NO_2 Modeling Techniques

Overview of Issue

The NO_2 modeling techniques currently available in AERMOD estimate the NO-to-NO_2 conversion via ozone in order to estimate total NO_2 impacts (which include both the converted NO and the emitted NO_2). The techniques available to estimate this conversion have three "tiers", with varying degrees of complexity, but even the most advanced Tier 3 techniques (*i.e.*, the Ozone Limiting Method, OLM, and the Plume Volume Molar Ratio Method, PVMRM), are considered screening rather than refined modeling techniques. As screening techniques, their use in regulatory applications should occur in agreement with the appropriate reviewing authority (paragraph 3.0(b) of Appendix W).

The EPA has not been able to identify either OLM nor PVMRM to be part of the preferred version of AERMOD modeling system for use as a refined model for all applications. This is due to two primary factors:

1. OLM and PVMRM both have known limitations as to which source types and configurations for which they work best. PVMRM is known to work best with relatively isolated sources, but it can potentially overestimate the NO-to-NO_2 conversion when plumes have significant overlap, as it can overestimate the amount of entrained ozone. OLM is somewhat less sophisticated than PVMRM as it does not estimate entrained ozone, but bases the NO-to-NO_2 conversion on the total amount of ozone present in the atmosphere. Thus, there appears to be a fundamental need for a refinement to PVMRM or OLM or an alternative Tier 3 model that addresses these limitations.
2. The databases available to evaluate NO_x emissions and NO-to-NO_2 conversion have several limitations, mainly uncertainty in the emissions and characterization of on-site ozone data. As a result, they are not of sufficient quality to make a determination of preference based on model performance. Thus, there is a need for additional field study databases with sufficient information to inform the preferred model selection process.

Current Implementation in AERMOD

AERMOD currently has multiple techniques to model NO_2 concentrations, all of which are considered screening techniques. Per Section 4.2.3.4 of the Guideline, the EPA recommends that NO_2 modeling should be done as a three-tiered screening approach, where each tier increases in complexity and decreases in conservativeness. The first tier is total conversion, so all emitted NO_X is immediately converted to NO_2. The second tier is the Ambient Ratio Method, ARM or ARM2. The ARM method and an updated ARM2 method are included in the most recent release of AERMOD, v16216r. [1] The ARM method uses a default ambient ratio to estimate NO-to-NO_2 conversion for all applications (0.75 as the default ratio for annual NO_2 and 0.80 as the default ratio for hourly NO_2). ARM2 adjusts the modeled NO_X concentrations based on an empirical relationship between ambient NO_X and ambient NO_2 concentrations. The third tier consists of two options: 1) the Ozone Limiting Method described by Cole and Summerhays (1979), and 2) the Plume Volume Molar Ratio Method developed by Hanrahan (1999).

[1] Though the original ARM method is included in the current version of AERMOD as an NOx conversion option, the updated *Guideline* specifies ARM2 as the preferred Tier 2 method.

OLM uses the assumption that either Ozone (O_3) or available NO_X is the limiting factor in the reaction of NO with O_3 to form NO_2. PVMRM estimates the amount of ozone entrained in the dispersion plume of a source to determine the amount of ozone that is available for oxidation of NO to form NO_2, then applies a limiting factor approach. Based on the recent revisions to the *Guideline*, the latest release of AERMOD, v16216r, includes a formulation update to PVMRM to provide more accurate calculations of dispersion plume volumes, especially for stable atmospheric conditions.

Summary of Current Literature or Research

Carruthers et al., 2017

This work documents the development of a technique to more accurately model chemical reactions to form NO_2, called the Atmospheric Dispersion Model Method, ADMSM. The ADMSM uses similar calculations for plume entrainment as PVMRM, but adds a “reaction rate” based on solar radiation and travel time from source to receptor. The reaction rate is based on the generic reaction set (GRS) chemistry scheme for multiple step conversions between NO, NO_2, and O_3. The authors provide comparisons of the two current AERMOD tier three methods, OLM and PVMRM (updated) to the ADMSM for four data sets. OLM showed the worst performance, because of its inherent method of maximum conversion. PVMRM showed better performance, because of the entrainment aspect of the calculation. ADMSM showed the best performance by including the entrainment methodology with the addition of travel time to calculate a reaction rate sing GRS.

Considerations for Updates in Model System

Updates to NO2 Tier 3 methods in the modeling system

The American Petroleum Institute (API) is currently working with the Atmospheric Dispersion Modeling System (ADMS) model developers (CERC) in the UK to implement the ADMS NO_2 chemistry scheme into AERMOD. This scheme is documented in the Carruthers (2017) article detailed above. An initial version of this NO_2 scheme integrated into AERMOD was shared with the EPA’s Air Quality Modeling Group in June of 2015. API is currently working with CERC to provide the EPA with an updated version of this approach. Once received, the EPA will evaluate this new method for consideration as an alternative model (i.e., beta option) for use as a Tier 3 method in AERMOD for NO_2 modeling. This could be available for public release in late 2018.

Database development and assessments of Tier 3 methods

Over the past several years, there have been several externally (non-EPA) funded field studies focused on NO_X emissions, some of which had the specific goal of providing a field database for model evaluation. The EPA is leading two workgroups that are evaluating these field studies for use as model evaluation databases. This evaluation will eventually result in new databases for public evaluations as well as peer-reviewed journal articles assessing model performance. It is hoped that these databases can be information that can help determine if the ADMS or other iterations of OLM or PVMRM can be considered as a refined model for specific cases, determine if a single model can be identified as a preferred model, or be used in the further development of an alternative Tier 3 method.

References

Carruthers, D.J., Stocker, J.R., Ellis, A., Seaton, M.D. and Smith, S.E. (2017). Evaluation of an explicit NO_X chemistry method in AERMOD. Journal of the Air & Waste Management Association, 67(6), pp.702-712.

Cole, H.S. and Summerhays, J.E. (1979). A review of techniques available for estimating short-term NO_2 concentrations. Journal of the Air Pollution Control Association, 29(8), pp.812-817.

Chu, S., Meyer, E. (1991). Use of ambient ratios to estimate impact of NOX sources on annual NO_2 concentration. In: Annual Meeting of the Air and Waste Management Association, Vancouver, British Columbia.

Hanrahan, P.L. (1999). The plume volume molar ratio method for determining NO_2/NO_X ratios in modeling—Part I: Methodology. Journal of the Air & Waste Management Association, 49(11), pp.1324-1331.

Podrez, M. (2015). An update to the ambient ratio method for 1-h NO_2 air quality standards dispersion modeling. Atmospheric Environment, 103, pp.163-170.