



UNITED STATES ENVIRONMENTAL PROTECTION AGENCY  
RESEARCH TRIANGLE PARK, NC 27711

SEP 30 2014

OFFICE OF  
AIR QUALITY PLANNING  
AND STANDARDS

**MEMORANDUM**

SUBJECT: Clarification on the Use of AERMOD Dispersion Modeling for Demonstrating Compliance with the NO<sub>2</sub> National Ambient Air Quality Standard

FROM: R. Chris Owen and Roger Brode *R. Chris Owen*  
Air Quality Modeling Group, C439-01 *Roger Brode*

TO: Regional Dispersion Modeling Contacts

**1. Introduction**

On January 22, 2010, the U.S. Environmental Protection Agency (EPA) announced a new 1-hour nitrogen dioxide (NO<sub>2</sub>) National Ambient Air Quality Standard (1-hour NO<sub>2</sub> NAAQS or 1-hour NO<sub>2</sub> standard). The new standard specifies attainment at a monitor when the 3-year average of the 98th-percentile of the annual distribution of daily maximum 1-hour concentrations is less than or equal to 100 ppb. The final rule for the new 1-hour NO<sub>2</sub> NAAQS was published in the Federal Register on February 9, 2010 (75 FR 6474-6537), and the standard became effective on April 2, 2010 (EPA, 2010a).

This memorandum clarifies the applicability of current guidance in the *Guideline on Air Quality Models* (40 CFR Part 51, Appendix W, generally referred to simply as Appendix W, U.S. EPA, 2005) for modeling NO<sub>2</sub> impacts in accordance with the Prevention of Significant Deterioration (PSD) permit requirements to demonstrate compliance with the new 1-hour NO<sub>2</sub> standard and the existing annual standard. The guidance provided here supplements the June 28, 2010 (U.S. EPA, 2010b) and March 1, 2011 (U.S. EPA, 2011) guidance memorandums by providing further clarification and guidance on the application of Appendix W for the 1-hour NO<sub>2</sub> standard. The topics clarified in this memorandum include:

- Tier 2 methods - The status of the Ambient Ratio Method (ARM) and Ambient Ratio Method 2 (ARM2) Tier 2 modeling approaches for demonstrating NAAQS compliance under the PSD program.

- $\text{NO}_2/\text{NO}_x$  in-stack ratio – The selection and application of the  $\text{NO}_2/\text{NO}_x$  in-stack ratio for use in Tier 3  $\text{NO}_2$  modeling applications.
- Tier 3 methods - The appropriate applications for the Ozone Limiting Method (OLM) and Plume Volume Molar Ratio Method (PVMRM) Tier 3  $\text{NO}_2$  modeling schemes.
- Background sources – The treatment of background sources and monitoring data in compliance demonstrations.

## 2. Summary of Current Guidance

Though the NAAQS is based on  $\text{NO}_2$  concentrations, the majority of nitrogen oxides ( $\text{NO}_x$ ) emissions are in the form of nitric oxide (NO) rather than  $\text{NO}_2$ . As noted in Section 5.1.j of the Appendix W, the resultant  $\text{NO}_2$  concentrations are largely driven by the ambient chemical environment (i.e., the reaction of NO with ambient ozone to form  $\text{NO}_2$ ) and the initial  $\text{NO}_2/\text{NO}_x$  ratio of the emissions (i.e., the in-stack ratio or ISR). As a result, Section 5.2.4 of Appendix W outlines a three tiered approach to estimating modeled  $\text{NO}_2$  concentrations. We note that these sections of Appendix W were written when there was only an annual  $\text{NO}_2$  standard, which necessitated U.S. EPA, 2010b and U.S. EPA, 2011 to clarify their application in the context of the new 1-hour standard. The current recommended tiered methods are:

- Tier 1 – assume full conversion of NO to  $\text{NO}_2$ , where total  $\text{NO}_x$  concentrations are computed with a refined modeling technique specified in Section 4.2.2 of Appendix W.
- Tier 2 – multiply Tier 1 results by empirically derived  $\text{NO}_2/\text{NO}_x$  ratios, with 0.75 as the national default ratio for annual  $\text{NO}_2$  (Chu and Meyer, 1991) and 0.80 as the national default ratio for hourly  $\text{NO}_2$  (Want, et al, 2011; Janssen, et al, 1991), as recommended in U.S. EPA, 2011.
- Tier 3 – detailed screening methods may be used on a case-by-cases basis. At this time, OLM (Cole and Summerhays, 1979) and the PVMRM (Hanrahan, 1999) are considered to be appropriate as detailed screening techniques.

As for EPA preferred models for  $\text{NO}_2$  modeling, AERMOD is specified as the preferred model for regulatory applications in Section 4.2.2 of Appendix W. It should also be noted that all three tiers of  $\text{NO}_2$  modeling are classified as screening techniques, and as such, negative emission rates should not be used to account for emission reductions when conducting dispersion modeling to determine net ambient impacts associated with emission changes for comparison to SILs, for NAAQS compliance demonstrations, nor for annual increment analysis. Questions regarding the application of the tiered approach for  $\text{NO}_2$  modeling for any specific permit action should be addressed to the appropriate permitting authority and EPA Regional Office modeling staff.

### **3. Tier 2 Methods**

#### **3.1 ARM**

The Tier 2 Ambient Ratio Method (ARM) applies a national default NO<sub>2</sub>/NO<sub>x</sub> ratio of 0.75 for the calculation of the annual standard and, as specified in U.S. EPA, 2011, 0.80 for the calculation of the hourly standard. Additionally, regional NO<sub>2</sub>/NO<sub>x</sub> ratios representative of area wide quasi-equilibrium conditions may be applied as default ratios under Tier 2, provided that the ambient data meets the guidelines specified in Sections 5.2.4.c and 5.2.4.d of Appendix W. The ratios should be applied only to the modeled concentrations, and the monitored NO<sub>2</sub> background levels should be added to the modeled concentrations to compute the design value. Prior to AERMOD version 13350, the application of the ARM method required the user to post-process the model data and monitored background to compute the design value. However, the ARM method has been incorporated into the AERMOD model code (version 13350 and later), such that monitored background data and ARM adjusted modeled NO<sub>2</sub> are combined within the model in order to eliminate the need for post-processing to compute the annual and hourly modeled design values. These options are invoked through the CO MODELOPT ARM and the CO ARMRATIO keywords and requires that BACKGRND is included in the SRCGROUP ALL specification. More details about these options can be found in the AERMOD User's Guide Addendum (U.S. EPA, 2014).

#### **3.2 ARM2**

AERMOD version 13350 introduced a new Tier 2 method, the Ambient Ratio Method 2 (ARM2), which is based on an evaluation of the ratios of NO<sub>2</sub>/NO<sub>x</sub> from the EPA's Air Quality System (AQS) record of ambient air quality data. The ARM2 development report (API, 2013) specifies that ARM2 was developed by binning all the AQS data into bins of 10 ppb increments for NO<sub>x</sub> values less than 200 ppb and into bins of 20 ppb for NO<sub>x</sub> in the range of 200-600 ppb. From each bin, the 98<sup>th</sup> percentile NO<sub>2</sub>/NO<sub>x</sub> ratio was determined and finally, a sixth-order polynomial regression was generated based on the 98<sup>th</sup> percentile ratios from each bin to obtain the ARM2 equation, which is used to compute a NO<sub>2</sub>/NO<sub>x</sub> ratio based on the total NO<sub>x</sub> levels. The ARM2 report presents three basic evaluations: (1) an overview of the temporal and spatial trends in the NO<sub>2</sub>/NO<sub>x</sub> ratio data, (2) a model intercomparison based on three field studies, and (3) model sensitivity tests based on hypothetical case studies, all of which are briefly summarized below.

##### **3.2.1 Spatial and Temporal Variation**

While the ARM2 development is based on the 98<sup>th</sup> percentile of binned NO<sub>2</sub>/NO<sub>x</sub> ratios from the nation-wide AQS data from 2001-2010, the ARM2 development report compares these ratios to

equivalent ratios based on regional and temporal subsets of the data. In most cases, the regional 98<sup>th</sup> percentile NO<sub>2</sub>/NO<sub>x</sub> ratio was more conservative than the one based on the nation-wide ratios. The most significant deviation from this occurred in the Midwest in the range of 420-480 ppb of NO<sub>x</sub>, where the regional 98<sup>th</sup> percentile was 4-14% higher. The temporal analysis, which compared data from multiple time periods (i.e., 2001-2003, 2004-2007, and 2008-2010) to the 10-year average, generally found that NO<sub>2</sub>/NO<sub>x</sub> ratios have been decreasing over time. The 2001-2003 ratios were on average 6.8% higher than the 10-year average and 2008-2010 ratios 1.2% were lower on average. However, all three temporal subsets showed a higher 98<sup>th</sup> percentile in the highest NO<sub>x</sub> bins. The higher 98<sup>th</sup> percentiles in the temporal subset bins and in the Midwest can generally be attributed to the relatively small number of samples and does not immediately indicate any issues with the broad application of the method across the U.S.

### **3.2.2 Field Measurement Based Model Evaluation**

The ARM2 report also presents several model performance evaluations, comparing modeled versus monitored NO<sub>2</sub> concentrations based on ARM, ARM2, PVMRM and OLM for three field studies: the Empire Abo gas plant in New Mexico, the Palaau Generating station in Hawaii, and a small power plant in Wainwright, Alaska. The evaluations considered the data from several aspects, including comparing the modeled and monitored concentrations paired in time and space, evaluations based on the ranked data (i.e., Q-Q plots and comparisons of the robust highest concentrations) and an evaluation of the behavior of the modeled and monitored NO<sub>2</sub>/NO<sub>x</sub> ratios as a function of the total NO<sub>x</sub> concentration (i.e., an evaluation similar to the fundamental development of ARM2). The evaluations demonstrated that ARM2 is generally less conservative than full conversion and ARM and generally more conservative than PVMRM and OLM when considering the highest concentrations (i.e., those most relevant for regulatory purposes).

### **3.2.3 Sensitivity Case Studies**

The report also includes the ARM2 results from sensitivity tests comparing hypothetical applications of the Tier 3 methods of OLM and PVRMR for a variety of source types (MACTEC, 2004, API, 2012). The sensitivity studies presented in the report generally indicate that ARM2 results are similar with or conservative relative to OLM and PVMRM. However, there are cases when the Tier 3 methods are known to be unrealistic as a screening tool due to an over estimation of the available ozone for NO conversion, resulting in an over-estimation of the total NO<sub>2</sub> and in cases where the Tier 3 methods were more conservative than ARM2.

### 3.2.4 EPA Analysis of ARM2

EPA believes that the evaluations indicate that the results from ARM2 are generally more conservative relative to the Tier 3 methods of OLM and PVMRM which is consistent with the tiered screening approach currently recommended in Appendix W for NO<sub>2</sub>. Additionally, section 5.2.4c of Appendix W, which addresses the Tier 2 methods, provides for the consideration of “alternative default NO<sub>2</sub>/NO<sub>x</sub> ratios” as an additional Tier 2 NO<sub>2</sub> modeling method, as long as the NO<sub>2</sub> and NO<sub>x</sub> data are considered accurate “within the range of typically measured values,” though this language was developed for an annual rather than an hourly standard. Given that the AQS data are used for NAAQS designations, this data should generally be considered to be accurate and covers all ranges of measured values, not just those that are “typical”. Thus, EPA finds that the application of ARM2 is generally supported by the current language in Appendix W and the model performance evaluations and other comparisons presented in the ARM2 development report make a strong case for broad acceptance of ARM2 as a Tier 2 method, with a few important exceptions:

1. It is not clear that the AQS data represent the direct impact from any specific source, much less the direct impact from any major NO<sub>2</sub> sources that have relatively high ISRs, as the AQS monitors are usually placed to determine the general background levels of air quality in an area. Thus, the AQS data alone does not necessarily represent the highest impacts that might occur near a major NO<sub>x</sub> source. As a result, ARM2 may not represent the behavior of these impacts. Unfortunately, an extensive analysis of the locations of the AQS monitors, major point sources, and transportation and other area sources would be required to better understand the representativeness of the AQS data in this respect.
2. The field evaluation databases and case studies were based on sources with a relatively low ISR (0.1-0.2), so the results from these evaluations do not show what types of impacts may be expected near a source that has a higher ISR (e.g., 0.5, the current default ISR specified for Tier 3 modeling). Fortunately, additional modeling studies can be completed to gain a better understanding of the ability of ARM2 to determine maximum, near-source impacts from sources with higher ISRs.

Attachment A of this memorandum details additional testing completed by the EPA to explore the relative impact of sources with ISRs greater than 0.2 on ARM2, OLM, and PVMRM modeling results. The general findings from this analysis show that the ISR can have a significant impact on the NO<sub>2</sub>/NO<sub>x</sub> ratios such that ARM2 is no longer conservative relative to the Tier 3 methods and could potentially underestimate the true NO<sub>2</sub>/NO<sub>x</sub> ratios and NO<sub>2</sub> concentrations. However, as described below, the analysis did indicate ranges of total NO<sub>x</sub> in which ARM2 is conservative relative to the Tier 3 methods and likely to produce more accurate NO<sub>2</sub>/NO<sub>x</sub> ratios as well.

### 3.2.5 Current implementation of ARM2

ARM2 is available as a non-DEFAULT BETA option in AERMOD, similar to the current OLM and PVMRM Tier 3 NO<sub>2</sub> screening options. As a result of their non-regulatory-default status, pursuant to Sections 3.1.2.c, 3.2.2.a, and A.1.a(2) of Appendix W, application of AERMOD with ARM2 is not a “preferred model” and, therefore, requires justification and approval by the Regional Office on a case-by-case basis. While EPA is continuing to evaluate the ARM2 option within AERMOD for use in compliance demonstrations for the 1-hour NO<sub>2</sub> standard, the analysis conducted by the EPA and information presented in the ARM2 documentation generally indicate that ARM2 is appropriate in many cases when the application of the ARM method is appropriate, with some potential exceptions as described below.

The implementation of ARM2 within AERMOD applies the ARM2 ratios to the modeled NO<sub>x</sub> concentration to determine the total modeled NO<sub>2</sub>. For a cumulative analysis, monitored NO<sub>2</sub> background levels should not be adjusted by the ARM2 ratio, but should be added to the modeled NO<sub>2</sub>, which can be done directly in the AERMOD simulation. The ARM2 method includes a default maximum NO<sub>2</sub>/NO<sub>x</sub> ratio of 0.9 at very low levels of NO<sub>x</sub> and a default minimum ratio of 0.2 at very high levels of NO<sub>x</sub>. The implementation of ARM2 in AERMOD allows the user to set the maximum and minimum ratios, when such a change is determined appropriate, through the use of the CO MODELOPT ARM2 and the CO ARMRATIO keywords. See the AERMOD User’s Guide Addendum (EPA, 2014) for more details on these options. Note that the CO ARMRATIO keyword is used in both the ARM and ARM2 MODELOPT keywords, specifying the maximum and minimum ratios for ARM2 and the 1-hour and annual ratios for ARM.

### 3.2.6 Approval of ARM2

The tests conducted by the EPA indicated two cases where application of ARM2 may not be appropriate, specifically when the NO<sub>2</sub>/NO<sub>x</sub> ISR of the source is relatively high and when there is remarkably high background ozone (leading to more complete and more rapid conversion of NO to NO<sub>2</sub>). Thus, the EPA recommends that the appropriate reviewing authorities (State/Local/Tribal Permitting authority and appropriate EPA Regional Office representatives) consider the follow conditions prior to approving the use of ARM2:

1. The Tier 1, total conversion, results from modeling the primary source can be used to determine if the primary source is likely to have ambient impacts that are appropriately conservative when using ARM2 regardless of the ISR of the primary source. The EPA sensitivity study indicates that this threshold is around 150-200 ppb of total modeled NO<sub>x</sub> concentrations. Given the role of ozone in the EPA tests, the lower end of the threshold (150 ppb NO<sub>x</sub>) would be appropriate in areas with higher background ozone concentrations and the higher end of the threshold (200 ppb NO<sub>x</sub>) may be appropriate in

areas with lower background ozone concentrations. In such a case, no documentation of the source's ISR would need to be provided, though it would be preferred.

2. If the total predicted NO<sub>x</sub> from a Tier 1, total conversion, analysis exceeds the 150-200 ppb threshold recommended above, then the representative background NO<sub>2</sub> concentration may also be considered to justify a higher NO<sub>x</sub> threshold. If representative background NO<sub>2</sub> levels are generally low (less than about 20-30 ppb), then it may be appropriate to consider a higher NO<sub>x</sub> threshold to justify use of ARM2. Details on this approach are provided in Attachment A of this memorandum.
3. If the total NO<sub>x</sub> from a Tier 1, total conversion analysis exceeds the 150-200 ppb threshold outlined above, then the NO<sub>2</sub>/NO<sub>x</sub> ISR of the primary source should be considered. If an adequate demonstration can be provided that the primary source has ISRs that are all below 0.2, then ARM2 should be appropriately conservative for a Tier 2 analysis. If the source has a known ISR greater than 0.2, then ARM2 may be used, but the minimum ARM2 ratio should be adjusted to match the source's ISR. If a source has multiple stacks with varying ISRs, then nominally, the minimum ARM2 ratio should be set to the maximum source ISR. However, the sensitivity tests indicate that there could be some leeway with the minimum ARM2 ratio based on the relative locations of the stacks and the receptors with the maximum modeled impact and the prevailing wind directions. This last approach would require a time consuming analysis of the incremental contribution of each stack to the receptors with the maximum modeled impact, so an applicant may find it easier to pursue Tier 3 modeling.
  - a. The EPA's preference for an adequate demonstration of a source's ISR is stack testing results from the actual source. However, this is not an option for new sources and may be burdensome for sources that do not already perform stack testing. In these cases, an adequate demonstration of a source's ISR may include, but is not limited to, use of source manufacturer test data, state or local agency guidance, data available through EPA's ISR database or other public database.
  - b. The EPA recommends that if stack test data is to be used for this demonstration, then the permitting agency should request that the source submit the data to the EPA's ISR database as part of the documentation process.
4. The EPA analysis indicated that particularly high background ozone concentrations could result in higher predicted NO<sub>2</sub>/NO<sub>x</sub> ratios even for sources that had an ISR of 0.2. While the background ozone was generally secondary to the ISR in terms of determining the estimated NO<sub>2</sub>/NO<sub>x</sub> ratios, it was nonetheless significant and thus the background ozone should be considered. The sensitivity tests indicated that background ozone concentrations of 80-90 ppb was an approximate threshold to determine when background ozone could cause Tier 3 and actual NO<sub>2</sub>/NO<sub>x</sub> ratios to exceed the ARM2

ratios. Thus, nominally, if there are frequently multiple days (e.g., more than 7) with hourly ozone greater than 80-90 ppb during a typical year, then caution should be used when applying ARM2. However, if additional analysis shows that these high ozone days or hours are not coincident with the maximum modeled NO<sub>x</sub> impacts, then the background ozone should not hinder the approval of ARM2.

#### **4. NO<sub>2</sub>/NO<sub>x</sub> In-Stack Ratios (ISR)**

The Tier 3 NO<sub>2</sub> screening methods, OLM and PVMRM, require the ISR as an input to the model. U.S. EPA, 2010b outlined scenarios where the ISR could potentially be the controlling factor in the speciation of NO<sub>x</sub> as NO<sub>2</sub>, particularly when considering maximum 1-hour concentrations. Thus, the overwhelming preference is for source-specific data. However, given the paucity of NO<sub>2</sub>/NO<sub>x</sub> ISR data, U.S. EPA, 2011 established a general acceptance of 0.5 as a default NO<sub>2</sub>/NO<sub>x</sub> in-stack ratio for usage with OLM and PVMRM when source-specific data or data from similar source types are not available. In order to address the need for additional NO<sub>2</sub>/NO<sub>x</sub> ISR data, in August, 2012, the EPA initiated an effort to formally collect source-test data. Submission of data is voluntary and open to all members of the community, including regulators, industry, equipment manufacturers, and environmental groups. Currently, there have been over two thousand records submitted, though they cover a fairly small range of source types. Additional details on the NO<sub>2</sub>/NO<sub>x</sub> in-stack ratio database can be found on the SCRAM website ([http://www.epa.gov/ttn/scram/no2\\_isr\\_database.htm](http://www.epa.gov/ttn/scram/no2_isr_database.htm)).

For compliance demonstrations of the 1-hour NO<sub>2</sub> standard in the context of the Tier 2 or 3 approaches, it is important to consider the cases which lead to the highest concentrations of NO<sub>2</sub>. U.S. EPA, 2010b identified the following two scenarios which may lead to high NO<sub>x</sub> concentrations:

- In the first scenario, a low-level source experiencing low wind speeds and limited vertical mixing was identified as a case that would most likely lead to high levels of surface NO<sub>x</sub>. In this case, mixing with ozone is expected to be limited, also limiting the conversion of NO to NO<sub>2</sub>. If the ISR of NO<sub>2</sub>/NO<sub>x</sub> is low, then the Tier 2 approaches are expected to be conservative, as most of the NO<sub>x</sub> will be in the form of NO. However, if the ISR is high, then ARM2 may not be conservative, as a larger percentage of the total NO<sub>x</sub> is already present as NO<sub>2</sub>. Based on evaluations of potential ambient NO<sub>2</sub>/NO<sub>x</sub> ratios for cases like these, as outlined above, EPA is currently recommending that some applications of ARM2 include a demonstration that the source's ISR is less than 0.2 for approval of ARM2.
- In the second scenario, a plume from an elevated source in flat terrain, during daytime convective conditions, would experience significant entrainment of ozone (for conversion of NO to NO<sub>2</sub>) as well as sufficient vertical mixing to bring the plume down to the surface. In this case, ARM2 may also not be conservative regardless of the NO<sub>2</sub>/NO<sub>x</sub> in-

stack-ratio, as there might be sufficient ozone to convert NO to NO<sub>2</sub> or there may already be a higher percentage of NO<sub>2</sub> if the NO<sub>2</sub>/NO<sub>x</sub> ISR is high.

Thus, even though the NO<sub>2</sub>/NO<sub>x</sub> ISR is not a required modeling input for the Tier 2 methods, it should still be considered when applying the ARM2 Tier 2 method, particularly when the NO<sub>2</sub>/NO<sub>x</sub> ISR is expected to be high or in the types of cases outlined above.

In the context of Tier 3 NO<sub>2</sub> screening, the NO<sub>2</sub>/NO<sub>x</sub> ISR is a required model input and must always be supplied for both the primary source and all nearby sources included in the modeling. As outlined above, when no source-specific data and no data for similar sources are available, a default ISR of 0.5 may be used for PVMRM and OLM. However, since there may be cases when the ISR is the controlling factor in the speciation of NO<sub>x</sub> as NO<sub>2</sub>, having accurate source-specific data is advantageous in accurately determining a source's impact. Since the receptors most affected by the scenarios where the ISR is most important are generally closest to the source, the importance of the ISR on the NO<sub>x</sub> partitioning will generally diminish with larger transport times and greater transport distances. There may be exceptions to this when there are other large sources that are close to one another and significantly impact the cumulative concentration gradients. Thus, the greatest need for accurate ISR, or when lacking source-specific data, the need for appropriately conservative ISR, is for the primary source and other large nearby sources rather than the smaller nearby and more distant sources included in cumulative modeling.

Given that the greatest impact of the NO<sub>2</sub>/NO<sub>x</sub> in-stack ratio is typically on the closest/closer receptors to the source and that the highest modeled impact also generally is close to the source, it is reasonable to consider a less conservative default ISR for sources more distant from the primary source. Thus, for cumulative modeling, the new EPA recommendation for default ISR is to use 0.5 as a default for the primary source and any sources in the immediate vicinity of the primary source, when source-specific data is not available, and 0.2 as a default for the more distant nearby sources. The EPA believes that the sources that can use a default of 0.2 will generally be greater than 1-3 km away from the primary source, with the distance dependent upon the relative strength of the primary and background sources as well as the relative location of the background sources with respect to the prominent wind direction and location of expected maximum impacts from the primary source. With EPA's effort to collect additional source test data, we hope that over time the range of source categories for which ISR information is readily available will increase and that the quality of such information will improve, at which time, additional recommendations may be made.

## **5. Tier 3 Methods**

Appendix W discusses the use of OLM and PVMRM as Tier 3 methods for point sources and though much of the historical documentation for these Tier 3 methods mentions only point

sources, the EPA supports the usage of both Tier 3 methods for non-point sources, as discussed below and in U.S. EPA, 2011. Both of these methods are based on the same basic chemical assumptions, the titration of NO by ozone to form NO<sub>2</sub>. Both use the NO<sub>2</sub>/NO<sub>x</sub> ISR and information about the ambient ozone in the determination of the amount of titration that will occur in the plume. However, there are important differences that should be considered when determining which method is most appropriate for a particular modeling scenario. The primary difference between the two methods is the way in which the amount of ozone available for conversion of NO to NO<sub>2</sub> is determined. OLM assumes that all the ambient ozone is available for NO titration (i.e., instantaneous complete mixing with background air), regardless of the source or plume characteristics. In contrast, PVMRM determines the amount of ozone within the plume volume (computed from the source to the receptor) and limits the conversion of NO to NO<sub>2</sub> based on the ozone entrained in the plume. The calculation of the plume volume is done for an individual source or group of sources and on an hourly basis for each source/receptor combination, taking into account the plume dispersion for that hour.

In many respects, PVMRM represents a more accurate representation of the potential titration of NO by ozone and for certain modeling scenarios, PVMRM has a number of advantages over OLM. By accounting for the ozone available within the plume volume, PVMRM can more accurately determine the amount of NO titration, particularly near the source. Additionally, PVMRM more readily accounts for conversion limitations when plumes overlap by computing a merged plume volume, rather than assuming NO titration computations on an individual plume basis. However, the method for estimating the plume volume can be problematic in certain scenarios. When considering multiple plumes, the plume volume at each receptor is computed by first identifying the primary source contributing to the NO<sub>x</sub> at the receptor. Then, all additional sources contributing at least half of the amount of NO<sub>x</sub> as the primary contributing source are identified as “major contributing sources.” Third, the maximum width between the major contributing sources is found. Finally, the maximum width found in the third step is added to the width of the primary contributing plume to determine the combined plume width. The approach to determine a combined plume width potentially incorporates a significant amount of empty space between the major contributing sources and thus could overestimate the plume size, the amount of available ozone, and the amount of NO titration. Similarly, for area sources, PVMRM uses the projected width of the area source as part of determining the combined plume width, which can exacerbate the problem of overestimating the plume volume and the amount of ozone available for NO titration. A similar effect occurs with sources at or near the surface because PVMRM does not account for ground reflection in the plume volume, again resulting in an over-prediction of the amount of ozone available for NO titration.

Therefore, PVMRM is not recommended for use with area (or line) sources or with near-surface releases or for groups of sources with moderate distances between them. U.S. EPA, 2011 suggests that roadway sources, which are often modeled as elongated area sources, may be better

modeled as a series of volume sources when using PVMRM. While PVMRM may be used for roadway sources, due to the issues with estimating plume volumes with PVMRM for near-surface releases, OLM may be the best option for modeling roadways. OLM with the OLMGROUP ALL has been used by the EPA for roadway sources to site near-road NO<sub>2</sub> monitors (Watkins & Baldauf, 2012) and has also been shown to provide generally good model performance for roadway sources as applied in the NO<sub>2</sub> Risk and Exposure Analysis (REA, U.S. EPA, 2008). In general, the OLMGROUP ALL option was recommended in U.S. EPA, 2010b as the best approach for using OLM in AERMOD, as the OLMGROUP ALL option allows for some competition for ozone when there are overlapping plumes.

## **6. Background Sources of NO<sub>2</sub> and Ambient Ozone Concentrations**

Each of the tiered NO<sub>x</sub> modeling methods require the identification of nearby NO<sub>x</sub> sources to include in cumulative modeling, a background NO<sub>2</sub> monitor to add to the modeled NO<sub>2</sub> for compliance demonstrations to account for natural background and non-modeled sources, and in the Tier 3 cases, a background ozone monitor for use in the NO titration schemes. U.S. EPA, 2010b briefly discusses the inclusion of nearby sources and the representativeness of ambient air quality data, while U.S. EPA, 2011 provides a significantly more detailed discussion. With respect to the number of nearby sources to be included in cumulative modeling, both memorandums cite Section 8.2.3 of Appendix W, which states “the number of such [nearby] sources is expected to be small except in unusual situations” and point to the “significant concentration gradient in the vicinity of the source” as the primary criterion for selection of these nearby sources. While the selection of nearby sources should also include a consideration of the representativeness of the available ambient monitoring data, including minimizing the potential double-counting of the modeled source impacts on the monitoring data. Here we reaffirm the previous guidance by reiterating that, in most cases, the number of nearby sources needed in cumulative modeling is expected to be far fewer than the past practice following section IV.C.1 of the EPA’s draft New Source Review manual, which specified an inventory that included all sources within the radius of influence plus 50 km (U.S. EPA, 1990). We also reemphasize that the determination will require sound professional judgment by the permit applicant and we recommend early consultation with the appropriate reviewing authorities.

Once the appropriate nearby sources and a representative background monitor have been identified, there are a number of ways that the background data can be combined with the cumulative modeling to determine compliance. U.S. EPA, 2010b outlines a “first tier” approach for demonstrating compliance with the 1-hr NO<sub>2</sub> standard, which combines the overall highest 1-hour background NO<sub>2</sub> concentration to the modeled design value. The EPA recognized that for many cases, this approach is too conservative and thus revised the “first tier” approach in U.S. EPA, 2011 with the recommendation that the monitored design value from the most recent three years of monitored data should be combined with the modeled design value, based on 5 years of

modeling. U.S. EPA, 2011 goes on to add a “second tier” approach, with more refined temporal pairing. The recommended refined method uses “multiyear averages of the 98th-percentile of the available background concentrations by season and hour-of-day, excluding periods when the source in question is expected to impact the monitored concentration.” When mobile sources are expected to significantly impact the monitor, the day-of-week variability may also be an appropriate consideration. It should also be noted that when determining the 98<sup>th</sup> percentile value, the ambient monitoring requirements (Appendix S to 40 CFR Part 50) specify the second-high value, given the number of values expected to be available for each season hour-of-day (90 to 92). However, the EPA recommends using the third-highest value in each season hour-of-day for modeling, which excludes the highest 8 values from the analysis rather than the highest 4 and thus more closely mimics the standard, which excludes the highest 7 values. U.S. EPA, 2011 provides an extensive discussion and supporting data for this “second tier” approach.

Based on the experience of the EPA since U.S. EPA, 2011 was issued, the EPA continues to support this “second tier” approach and generally recommends that it should be routinely accepted by the permitting authority, provided that an adequate demonstration of the appropriateness of the monitoring data has been provided. However, the EPA maintains that pairing the monitoring data on an hourly basis with modeled data paired in time (i.e., the “paired sums” approach) is not appropriate for the majority of modeling applications.

Whether using the first or second “tier” approach for combining monitoring data with modeled concentrations, it is important to insure that the monitoring data is adequately representative. Section 8.2.2b of Appendix W specifies for an Isolated Single Source analysis that the monitor should exclude “values when the source in question is impacting the monitor.” For an hourly standard and where there are 2 monitors in the vicinity of the Isolated Single Source, this may mean selectively using data from the monitor that is upwind of the source at each hour. This could be accomplished by manually editing the background file to splice together a wind-direction dependent monitored value. However, starting with version 13350, AERMOD includes the option to specify multiple background files, based on their geographic relation to the monitor and AERMOD will automatically apply the monitoring data from the appropriate downwind monitor on an hourly basis. This is implemented with the SO BGSECTOR keyword, which determines the applicable sector based on the flow vector (i.e. downwind direction) derived from the wind direction in the hourly surface meteorological file. While the BGSECTOR option is generally applicable to all pollutants, a similar NO<sub>2</sub>-specific option has also been incorporated in AERMOD (beginning with version 13350) for supplying background ozone concentrations for Tier 3 NO<sub>2</sub> assessments. The CO O3SECTOR keyword allows the specification of multiple background ozone files, which are also selected based on the flow vector. However, it should be noted that the implementation in AERMOD of the selection of the background monitor (i.e., specifying the flow vector) is not meant to imply that the downwind monitor should always be used for either ozone or NO<sub>2</sub>. U.S. EPA, 2011 provides various examples of when an upwind

versus downwind monitor should be used. The example provided here, when a monitor is impacted by an existing isolated source's emissions, is a scenario when the upwind monitor would be preferred and thus the user-specified sectors should be adjusted by 180 degrees, such that the upwind monitor would be selected. Modeling a new source that does not include nearby sources in the cumulative modeling is an example of a scenario when the downwind monitor might be the preferred option.

## 7. Summary

The primary purpose of this memorandum was to provide an assessment of the appropriateness of the new ARM2 NO<sub>x</sub> speciation method and to provide guidance on its application and acceptance as an alternative Tier 2 modeling approach under Appendix W. A number of other NO<sub>2</sub>-related modeling issues for regulatory purposes with the AERMOD air quality model were also addressed. In summary, the recommendations and findings presented in this memorandum include:

- The EPA testing and evaluation of the ARM2 method indicates that ARM2 appears to be an appropriate Tier 2 NO<sub>2</sub> modeling method in some cases and should be approved for usage as an alternative modeling option in these cases. These cases are:
  1. The primary source/facility has made a demonstration that the source/facility has a NO<sub>2</sub>/NO<sub>x</sub> in-stack ratio (ISR) of less than 0.2 (for 95% or more of the short-term NO<sub>x</sub> emissions).
  2. The primary source/facility has made a demonstration that the total modeled NO<sub>x</sub> from the source/facility is less than 150-200 ppb.
  3. The background ozone is not persistently above approximately 80-90 ppb.

If these conditions are not met, then ARM2 may underestimate ambient NO<sub>2</sub>/NO<sub>x</sub> ratios and so either a Tier III approach should be utilized or ARM2 should be applied with additional caution/considerations.

- The NO<sub>2</sub>/NO<sub>x</sub> ISR is an important input to the OLM and PVMRM Tier 3 methods and should also be considered in determining the appropriateness of application of the Tier 2 ARM2 method. Site or source specific values of the ISR are the preferred input and to facilitate the increased availability of more representative ISRs, the EPA launched a voluntary effort to collect and make available ISRs from a wide variety of sources. However, when site or source specific values are not available, a default ISR of 0.5 may be used for the primary source and a default ISR of 0.2 may be used for more distant sources (greater than 1-3 km) in the cumulative modeling applications of OLM and PVMRM.

- Both PVMRM and OLM Tier 3 methods may be used for non-point sources, including roadways. However, PVMRM is most appropriate with relatively isolated and elevated sources, while OLM is more appropriate for area sources, near-surface releases, or scenarios with multiple sources where plume overlap is likely to occur. In these cases, the OLMGROUP ALL option is recommended to better account for competition of ozone.
- AERMOD now includes directional-varying background options for both the primary pollutant (e.g., NO<sub>2</sub>) and ozone in the Tier 3 methods. The general recommendation is that background data located downwind of the isolated source and near the receptor should be used for new sources and background data upwind of the isolated source should be used for non-nearby existing sources in order to minimize double-counting the impact of the existing source on the background data. U.S. EPA, 2011 provides a more comprehensive discussion of the selection and treatment of background monitoring data and should also be consulted.

## 8. References

Cole, H.S. and J.E. Summerhays, 1979. A Review of Techniques Available for Estimation of Short-Term NO<sub>2</sub> Concentrations. *Journal of the Air Pollution Control Association*, 29(8): 812–817.

Chu, S.H. and E.L. Meyer, 1991. Use of Ambient Ratios to Estimate Impact of NO<sub>x</sub> Sources on Annual NO<sub>2</sub> Concentrations. *Proceedings, 84th Annual Meeting & Exhibition of the Air & Waste Management Association, Vancouver, B.C.; 16–21 June 1991. (16pp.) (Docket No. A–92–65, II–A–9)*

Hanrahan, P.L., 1999. The Plume Volume Molar Ratio Method for Determining NO<sub>2</sub>/NO<sub>x</sub> Ratios in Modeling – Part I: Methodology. *J. Air & Waste Manage. Assoc.*, 49, 1324–1331.

MACTEC, 2004. Sensitivity Analysis of PVMRM and OLM in AERMOD. Final Report, Alaska DEC Contract No. 18-8018-04. MACTEC Federal Programs, Inc., Research Triangle Park, NC.

Podrez, M., 2012, Updated Tier 2 Ambient Ratio Method (ARM) for 1-hr NO<sub>2</sub> NAAQS Analyses, presented at the 10th Modeling Conference, Research Triangle Park, NC on March 14, 2012.

U.S. EPA, 1990, New Source Review Workshop Manual for Prevention of Significant of Deterioration and Nonattainment Area Permitting, Draft, October, 1990.

U. S. EPA, 2008. Risk and Exposure Assessment to Support the Review of the NO<sub>2</sub> Primary National Ambient Air Quality Standard. EPA-452/R-08-008a. U.S. Environmental Protection Agency, Research Triangle Park, NC.

U. S. EPA, 2010a. Applicability of the Federal Prevention of Significant Deterioration Permit Requirements to New and Revised National Ambient Air Quality Standards. Stephen D. Page Memorandum, dated April 1, 2010. U.S. EPA, Research Triangle Park, NC.

U.S. EPA, 2010b. Applicability of Appendix W Modeling Guidance for the 1-hour NO<sub>2</sub> NAAQS. Tyler Fox Memorandum, dated June 28, 2010. U.S. EPA, Research Triangle Park, NC.

U. S. EPA, 2011, "Additional Clarification Regarding Application of Appendix W Modeling Guidance for the 1-hour NO<sub>2</sub> NAAQS", U.S. EPA, March 1, 2011.

U.S. EPA, 2014. Addendum – User's Guide for the AMS/EPA Regulatory Model – AERMOD. EPA-454/B-03-001, Research Triangle Park, North Carolina 27711.

Wang, Y.J., A. DenBleyker, E. McDonald-Buller, D. Allen and K. Zhang, 2011. Modeling the chemical evolution of nitrogen oxides near roadways. *Atmos. Env.*, 45, 43-52.

Watkins, N. and R. Baldauf, 2012. Near-road NO<sub>2</sub> Monitoring Technical Assistance Document, U.S. EPA, June, 2012.

*This Page Intentionally Left Blank*

## **ATTACHMENT A. – EPA EVALUATION OF ARM2 PERFORMANCE**

To address these potential limitations of the ARM2 evaluation, the EPA has conducted additional testing to inform the application and approval of ARM2. Specifically, the EPA has considered theoretical maximum concentrations of NO<sub>2</sub> based on combinations of chemical pathways for NO<sub>2</sub>. The first is based on the simple, but total titration of NO to NO<sub>2</sub> by ozone (TT). The second is based on the partial titration of NO considering the “pseudo-steady state” of NO, NO<sub>2</sub>, and ozone (PSS). The third is based on a theoretical Lagrangian plume that combines complete TT and PSS for NO titration, but also takes into account the volume of the plume and mixing with background air (PV). Additionally, the EPA has conducted modeling sensitivity tests based on a modifications of the ARM2 development report case studies, with a higher ISR, higher default background ozone, and with various receptor heights, including placing the receptors at stack height in order to capture the impacts closer to the plume centerline.

### **1. Theoretical Applications of Total Titration and the Pseudo-Steady State Approximation**

For these evaluations, the EPA considered a wide range of ambient conditions to determine the potential maximum NO<sub>2</sub> concentrations resulting from various NO<sub>x</sub> levels based on two fundamental assumptions about NO conversion to NO<sub>2</sub> by ozone. The first assumption is total titration of NO by ozone, which assumes that all available ozone is consumed for NO conversion, where availability is considered on the basis of ambient mixing ratios, ignoring plume volumes. The second assumption is based on the pseudo-steady state assumption, which determines an equilibrium ratio between ozone, NO and NO<sub>2</sub>. This equilibrium is driven by the NO<sub>x</sub> and ozone concentrations as well as ambient temperature, solar zenith angle (SZA), and cloud cover. The PSS equation is normally used to evaluate ozone formation and is formulated to determine ozone levels based on the speciation of NO and NO<sub>2</sub>. For the purposes of the tests conducted here, the PSS equation was rearranged to use constant ozone and determine the NO and NO<sub>2</sub> speciation instead. The result of this assumption is that NO titration is never ozone limited and can thus overestimate the NO<sub>2</sub>/NO<sub>x</sub> ratio when the total NO<sub>x</sub> is greater than the ozone concentration. To mitigate this aspect of the PSS approach, when evaluating a specific range of NO<sub>x</sub> with accompanying ozone and meteorological conditions, the PSS assumption was used to determine the NO<sub>2</sub>/NO<sub>x</sub> ratio when the total NO<sub>x</sub> was less than the ozone concentration and the TT assumption was used when the total NO<sub>x</sub> was greater than the ozone concentration. Because of the combination of assumptions listed above, plus an assumption of complete mixing of the plume with background, the computed NO<sub>2</sub>/NO<sub>x</sub> ratios likely overestimate typical NO<sub>2</sub>/NO<sub>x</sub> ratios. However, this approach is attractive as it allows for a conservative assessment of theoretical NO<sub>2</sub>/NO<sub>x</sub> ratios across a wide range of ambient conditions. While the EPA considered many meteorological and emissions scenarios for this evaluation, only small subset are presented here, with the specific plume and meteorological assumptions for each scenario detailed in Table 1.

Scenario	ISR	Ozone (ppb)	Temperature (F)	Solar zenith angle (SZA, degrees)	Cloud cover	NO <sub>x</sub> conversion
U.S. extreme,ST	0.0	150 <sup>1</sup>	97 <sup>2</sup>	25 (Texas or Florida)	0%	TT/PSS
U.S. mean, ST	0.0	30 <sup>3</sup>	56 <sup>4</sup>	37.5 (e.g., Kansas)	50%	TT/PSS
U.S. high, ST	0.0	84 <sup>5</sup>	76 <sup>6</sup>	37.5 (e.g., Kansas)	50%	TT/PSS
PV, 0.2 high	0.2	84	76	37.5 (e.g., Kansas)	50%	Mixing volumes with TT/PSS
PV, 0.2 mean	0.2	30	76	37.5 (e.g., Kansas)	50%	Mixing volumes with TT/PSS
PV, 0.5 mean	0.5	30	76	37.5 (e.g., Kansas)	50%	Mixing volumes with TT/PSS
PV, 0.5 high	0.5	84	76	37.5 (e.g., Kansas)	50%	Mixing volumes with TT/PSS
PVMRM, 0.5 max/DV	0.5	Actual (85) <sup>7</sup>	Actual <sup>7</sup>	NA	Actual <sup>7</sup>	PVMRM
PVMRM, 0.2 max/DV	0.2	Actual (85) <sup>7</sup>	Actual <sup>7</sup>	NA	Actual <sup>7</sup>	PVMRM

Table 1: Ambient conditions and source configurations for EPA test cases

Figure 1 shows the results from the three scenarios using the combined PSS/TT approach, based on a source with pure NO emissions (i.e., an ISR of 0). The scenario “U.S. extreme, ST” shows the NO<sub>2</sub>/NO<sub>x</sub> ratios from NO<sub>x</sub> concentrations determined from the most extreme conditions for the U.S. and thus indicate the highest 1-hr NO<sub>2</sub>/NO<sub>x</sub> ratios possible for a source of this type. The results from this extreme scenario give higher NO<sub>2</sub> concentrations at basically all NO<sub>x</sub> levels than ARM2 and indicate that there could be times when a source with only NO emissions could produce NO<sub>2</sub> concentrations larger than ARM2. In contrast to these extreme conditions, the scenarios, “U.S. high, ST” and “U.S. mean, ST” consider less extreme values, using roughly maximum and mean monthly summertime temperatures for the continental U.S., and mean and more representative maximum ozone from AQS. The mean conditions produce NO<sub>2</sub>/NO<sub>x</sub> ratios notably lower than ARM2, which is expected, as ARM2 uses the highest NO<sub>2</sub>/NO<sub>x</sub> ratios from each NO<sub>x</sub> bin rather than the mean ratios from each bin. The “U.S. high, ST” scenario gives NO<sub>2</sub>/NO<sub>x</sub> ratios that are closer to the ARM ratios, with the ratios from the “high” scenario less than the ARM2 ratios in the higher NO<sub>x</sub> levels (above 300 ppb of NO<sub>x</sub>).

<sup>1</sup> Roughly the maximum ozone from AQS data from 2008-2012

<sup>2</sup> Maximum monthly mean maximum summertime temperature from Austin, TX

<sup>3</sup> Mean ozone concentrations from AQS from 2008-2012, including nighttime and daytime samples.

<sup>4</sup> Mean temperature in July for the contiguous U.S.

<sup>5</sup> Mean ozone concentration plus 3 standard deviations of the mean from AQS from 2008-2012

<sup>6</sup> Mean maximum temperature in July for the contiguous U.S.

<sup>7</sup> Actual ozone and meteorological data from Anchorage, AK from 1991-1995, with 85 ppb used to fill missing hours.

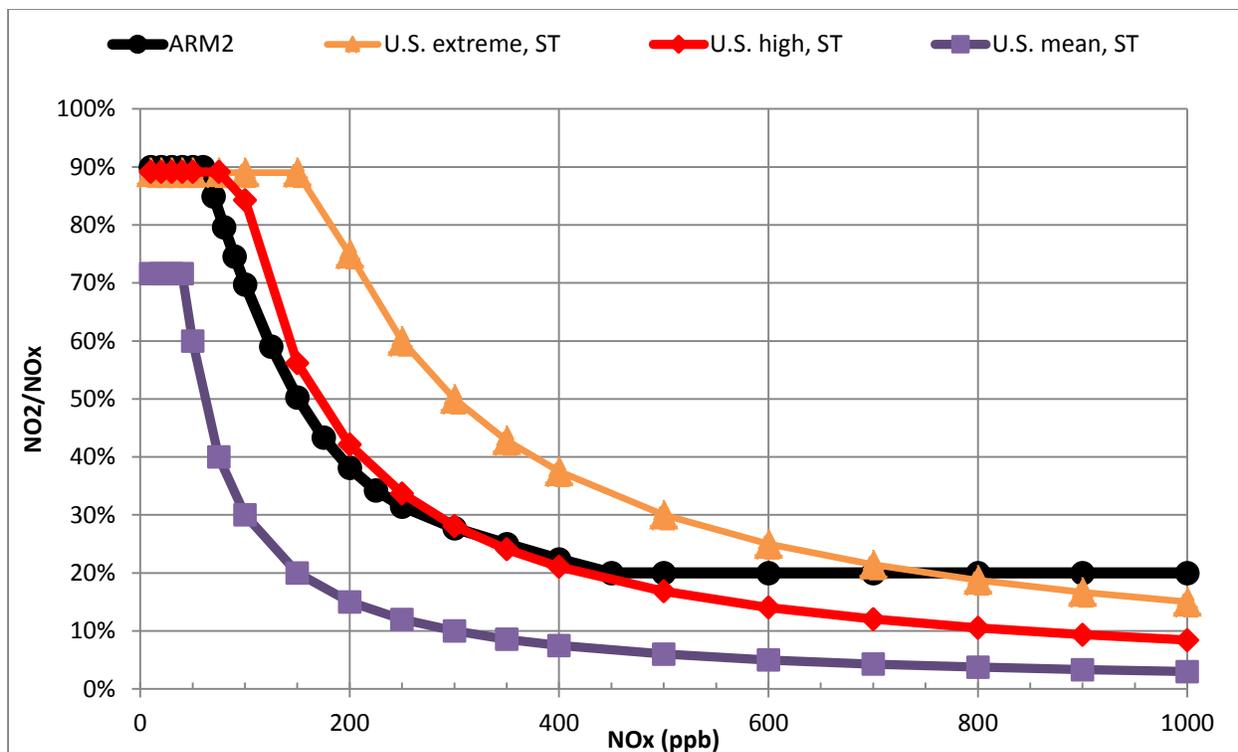


Figure 1: NO<sub>2</sub>/NO<sub>x</sub> ratios for ARM2 and the EPA PSS/TT sensitivity studies

It should be noted that while the “high” scenario is close to the ARM2 values in the range of 50-300 ppb NO<sub>x</sub>, the curves are very steep in this range, such that at any specific NO<sub>x</sub> level, the difference between the two curves can still be large (e.g., ARM2 indicates 70 ppb of NO<sub>2</sub> at 100 ppb of NO<sub>x</sub> while the “U.S. high, ST” curve indicates 84 ppb of NO<sub>2</sub>). Thus, the “high” scenario also indicates that there are times when a source with only NO emissions could produce NO<sub>2</sub> concentrations larger than ARM2. It should also be noted that surface ozone typically has a strong diurnal pattern, with higher ozone levels during the day, when photochemistry produces ozone, and lower ozone levels at night, when scavenging by NO tends to dominate ozone chemistry. The ozone levels include both nighttime and daytime measurements, which certainly affect the average and standard deviations computed for the dataset used here. Background ozone concentrations are typically assumed to be closer to 40 ppb for the continental US rather than the 30 used here. While 40 ppb of ozone would increase the NO<sub>2</sub>/NO<sub>x</sub> ratios for the “mean” scenario, the ratios would still be substantially less than the ARM2 ratios. Furthermore, while using only the daytime ozone data would provide a higher mean concentration, it would also give a lower standard deviation, which is likely to result in concentrations for a “high” scenario on the order of 80-90 ppb. Thus, it is not likely that the inclusion of nighttime and daytime ozone in the computations here will have a significant impact on the findings.

In order to account for the ISR of NO<sub>2</sub>/NO<sub>x</sub> and a more realistic consideration of ozone availability, another set of scenarios were constructed that use the TT and PSS assumptions but also uses a hypothetical ISR to initially proportion the total NO<sub>x</sub> according to the ISR. These

plume volume scenarios (PV) take into account ozone availability, by using an initial plume volume, which mixes with background air as the plume volume increases, limiting the amount of ozone available to react with the remaining NO. This approach is similar to PVMRM in that the initial NO<sub>2</sub> remains as NO<sub>2</sub> and only the initial NO is available for titration and that ozone availability is considered. This assumption simplifies the calculation by using the mixing ratios of the plume and background air, rather than computing the moles of NO<sub>x</sub> and ozone. This approach also assumes a uniform puff, rather than a Gaussian plume, as would be used in PVMRM.

For this analysis, four PV scenarios are shown in Figure 2, two with an ISR of 0.2 and two with an ISR of 0.5. For each ISR, “mean” and “high” ozone scenarios are examined, with 30 and 84 ppb of ozone, matching the PSS/TT scenarios above. In contrast to the PSS/TT scenarios, the NO<sub>2</sub>/NO<sub>x</sub> ratios from the PV tests are generally higher than those from ARM2, with the major exception occurring in the 0.2 ISR PV scenario with mean ozone, where ARM2 has higher ratios up until 300 ppb NO<sub>x</sub>. Without the inclusion of the initial NO<sub>2</sub>, these curves would closely match the TT/PSS cases discussed above when equivalent ambient conditions are used. The addition of the ISR clearly has a significant impact on the resulting NO<sub>2</sub>/NO<sub>x</sub> ratios, such that the NO<sub>2</sub>/NO<sub>x</sub> ISR is the controlling factor rather than the ambient conditions on the maximum potential impacts. It is important to keep in mind that the PSS/TT approach used in these scenarios are near theoretical maximum and presents a conservative assessment of theoretical NO<sub>2</sub>/NO<sub>x</sub> ratios.

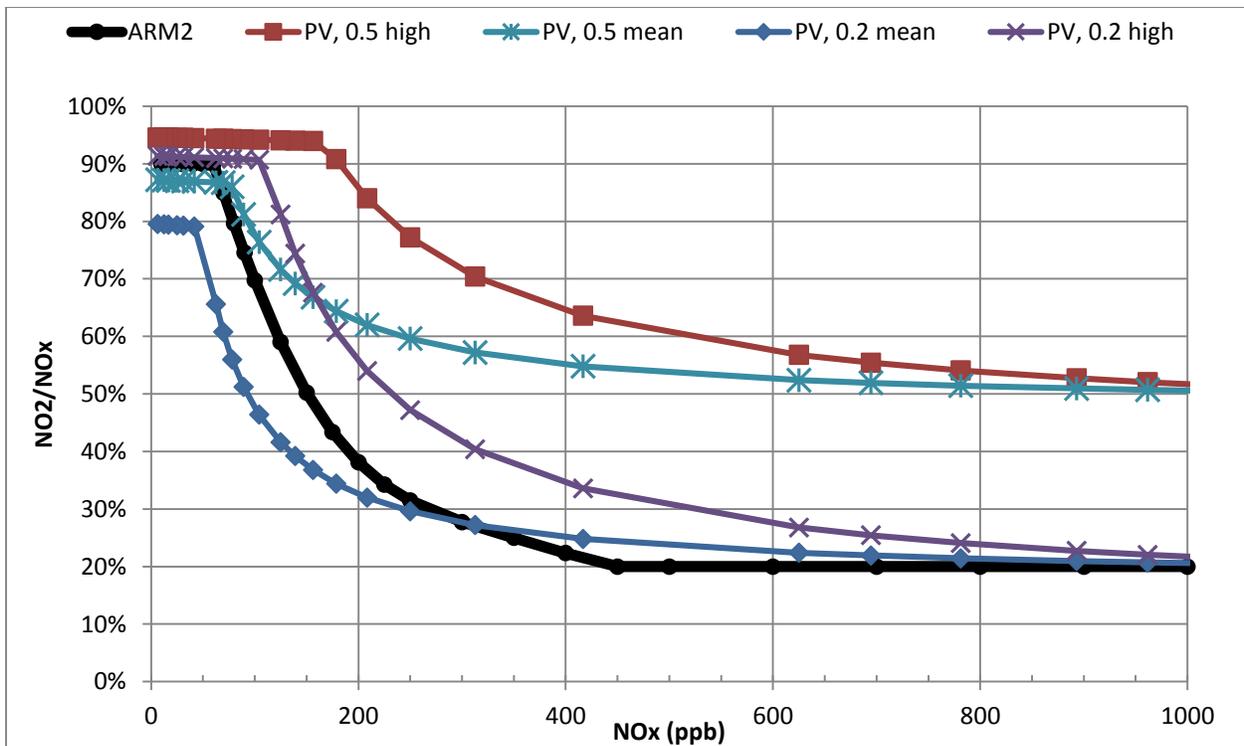


Figure 2: NO<sub>2</sub>/NO<sub>x</sub> ratios for ARM2 and the EPA PV sensitivity studies

## 2. Expanded Single-Source PVMRM Case Study

Since the theoretical “PV” tests conducted by the EPA indicate that a high NO<sub>2</sub>/NO<sub>x</sub> ISR can produce NO<sub>2</sub>/NO<sub>x</sub> ratios well above those determined from ARM2 and the API (2013) ARM2 cases all included a relatively low ISR or 0.1-0.2, one of the single-source cases from the ARM2 development report was modified for further investigation. The case includes a single point source, with a stack height of 35 m, an emission rate of 50 g/s, and an ISR of 0.1. The source was modified to have an ISR of 0.5 and 0.2, the receptor grid was raised from ground level to 35 m, in order to sample closer to the plume centerline, and the closest receptor was placed 1 m from the source.

The four sets of results from two full 5-year model simulations are shown in Figure 3. The resulting design values (5-year average of the 98<sup>th</sup> percentile daily 1-hour maximum at each receptor) and maximum (5-year average of the highest daily 1-hour maximum at each receptor) are shown. The design values from an OLM model simulation of the 0.5 ISR source are also included for additional reference. While the ambient ratios of the PVMRM design values (e.g., 98<sup>th</sup> percentile) for the 0.2 and 0.5 ISR sources are notably lower than the ambient ratios for the maximum impacts, all three simulations have NO<sub>2</sub>/NO<sub>x</sub> ratios at the highest NO<sub>x</sub> levels that approach the ISR for each source. The result of the minimum NO<sub>2</sub>/NO<sub>x</sub> ratio being equal to the ISR is similar to the hypothetical results from the PV scenarios and is not a particularly surprising result – a source with a high ISR will have near-source, maximum impacts that heavily reflect the initial partitioning of NO and NO<sub>2</sub>. Even when the plume becomes diluted, the generic assumption for NO<sub>2</sub> modeling is that NO titration is irreversible and the NO<sub>2</sub>/NO<sub>x</sub> ratio can only increase as the plume becomes mixed with background air providing more ozone for NO titration. The differences between the OLM and PVMRM results are interesting and informative. Though the OLM results more closely reflect the results from the PV scenarios presented above, as outlined in the memorandum, the expectation is that PVMRM more accurately represents NO titration by accounting for the actual volume of the plume. The fact that the PVMRM ratios are lower than the OLM ratios indicate that the plume volume is limiting more ozone entrainment than would be inferred from OLM conversion based solely on the ambient mixing ratio, though the truth is likely somewhere in between the two model results. Nonetheless, these PVMRM results indicate that ARM2 could potentially underestimate the maximum 1-hour impacts from a source with an ISR above 0.2 and that ARM2 is likely not conservative for a 1-hour standard relative to PVMRM in such a scenario.

While the PVMRM results presented above are from a source with a high, but not unrealistic, NO<sub>x</sub> emission rate, the receptor placement is clearly not appropriate for a typical NSR/PSD application (unless plume impaction on nearby terrain occurs). Thus, we have repeated the two PVMRM runs, but with a receptor height of 1.8 meters, to capture impacts closer to the ground. These results are not shown, but there is not surprisingly a major difference in the calculated

total  $\text{NO}_x$  and  $\text{NO}_2$  concentrations, with the maximum  $\text{NO}_x$  impact reduced by several orders of magnitude from the 35 m receptors to the 1.8 m receptors. Since the maximum  $\text{NO}_x$  impacts are much lower, the  $\text{NO}_2/\text{NO}_x$  ratios for these 1.8 m receptors are in the range where the ARM2 ratios are higher than the PVMRM ratios. For both sources, the average ARM2 ratio for the design values at 1.8 m is 0.9 versus an average ratio of 0.63 for the 0.5 ISR source and 0.37 for the 0.2 ISR source from PVMRM. The implication for the difference in the 35 m and 1.8 m receptor results is that a source with a high ISR can be modeled with ARM2 and the resulting concentrations can be conservative relative to PVMRM and OLM. However, there is a clear dividing line where ARM2 becomes less conservative than PVMRM. For the 0.5 ISR source, this occurs around 150-200 ppb of total  $\text{NO}_x$ , indicating that if the impacts for the source are less than this threshold, then ARM2 will be likely be conservative relative to PVMRM, regardless of the ISR of the source (assuming a maximum default ISR of 0.5, as specified for Tier 3 sources). While the expectation is not that ARM2 should always be conservative relative to either of the Tier 3 methods, this particular modeling scenario is one in which PVMRM is expected to perform particularly well, indicating that any under prediction of ARM2 relative to PVMRM for these cases likely indicates ARM2 would also under predict a similar source's true impacts.

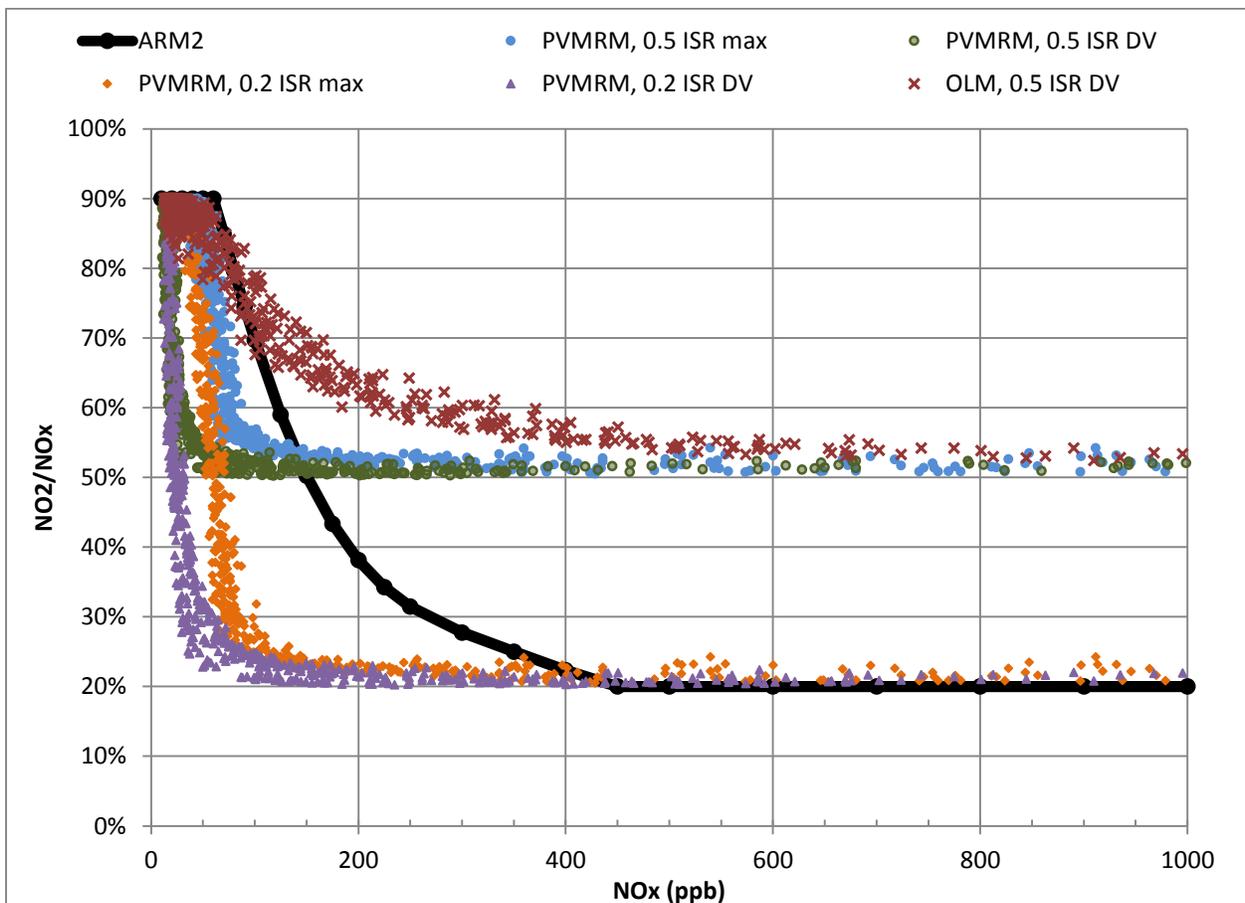


Figure 3:  $\text{NO}_2/\text{NO}_x$  ratios for ARM2 and the EPA PVMRM sensitivity studies

### 3.0 Multi-Source Scenarios

Given the potential importance of the ISR on the modeling results, the EPA also conducted some limited testing of multi-source scenarios. There was one multi-source scenario included in the ARM2 development report, based on oil and gas sampling in Alaska and originally included 64 sources, some of which experienced downwash, and all had an ISR of 0.1. In order to gauge the effect of multiple sources and varying ISRs, additional testing was done with a modified version of this multi-source scenario. For the testing done here, the scenario was scaled down to only 4 of the larger sources, all of which included downwash influences, and also covered the general extent of the original project area. The test results shown in Figure 4 are based on modifying two of the four sources to have an ISR of 0.5, such that there were 2 simulations with 1 source with an ISR of 0.5 and 1 simulation with 2 sources with an ISR of 0.5.

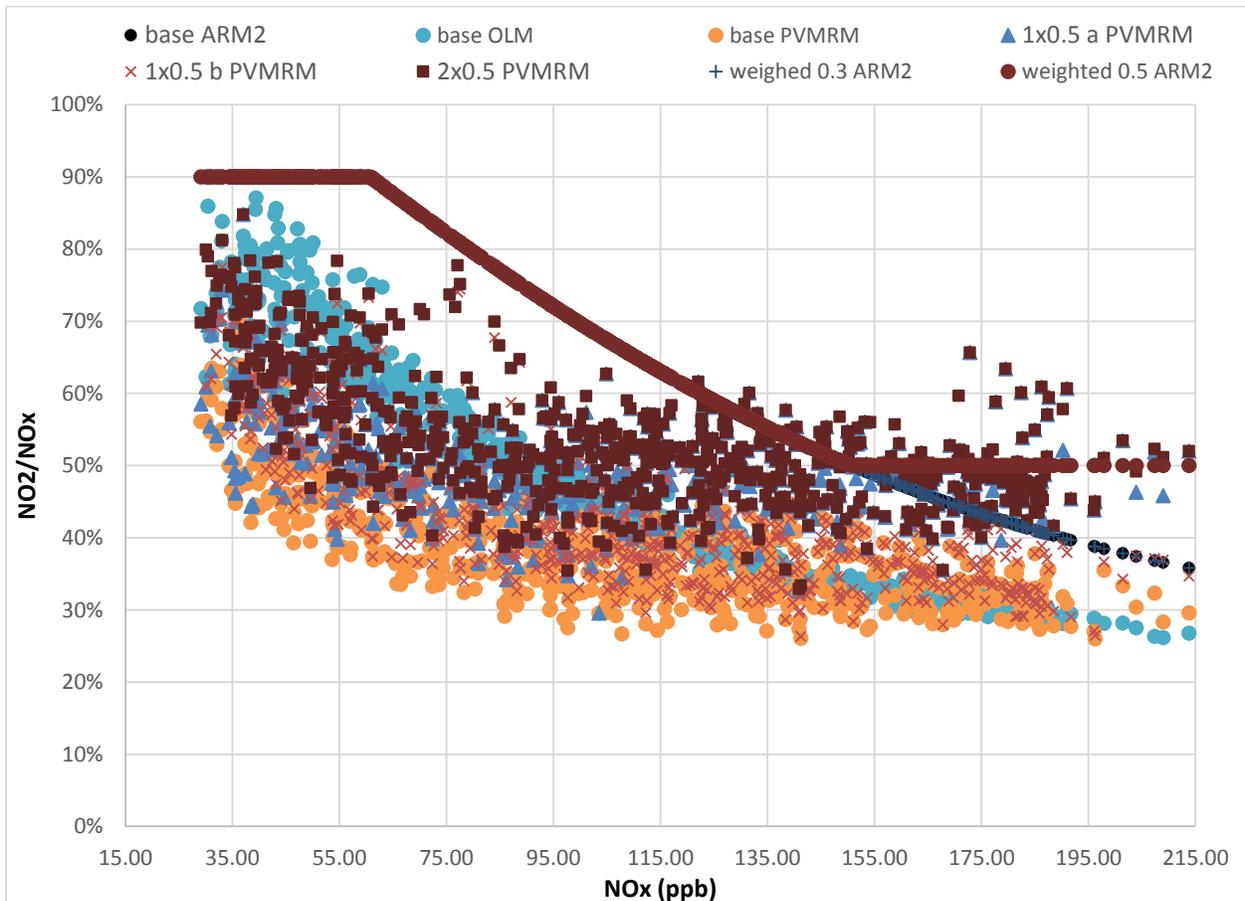


Figure 4: NO<sub>2</sub>/NO<sub>x</sub> ratios for the multi-source scenario sensitivity studies

These tests provide several interesting results. First, there is once again a NO<sub>x</sub> threshold where ARM2 becomes less conservative than the Tier 3 methods occurring around 150 ppb of NO<sub>x</sub>. Second, the two scenarios based on increasing the ISR to 0.5 for one of the sources are remarkably different, with the “1x0.5 b” case results more similar to the base case than the

“1x0.5 a” case. Similarly, the “1x0.5 a” case results are more similar to the “2x0.5” scenario that has 2 sources with an ISR of 0.5. These findings are due to the relative location of the receptors with the maximum concentrations to the 0.5 ISR source and the predominant wind conditions. The 0.5 ISR source in the “1x0.5 a” scenario is closer to and immediately upwind of the receptors with the maximum concentrations, while the 0.5 ISR source in the “1x0.5 b” scenario is farther upwind from these receptors. Ultimately, the results clearly demonstrate that when one source in a multi-source scenario has an ISR above the minimum ARM2 NO<sub>2</sub>/NO<sub>x</sub> ratio, then the ARM2 results may still be less conservative relative the Tier 3 methods.

Since the implementation of ARM2 in AERMOD allows the user to specify the minimum and maximum NO<sub>2</sub>/NO<sub>x</sub> ratio, the ARM2 settings can be adjusted to eliminate the NO<sub>2</sub>/NO<sub>x</sub> ratio under prediction when sources with an ISR greater than 0.2 are included in the modeling scenario. To explore this possibility, two additional scenarios were considered. For these simulations the minimum ARM2 ratio was adjusted to match the emission-weighted mean ISR from the four sources included (resulting in an ISR of 0.3066) and the maximum ISR from all sources (0.5). The results from these two additional ARM2-based runs are shown in Figure 4. Since the modified ARM2 runs do not change the source properties, the ARM2 results in the lower NO<sub>x</sub> levels are identical in all three ARM2 runs. For the base case and weighted ARM2 case, the NO<sub>2</sub>/NO<sub>x</sub> ratios are identical at all NO<sub>x</sub> levels because the minimum modeled NO<sub>2</sub>/NO<sub>x</sub> ratio from the base case (0.36) was greater than the emission weighted minimum ratio of 0.3066. In contrast, the “0.5” ARM2 run has substantially higher NO<sub>2</sub>/NO<sub>x</sub> ratios at the higher NO<sub>x</sub> levels. However, the maximum Tier 3 results have higher NO<sub>2</sub>/NO<sub>x</sub> ratios than the “0.5” ARM2 run. These additional tests demonstrate that simply adjusting the minimum ARM2 ratio does not insure that the ARM2 NO<sub>2</sub>/NO<sub>x</sub> ratio will be conservative relative to the Tier 3 methods.

#### **4.0 Conclusions of Additional EPA ARM2 Analysis**

The additional EPA analysis of the ARM2 method expands considerably on the evaluation provided in the ARM2 development report, specifically highlighting when true ambient NO<sub>2</sub>/NO<sub>x</sub> ratios may be well above those computed by ARM2. While the ARM2 development report focused on modeled design values (i.e., 98<sup>th</sup> percentiles), the EPA analysis also considered single, high NO<sub>x</sub> values to target the highest potential NO<sub>2</sub>/NO<sub>x</sub> ratios from a variety of scenarios. The EPA analysis indicates that there are several scenarios where ARM2 may not be appropriate or should be applied with caution. The first case is when there may be very high ozone present in the area of the project source. The second case, and biggest shortcoming of ARM2, is when one or more sources have ISRs greater than 0.2. This deficiency was highlighted in theoretical PV tests and the single and multi-source Tier 3 modeling results. Unfortunately, these findings complicate the implementation of ARM2 as a Tier 2 screening technique by requiring more consideration to justify for its usage than the existing ARM. However, there is a strong indication that below a certain total NO<sub>x</sub> threshold, in the range of 150-200 ppb of NO<sub>x</sub>,

ARM2 is likely to be conservative relative to the Tier 3 methods regardless of the source’s ISR and therefore may be used as a safe harbor for the application of ARM2. It thus stands to reason that if a source or group of sources has a maximum modeled design value from the Tier 1 full conversion assumption below this threshold, then there should be no reason to restrict the usage of ARM2 or require a demonstration of the source’s ISR.

When performing cumulative modeling, a similar threshold consideration could be made when background is added. Since the goal of the Tier 2 screening method is to determine if a violation will occur, the impact of the addition of the background NO<sub>2</sub> can also be considered. For example, in order to model a NO<sub>2</sub> concentration above the 1-hour standard with ARM2 absent any background, the total modeled NO<sub>x</sub> would have to be 500 ppb (at 500 ppb NO<sub>x</sub>, the ARM2 ratio is 0.2, giving a NO<sub>2</sub> concentration of 100 ppb). In contrast, if the background level of NO<sub>2</sub> is 35 ppb, then the total modeled NO<sub>x</sub> needed to exceed the 1-hour NAAQS would only have to be 85 ppb (the ARM2 ratio at 85 ppb of NO<sub>x</sub> is 0.77, giving a NO<sub>2</sub> concentration of 65, for a cumulative NO<sub>2</sub> concentration of 100 ppb). For the ARM2 “approval threshold” of about 150 ppb of NO<sub>x</sub>, the resultant NO<sub>2</sub> concentration is 75 ppb and the background needed to produce a violation is only 25 ppb. Table 2 outlines benchmarks for modeling a violation for a number of background levels of NO<sub>2</sub>. Based on the values in this table, it could reasonably be expected that a model violation would correctly be identified if the total NO<sub>x</sub> of the 98<sup>th</sup> percentile values is below the level corresponding to the background values provided. For example, if the background NO<sub>2</sub> is 15 ppb, then the threshold for violation-identification would be 320 ppb NO<sub>x</sub>, implying that ARM2 might be appropriate for use regardless of the ISR as long as the full conversion modeled design value (98<sup>th</sup> percentile) at any receptor is below this threshold.

NO <sub>x</sub>	ARM2 NO <sub>2</sub> /NO <sub>x</sub>	NO <sub>2</sub>	Background	Cumulative NO <sub>2</sub>
105	67%	70.81	30	100.81
145	52%	75.17	25	100.17
270	30%	80.33	20	100.33
320	27%	85.14	15	100.14
455	20%	91.00	10	101.00
500	19%	100.00	0	100.00

Table 2: Modeled violation thresholds for various background levels of NO<sub>2</sub> and NO<sub>2</sub>/NO<sub>x</sub> ratios

There are also indications that when ozone levels are particularly high, ARM2 may underestimate NO<sub>2</sub> concentrations even when the source has a low ISR. The threshold for ozone effects being important appears to be approximately 90 ppb. When ozone levels are this high, the PV and PSS/TT tests indicated high NO<sub>2</sub>/NO<sub>x</sub> ratios could occur even when the source has no direct NO<sub>2</sub> emissions. PVMRM tests of a single source indicate a source with an ISR of 0.2 and 90 ppb of background ozone will model higher NO<sub>2</sub> than ARM2 when the total NO<sub>x</sub> is above 250 ppb. Tests also indicate that lower ozone would produce PVMRM NO<sub>2</sub> results less than ARM2 NO<sub>2</sub> results up until 500 ppb of NO<sub>x</sub>, above which, PVMRM and ARM2 would have

roughly equal  $\text{NO}_2/\text{NO}_x$  ratios. Thus, areas that regularly experience exceptionally high hourly ozone levels should use ARM2 with caution.