Modeling Challenges Posed by the New NAAQS for Nitrogen Dioxide and $PM_{2.5}$





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Compliance Challenges Issues for NO_2 and $PM_{2.5}$

- Very low ambient standards for NO_2 and $PM_{2.5}$ are resulting in new nonattainment areas
- Emission limitations in these areas must be solved with dispersion modeling
- Modeling is also used for permitting new sources
- NO_2 modeled compliance is complicated by secondary formation of NO_2 from NO and a new, strict 1-hour standard
- $PM_{2.5}$ modeled compliance is complicated by high existing concentrations and secondary formation of $PM_{2.5}$ from SO_2 and NO_X emissions
- There are many conservative modeling approaches that lead to concentration overpredictions

1-hr NO_2 National Ambient Air Quality Standard (NAAQS)

- 100 ppb for 98th percentile highest daily maximum averaged over three years
- EPA also has plans for NO_2 monitoring within 50 meters of major roads in cities with at least 500,000 residents
  - Likely a much higher level of NO_2 (factor of ~2 or more) concentrations within 100 meters of a major roadway
- As monitoring is expanded, the likelihood of new nonattainment areas is high
- Difficulties in showing modeled attainment due to conservative model approaches is also a problem

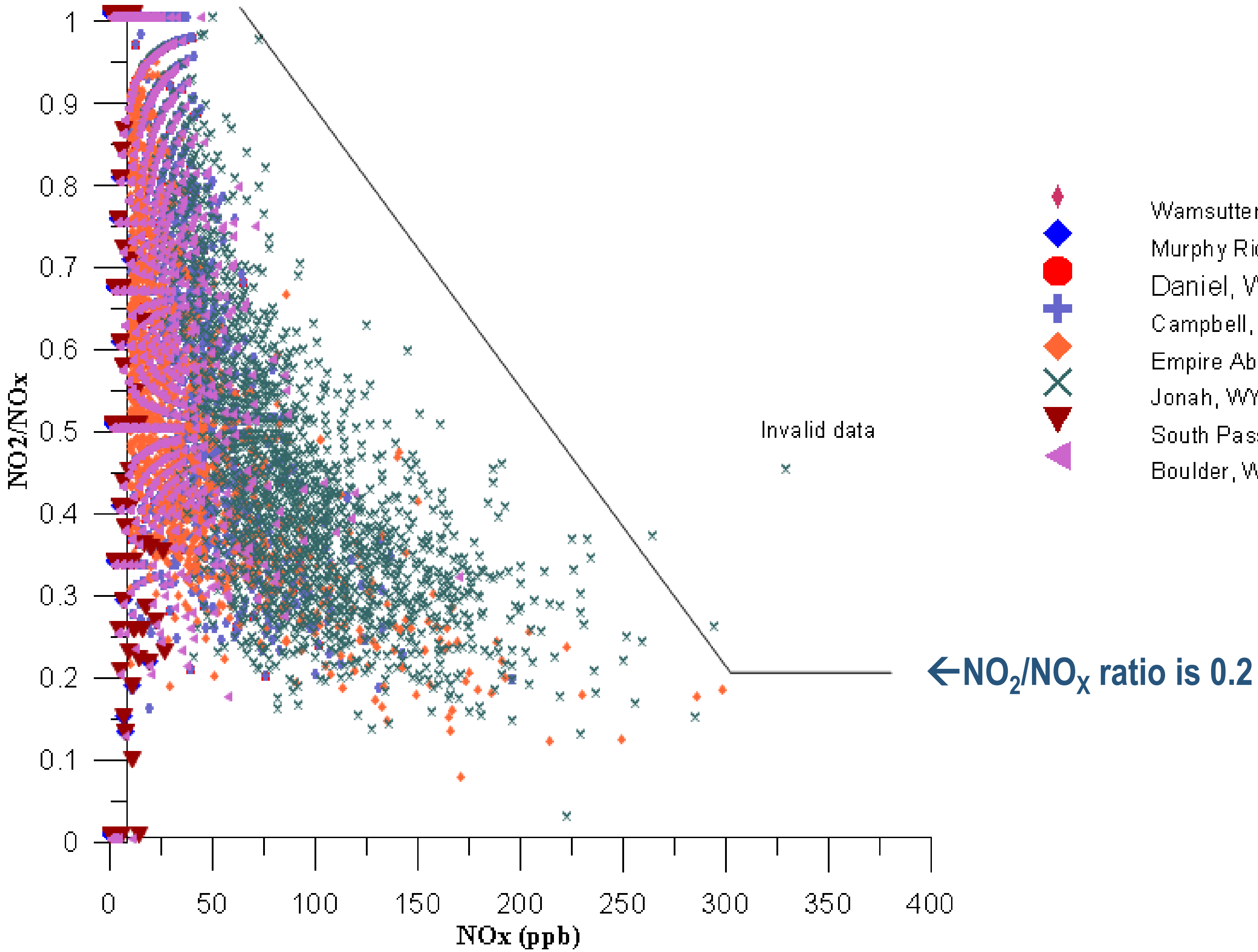
NO_2 Modeling Refinements Needed

- NO_2 is a secondary pollutant that depends upon the interaction between NO, ozone, and NO_2
- Most NO_x emitted as NO, which can be oxidized by ozone

$$NO + O_3 \rightarrow NO_2 + O_2$$

- Modeling assumes ambient air and plume to be well-mixed
- It is important to carefully characterize the emissions in terms of NO versus NO_2 components – need stack testing
- Conversion rate of NO to NO_2 needs refinement – near-field impacts can be the limiting case
- Models like AERMOD generally overpredict the rate of conversion of NO to NO_2
- Roadway emissions and ozone estimates near roadways are very challenging for modeling applications

Field Data Shows a Consistent Picture of NO_2/NO_X Ratios for High NO_X Concentrations



From Blewitt et al., 2011 A&WMA Annual Conference presentation

Limited Conversion of NO to NO_2

- Analysis of 30 years of NO/NO_2 rural monitoring data indicates that an upper bound for NO_2 conversion can be defined based on NO_X concentrations
- Based on this review (27,000 hours of data), at elevated NO_X concentrations the conversion fraction of NO_2 is low (~ 20%), but EPA uses an 80% conversion rate!
- For high NO_X concentrations (close to the source), there is insufficient time for conversion of NO into NO_2
- Modeling improvements needed for NO to NO_2 reaction:
  - Finite time for mixing of ozone into plume
  - Finite time for chemical conversion of NO to NO_2

Summary of Problems with 1-hour NO_2 Standard

- Very restrictive for permitting of new sources, even natural-gas fired sources
- Time required to resolve modeling problems can make permitting infeasible (a “permit killer”)
- When many sources are modeled together, the overprediction of actual concentrations can exceed two orders of magnitude!
- Modeling approaches need considerable refinement, but field databases for evaluation are lacking
- New monitoring could greatly expand the extent of nonattainment areas and result in even more modeling requirements

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Components of $PM_{2.5}$

- Direct $PM_{2.5}$ emissions consist of two components:
  - "Filterable" or "front half" – collected on filter
  - "Condensable" or "back half" (CPM) – condenses in ambient conditions
- Secondary particles that form in the atmosphere from chemical reactions
  - Precursors that react to form secondary emissions are SO_2, NO_X, VOC, and NH_3
  - Sulfates and nitrates most common, but they take some time to form after gases are emitted – difficult process to model

Regulatory Timeline for $PM_{2.5}$

- 1997: $PM_{2.5}$ NAAQS promulgated
  - 65 µg/m^3 24-hour average
  - 15 µg/m^3 annual average
- 1997 to 2010: Transitional NSR implementation guidance
  - Use PM_{10} as surrogate
- 2006: $PM_{2.5}$ NAAQS revised
  - 24-hour standard lowered to 35 µg/m^3
- October 2010: Final rule on PSD modeling SILs, SMCs and increments
- 2011: annual NAAQS review staff policy assessment: suggest lowering annual NAAQS to 11-12 µg/m^3
- Late 2011: states and activists ask DC District Court of Appeals to force EPA to issue a proposed revision to the $PM_{2.5}$ annual NAAQS

Modeling is Needed to Resolve Nonattainment Areas and for New Source Review Permitting

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- Many more nonattainment areas could occur with more stringent annual $PM_{2.5}$ NAAQS
- EPA has not updated their modeling guidance for $PM_{2.5}$ (draft expected in early 2012)
- Method for adding modeled and background concentrations is still not settled
- Short-range models only deal with direct $PM_{2.5}$ emissions, but EPA must deal with secondary emissions due to Sierra Club legal challenge
- Long-range models can predict secondary $PM_{2.5}$
  - But CALPUFF critiqued for simplistic secondary PM chemistry; new version 6.4 has improved chemistry
  - Regional models (CMAQ, CAMx)
    - not evaluated for single source modeling
    - significant resource requirements

General Model Overprediction Issue #1: Adding Source Impacts and Background Concentrations

- If many sources are modeled, then modeling overpredictions are additive – need to restrict extent of modeled sources
- If peak monitoring concentrations are added to account for unmodeled sources, that will result in overly high total predictions
- Best approach is to add background concentrations and modeled concentrations on a concurrent, hourly basis
- EPA is resistant to these practical suggestions and prefers conservative approaches that can lead to false nonattainment issues

Model Overprediction Issue #2: Need for Refined Input Data

- Especially in high terrain areas, AERMOD is designed to be conservative without use of multiple-level meteorological data
- Use of low-level meteorological data for tall stack releases in terrain can lead to large overpredictions
- Lack of representative concurrent monitoring data can also result in use of peak background values from monitors in urban areas
- Acquisition of site-specific meteorological and ambient data can substantially affect modeling results

Model Overprediction Issue #3: Selection of Emission Rates

- Large emission variation possible over the course of a year
- Highly intermittent sources (e.g., emergency backup engines) present important modeling challenges
- For these sources, assuming fixed peak 1-hour emissions on a continuous basis will result in unrealistic modeled results, even using a theoretically perfect dispersion model
- Better approach is to assume a distribution of emission rates and use a Monte-Carlo emission selection procedure
- EMVAP (Emissions Variability Processor), being developed for EPRI by AECOM, could fit well with the probabilistic forms of the short-term NAAQS

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EMVAP Overview and Summary

- Use of peak emission rates for intermittent or variable emissions sources can result in unrealistic peak predictions
- This is evident in evaluations conducted on AERMOD validation databases
- Use of emission rates selected using actual probability of their occurrence results in improved model performance
- This process is currently being tested as a Monte-Carlo technique that is a post-processor to AERMOD – creates hundreds or thousands of simulated years of concentrations - averaged to determine the expected result
- EMVAP can result in a more reasonable estimate of the distribution of 98th or 99th percentile values over a given simulation period (e.g., 1000 or more realizations)

Summary of Issues for NO_2 and $PM_{2.5}$

- Both NO_2 and $PM_{2.5}$ NAAQS are stringent and involve complex modeling challenges with secondary formation
- Current and future nonattainment areas will increase need for modeling applications
- New Source Review permitting is very difficult with these new NAAQS and conservative modeling approaches
- More realistic and unbiased modeling assessment methods are needed in light of tightening standards
- Even if the models were perfect (which they aren't), substantial challenges are present for areas of how background is accounted for, need for refined input data, and consideration of emission input data