



Review of Plume Volume Molar Ratio Method (PVMRM) and Ozone Limiting Method (OLM) for Predicting Short-term NO₂ Impacts

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Topics for Discussion

- ISC and AERMOD PVMRM and OLM code review
- Improving plume models based on scientific principles
- Data sets for PVMRM and OLM model evaluations
- Conclusions



Review of the OLM and PVMRM Codes

- The purpose of the code review was to:
 - Determine if the AERMOD and ISC models were coded in a manner consistent with the formulation
 - Assess if the model algorithms are well founded

- Reviewed:
 - Cole and Summerhays (1979) for the OLM formulation
 - Hanrahan (1999a and b) and EPA (2004) Addendum to the AERMOD Model Formulation Document for PVMRM
 - Other related documents



Structure of the Ozone Limiting Method (OLM)

- The OLM involves an initial comparison of the estimated maximum NO_x concentration and the ambient ozone concentration to determine which is the limiting factor to NO_2 formation
- If the O_3 concentration is greater than $[\text{NO}_x]_{\text{max}}$, then total conversion is assumed
- If $[\text{NO}_x]_{\text{max}}$ is greater than the O_3 concentration the formation of NO_2 is limited by the ambient O_3 concentration



Results of the OLM Review in the ISC and AERMOD Codes

- The OLM was implemented in both the ISCST3 model and AERMOD model (09292) according to the method formulation as described in Cole and Summerhays (1979)
- The OLM method does not account for the molar ratio of NO_x to ozone mixed into the plume



Structure of the PVMRM

- The PVMRM routine calculates the molar ratio of ozone to NO_x in an effluent plume at receptor locations using dispersion (quasi - instantaneous) rates that differ from those that are being used by AERMOD to calculate the NO_x concentration. These are described as relative vs. continuous diffusion rates.
- This molar ratio is multiplied by the NO_x concentrations provided by AERMOD to calculate the NO_2 concentrations in the plume.
- PVMRM includes a method to simulate multiple NO_x sources by accounting for how the plumes merge and combine.
- Neither OLM nor PVMRM account for the gradual entrainment and mixing of ambient ozone in the plume. Fresh ozone is assumed to be uniformly mixed across the cross section.



Structure of the PVMRM Routine in the ISC and AERMOD Models

- As implemented for use with ISC predicted NO_x concentrations, the PVMRM routine is in a separate post-processor code (Hanrahan, 1999)
- PVMRM is a non-default option in AERMOD
 - Calculations are part of the internal AERMOD Fortran code.



AERMOD PVMRM – Technical Issues

Number of AERMOD standard deviations from plume centerline that define the plume volume (value of “ n_z ”)

- The PVMRM method has its own dispersion parameter formulas (different from AERMOD) that assume $\sigma_{y \text{ PVMRM}} = \sigma_{z \text{ PVMRM}}$ and that $R = n_z \sigma_{y \text{ PVMRM}} = n_z \sigma_{z \text{ PVMRM}}$
 - AERMOD/PVMRM employs a top hat type distribution (concentration constant across the plume radius R) of contaminants within a plume
 - AERMOD itself employs a Gaussian distribution with standard deviation σ_y and σ_z



AERMOD PVMRM – Technical Issues

Number of AERMOD standard deviations from plume centerline that define the plume volume (value of “ n_z ”)

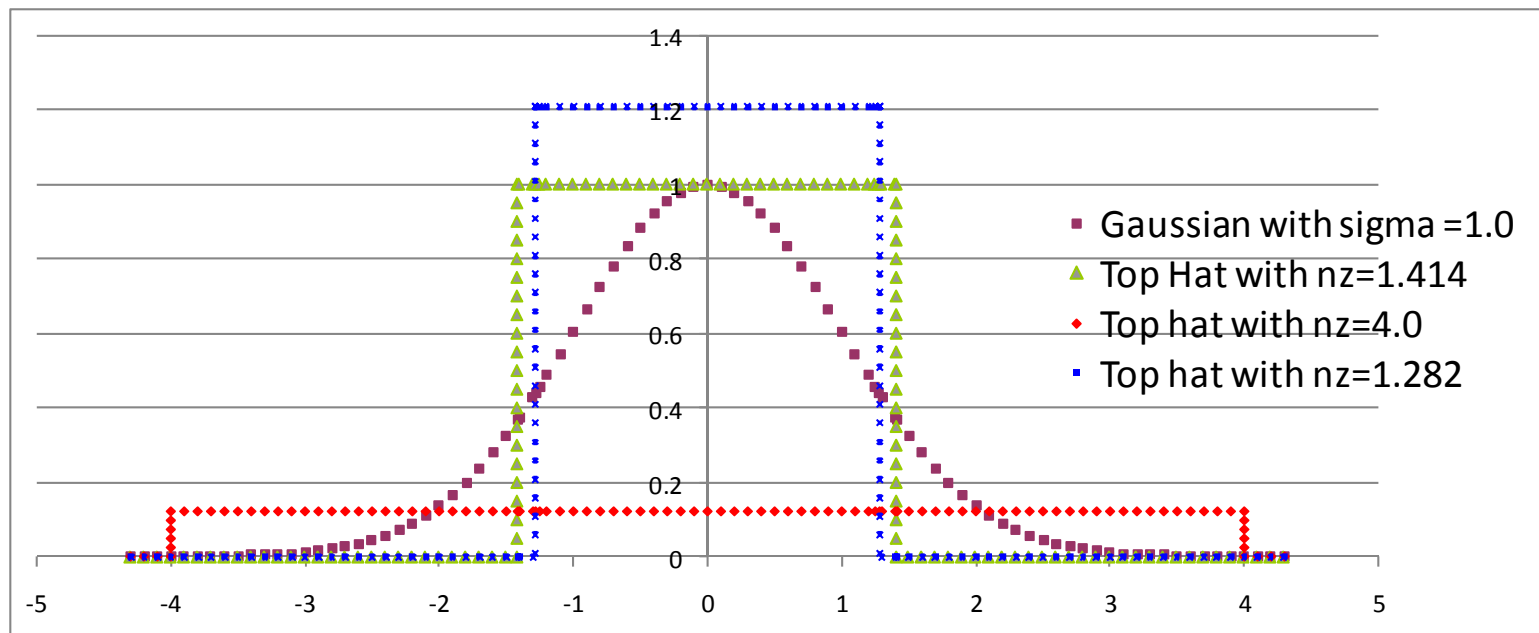
- Hanrahan notes that the choice of n_z “is somewhat arbitrary” since the intent is to fit a top hat over a Gaussian shape, and chose a value of $n_z = 1.282$, noting that 80% of the area under the normal curve is between ± 1.282 standard deviations of the mean value.
- In the AERMOD/PVMRM model, a value of $n_z = 4.0$ was chosen which corresponds to “about 99.99% of the volume under the normal curve”.
 - $n_z = 4.0$ results in a poor “fit” since the top hat is a shallow pancake compared to the Gaussian shape.



AERMOD PVMRM – Technical Issues

2-D representation of the number of AERMOD standard deviations from plume centerline that define the plume volume (value of “ n_z ”)

Cross sections of equivalent Top Hat and Gaussian distributions:





AERMOD PVMRM – Technical Issues

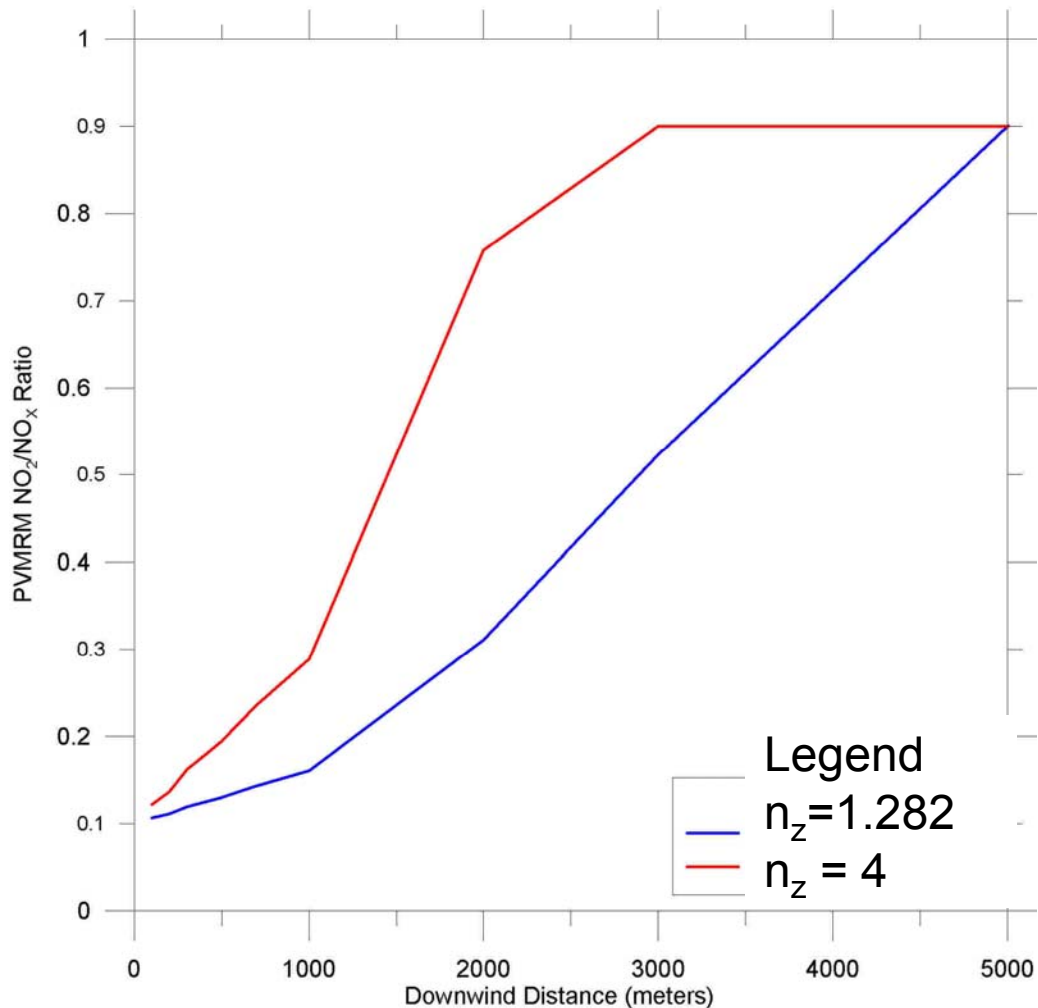
Number of AERMOD standard deviations from plume centerline that define the plume volume (value of “ n_z ”)

- Equating the mass flux in a Gaussian distribution with that in a top hat distribution and assuming that the centerline concentrations are about the same would result in a “best-estimate” of n_z taking on a value of between about 1.25 and 1.5. (That is $R = 1.25 \sigma$ to 1.5σ)
- Conclusion: The value of n_z should be in the range of 1.25 to 1.5. The value used by Hanrahan was within this range, and it should be retained. A value of 4 is much too large and results in too much ozone being mixed into the plume and hence too much conversion of NO to NO₂.



PVMRM – Implications of n_z Choice

NO₂/NO_x Ratio vs. Downwind Distance



Conditions

Ozone = 100 ppb

NO_x = 100 g/s

U = 3 m/s

Downwind plume volume fluxes based on ISC sigmas

Ratio values based on Excel emulator of ISC PVMRM

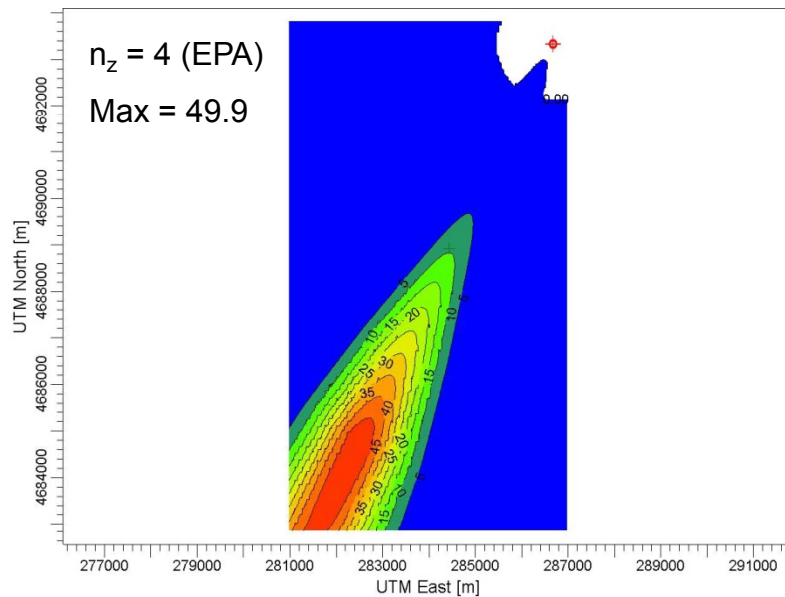
Instack NO₂ / NO_x = 0.1

Ambient Equilibrium = 0.9

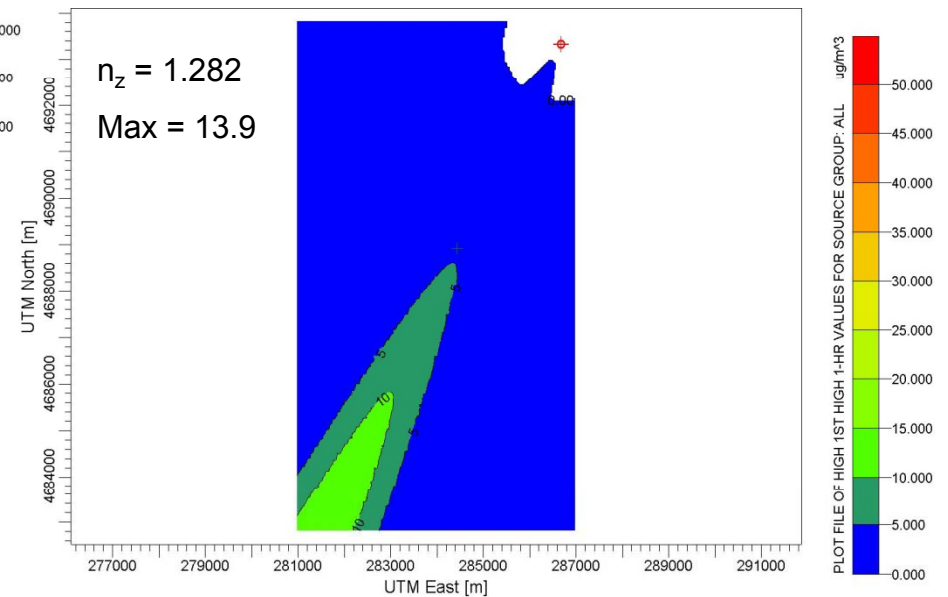


AERMOD PVMRM

1-hour NO₂ conc (ug/m³) as a function of n_z



1-hour NO₂ concentrations
2 stacks, tall, buoyant,
approximately co-located
26,000 receptors spaced 50m apart
4.1 m/s wind from 26°
Relatively stable atmosphere



NOTE:

Near field almost identical
Factor of 3.5 difference in maximum



AERMOD PVMRM – Technical Issues

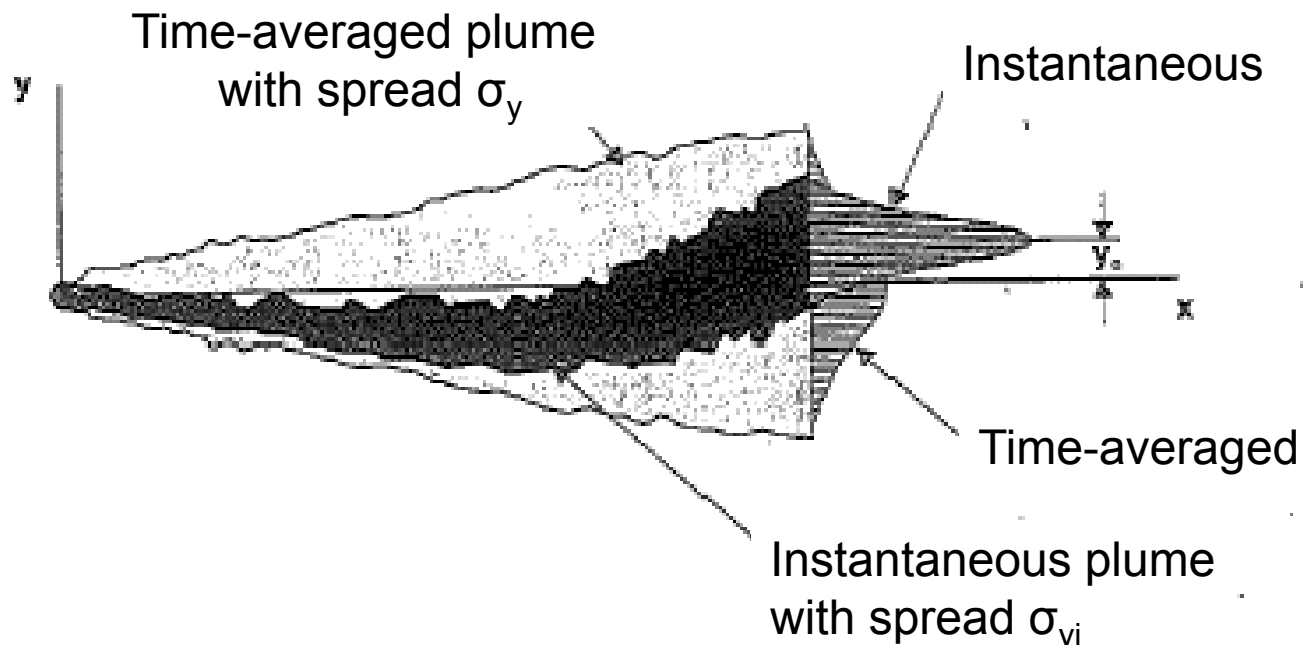
Definition of the Time-Averaged (AERMOD) Ensemble Plume Volume Compared to the Relative (PVMRM) Plume Volume

- In AERMOD the PVMRM plume relative σ_r (same in all directions) is based on Weil's (1996, 1998) relative dispersion formulation that was suggested for the U.S. Army SOBODM puff dispersion model for daytime conditions.
 - Weil's formula is for unstable conditions and does not account for neutral or stable conditions.
 - The lateral and vertical dispersion parameters are assumed equal (i.e., $\sigma_r = \sigma_y = \sigma_z$) in PVMRM, an assumption that is not valid for stable conditions, when vertical dispersion is less.
 - Spot checks of the σ 's calculated by PVMRM and AERMOD show large differences (more than a factor of two) in many combinations of meteorological scenarios. Sometimes the differences are positive and sometimes negative.
 - As explained in fundamental texts such as Pasquill (1974), the relative σ should never exceed the continuous plume σ .



AERMOD PVMRM – Technical Issues

Definition of the Time-Averaged (AERMOD) Ensemble Plume Volume Compared to the Relative (PVMRM) Instantaneous Plume Volume



Dr. D. J. Wilson 1995, "Concentration Fluctuations and Averaging Time in Vapor Clouds"
(CCPS Concept Book)



AERMOD PVMRM – Technical Issues

Definition of the Time-Averaged (AERMOD) Ensemble Plume Volume Compared to the Relative (PVMRM) Plume Volume

POTENTIAL SOLUTIONS to IDENTIFIED PROBLEMS

For Current Structure:

- 1) Add a relative dispersion formula for neutral and stable conditions,
- 2) Impose a condition that the relative and time-averaged sigma formulas have consistent relations to each other, so that the relative sigma is never larger than the time-averaged sigma, and
- 3) Eliminate the isotropic condition for stable plumes which we know have smaller depths than widths.



AERMOD PVMRM – Technical Issues

Definition of the Time-Averaged (AERMOD) Ensemble Plume Volume Compared to the Relative (PVMRM) Plume Volume

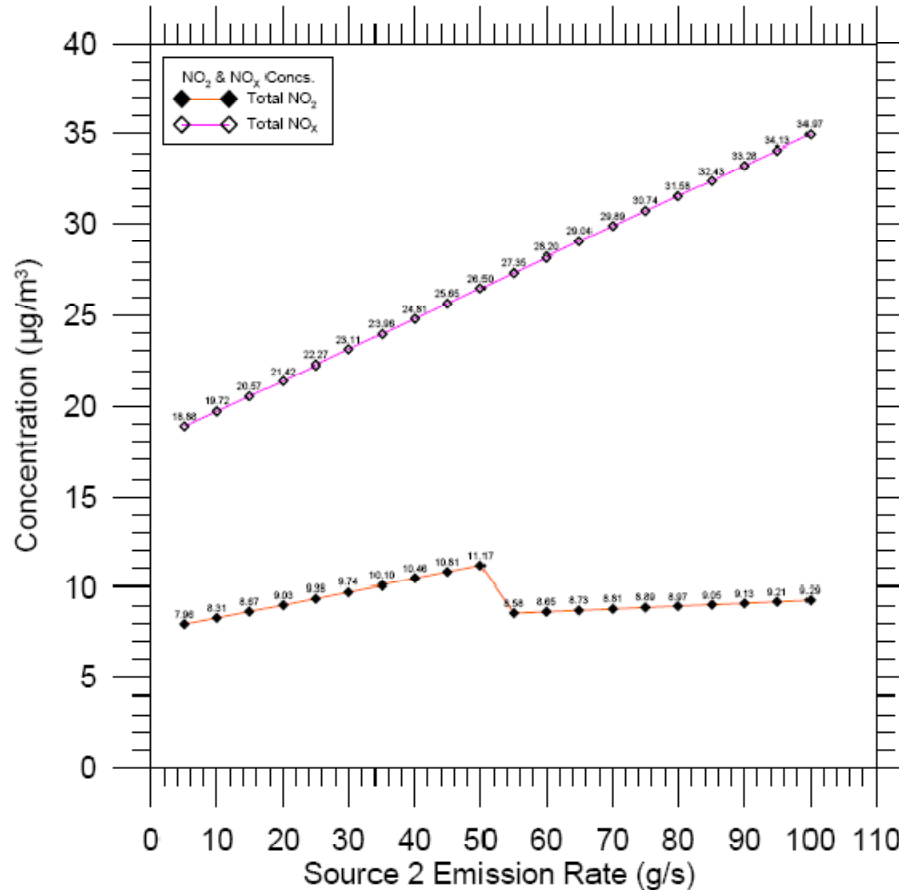
SUGGESTED ALTERNATIVE RELATIVE DISPERSION FORMULAS TO BE INVESTIGATED:

- 1) Basic theory of effects of averaging time on dispersion, in book chapters on fundamentals of atmospheric dispersion by Gifford (1968) and Pasquill (1974)
- 2) D. J. Wilson (1995) CCPS Book entitled “Concentration Fluctuations and Averaging Time in Vapor Clouds”
- 3) Integrating theory (Langevin model) on puff dispersion and its approach to continuous plume dispersion, and its validation with observations as described in a series of journal articles by Gifford in the 1990s
- 4) SCICHEM model approach (several journal articles by Sykes et al.)



AERMOD PVMRM – Other Issues

Discontinuities in predictions when multiple plume volumes are combined. The emission rate of 2nd source is shown (below 50 g/s, source #1 is dominant alone; above 50 g/s, both sources are considered in a combined plume volume.)



When the emission rate of a second source is such that it contributes at least half of the dominant plume impact at a receptor, the multiple plumes will combine. This can result in discontinuities of predicted NO₂ concentrations.



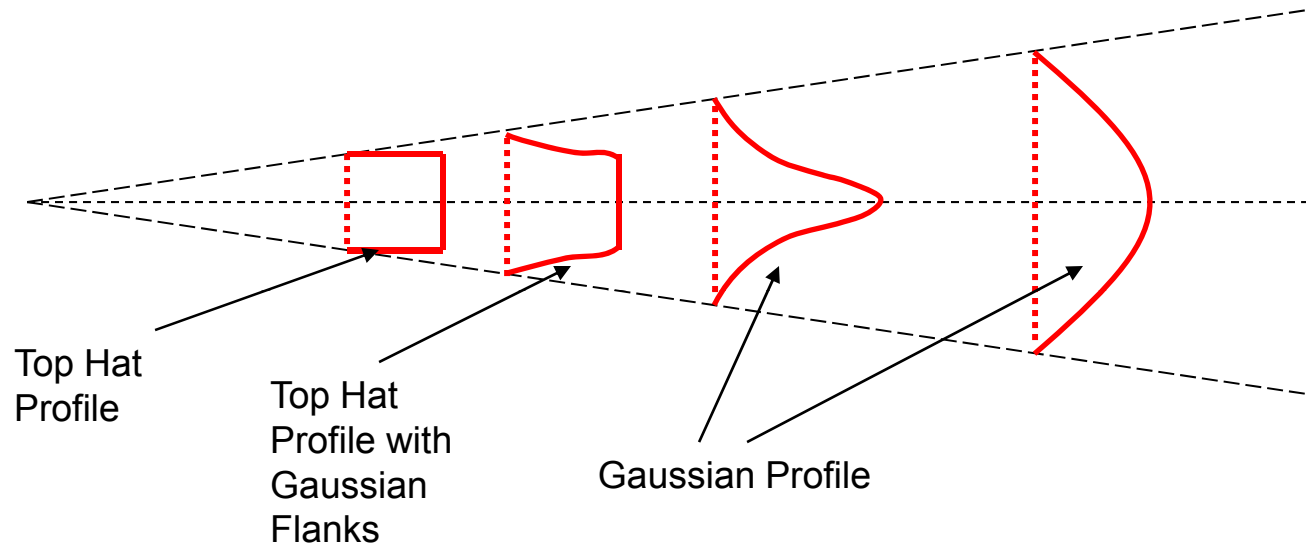
AERMOD PVMRM – Other Issues

Downwash Conditions

- PVMRM does not appear to adjust the plume σ_r to account for downwash. Downwash should be considered in both the relative diffusion and total diffusion categories because it occurs close to the source.
- Net effect would be more entrainment of ambient ozone and hence more production of NO_2
- Downwash is already considered in the AERMOD main plume model (i.e., total diffusion)



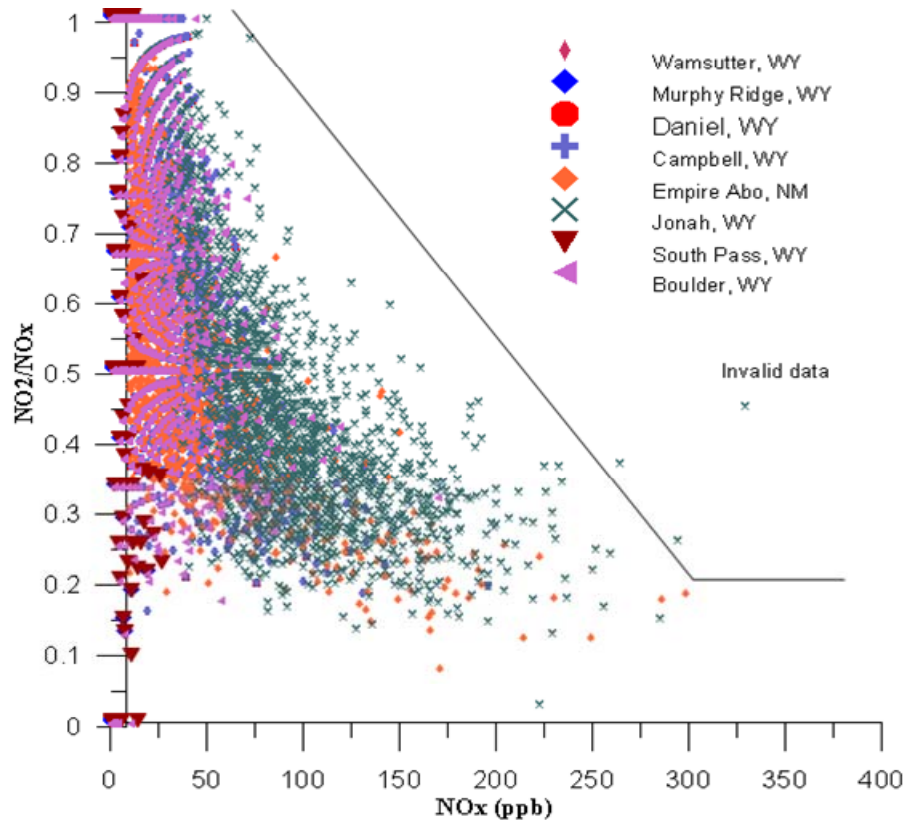
Possible Modification to Plume Model to Better Account for Plume Edge Effects



- Ozone limited
- Entrainment limited – fresh ozone is mixed into the edges of the plume leaving a core of NO (currently assumed that the entrained air is instantaneously mixed across the plume)
- Reaction time limited (currently assumed to be instantaneous)

NOTE: The SCICHEM and RPM-IV models already account for these effects

Monitoring Data are Consistent with more Complicated Ozone Entrainment Assumptions



- 30 years of hourly NO_x/NO₂ sampling, 200 to 5000 feet downwind
- If the sampler is on the plume centerline (NO_x conc is higher), the fraction of NO₂ is low
- If the sampler is on the edge of the plume (NO_x conc is lower) the conversion fraction is high
- This suggests that at these downwind distances, fresh ozone is not mixing much into the core of the plume
- This contrasts with OLM and PVMRM assumption of uniform mixing of fresh ozone across the plume

Cumulative Analysis of Empire Abo, NM and Wyoming NO₂ Monitoring Data

Source: Blewitt et. al., 2011, "Analysis of Near Field NO₂ Conversion Rates and the Development of a NO₂ Repartitioning Modeling Approach for Demonstrating Compliance with the 1-Hour NO₂ Standard"
Paper 2011-A-626-AWMA



Data Sets for OLM and PVMRM Evaluation

To conduct an appropriate model evaluation, one needs complete emissions and source parameters, ambient pollutant monitoring data and meteorology

- **Limited number of data sets used by EPA for OLM and PVMRM 1-hr evaluations:**
 - *Empire Abo, NM* - gas plant (emissions are based on PTE; no data on hourly load or fuel consumption)
 - *Palaau, HI* – oil fired turbine (data set uncertainties unknown)
- **We would like to perform an independent evaluation of the above data sets**
- **Potential data sets we are investigating:**
 - *KEMA - Aircraft measurements, Arellano and Bange* (source parameters were estimated)
 - *Alaskan Power Plant*
 - *San Juan, NM Power Plant*
 - *Others?* Please help us find other data bases.



New Model Evaluation Data Set – Alaskan Power Plant

- Remote location: small village north of the arctic circle
- Ambient monitoring station measuring hourly NO_x , NO_2 and O_3 concentrations and meteorological parameters (wind speed, wind direction, temperature)
- Local Power Plant located approximately 500 meters from the ambient monitoring station
- The power plant consists of 5 diesel generators (3 CAT 3508 and 2 CAT 3512). Each generator is vented through its own stack.
- Hourly operators logs are available that specify which engines are operating and the kilowatt output from each engine for each hour. An hourly emissions file and stack parameters have been generated based on the operator logs and the Caterpillar engine performance data.
- *Limitations* - No stack testing has been conducted.



Potential Model Evaluation Data Set – San Juan, NM Power Plant

- Isolated coal fired power plant near Farmington, NM
- Large stack height
- Title IV facility – CEMS data for NO_x
- Monitored NO , NO_2 , NO_x and O_3 data
- Monitored NO_2 concentrations can be traceable to the facility
- Meteorological data available from State of New Mexico
- Modeling files (downwash analysis) provided by State of New Mexico



Conclusions

- There are some technical issues and some inconsistencies in the AERMOD PVMRM formulation for short term NO₂ modeling:
 - The number of AERMOD standard deviations from the plume centerline that define the plume volume (value of “n_z”) is too high by about a factor of 3 or more
 - No relative dispersion formulas are provided for stable and neutral conditions
 - Currently, the relative (instantaneous) σ can exceed the continuous plume (time-averaged) σ .
 - Discontinuities in concentration can occur for multiple plumes, with the magnitude depending on the scenario modeled
 - Downwash is not considered
- OLM and PVMRM do not address the fact that ambient ozone is entrained at the edges of the plume and is not immediately mixed to the center of the plume.

We have suggested approaches to address some of these issues



Recommendations

- Additional complete data sets should be evaluated
 - One of the field data sets previously used for EPA 1-hr evaluations is missing key inputs such as detailed stack emissions and stack dimensions

- External and independent peer review of the model science, field data sets and evaluations should be completed

- Other currently-available models and approaches should be evaluated for short-term NO₂ modeling such as SCICHEM, RPM-IV, and the Monitored Ratio Method/Ambient Ratio Method 2



Want More Information?

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<http://mycommittees.api.org/rasa/amp/default.aspx>

- Final technical report for the OLM and PVMRM code review (to be posted by 7/31/2011)
- Information on the Ambient Ratio Method 2 Study – Use of ambient monitoring data to empirically predict NO₂/NO_x ratio based on NO_x concentration
- AERMOD Low Wind Speed Study - Final Report

or

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