all stack heights, and in buoyant and non-buoyant releases.
Figure 1. Comparison of Average Maximum 1-Hour Modeled NO2 Concentrations at Each Ozone Monitor

Based on the results presented above, performing a comparison of monitored concentrations determines the similarities between the data recorded at each of the ozone monitors throughout the state. Figure 2 shows this comparison for the filled 1-hour ozone data recorded from 2005-2009.

Figure 2. Comparison of Observed Ozone Data at Each Monitor Location
The limited variability in the modeled concentrations between each of the monitors (Figure 1) indicates that the range of monitored ozone concentrations recorded across the state during the time period analyzed (Figure 2) is not significant.

**Background Ozone Data File Differences**

AERMOD allows for various choices in incorporating ozone data into the model when using OLM and PVMRM. The model can read in hourly ozone data files and add a fill value to missing data if selected. The model can also use a single user specified value for all hours included in the modeling analysis. This analysis looked at using the monitored hourly ozone data files with both missing data filled in and as originally recorded (non-filled), as well as applying a single user-specified background concentration. As shown in Figure 3, the non-filled data yields significantly higher concentrations than the filled data and single concentration data. Additionally, the filled data results, though similar in magnitude to the single concentration data with respect to the non-filled data results, had consistently lower modeled concentrations than the data using a single ozone value.

**Figure 3. Average Modeled NO\textsubscript{2} Concentrations by Ozone Monitor and Data Type**

![Diagram showing modeled NO\textsubscript{2} concentrations by ozone monitor and data type.]

The substantial difference in non-filled data versus filled and single value data predicted concentrations might result from the model assuming full conversion of NO to NO\textsubscript{2} for the hours with missing ozone data. There is also very little difference in this trend when looking at the results for each of the stack heights modeled individually as well as for the buoyant and non-buoyant discharge styles. Additionally, substituting the single concentration value as the backup for missing hourly data is assumed to result in concentrations somewhere between the “single” and “filled” results shown above. This could be considered as another less conservative option for filling missing data hours instead of allowing the model to assume 100% conversion during these times.
Conclusions

The results of the ozone sensitivity analysis revealed little variability in predicted NO$_2$ concentrations between the 12 ozone-monitoring sites in the state of Iowa. There is greater variability between the various meteorological datasets used in conjunction with the monitoring data. The results also revealed that the data as originally recorded by the ozone monitor (non-filled) had predicted NO$_2$ concentrations considerably higher than the year-round (filled) and single ozone value scenarios.

Given these results, it would be better to use filled ozone monitor data or a single background ozone concentration in lieu of data that only covers the ozone season to deter overly conservative predicted NO$_2$ concentrations. In addition, the similarity in results across the 12 monitoring sites supports the creation of a single statewide ozone background file for use across the entire state (Appendix A).
Appendix A

The results of the ozone sensitivity analysis demonstrated little variability in the model predicted concentrations for each of the 12 monitoring sites. Based on these results as shown in Figure 1 of the above document, a combined statewide ozone background file was created. The following presents the steps and assumptions made in preparing the combined ozone data file.

- The raw monitored data is used for each of the twelve Iowa monitoring sites and the year-round Moline, IL monitor.
- For the Cedar Rapids, Des Moines, and Pisgah sites, the combined raw monitoring data is utilized.
- Missing data was not filled in prior to the averaging of the monitored values since there were no individual hours in which all monitors were missing data. Therefore, the process of averaging the monitor values results in a complete five year set of hourly ozone data with no missing hours.
- An average of all 12 monitors and the Moline monitor was determined for each hour of the five-year data set, 2005-2009.

Below are figures showing the comparison of the combined statewide ozone background with the individual ozone background results for the filled ozone data set. The results reflect a filled ozone data set for 2005-2009, and the average modeled concentrations for both PVMRM and OLM, H1H and H8H, all 5 stack heights and buoyant and non-buoyant point sources. Results further justify the creation of a combined statewide ozone background file.

Model Predicted 1-hour NO₂ Concentrations – Combined vs. Individual Filled Monitor Data

*Combined monitor data represented by blue dashed line, individual monitor data represented by solid graduated red lines