



NO₂ Conversion Model Development

EPA RSL Workshop

U.S. EPA / OAQPS / Air Quality Modeling Group

Monday, June 21, 2021

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NO₂ Conversion - Development

- **Purpose/Goal:** Improve NO₂ predictions for a wide variety of sources
- **External Collaboration:** API, PRCI, AECOM, ERM, CERC, WRAP/WESTAR, R2 & R6, BLM, EPRI
- **AERMOD v.21112:** Two new **alpha** options; developed by CERC and AECOM/ERM/EPA
 - Travel Time Reaction Method (TTRM), conversion of NO to NO₂ based on reaction time limitations calculated from the travel time from source to receptor.
 - General Reaction Set Method (GRSM), conversion based on equilibrium chemistry between NO, NO₂, and ozone.
- **Two near-field NO₂ field datasets finalized in 2019-2020**
 - Balko, OK: 4 monitors, ~12 months of data
 - Denver-Julesburg Basin, CO: 12 monitors, ~2 months of data
- **Additional datasets for evaluations**
 - Existing NO₂ datasets, Palaau, Empire Abo, Wainwright, & Prudhoe Bay
 - Identify any supplemental datasets from NO₂ network



NO₂ Conversion - Work Needed

- **Testing for TTRM and GRSM**
 - Both were added to the AERMOD code relatively late in the development process, need to be tested to verify functionality
- **Determine the appropriate application of TTRM**
 - Unclear if TTRM is a stand-alone method (unlikely) or needs to be paired with ARM2, OLM, or PVMRM for near-field
- **Evaluation with new and old datasets**
 - Comprehensive model evaluations of all methods with all datasets
 - Determine if there is a best performing model & that there is no bias to underpredict
 - Add best performing model to newer source types (e.g., RLINE)



NO₂ Conversion – NO₂/NO_x ISRs

- NO₂/NO_x in-stack ratio database updated Oct 2020
 - Database combined with old “alpha” database
 - Added new survey data from EPRI and PRCI
 - Four different tabs of data in the spreadsheet
- Varying levels of detail provided in each dataset
 - “Alpha” dataset not associated with alpha/beta options in AERMOD, data was just the first round collected prior to the formal data collection (2074 entries)
 - “NO₂_ratio_dataset” has extensive meta-data, intended to provide traceability and some QA (2379 entries)
 - “PRCI” (3199 entries) and “EPRI” (123 entries) result of surveys conducted by each trade group
- No hierarchy to the data, all data is provided as-is
 - Up to the regulating agency to determine the applicability of any data in the database

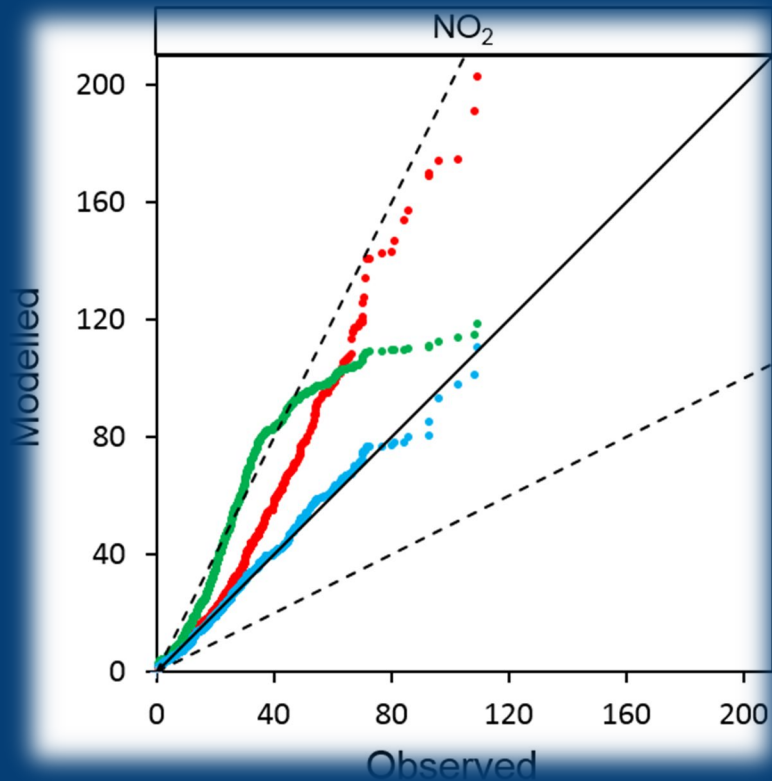
Theory, application and evaluation of the Generic Reaction Set Method (GRSM) for NO₂ chemistry

Dr. Jenny Stocker

2021 EPA Regional/State/Local
Dispersion Modelers' Workshop

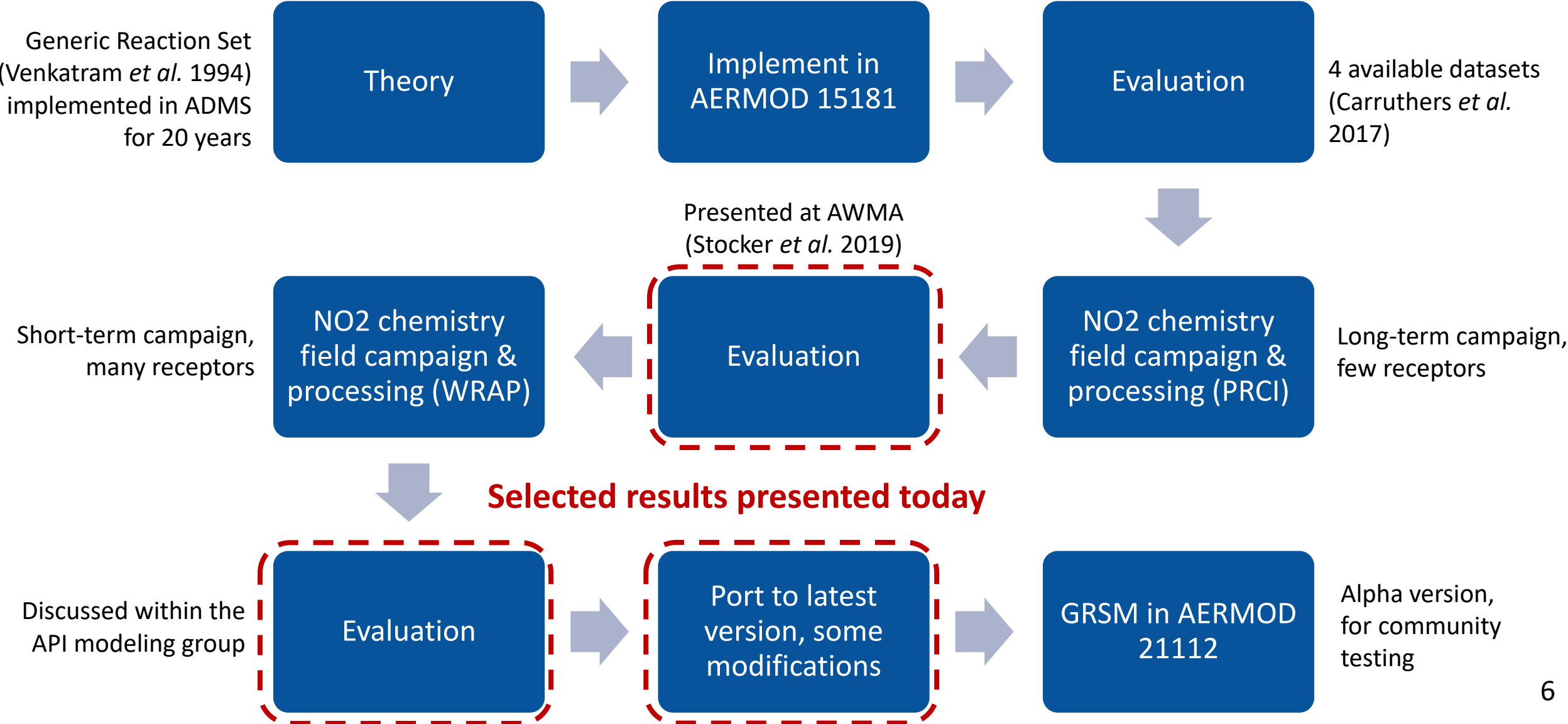
21 June 2021

Online



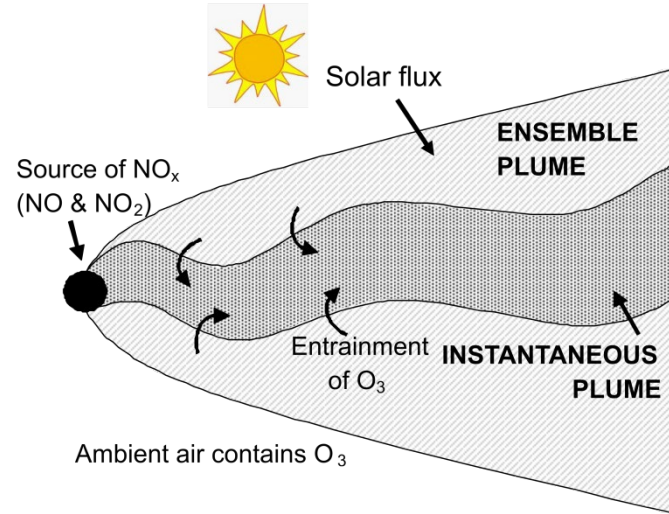
GRSM development

Development of GRSM (2015-2021, funded by API)



AERMOD chemistry schemes

Comparison of *regulatory* NO_2 conversion options that require O_3 background compared to *GRSM alpha* option



NO_x chemistry

'Ozone titration'



'Photolysis'



Fast reactions
(seconds - minutes)

| Item | OLM (Ozone-Limiting Method) <i>regulatory</i> | PVMRM (Plume Volume Molar Ratio Method) <i>regulatory</i> | GRSM (GRS Method) <i>alpha</i> |
|---|---|---|---|
| Hourly background | O_3 | O_3 | O_3 , NO_x , NO_2 |
| Method for 'O ₃ titration' | 100% conversion | 100% conversion | Explicit calculation |
| Method for 'photolysis' | Neglects | Neglects | Explicit calculation |
| Method for entrainment of O_3 into the plume | Fully entrained into <i>ensemble</i> plume | Limited entrainment (volume-based approach) into <i>instantaneous</i> plume | Limited entrainment (cross-sectional area-based approach) into <i>instantaneous</i> plume |
| Main sources of inaccuracy of predicted NO_2 | Full entrainment into ensemble plume so upper bound for NO_2 | Neglects reaction rates; assumptions relating to entrainment method | Reaction rates; assumptions relating to entrainment method |

Evaluation methodology

- Configure AERMOD to model NO_x concentrations (*initial model set up by API contractor, AECOM*)
- Evaluate NO_x model performance
- Modify configuration to ensure best NO_x performance - e.g., evaluate different met options
- Configure AERMOD to model NO₂ concentrations using OLM, PVMRM and GRSM
- Evaluate NO₂ model performance in terms of:
 - Performance relative to NO_x - e.g., if NO_x is under-predicting, so should NO₂ and vice versa
 - Chemistry performance - e.g., compare measured and observed NO₂/NO_x
 - Near-field and far field performance

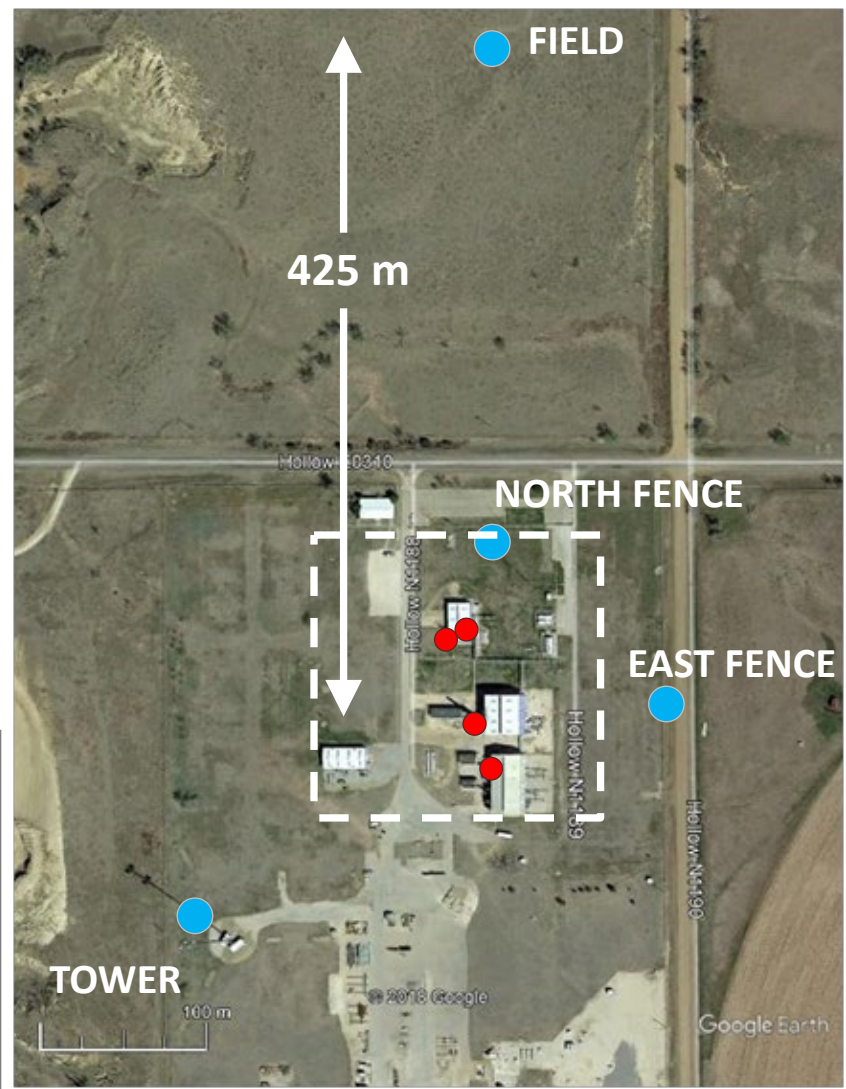
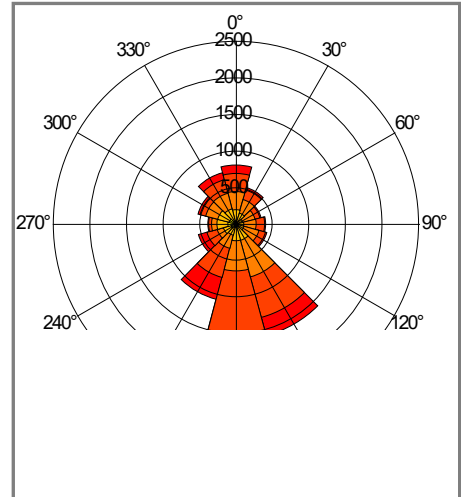
Ensure data paired in space and time

PRCI NO₂ chemistry field campaign (1 of 3)

13 month campaign at Balko, Oklahoma

- 4 main NO₂ sources:
 - 2 compressor engine stacks
 - 1 boiler
 - 1 emergency generator

Meteorological instruments on 30 m tower



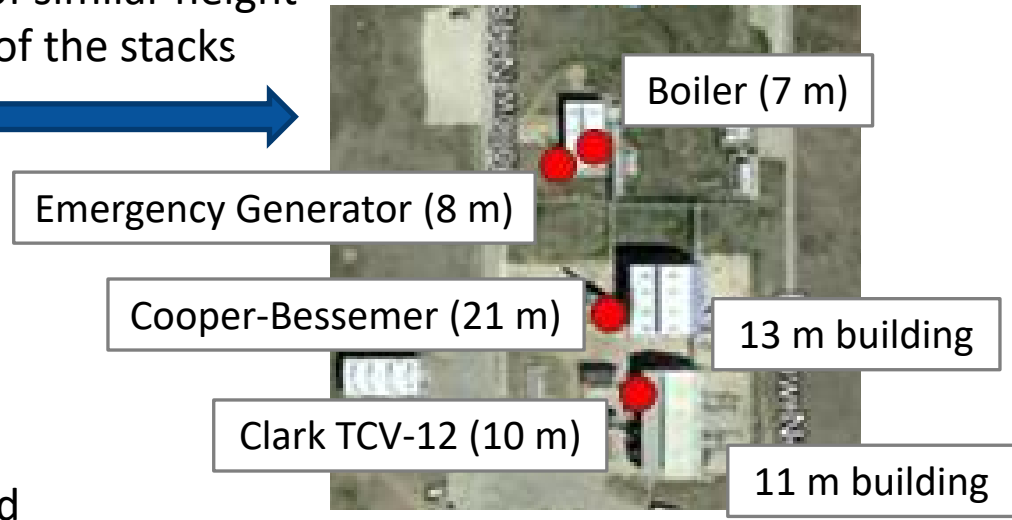
Parametric Emissions Monitoring Systems (PEMS) recorded hourly engine parameters (compressor engines only)

- 4 monitors:
 - 'North Fence' and 'Field' in alignment with the stacks and the prevailing wind
 - 'East Fence'
 - 'Tower'

Buildings adjacent to compressor engine stacks of similar height to one of the stacks



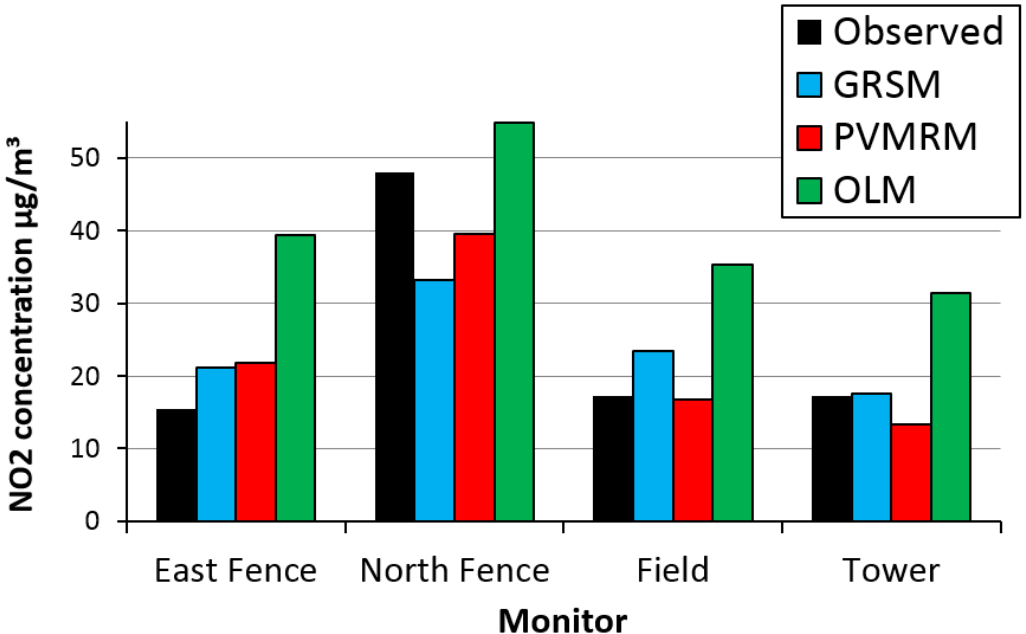
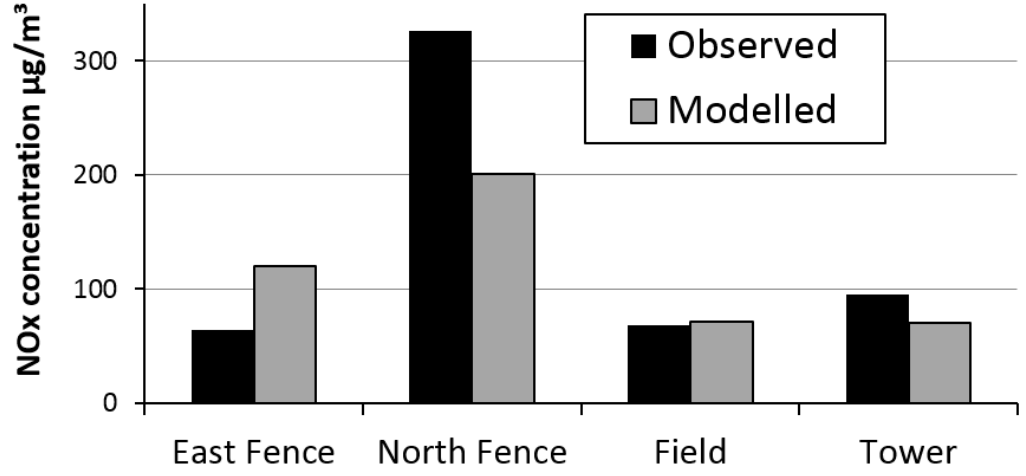
'Downwind sector' datasets analysed



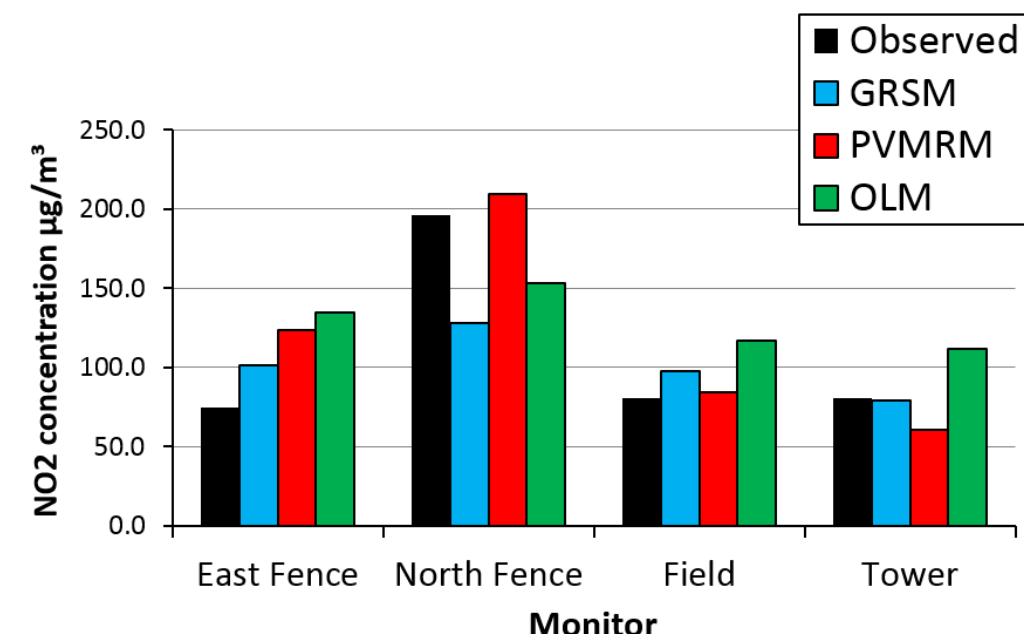
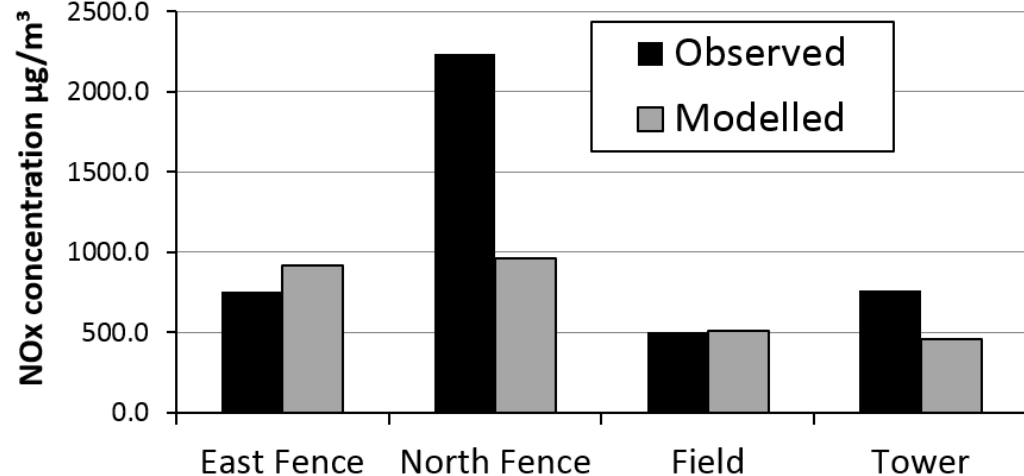
Clark TCV-12 compressor engine emissions dominate

PRCI NO₂ chemistry field campaign (2 of 3)

Period average: all monitors



Highest 10 values: all monitors

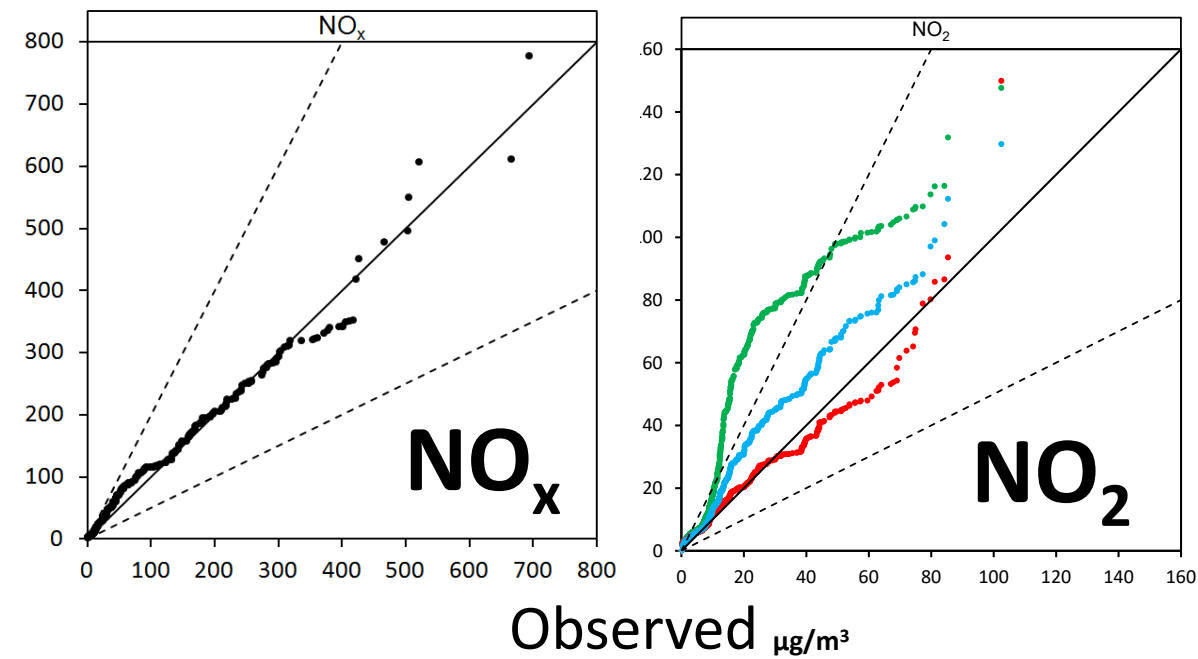
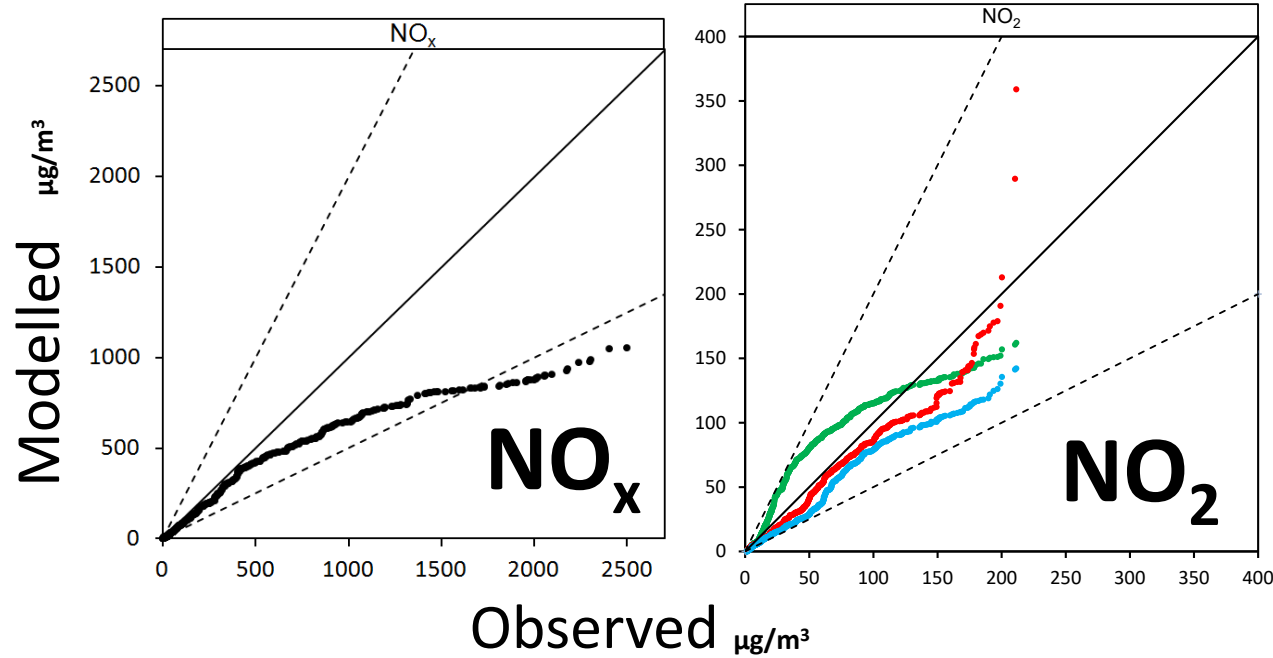


PRCI NO₂ chemistry field campaign (3 of 3)

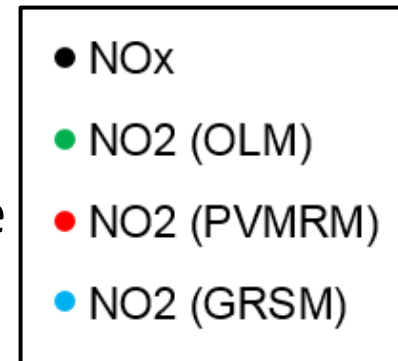
QQ plots:

North Fence (140 m)

Field (425 m)



- For high concentrations, GRSM NO₂ slightly over-predicted relative to NO_x at 140 m & 425 m downwind - may be related to uncertainty in ISR
- GRSM demonstrates consistency between NO_x & NO₂ with downwind distance
- PVMRM NO₂ over-predicts at 140 m & slightly under-predicts at 425 m



WRAP NO₂ chemistry field campaign (1 of 4)

2 sequential campaigns at adjacent Colorado drill rig sites ~ 5 weeks in total (October-November)

12 monitors (~ 100 m from main stacks) record NO_x and NO₂, 2 monitors also record O₃

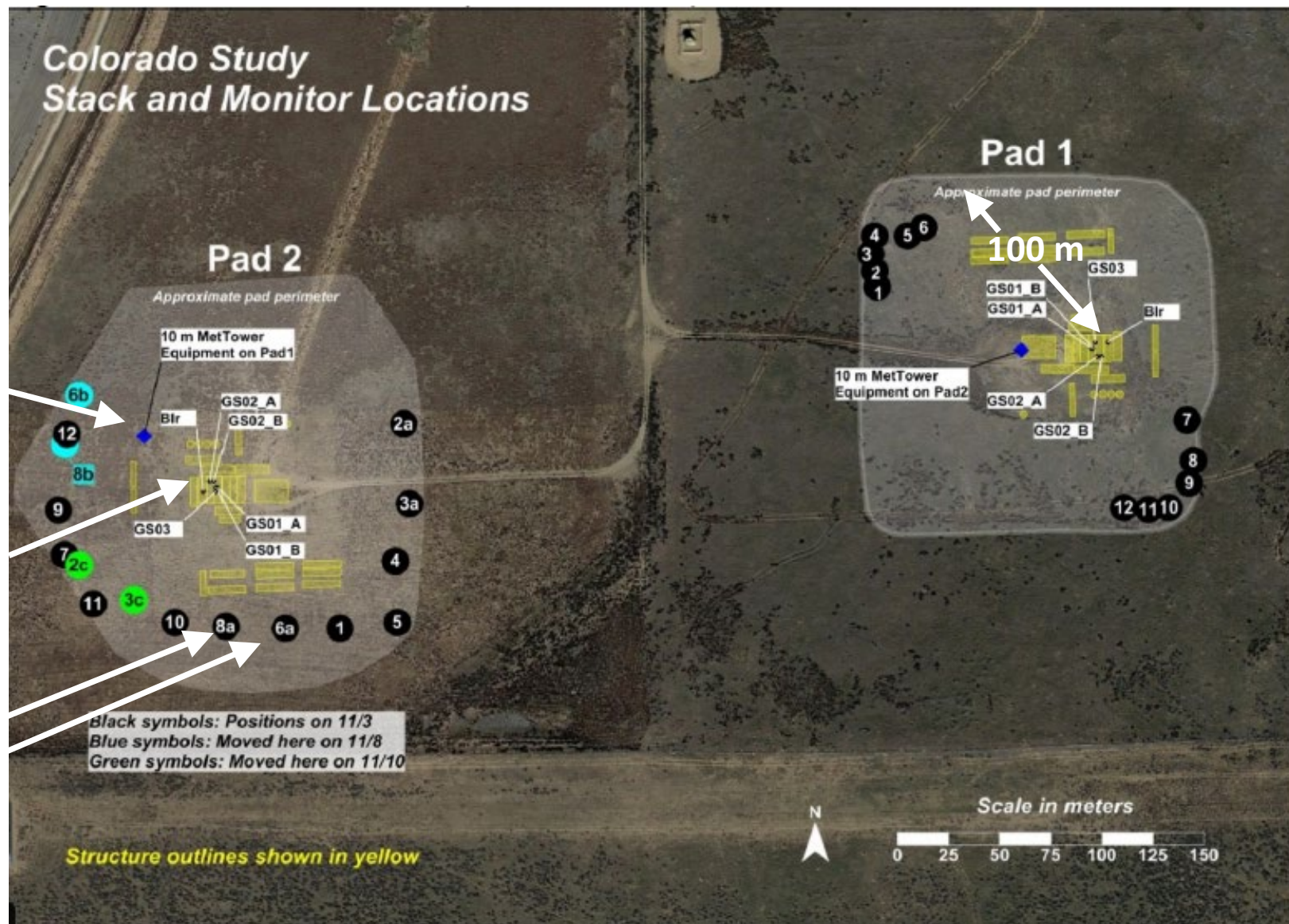
Meteorological instruments on 10 m onsite tower

Two diesel fired Caterpillar 3512B generators, one diesel fired Caterpillar C27 generator (all 5.5 m, EPA Tier 2 engines) + cold weather boiler

Sudden change in wind direction at Pad 2: some monitors moved

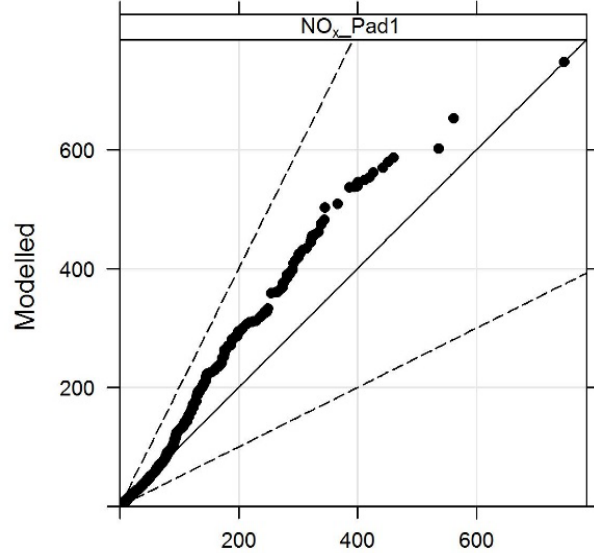
Flat terrain

‘Downwind sector’ datasets analysed

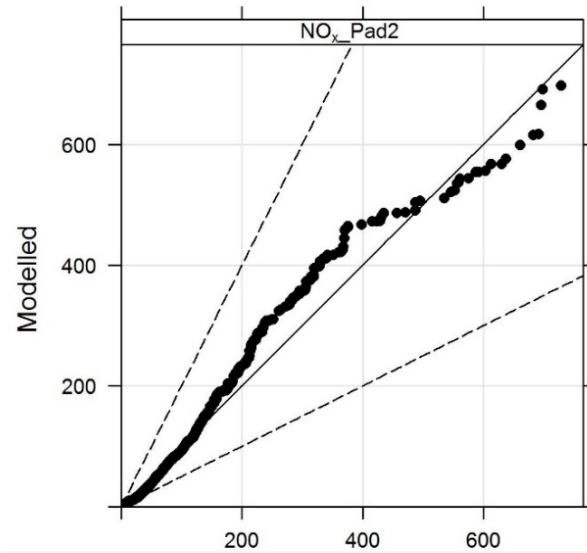


WRAP NO₂ chemistry field campaign (2 of 4)

QQ plots: Pad 1

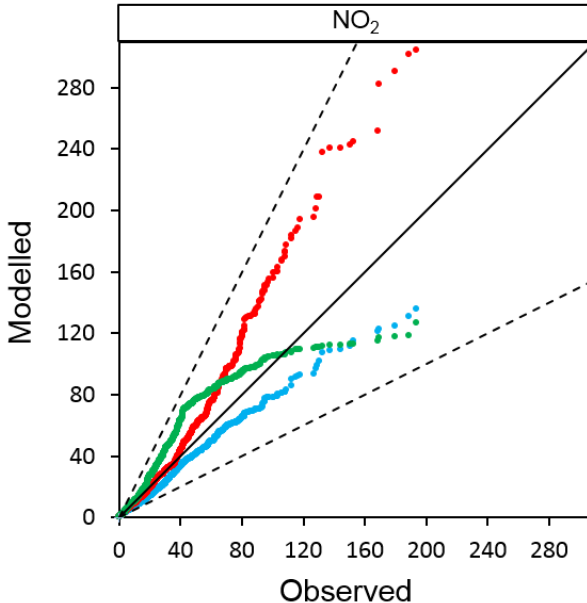
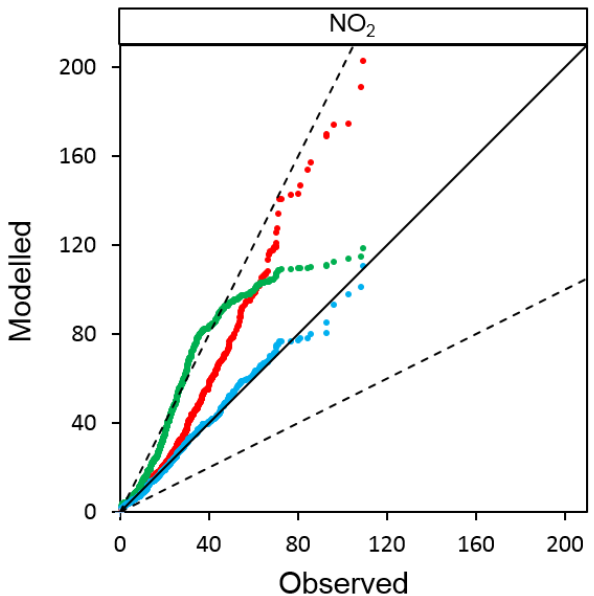


Pad 2

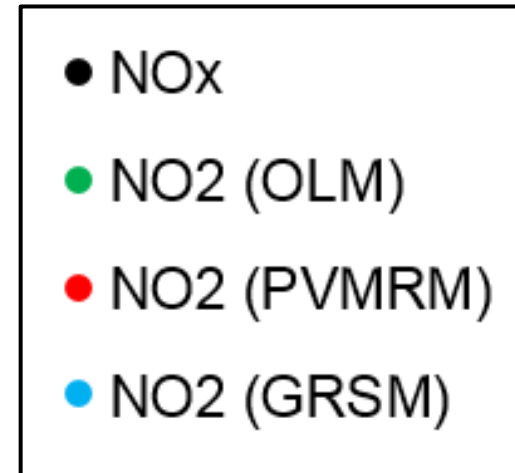


NO_x

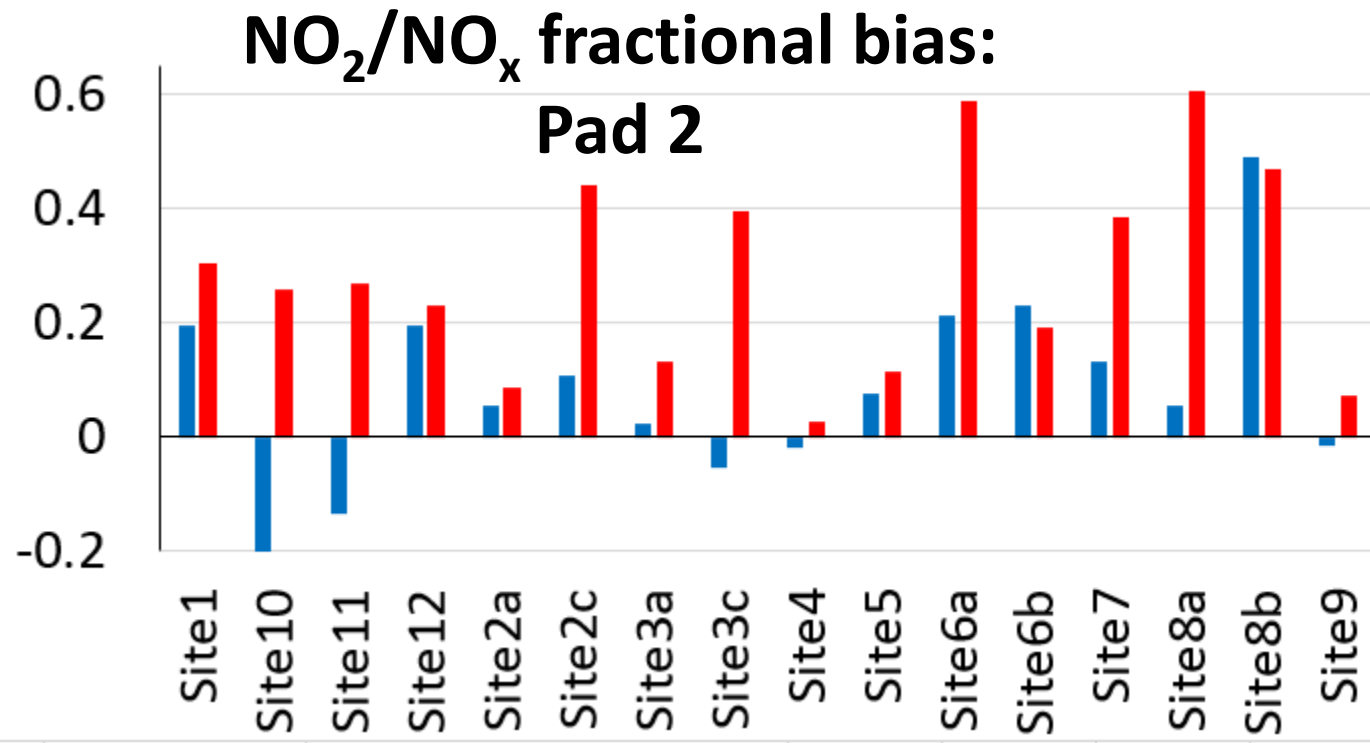
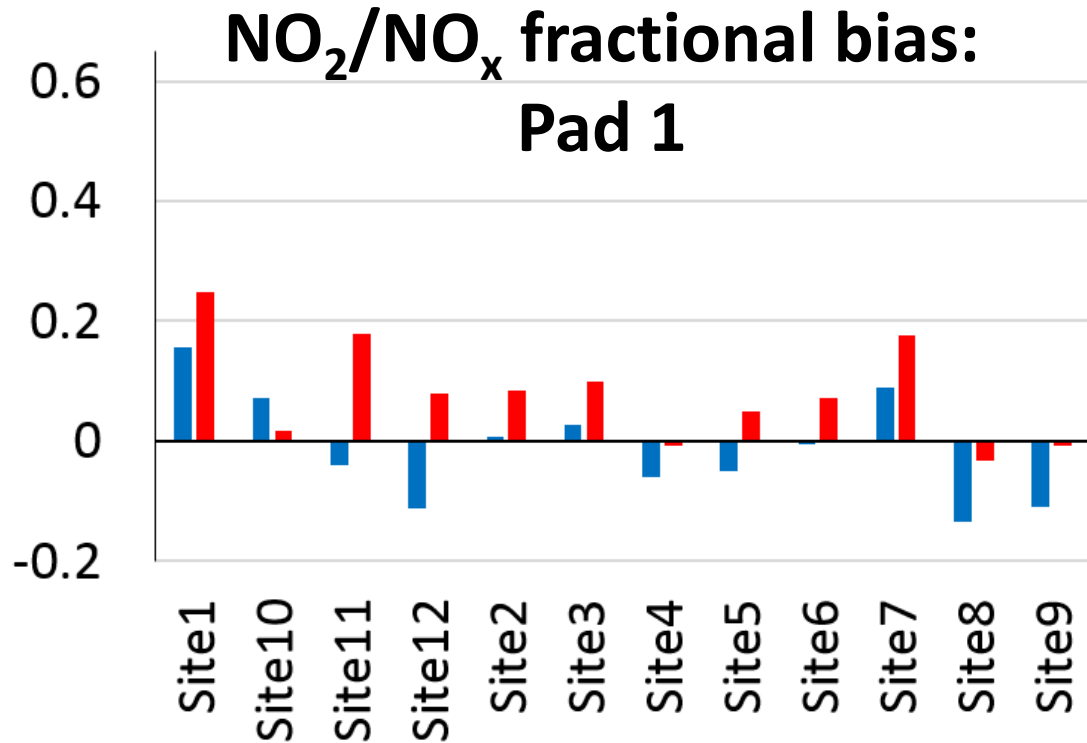
NO₂



- For high concentrations, GRSM NO₂ slightly under-predicted relative to NO_x at Pads 1 & 2 - may be related to uncertainty in ISR
- All models demonstrate consistency between NO_x and NO₂ for the two Pads
- PVMRM over-predicts NO₂ at high concentrations



WRAP NO₂ chemistry field campaign (3 of 4)



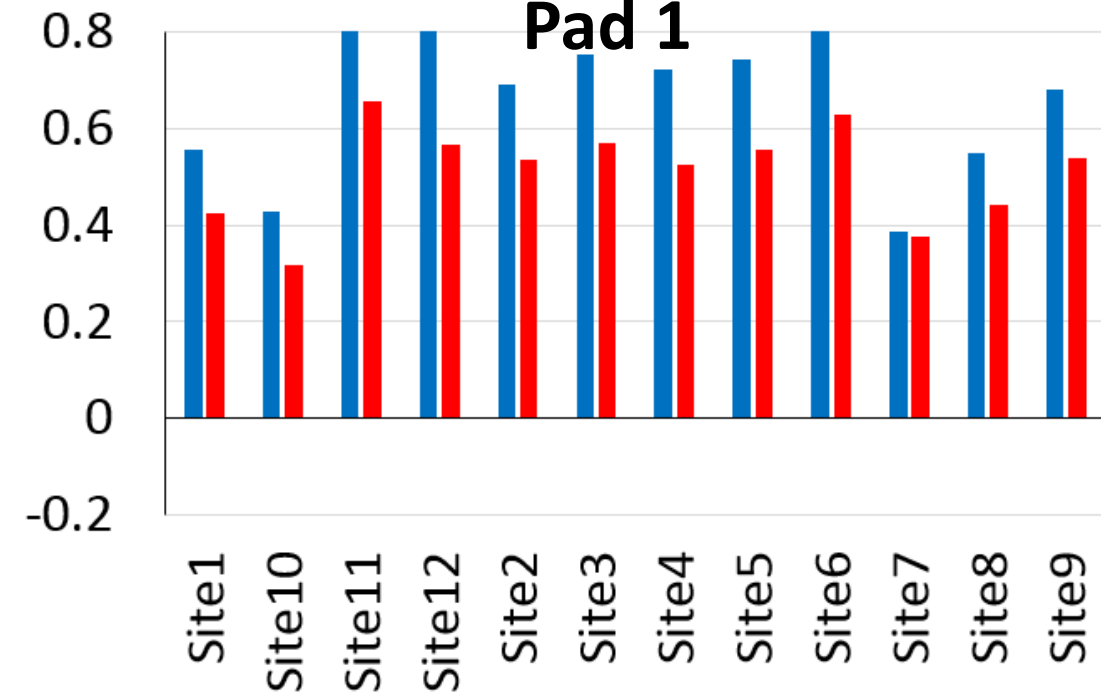
- NO₂/NO_x is a good indicator of chemistry performance
- Fractional bias has **an ideal value of 0**
- Looking in detail (monitor-by-monitor), for GRSM some sites over-predict and some under-predict (PVMRM almost always over-predicts NO₂ concentrations relative to NO_x concentrations)



WRAP NO₂ chemistry field campaign (4 of 4)

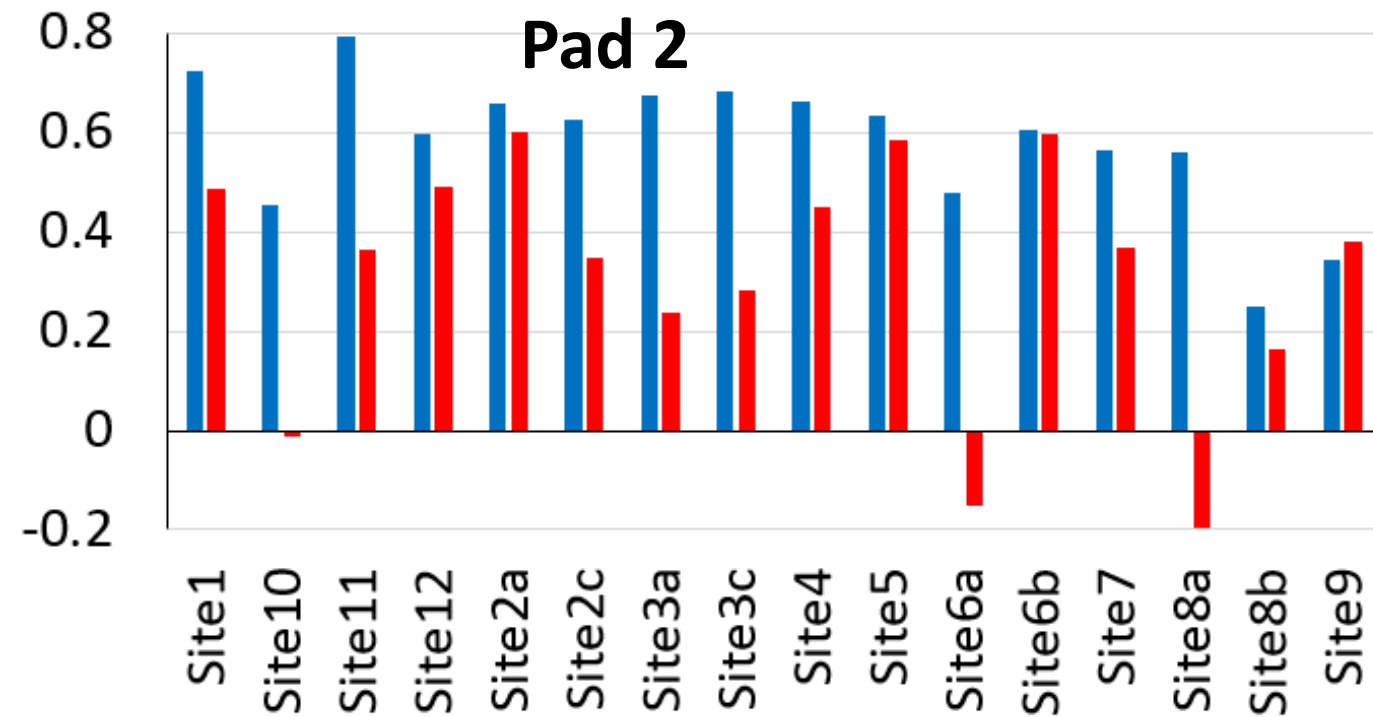
NO₂/NO_x correlation:

Pad 1



NO₂/NO_x correlation:

Pad 2



- NO₂/NO_x is a good indicator of chemistry performance

- Correlation has an **ideal value of 1**

- Looking in detail (monitor-by-monitor), for GRSM, correlations almost always higher (PVMRM has some negative correlations, likely related to few data points)



Generic Reaction Set Method (GRSM): Summary

- GRSM has been extensively evaluated using a range of datasets
- Model performance is generally good:
 - Consistency between modelled NO_x and NO_2 concentrations across both studies presented
 - Better NO_2 chemistry scheme performance than PVMRM
- The scheme developers are looking forward to feedback from the community regarding this AERMOD alpha option

References

- Venkatram A., P. Karamchandani, P. Pai, and R. Goldstein. 1994 The development and application of a simplified ozone modelling system (SOMS). *Atmos. Environ.* 28(22): 3365–78
- Carruthers, D.J.; Stocker, J.R.; Ellis, A.; Seaton, M.D.; Smith, S.E., Evaluation of an explicit NO_x chemistry method in AERMOD; *Journal of the Air and Waste Management Association.* 2017, 67:6, 702-712
- Stocker J, Carruthers D, Kalisz C, Paine R, Seaton M, Smith S and Warren C, 2019: Evaluation of explicit NO_x chemistry methods in AERMOD using a new compressor station dataset. *Guideline on Air Quality Models: Planning Ahead*, Durham, North Carolina, USA, March 2019
- Innovative Environmental Solutions, 2017. Balko OK Compressor Station 102: Data Summary and Initial AERMOD Performance Assessment, Report no. PR-312-15201-R01
- Colorado Field Study Workgroup, 2020: 2014 Colorado Oil and Gas Drill Rig Field Study Model Evaluation Database - Technical Support Document

Acknowledgments

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API

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Cathe Kalisz

ERM

Mark Garrison

Questions?

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Travel Time Reaction Method (TTRM) Procedure and Evaluation for AERMOD NO₂ Modeling

Presentation at EPA's 2021 Modeling Workshop June 21, 2021

The AECOM logo is displayed in a bold, black, sans-serif font on a light blue background in the bottom right corner of the slide.

Overview of Travel Time Reaction Method

- High level review Travel Time Reaction Method formulation
- Initial implementation
- Evaluation with Colorado drill rig and Balko, OK studies
- Conclusions
- Appendix with details of the Balko evaluation

- Acknowledgements: funding for the documentation, coding, and evaluation of TTRM was provided in large part by the American Petroleum Institute. Coding and evaluation of the TTRM option were conducted by Carlos Szembek and Chris Warren.

TTRM Formulation

- A refined approach to supplement the Tier 2 (ARM2) and Tier 3 (OLM and PVMRM) methods for converting NO to NO₂ is available for very short travel times in the near-field (e.g., fence line impacts)
- The full reaction of ozone with NO can be represented as such:
 - $NO + O_3 \rightarrow NO_2 + O_2$
- Simplified to the forward reaction yields a scaling factor for NO:
 - $NO_{2-frac} = 1 - e^{\{-k[O_3] t\}}$
where t is the *travel time* to a receptor from the source and k is the *reaction rate* represented as (from Hanrahan, 1999):
 - $k = (15.33/T_a) e^{(-1450/T_a)}$ in ppb⁻¹ sec⁻¹ where T_a is the *hourly ambient temperature*
- The conversion factor is capped at 0.9 and would scale any available NO remaining that is released from the stack
- This fractional NO₂ would then be added to the in-stack converted NO₂ to calculate the final NO₂ concentration.

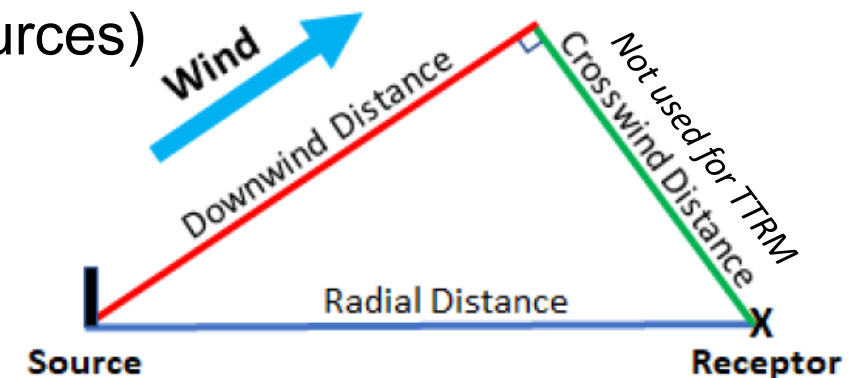
TTRM Example Spreadsheet Calculation Table

Conversion Fraction of NO to NO₂ as a function of Ozone Concentration and Transport Time (at Standard Temperature)

| Travel time (sec) | Ozone = 35 ppb | Ozone = 55 ppb | Ozone = 75 ppb |
|-------------------|----------------|----------------|----------------|
| 10 | 0.130 | 0.196 | 0.257 |
| 20 | 0.242 | 0.353 | 0.448 |
| 30 | 0.340 | 0.480 | 0.590 |
| 40 | 0.426 | 0.582 | 0.696 |
| 50 | 0.500 | 0.664 | 0.774 |
| 60 | 0.565 | 0.730 | 0.832 |

Travel Time Reaction Rate (TTRM) Procedure: Step 1

- TTRM is designed to supplement the results of an existing NO₂ modeling option
- **Step 1a:** Run AERMOD using a Tier 2 or Tier 3 option
- **Step 1b:** Also run AERMOD using the TTRM option for the same sources/receptors
- TTRM calculates travel time by selecting the “type” of distance and effective wind speed based on the dominant plume type.
- Distances vary between coherent or random plumes
 - Downwind (coherent plume for point and volume)
 - Radial (random plume for point/volume and all area sources)
- Effective wind speed (based on plume treatment):
 - U_{eff}: stable hours and indirect plumes
 - U_{effd}: direct plumes
 - U_{eff3}: penetrated plumes



Travel Time Reaction Method (TTRM) Procedure: Step 2

- **Optional Step 2:** Import both sets of modeling results (TTRM and a Tier 2 or 3 method) into a spreadsheet for each hour and receptor (or use your own post-processing software)
- In the very near-field, TTRM results are likely to be lower
- After the “crossover” where travel time is larger, the TTRM NO₂/NO_x ratio approaches 0.9, and the Tier 2 or 3 approaches are then applicable
- Recommendation: take the lower of the two results for each hour and receptor as the appropriate concentration
- At some point in the future, Steps 1 and 2 could be done within one AERMOD run, but for this implementation, two model runs must be done and post-processed manually (or by using post-processing software)



Model Evaluations of TTRM

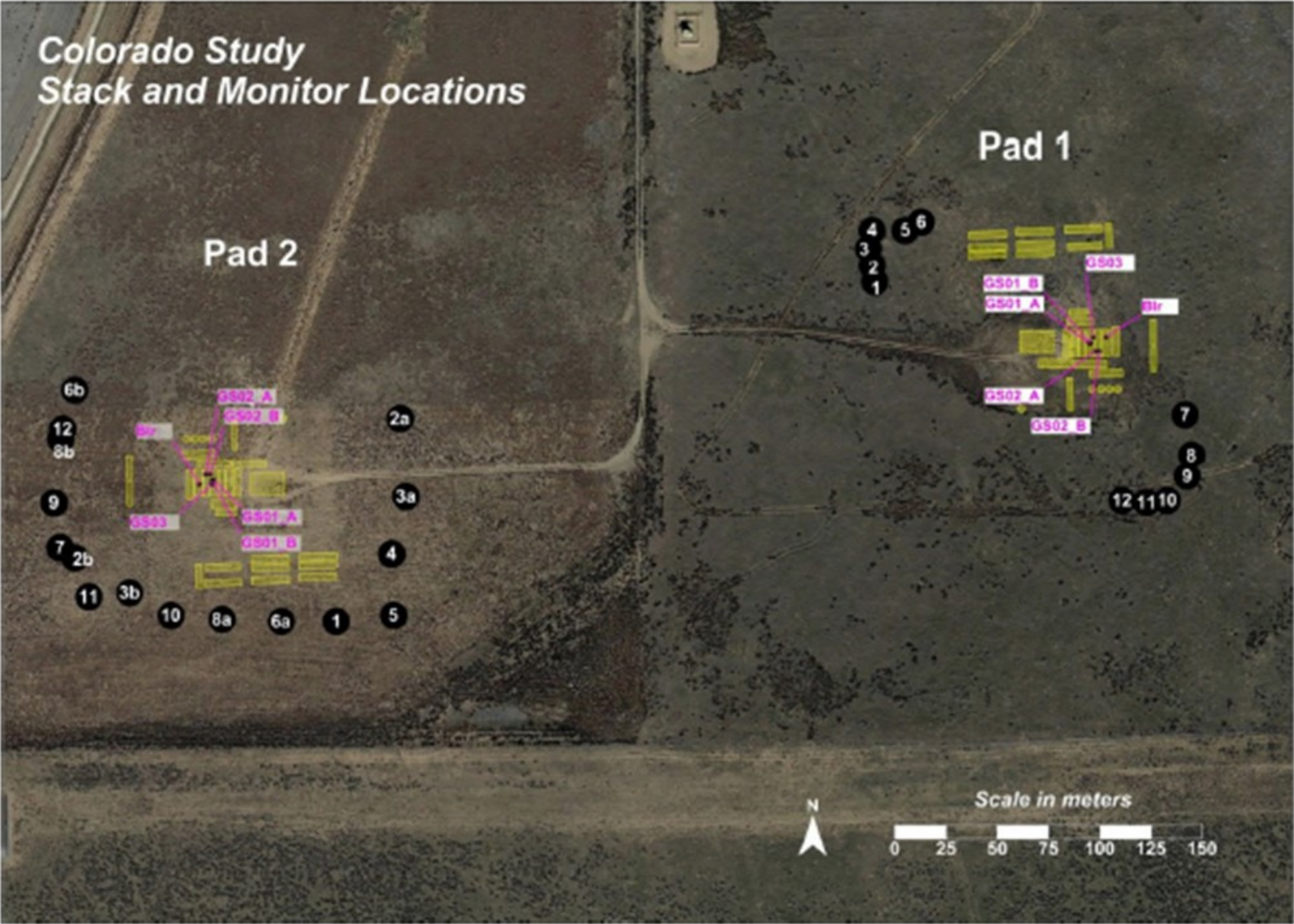
- Denver-Julesburg, CO
- Balko, OK

Evaluation Using 2014 Colorado Drill Rig Study Plume Capture Hours

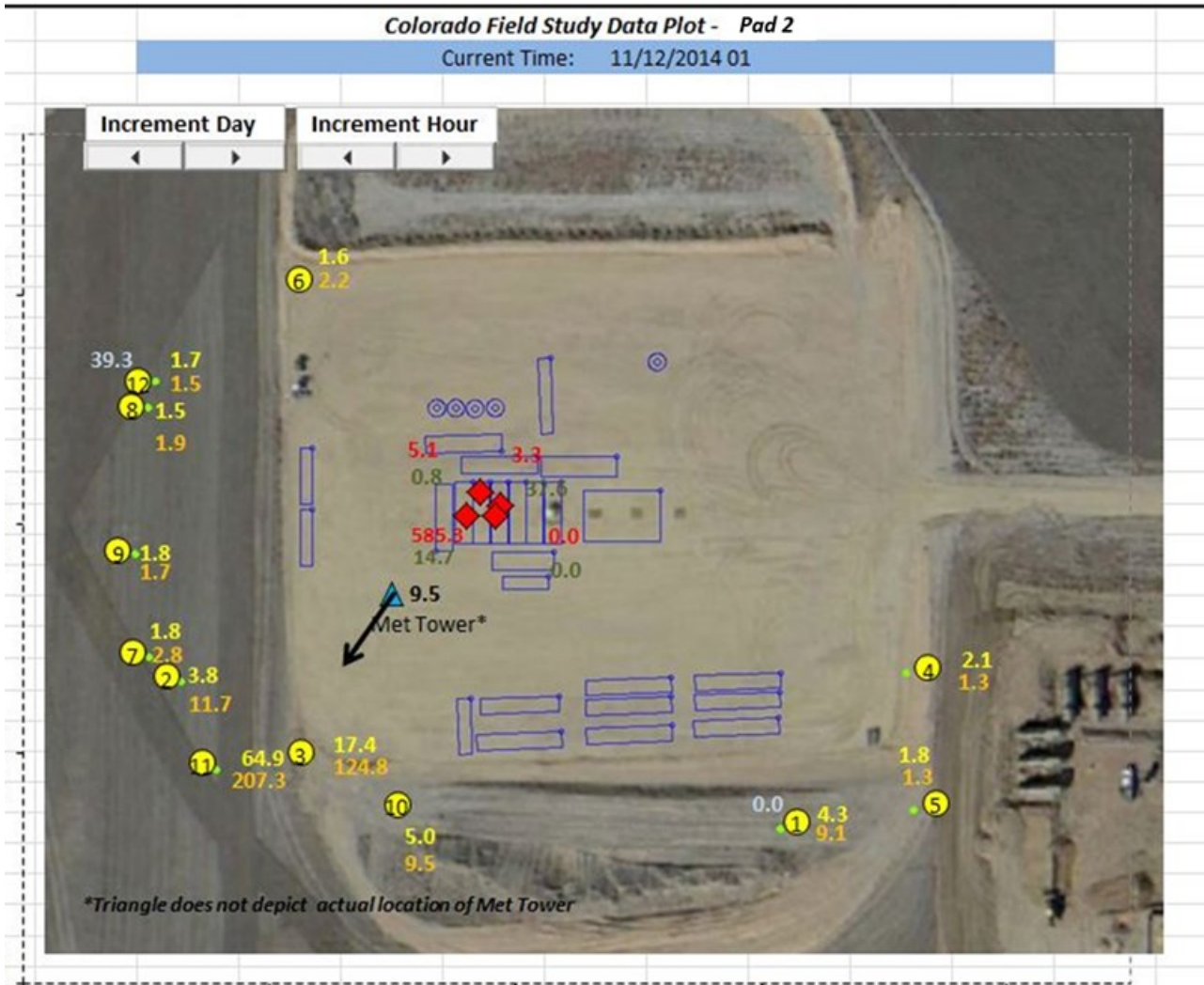
- Located north-northeast of Denver, CO.
- October 10 – November 16, 2014
- Adjacent well pads
 - (Pad 1, Pad 2)
- 12 ambient AQ monitors generally within 100 m.
- CEMS were used to measure exhaust level at six stack sources (5 generators, 1 boiler) on the drill rig.
- ISR values ranged from 0.04 to 0.09 for most sources.



Colorado Drill Rig Study – Pad Layouts at Two Locations



Colorado Drill Rig Study – Sample Ambient Monitor Plot



“Plume Capture” Modeling Hours:

These 160 hours feature a monitor with a peak concentration with lower monitored values available on either side of the peak measurement.

| Pad Layout | Plume Capture Hours |
|------------|---------------------|
| Pad 1 | 48 |
| Pad 2-A | 29 |
| Pad 2-B* | 83 |

* monitors relocated to provide more plume capture hours.

Model Evaluation Analysis

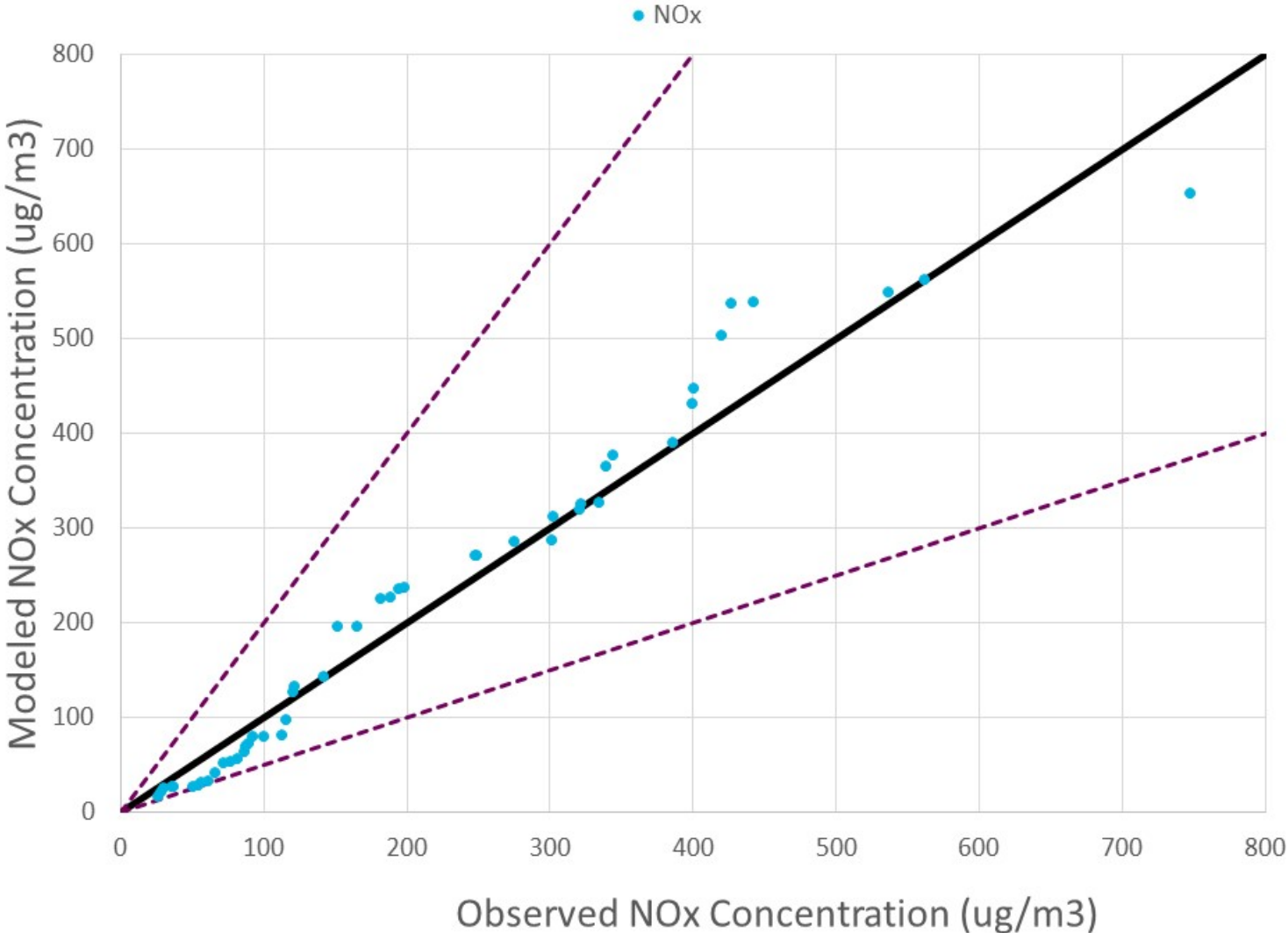
- Use one observation and prediction for each plume capture hour (paired for the peak plume capture monitor location)
- Model with the following AERMOD options:
 - NO_x (Tier 1 approach; tests AERMOD without NO₂ chemistry)
 - ARM2 (Tier 2)
 - OLM (Tier 3), using OLMGROUP ALL
 - PVMRM (Tier 3)
 - TTRM, then post-processed with ARM2, OLM, and PVMRM
- After TTRM is run, the hourly concentrations at each receptor were compared to those from another option, and the lower of the two values was used
- TTRM results are only applicable for near-field locations, where the fraction of NO₂/NO_x is low due to incomplete ozone reaction

Focus is on NO₂/NO_x Ratio for Evaluation

- Key difference for these modeling approaches is the conversion of NO to NO₂
- That fraction (NO₂/NO_x) should be the focus of the evaluation, not simply the magnitude of the NO₂ concentrations, because...
- If NO_x is underpredicted, then NO₂ will be underpredicted by an unbiased chemistry model
- Evaluation results are given for each pad separately due to different model performances for NO_x predictions
- Each modeled hour produced just a single observation – prediction pair
- For quantile-quantile plots, the hourly values were ascribed to a single “downwind” receptor (peak impact site)
- Meteorological / model option: cloud cover, no turbulence, ADJ_U*, actual wind directions

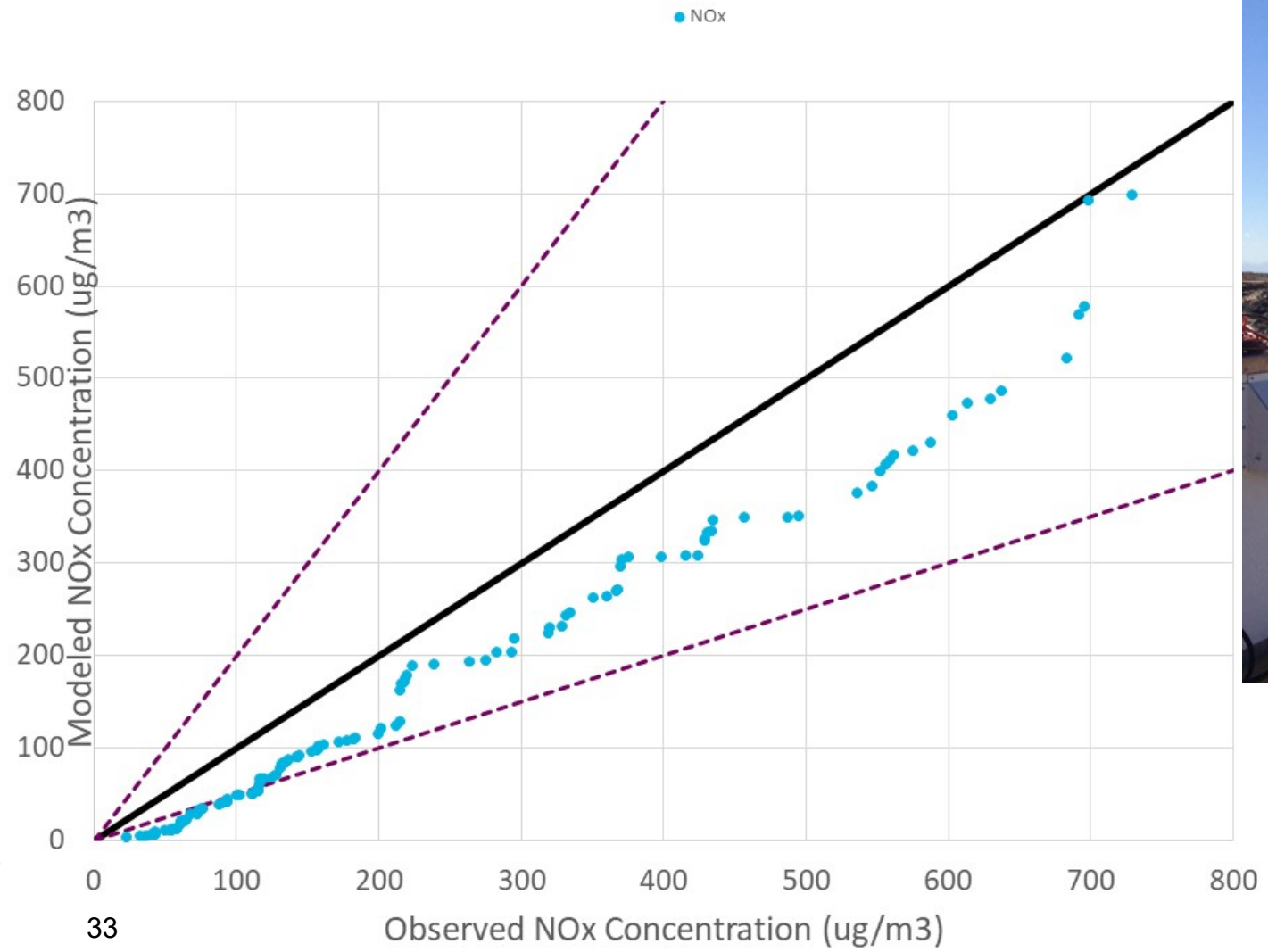
NOx Q-Q Plot for Pad 1 – Nearly Unbiased

Pad 1 NOx Plume Capture Hours (CC, no $\sigma\theta$, ADJ-U*)



NOx Q-Q Plot for Pad 2 – Underprediction – perhaps due to receptor elevation heights being misrepresented

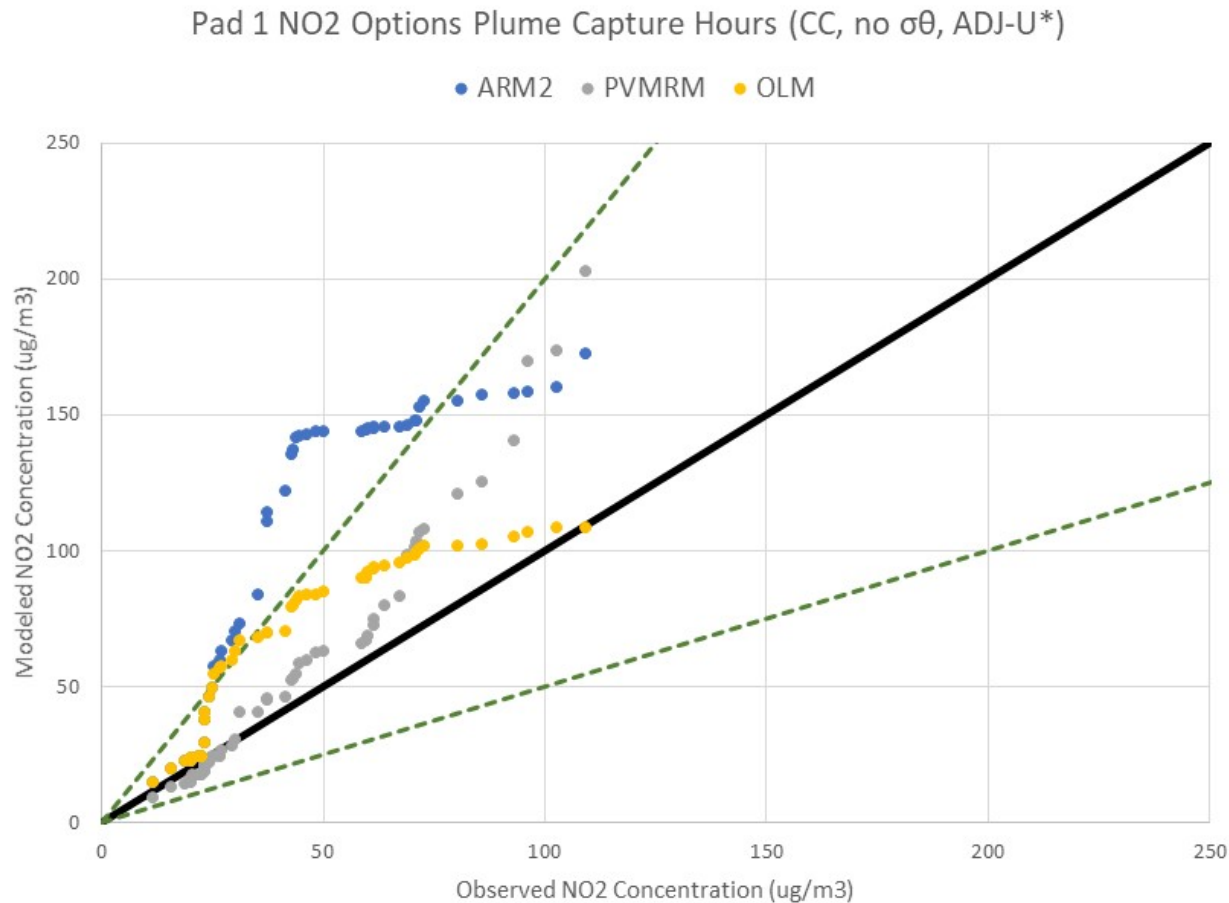
Pad 2 NOx Plume Capture Hours (CC, no $\sigma\theta$, ADJ-U*)



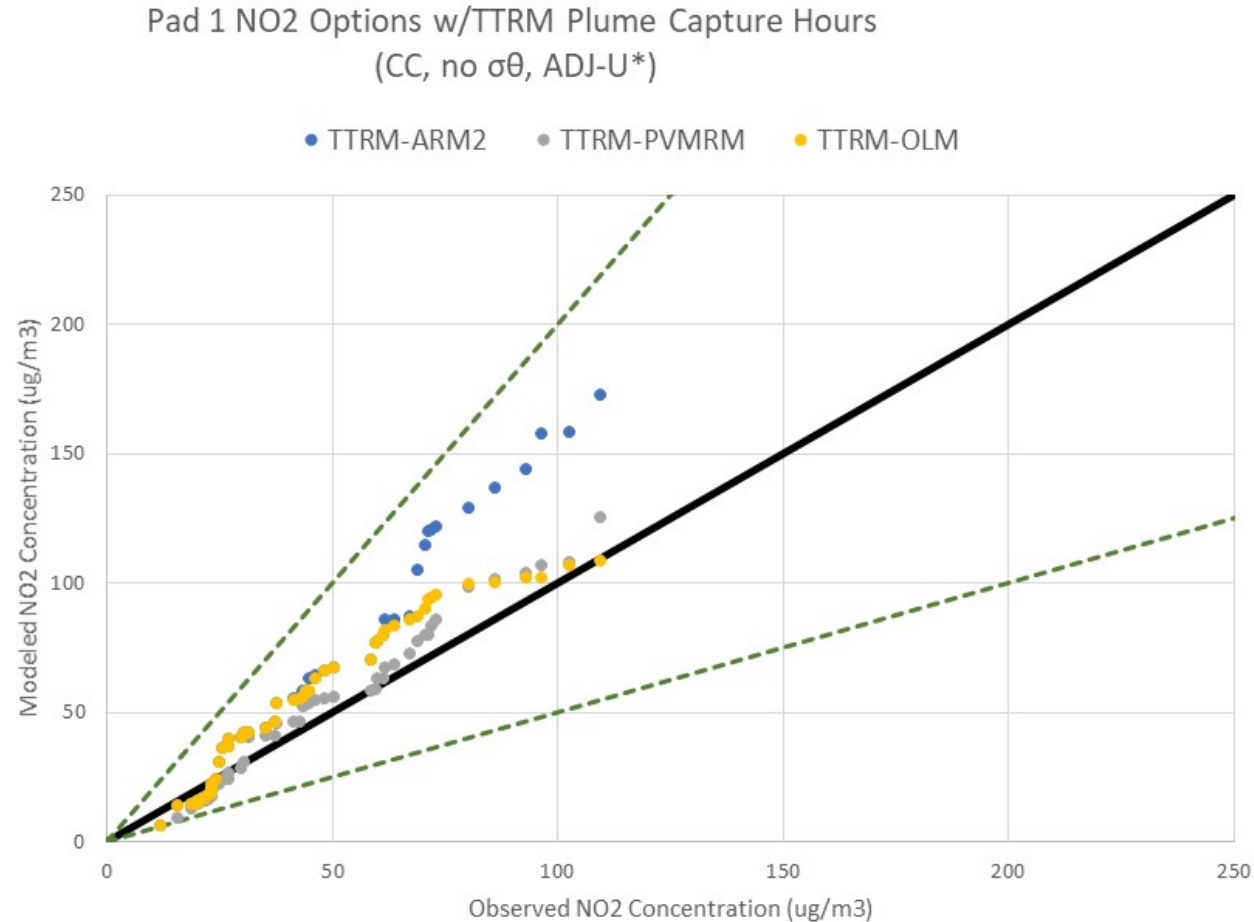
Monitors on southern berm should be modeled with increased elevation; this might mitigate the underprediction.

Q-Q Plot for Pad 1: NO₂ with TTRM Added on the Right

Without TTRM



Includes TTRM Enhancement

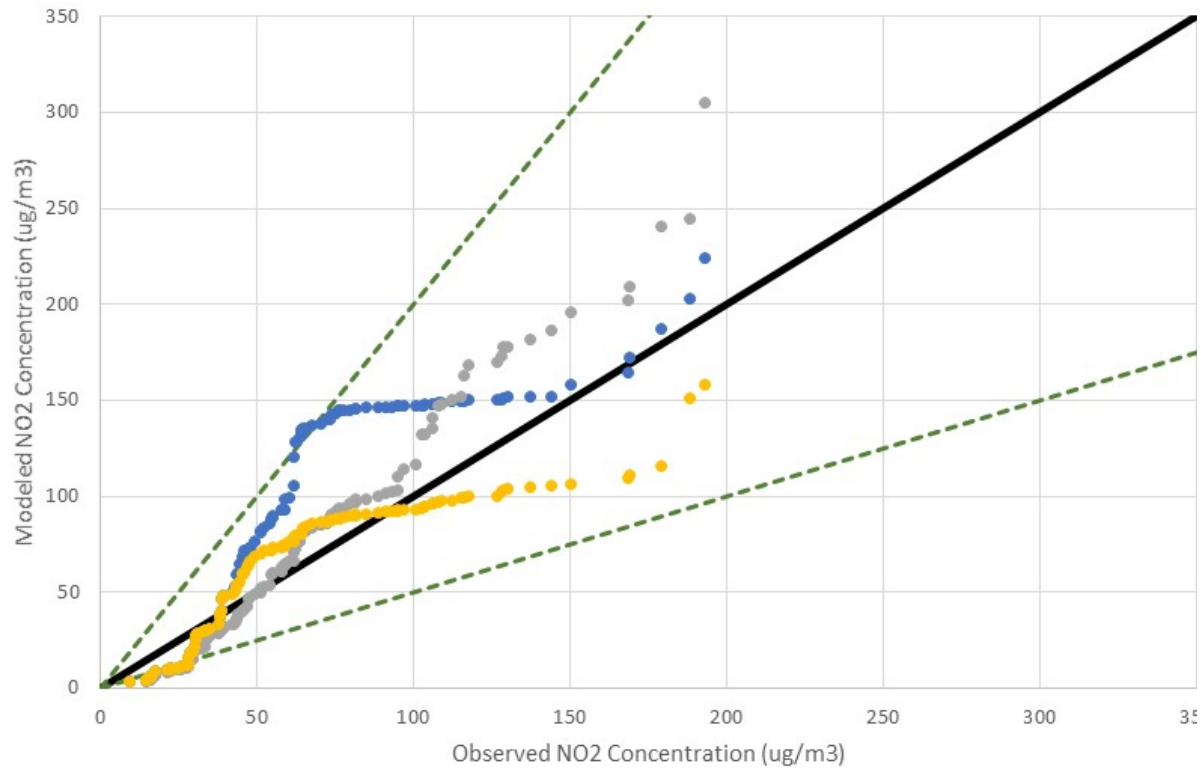


Q-Q Plot for Pad 2: NO₂ with TTRM Added on the Right

Without TTRM

Pad 2 NO₂ Options Plume Capture Hours (CC, no $\sigma\theta$, ADJ-U*)

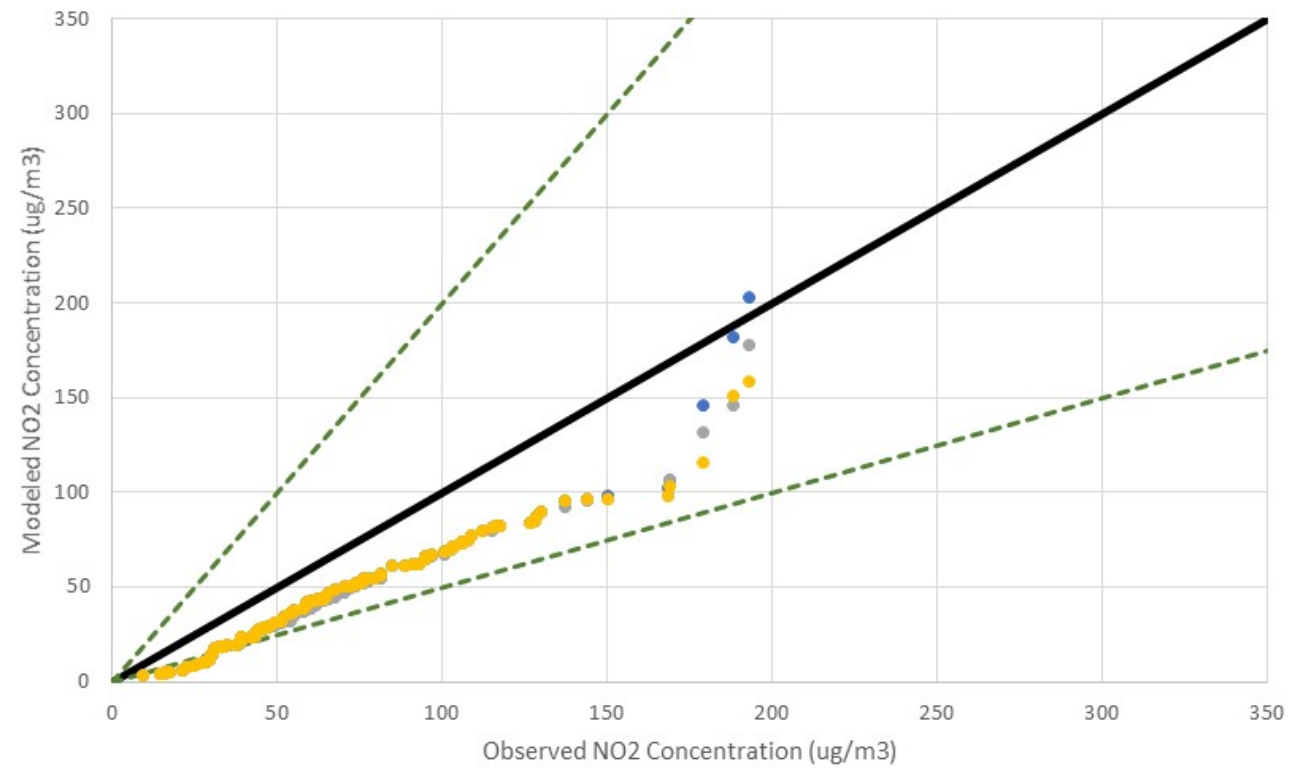
● ARM2 ● PVMRM ● OLM



Includes TTRM Enhancement

Pad 2 NO₂ Options w/TTRM Plume Capture Hours (CC, no $\sigma\theta$, ADJ-U*)

● TTRM-ARM2 ● TTRM-PVMRM ● TTRM-OLM



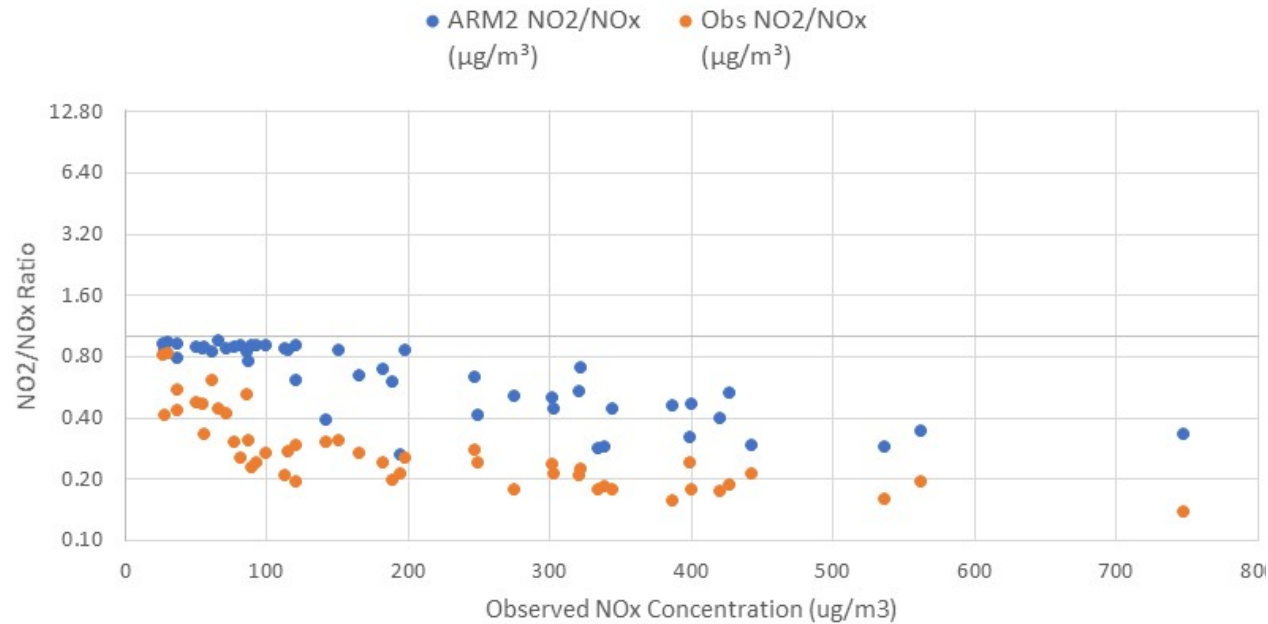
Further Analysis to Remove Effect of NO_x Bias

- The real model performance issue is the ratio of NO₂/NO_x
- We next show plots of observed as well as predicted NO₂/NO_x ratio for each model
- The NO₂/NO_x ratio is expected to decrease as observed NO_x increases
- The plots show the NO₂/NO_x ratio on the y axis and observed NO_x on the x axis

Pad 1: NO₂/NO_x Ratio vs. NO_x for ARM2 and ARM2 + TTRM

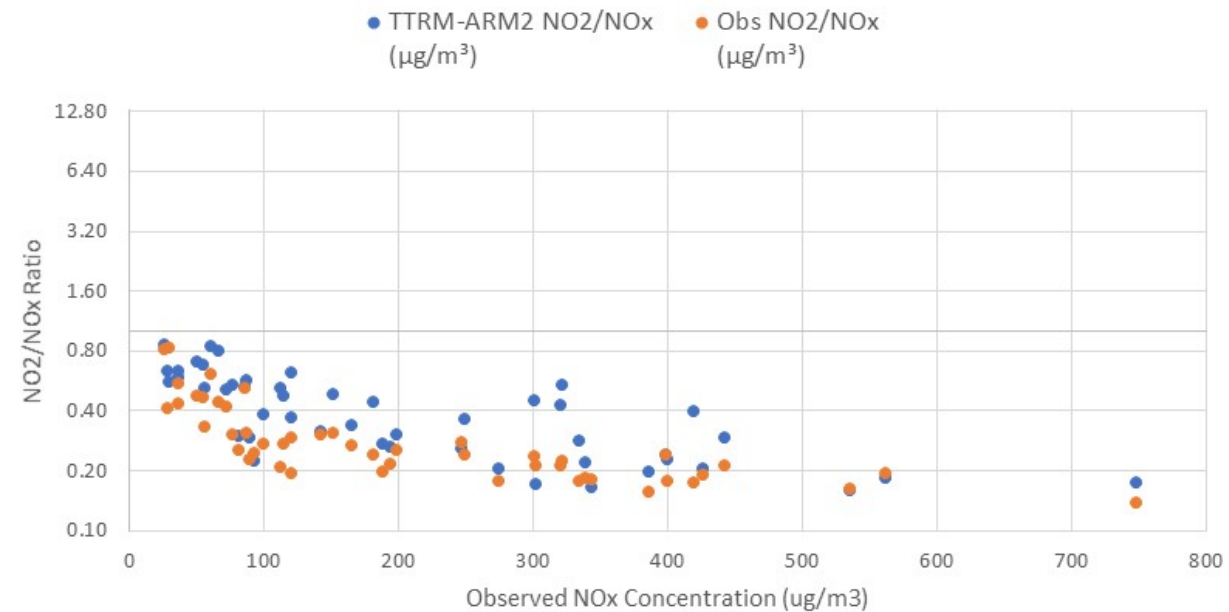
ARM2

Pad 1 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)



ARM2 + TTRM

Pad 1 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)



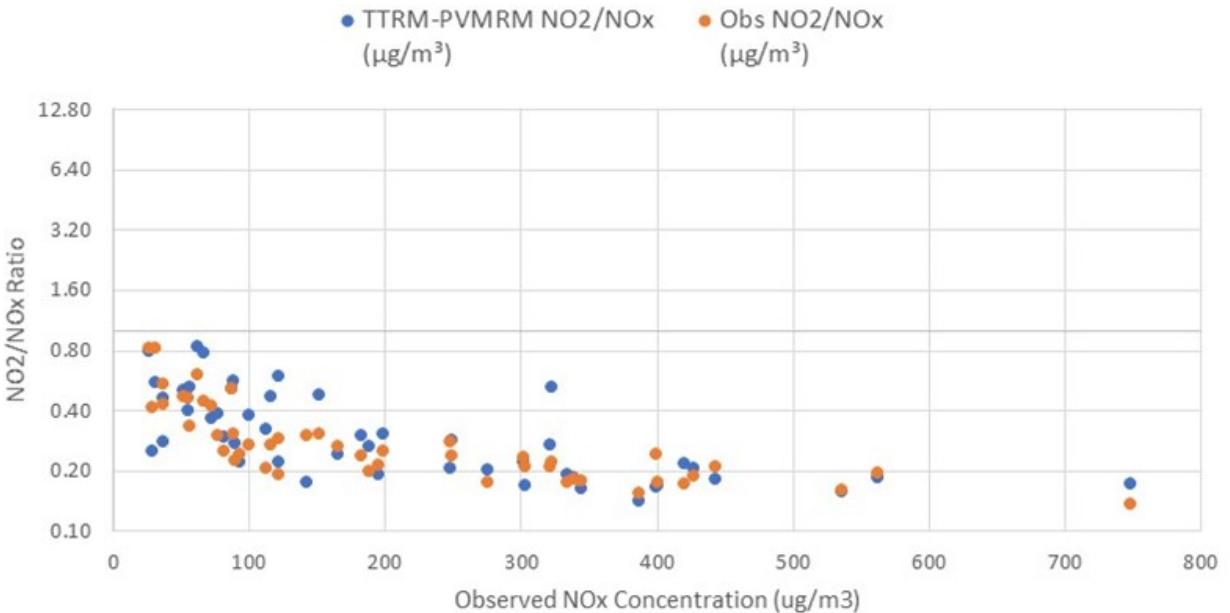
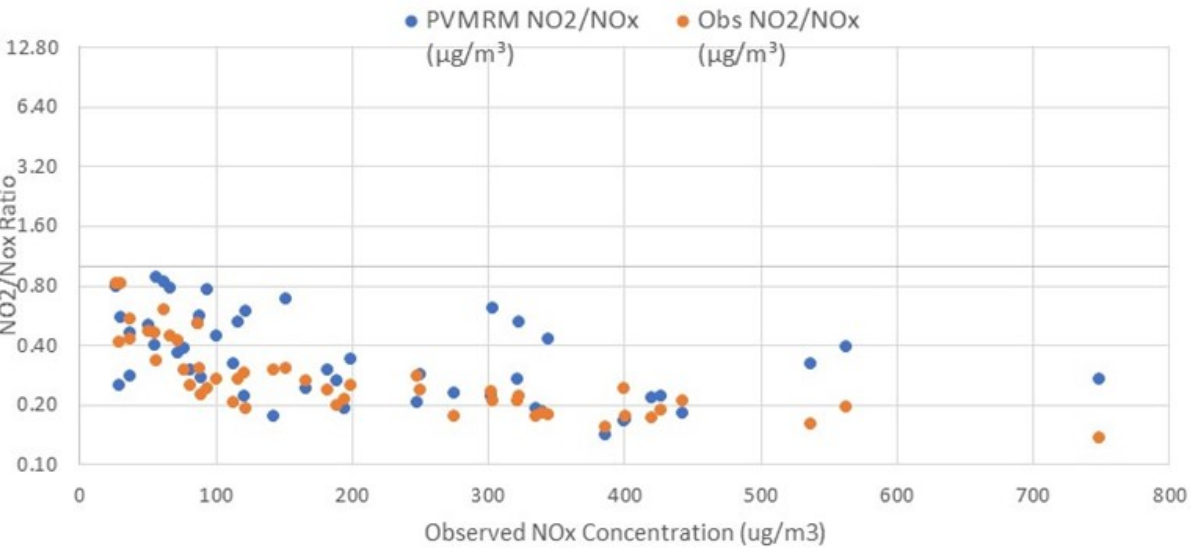
Pad 1: NO₂/NO_x Ratio vs. NO_x for PVMRM and PVMRM + TTRM

PVMRM

PVMRM + TTRM

Pad 1 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

Pad 1 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

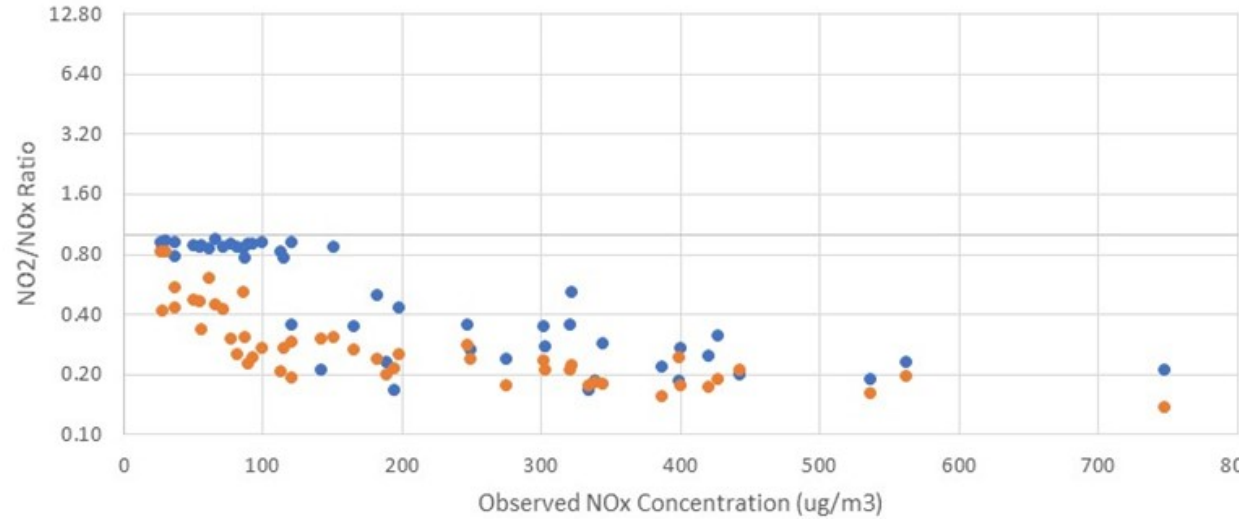


Pad 1: NO₂/NO_x Ratio vs. NO_x for OLM and OLM + TTRM

OLM

Pad 1 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

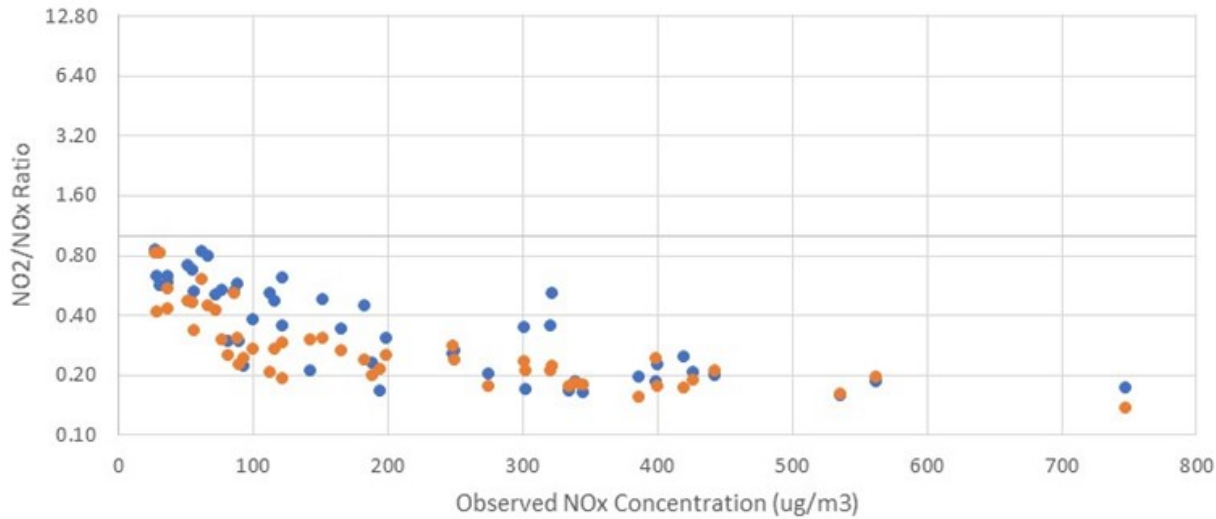
● OLM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



OLM + TTRM

Pad 1 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

● TTRM-OLM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)

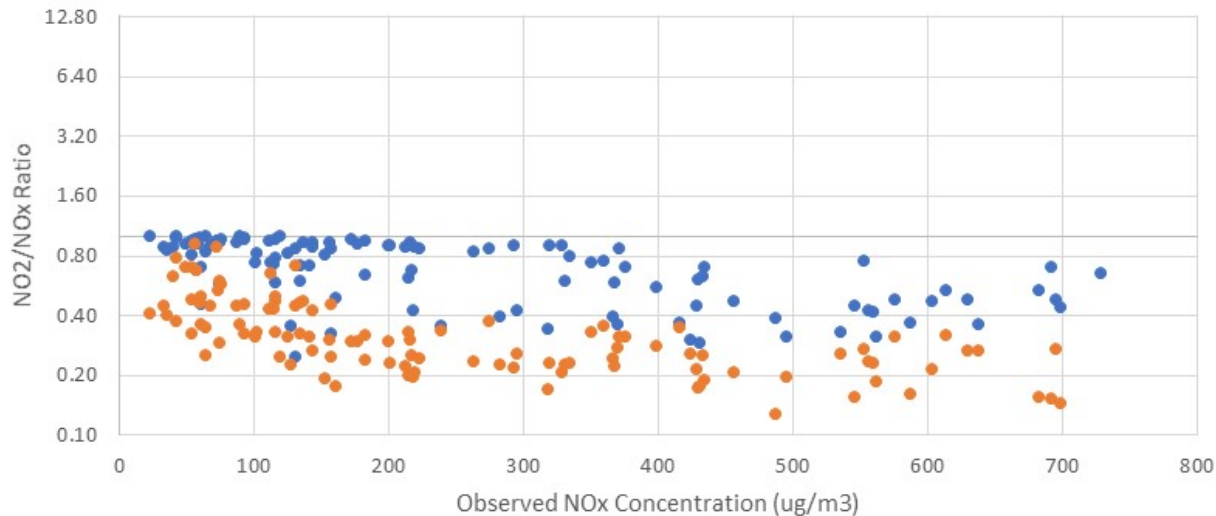


Pad 2: NO₂/NO_x Ratio vs. NO_x for ARM2 and ARM2 + TTRM

ARM2

Pad 2 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

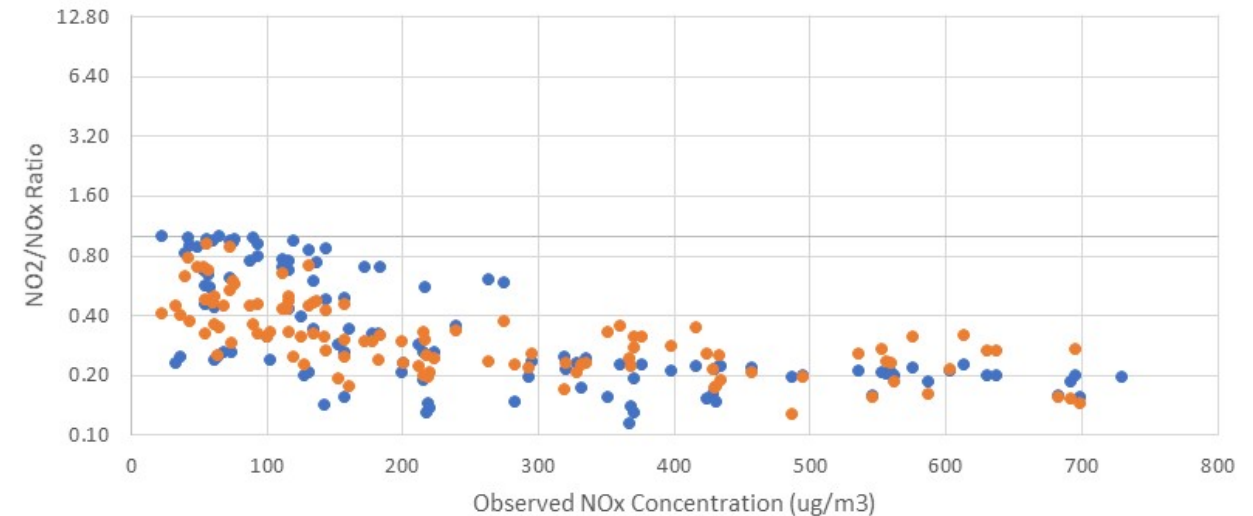
● ARM2 NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



ARM2 + TTRM

Pad 2 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

● TTRM-ARM2 NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)

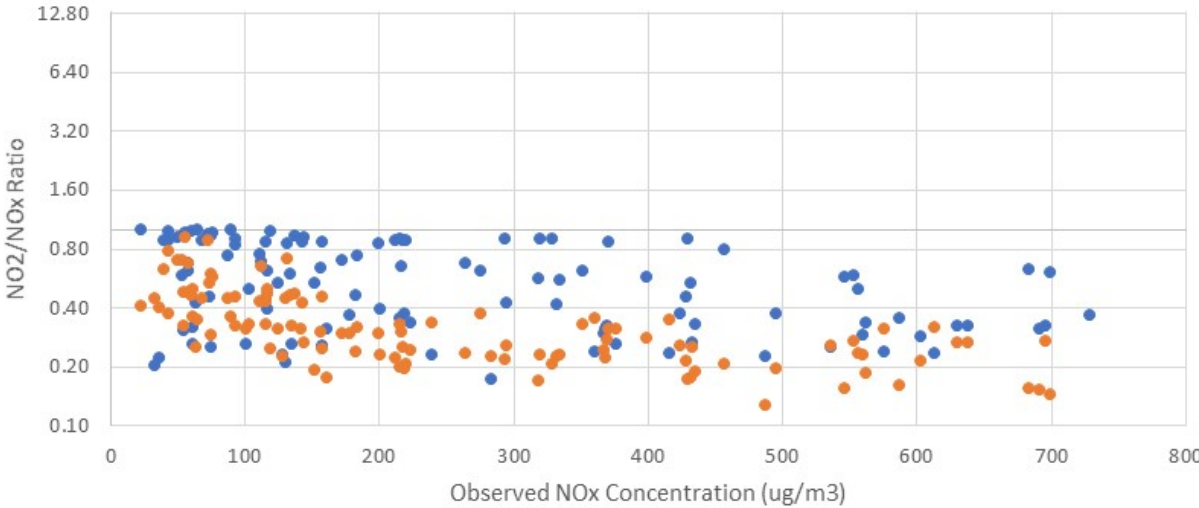


Pad 2: NO₂/NO_x Ratio vs. NO_x for PVMRM and PVMRM + TTRM

PVMRM

Pad 2 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

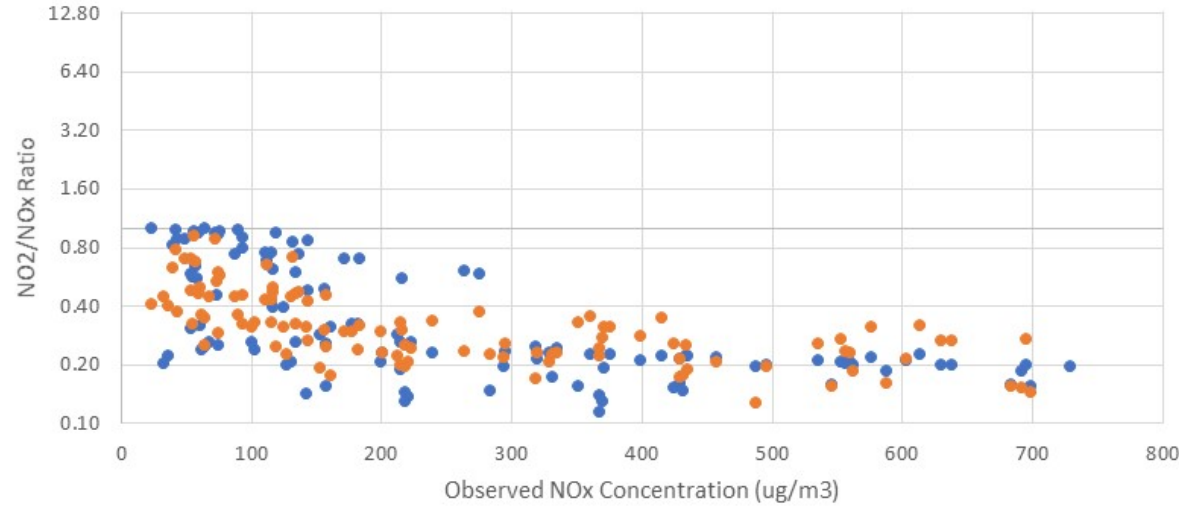
● PVMRM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



PVMRM + TTRM

Pad 2 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)

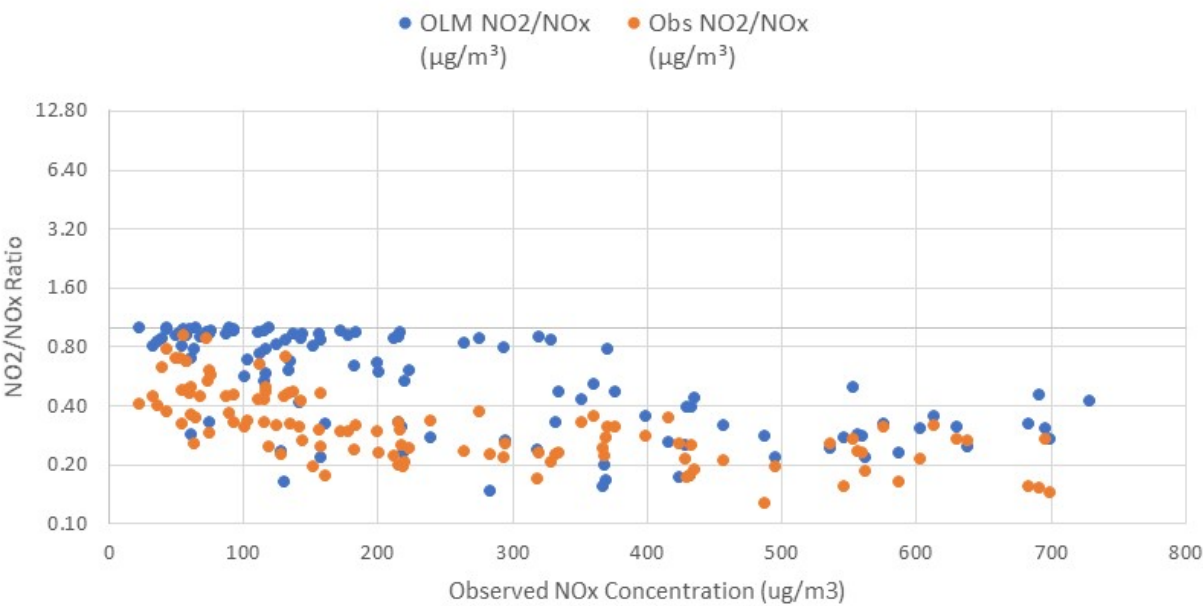
● TTRM-PVMRM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



Pad 2: NO₂/NO_x Ratio vs. NO_x for OLM and OLM + TTRM

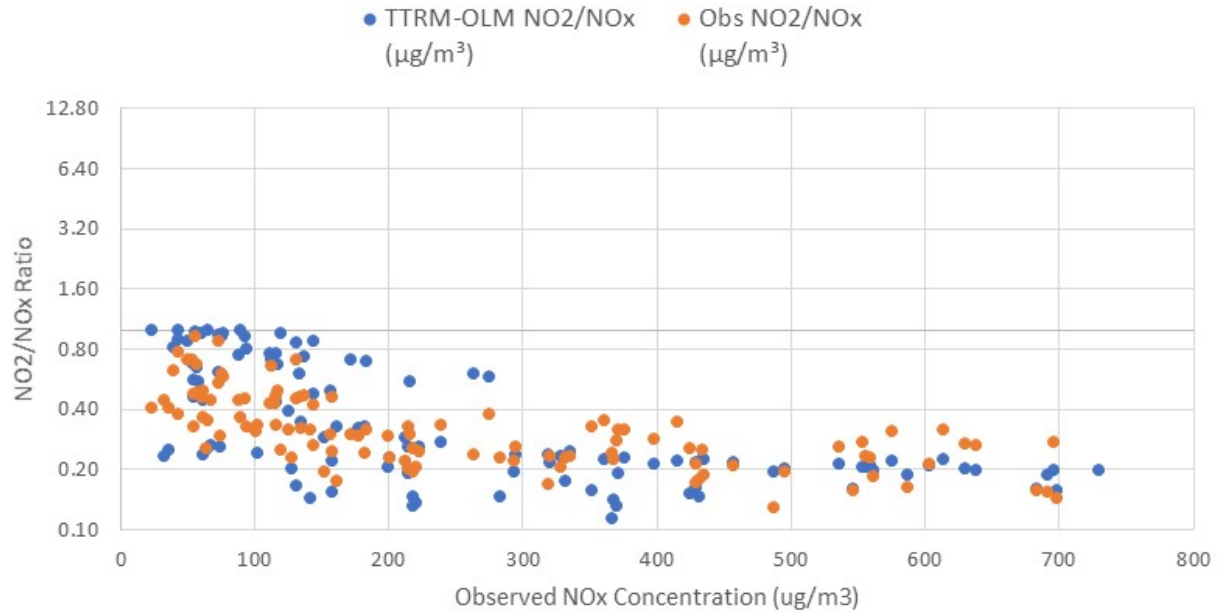
OLM

Pad 2 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)



OLM + TTRM

Pad 2 Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x Plume Capture Hours (CC, no σθ, ADJ-U*)



Summary of Colorado Evaluation with TTRM

- AERMOD NO_x predictions are relatively unbiased for Pad 1, underpredicting for Pad 2
- Reason for underpredicting at Pad 2 still unclear; might be due in part to corner vortex downwash issues or elevated berm for monitor placement that needs to be modeled more accurately
- Key performance issue is predicting the ratio of NO₂/NO_x
- Before applying TTRM, we find that ARM2 overpredicts more than OLM and PVMRM for that ratio
- OLM (with OLMGROUP) performs the best (PVMRM a close second), but they still overpredict the NO₂/NO_x ratio
- With TTRM added, all of these options perform better for both pads
- PVMRM and OLM with TTRM are close to unbiased, especially for high NO_x

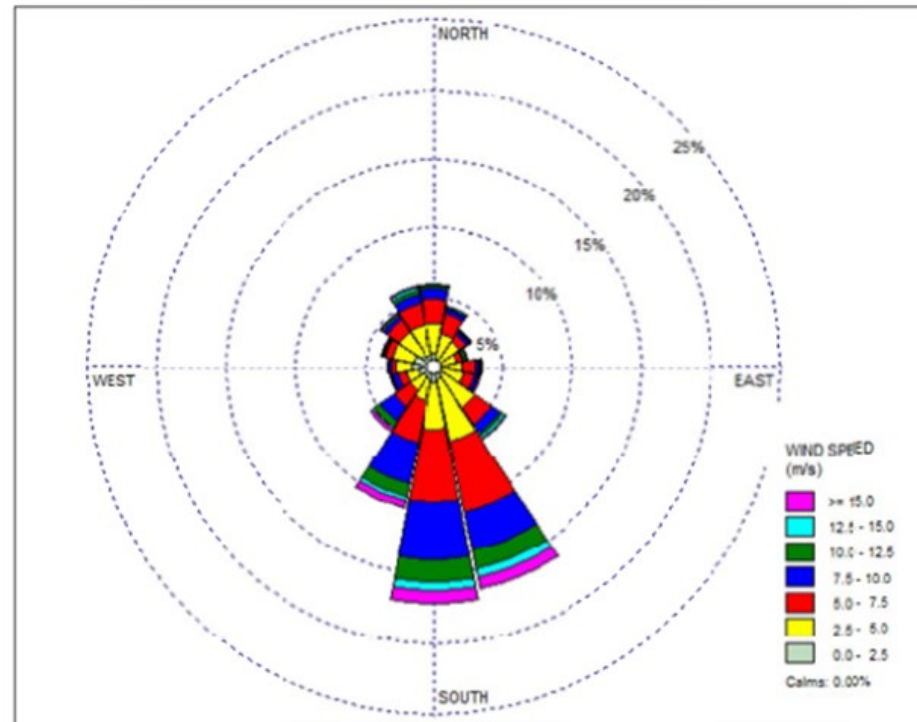
Balko, OK Database – Compressor Station

Figure 5-1. Four Ambient Monitoring Sites at Balko Compressor Station



- Monitor 1: North Field (~425 m from Clark TCV-12)
 - Monitor 2: North Fence (~140 m from Clark TCV-12)
 - Monitor 3: East Fence (~100 m from Clark TCV-12)
 - Monitor 4: Tower (~190 m from Clark TCV-12)
- These monitors are more distant than those from CO database

Annual 10-meter On-site Wind Rose December 2015 – December 2016



Model Evaluation for Sources of NO₂

- Primary sources of NO₂ associated with Clark-12 (C9) and to a lesser extent Cooper Bessemer (C10).
- An emergency generator and small boiler were also included in the modeling.
- Used observed NO_x and NO₂ data files provided by CERC for model evaluation.
- Most sources had an ISR=0.1.

Figure 2-6. Station 102 Compressor Buildings and Stacks



Model Evaluation Analysis

- Each monitor site was evaluated independently
- Model with the following AERMOD options:
 - NO_x (Tier 1 approach; tests AERMOD without NO₂ chemistry)
 - ARM2 (Tier 2)
 - OLM (Tier 3), using OLMGROUP ALL
 - PVMRM (Tier 3)
 - TTRM supplemented with runs using ARM2, OLM, and PVMRM
- When TTRM was run, the hourly concentrations at each receptor were compared to those from another option, and the lower of the two was used
- TTRM only affects concentrations for near-field locations, where the fraction of NO₂/NO_x is low due to incomplete ozone reaction
- See Appendix for details on the model evaluation results for TTRM

Summary of Balko, OK Evaluation with TTRM

- AERMOD NO_x predictions are relatively unbiased for North Field, underpredicted for North Field and Tower, and overpredicted for the East Fence monitor.
- Before applying TTRM, for the closer monitors (North and East Fences) PVMRM overpredicted the most, while ARM2 overpredicted the most at the far-field monitors.
- With TTRM added, biggest model improvements seen at North Fence monitor.
- In general, due to the larger distance to these monitors vs. the Colorado database, the effect of TTRM was less.
- PVMRM+TTRM has the best performance with some overprediction tendency.
- Use of TTRM does not result in an underprediction tendency for the NO₂/NO_x ratio, and it either reduces overprediction or results in little change for the peak predictions at the more distant monitors.

Overall Results and Conclusions

- In general, the use of the TTRM option results in better performance for monitors close to the source; lower or no effect at more distant monitors as expected
- TTRM generally results in unbiased predictions or modest overpredictions for the NO₂/NO_x ratio for very near-field receptors
- TTRM improves NO₂/NO_x ratio over a large range of NO_x concentrations for affected monitors
- The Tier 3 approaches (without TTRM) overpredict the NO₂/NO_x ratio less than ARM2, as expected
- TTRM should be paired with another method (e.g., a Tier 3 method) and then lower of the two concentrations should be used on an hourly / source / receptor basis

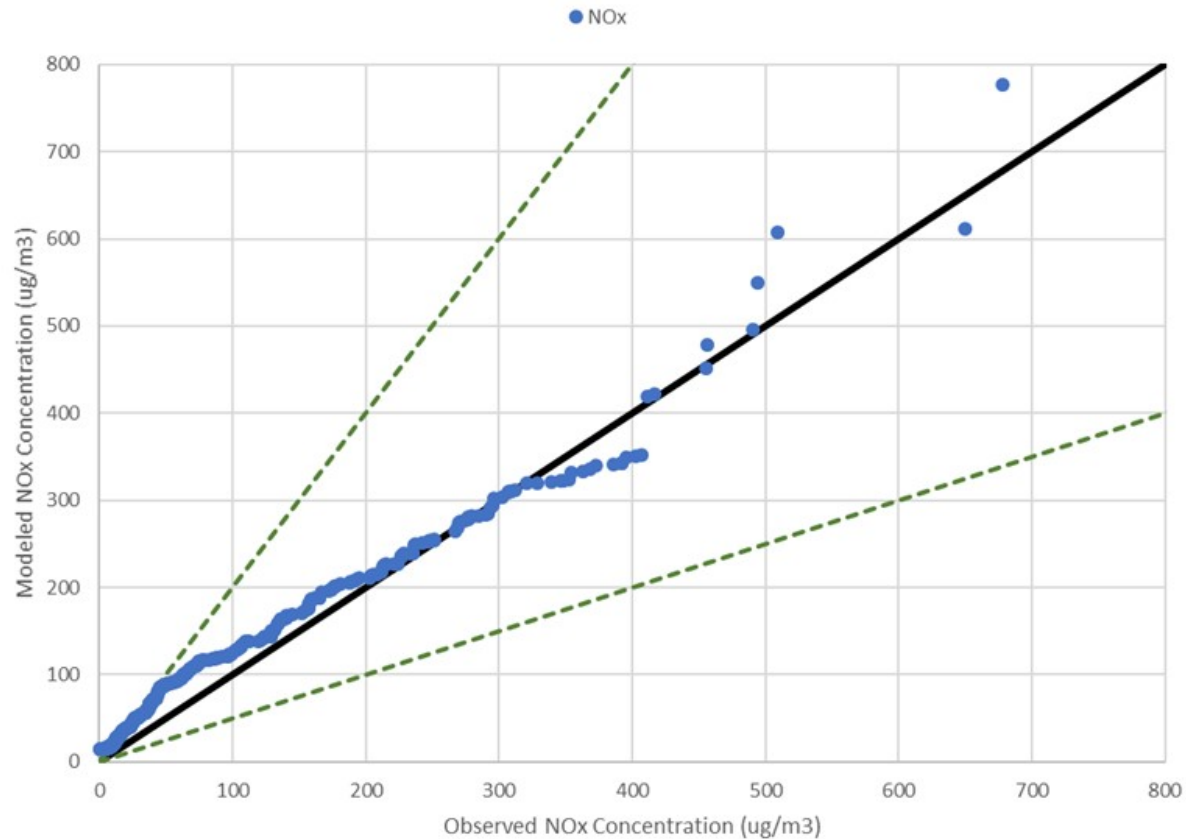
Appendix

- Details of the modeling results for Balko with the addition of TTRM are provided in this appendix.

Q-Q Plots for North Field: NO_x and NO₂

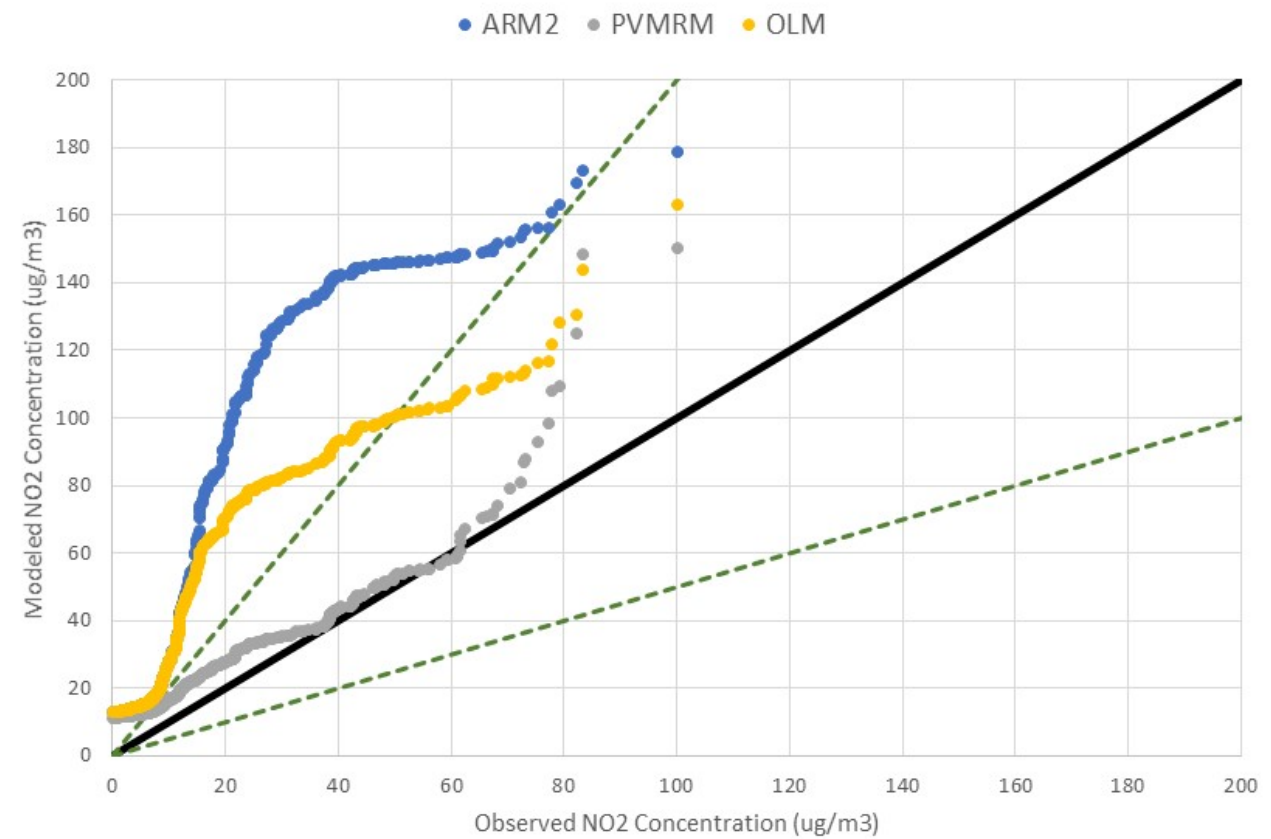
NO_x

North Field Monitor NO_x (Bulk RI, $\sigma\theta$)



NO₂

North Field Monitor NO₂ Options (Bulk RI, $\sigma\theta$)

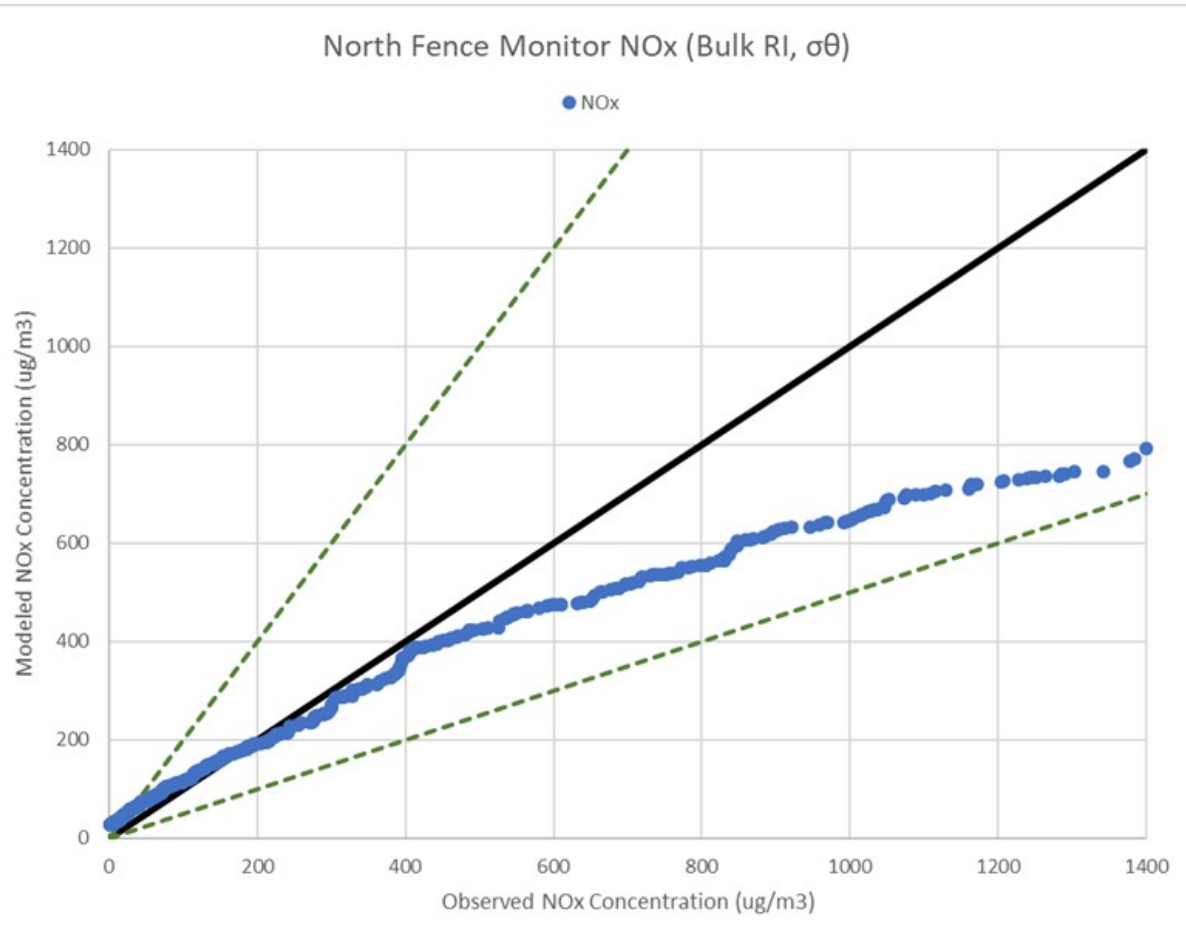


Note: for this monitor, TTRM does not change the Q-Q plot results for NO₂.

Q-Q Plots for North Fence: NO_x and NO₂

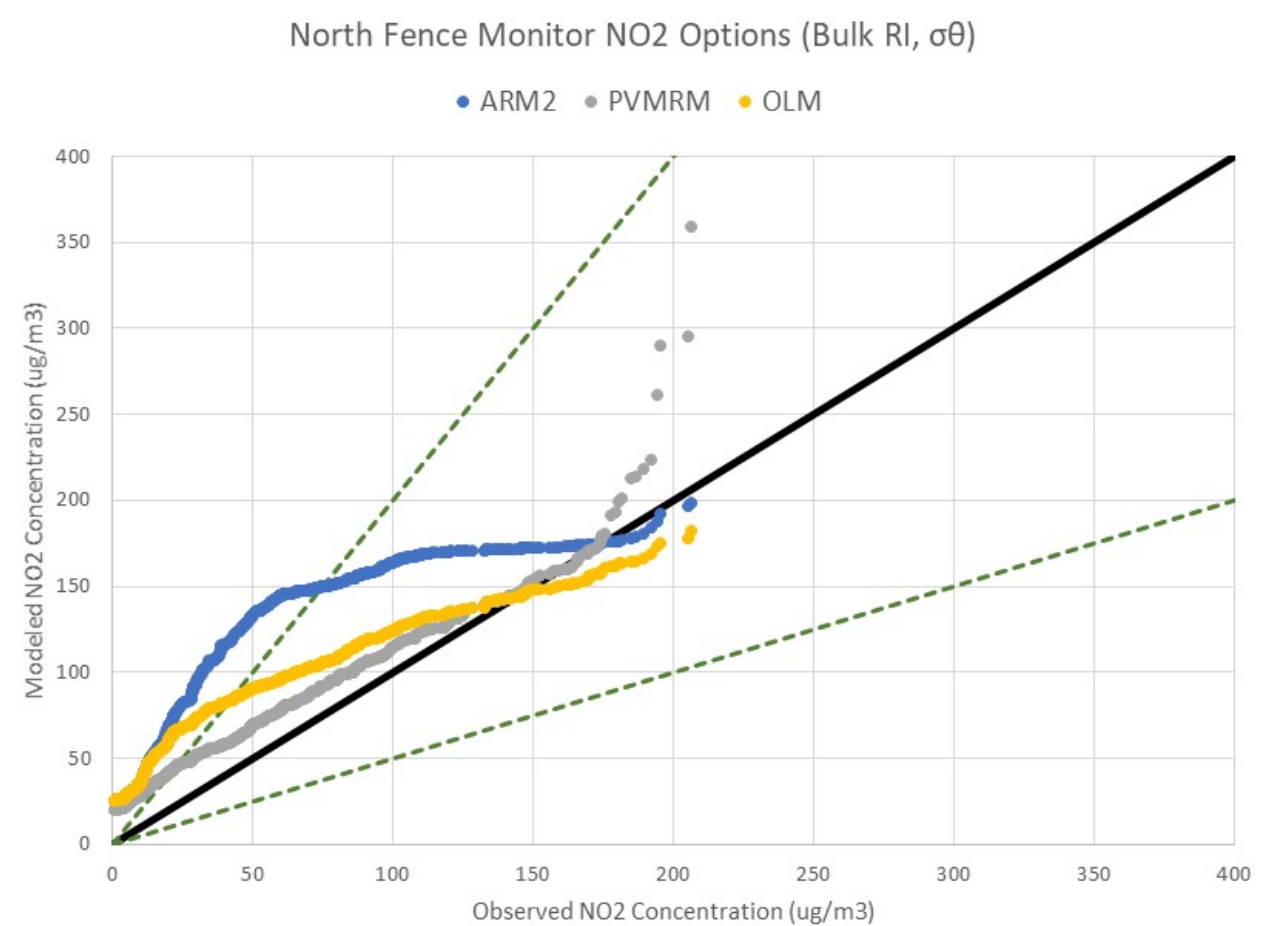
NO_x

North Fence Monitor NO_x (Bulk RI, $\sigma\theta$)



NO₂

North Fence Monitor NO₂ Options (Bulk RI, $\sigma\theta$)

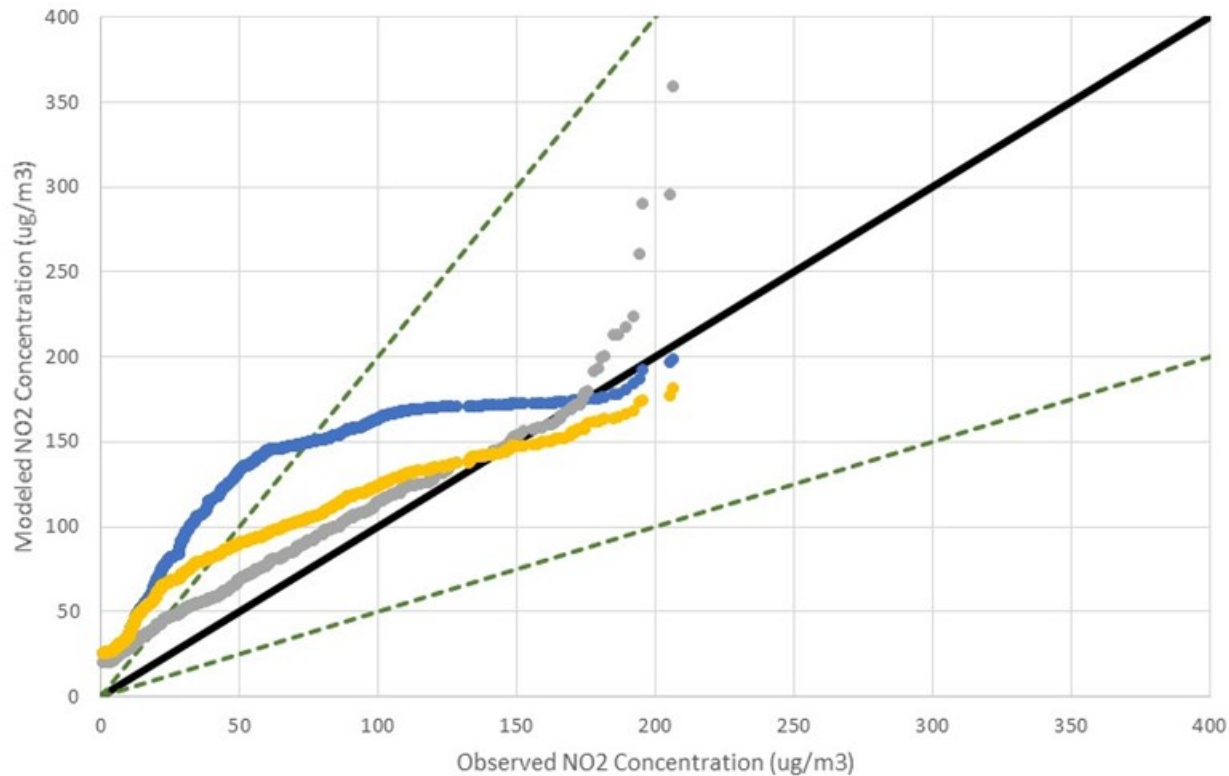


Q-Q Plot for North Fence: NO₂ with TTRM Added on the Right

Without TTRM

North Fence Monitor NO₂ Options (Bulk RI, $\sigma\theta$)

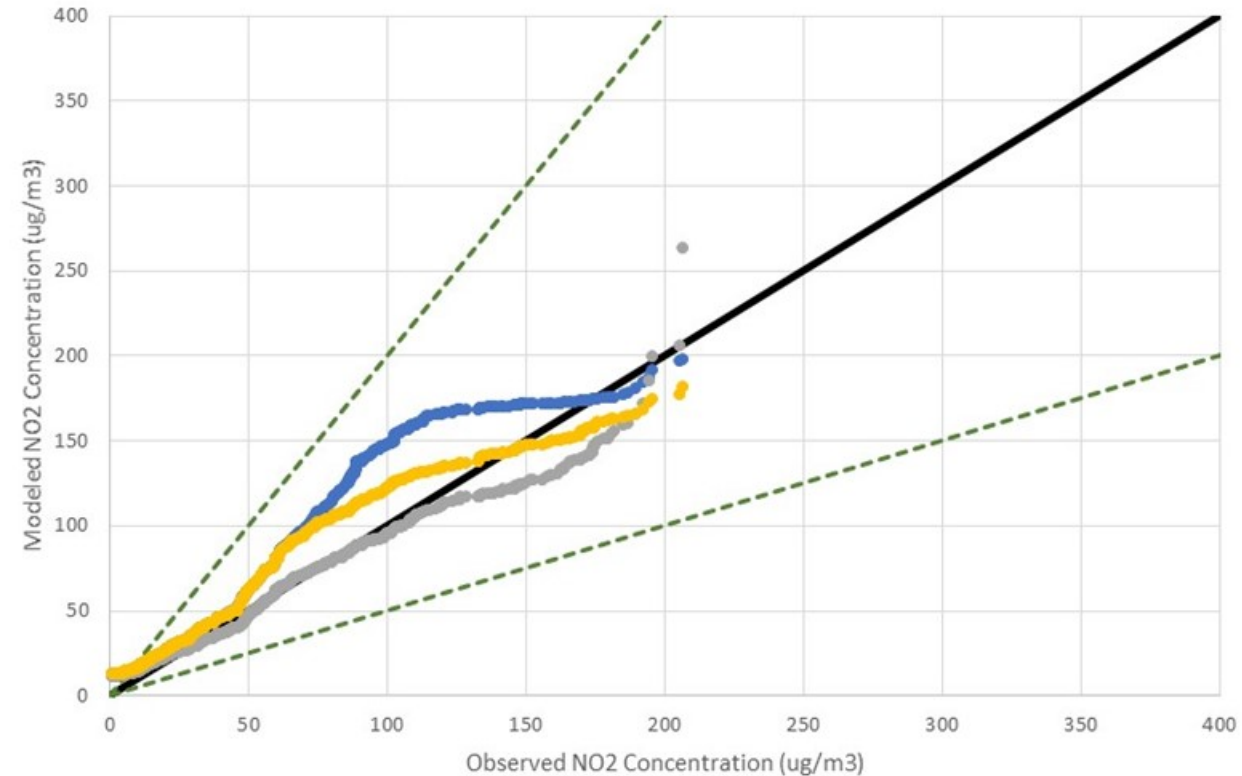
• ARM2 • PVMRM • OLM



Includes TTRM Enhancement

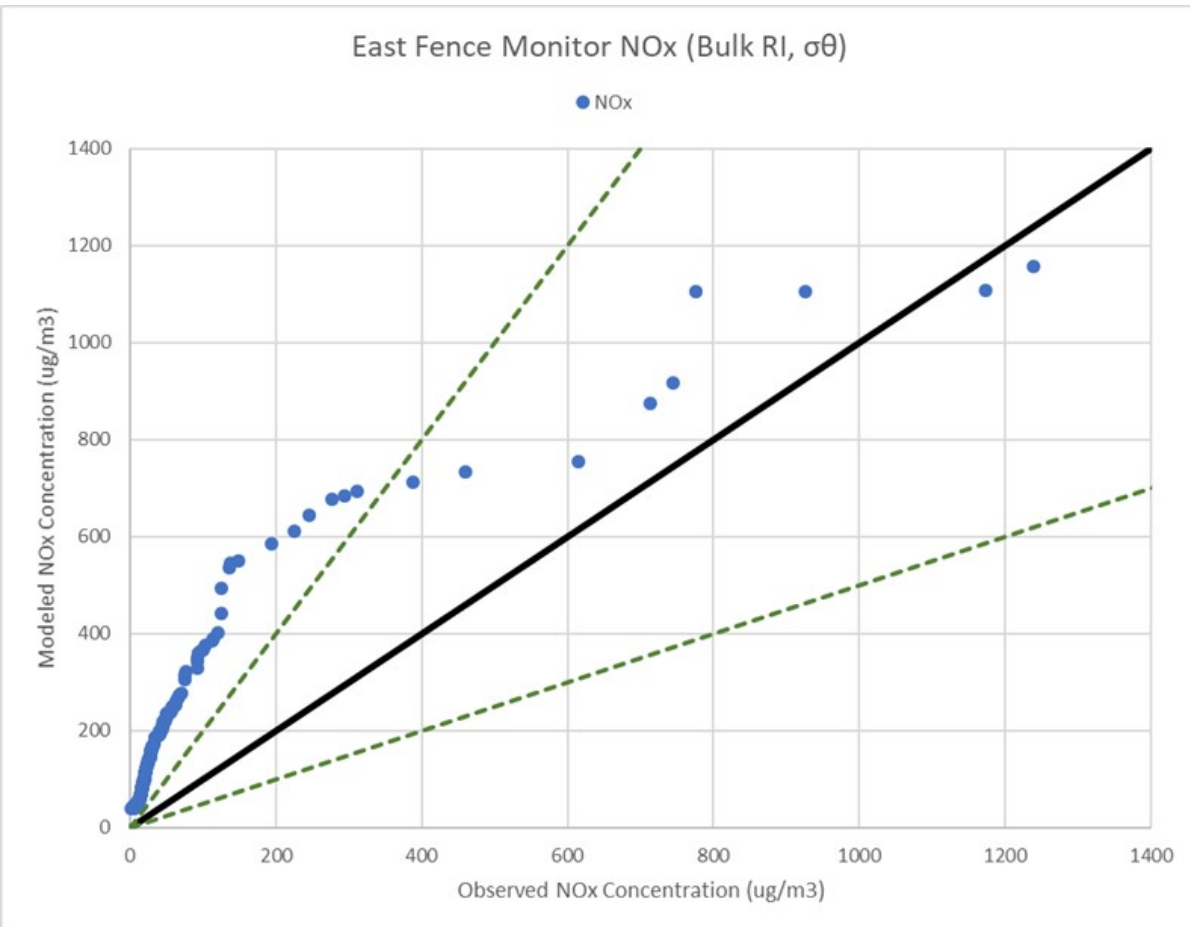
North Fence Monitor NO₂ Options with TTRM (Bulk RI, $\sigma\theta$)

• TTRM-ARM2 • TTRM-PVMRM • TTRM-OLM

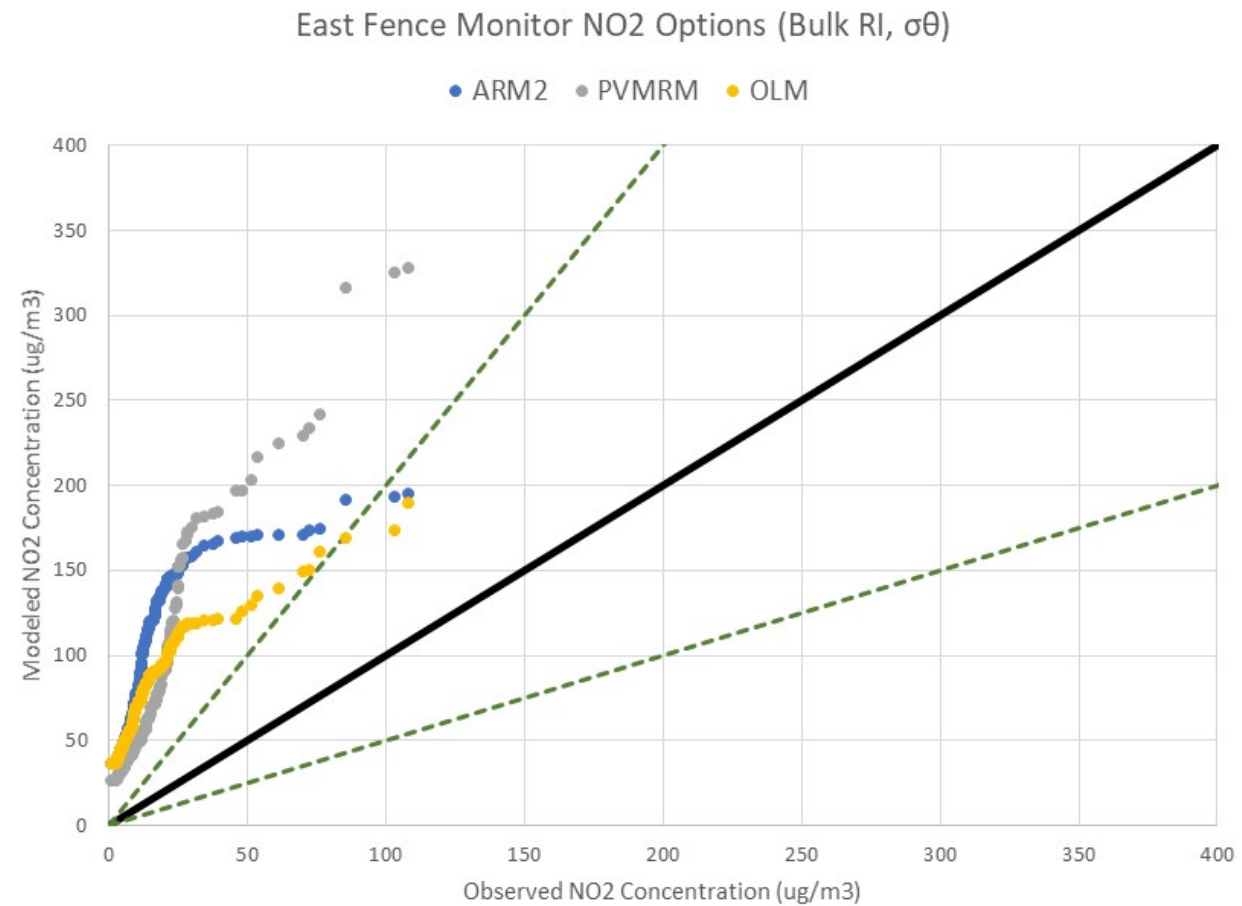


Q-Q Plots for East Fence: NOx and NO₂

NOx



NO₂

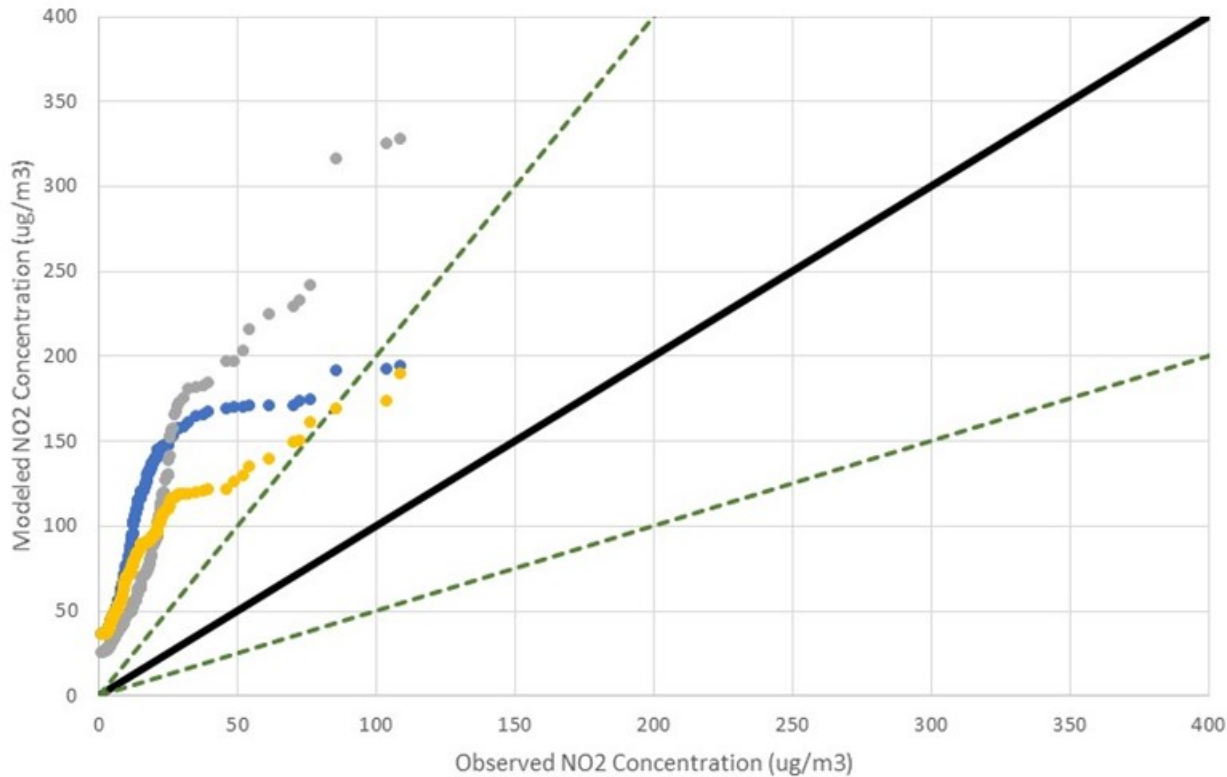


Q-Q Plot for East Fence: NO₂ with TTRM Added on the Right

Without TTRM

East Fence Monitor NO₂ Options (Bulk RI, $\sigma\theta$)

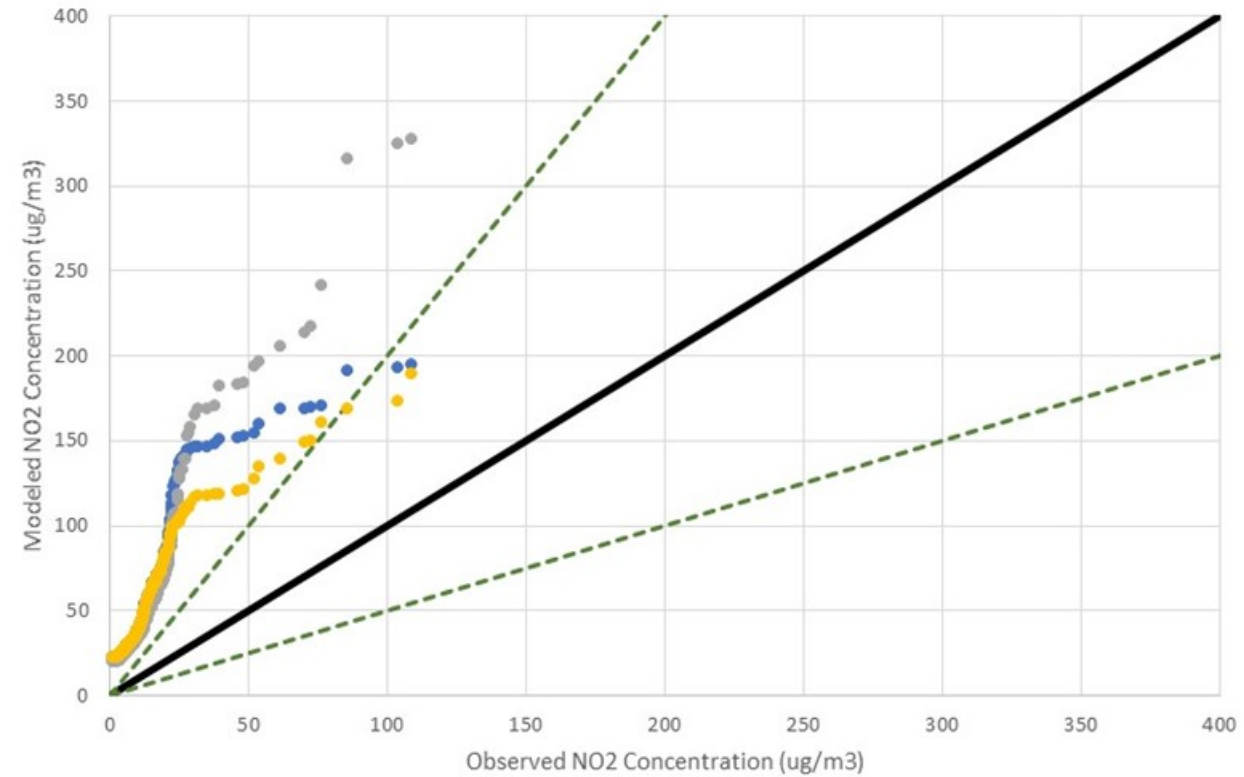
• ARM2 • PVMRM • OLM



Includes TTRM Enhancement

East Fence Monitor NO₂ Options with TTRM (Bulk RI, $\sigma\theta$)

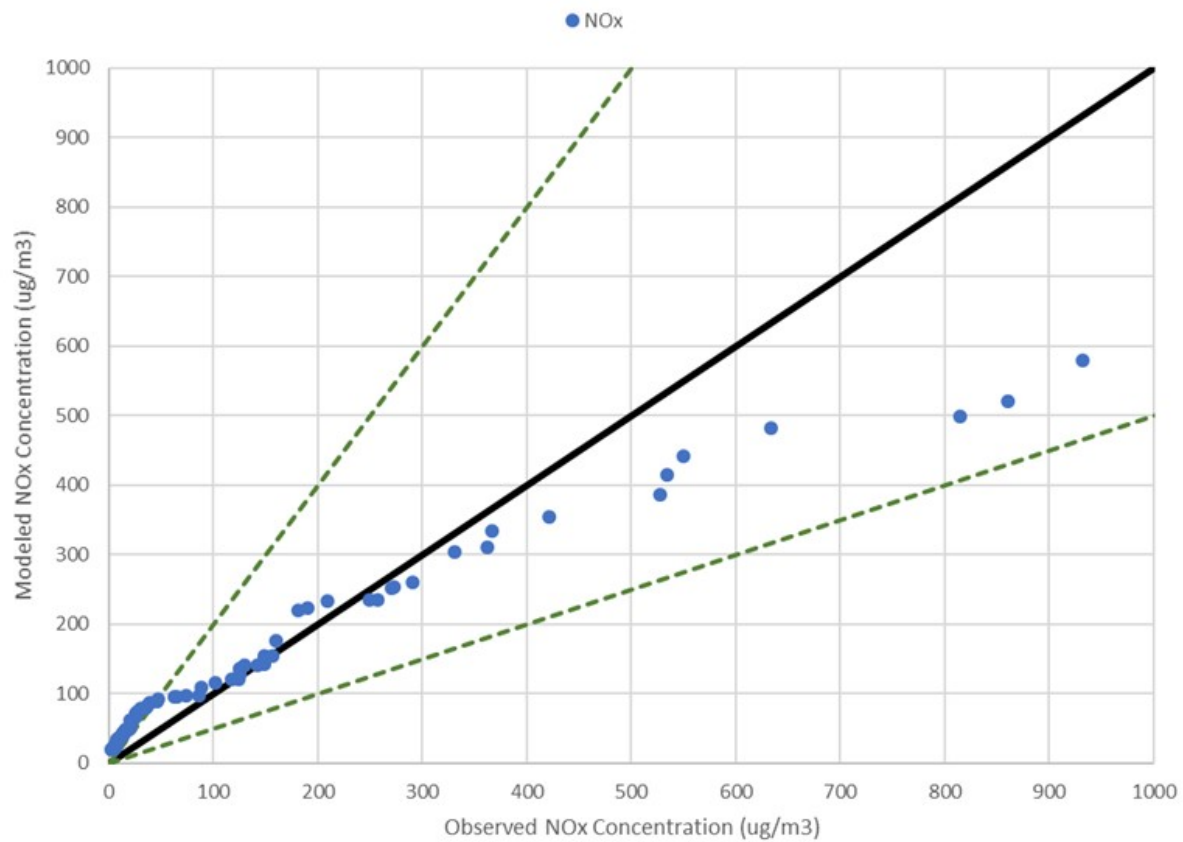
• TTRM-ARM2 • TTRM-PVMRM • TTRM-OLM



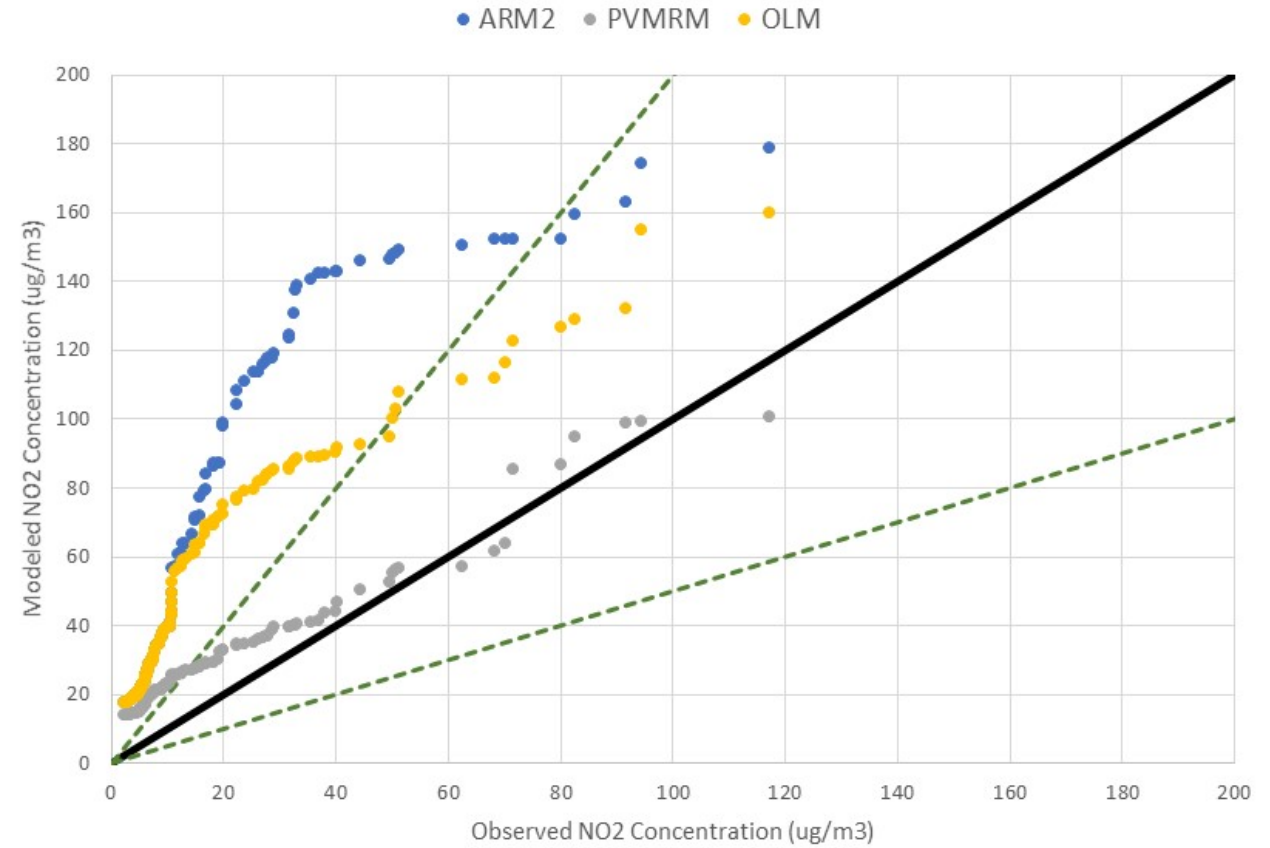
Q-Q Plots for Tower: NO_x and NO₂

NO₂

Tower Monitor NO_x (Bulk RI, $\sigma\theta$)

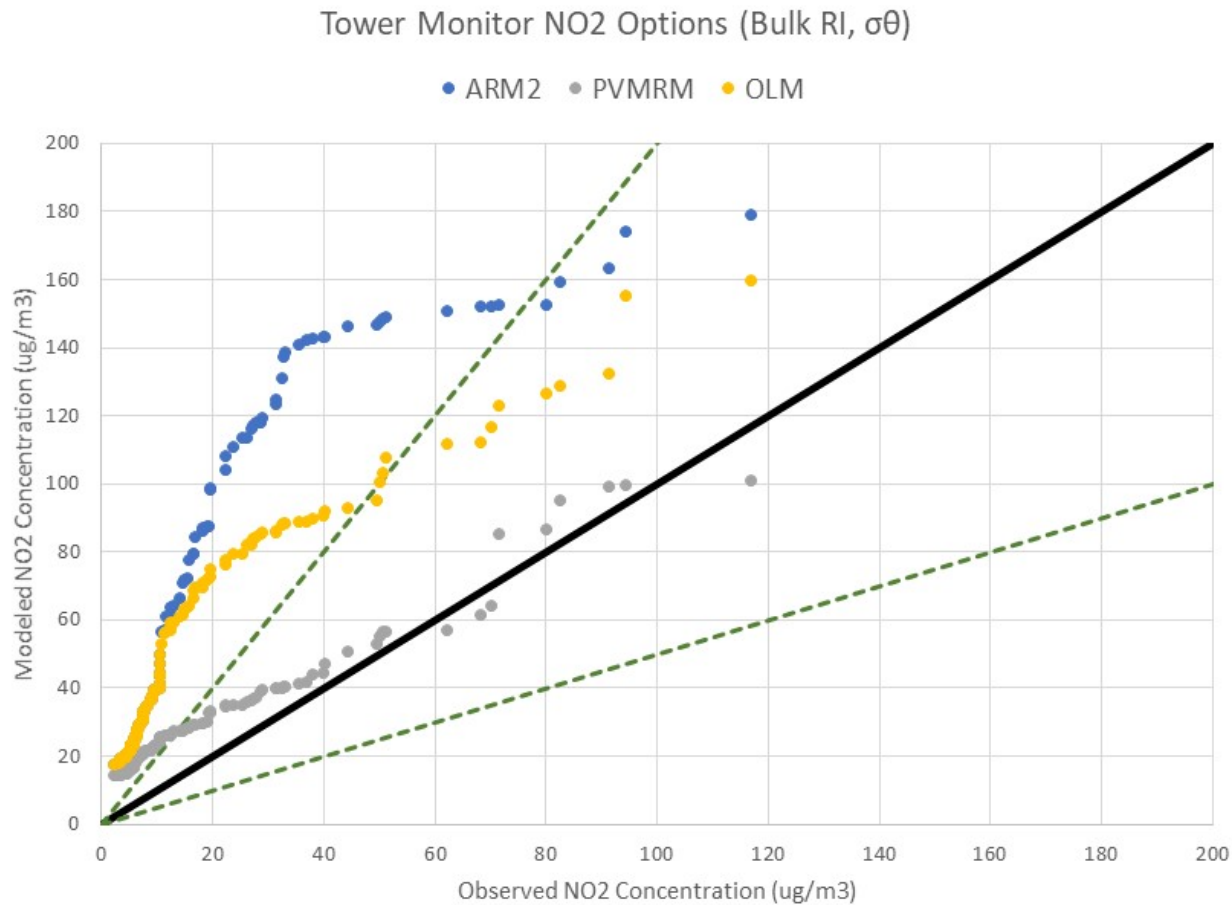


Tower Monitor NO₂ Options (Bulk RI, $\sigma\theta$)

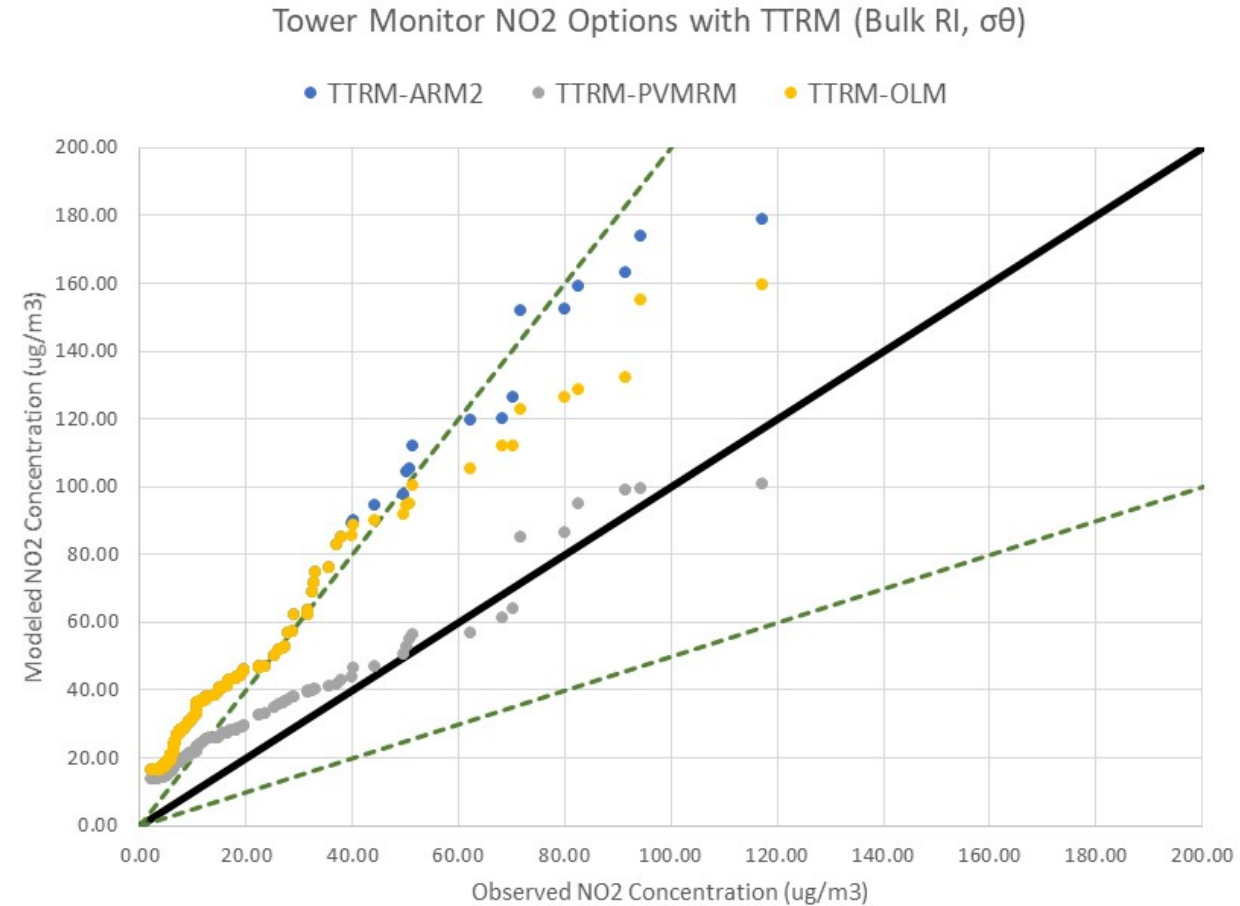


Q-Q Plot for Tower: NO₂ with TTRM Added on the Right

Without TTRM



Includes TTRM Enhancement



Further Analysis to Remove Effect of NO_x Bias

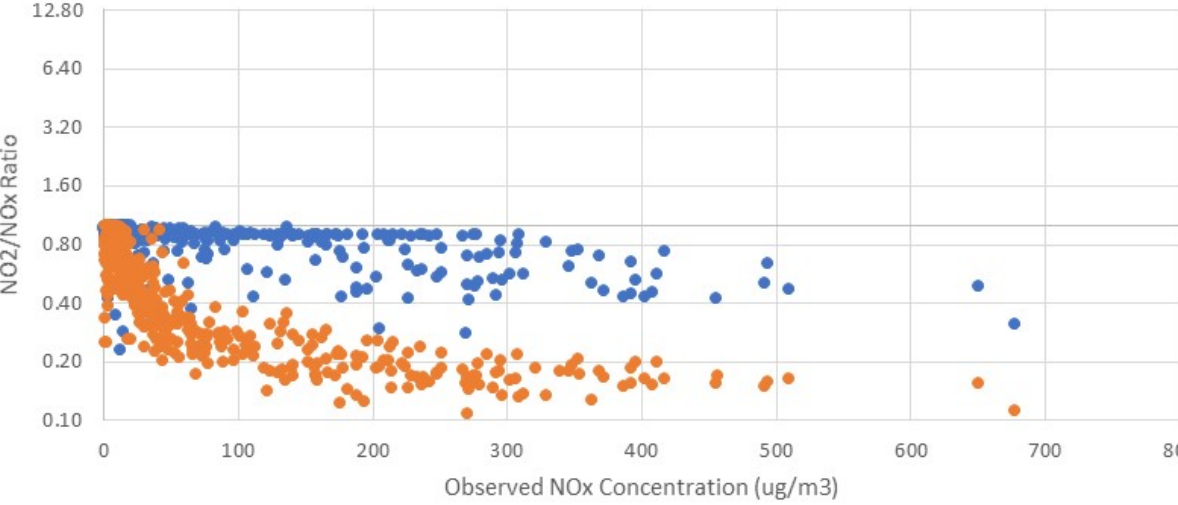
- The real model performance issue is the ratio of NO₂/NO_x
- We show plots of observed as well as predicted NO₂/NO_x for each model
- The NO₂/NO_x ratio is expected to decrease as observed NO_x increases
- The plots show the NO₂/NO_x ratio on the y axis and observed NO_x on the x axis

North Field: NO₂/NO_x Ratio vs. NO_x for ARM2 and ARM2 + TTRM

ARM2

North Field Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

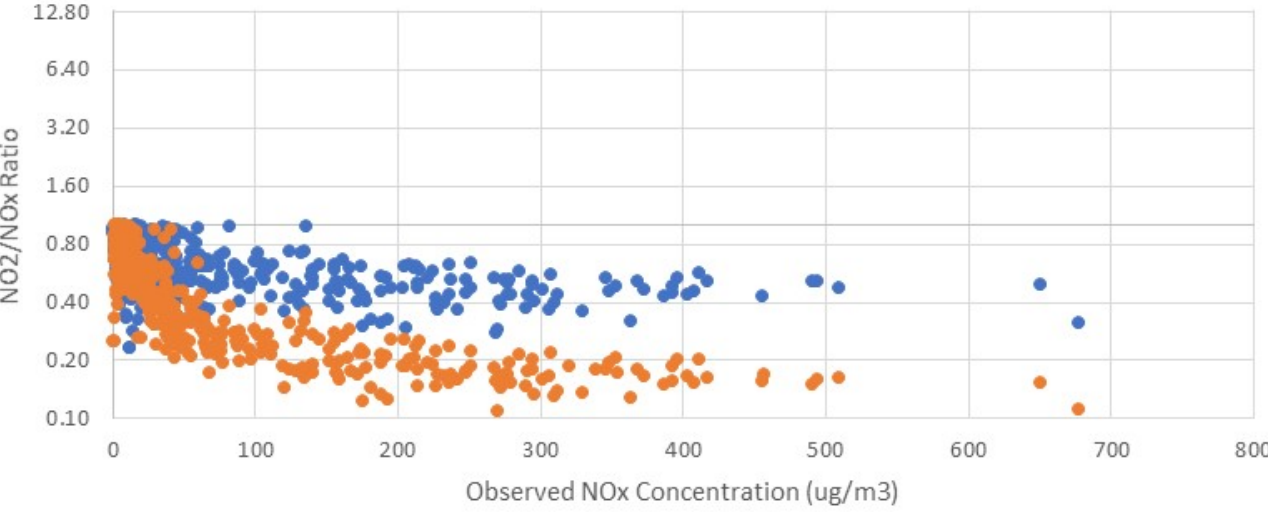
- ARM2 NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)



ARM2 + TTRM

North Field Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

- TTRM-ARM2 NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)



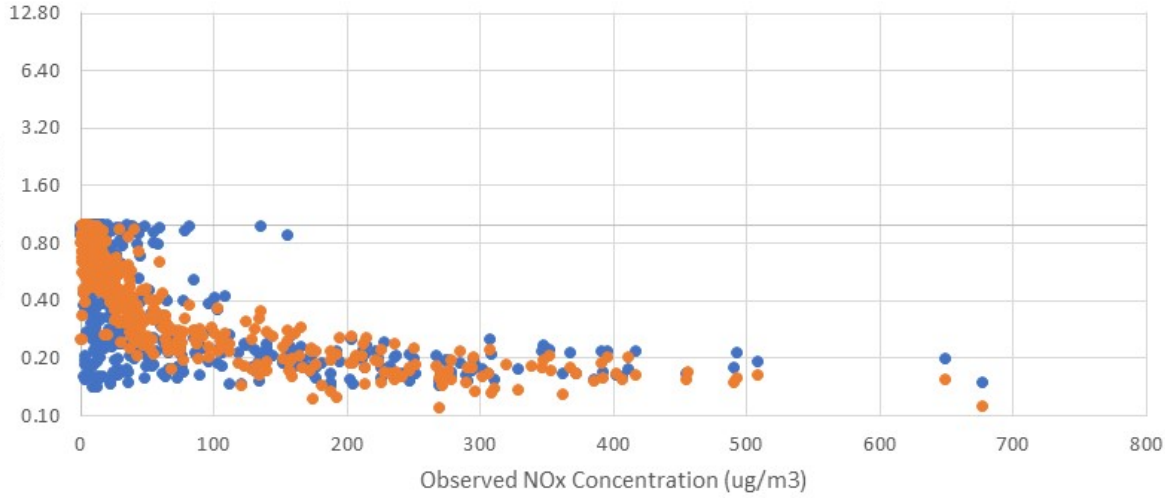
North Field: NO₂/NO_x Ratio vs. NO_x for PVMRM and PVMRM + TTRM

PVMRM

PVMRM + TTRM

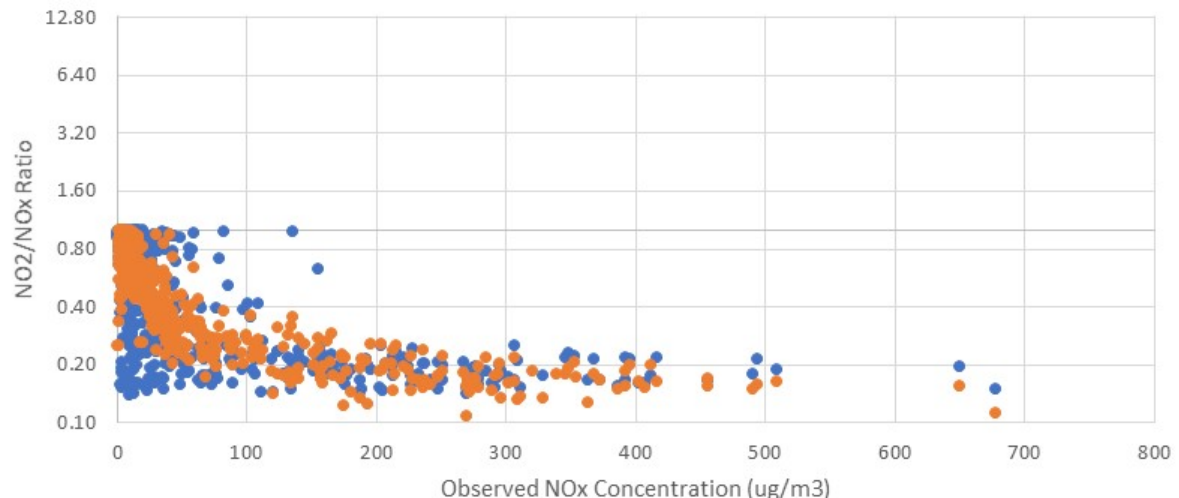
North Field Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

- PVMRM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)



North Field Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

- TTRM-PVMRM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)

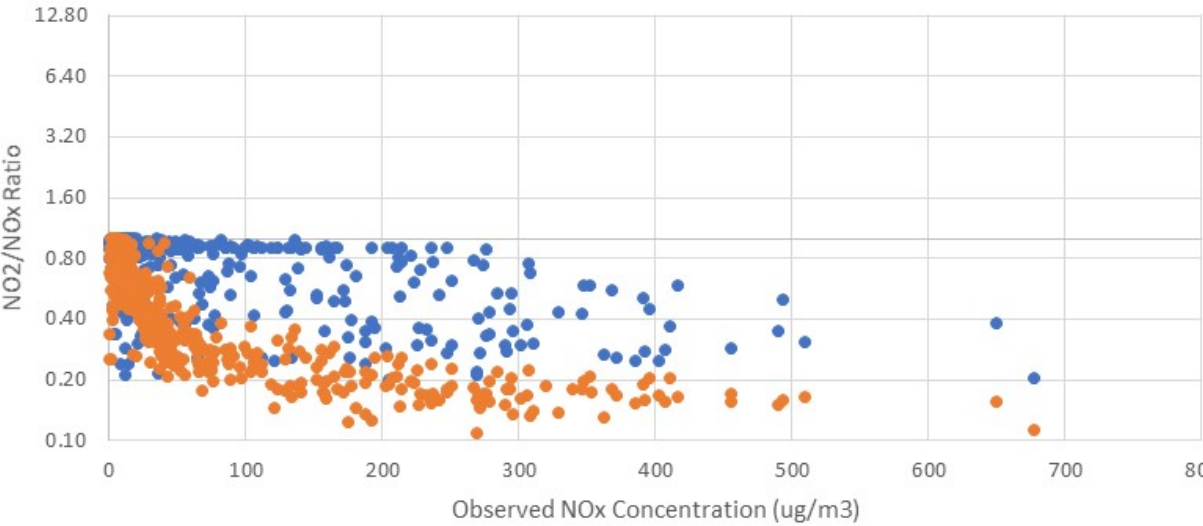


North Field: NO₂/NO_x Ratio vs. NO_x for OLM and OLM + TTRM

OLM

North Field Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

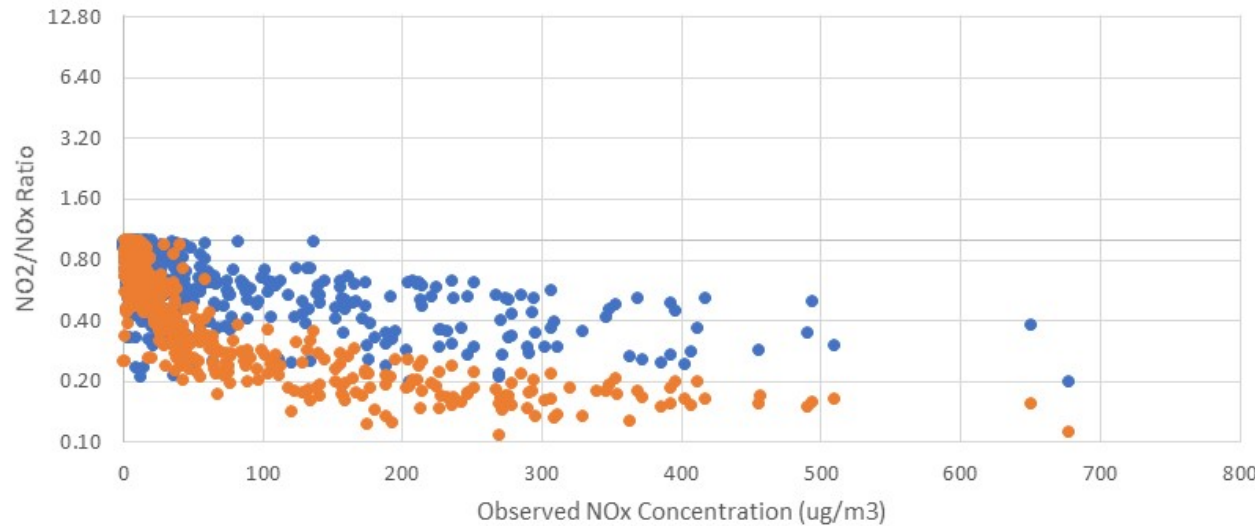
- OLM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)



OLM + TTRM

North Field Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

- TTRM-OLM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)



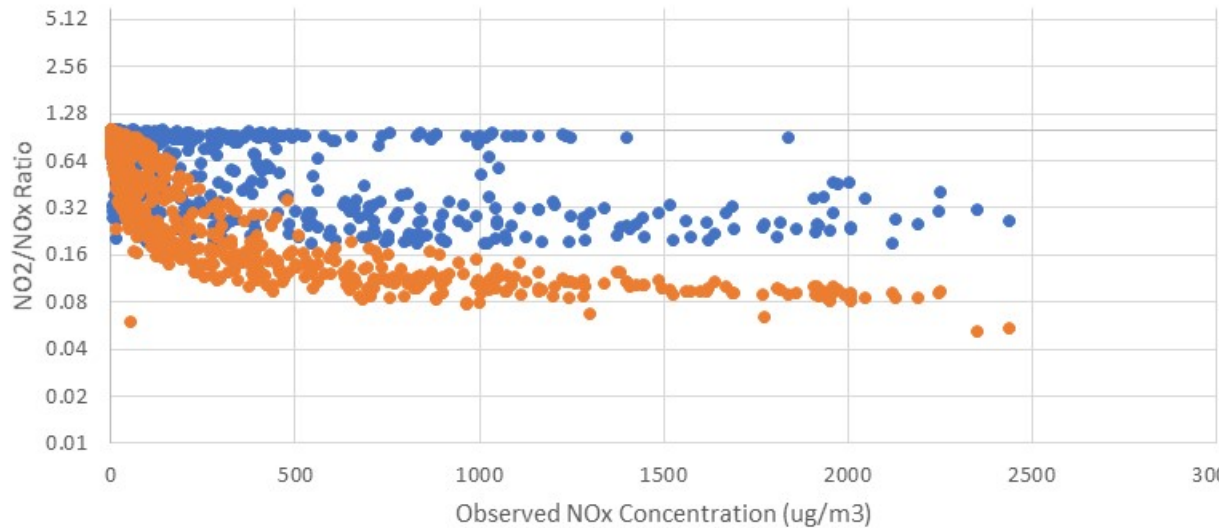
North Fence: NO₂/NO_x Ratio vs. NO_x for ARM2 and ARM2 + TTRM

ARM2

ARM2 + TTRM

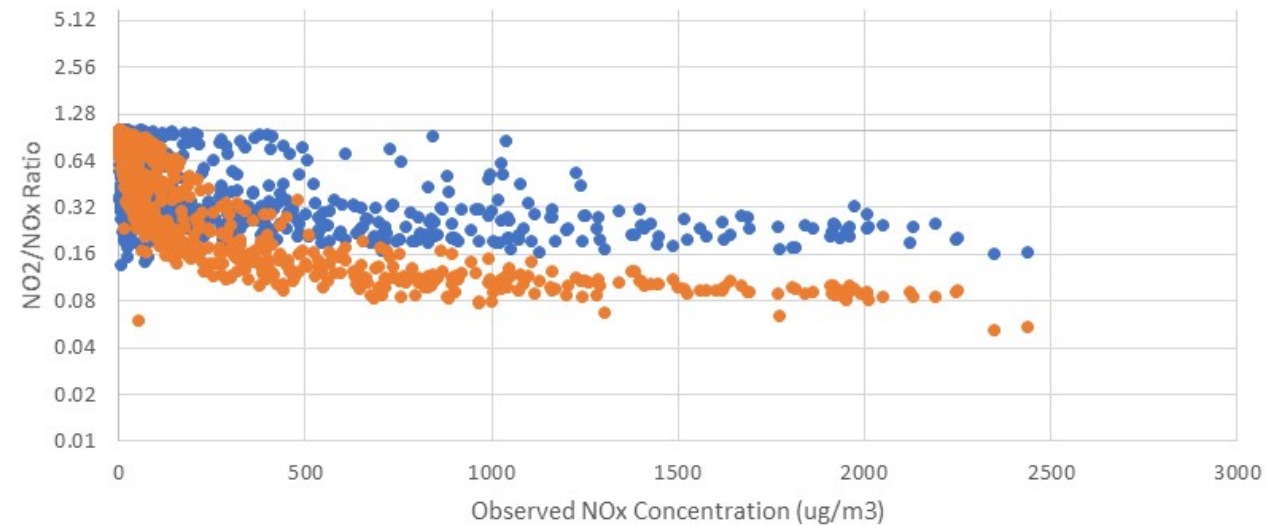
North Fence Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

● ARM2 NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



North Fence Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

● TTRM-ARM2 NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)

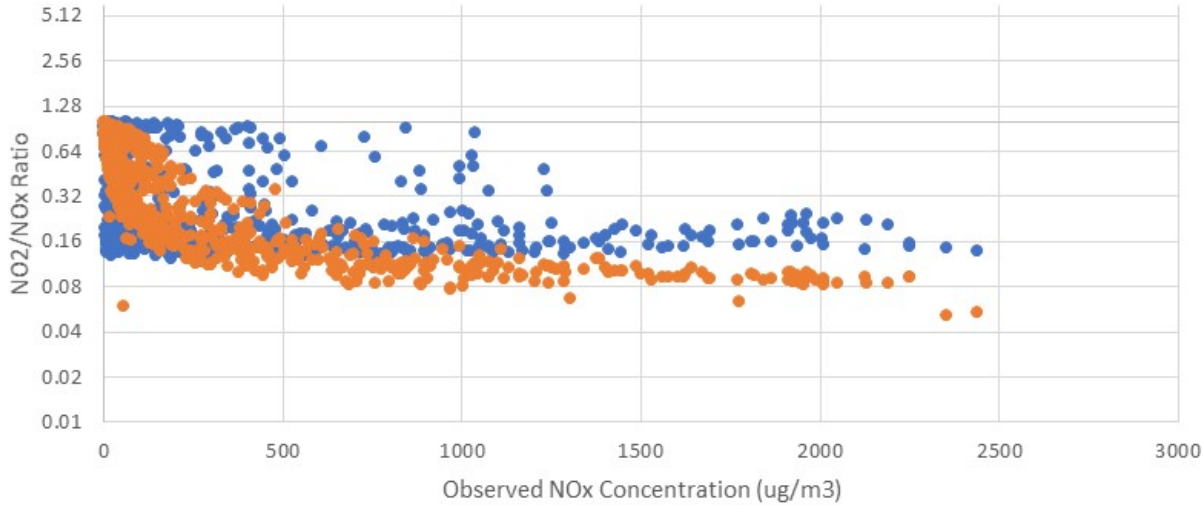


North Fence: NO₂/NO_x Ratio vs. NO_x for PVMRM and PVMRM + TTRM

PVMRM

North Fence Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

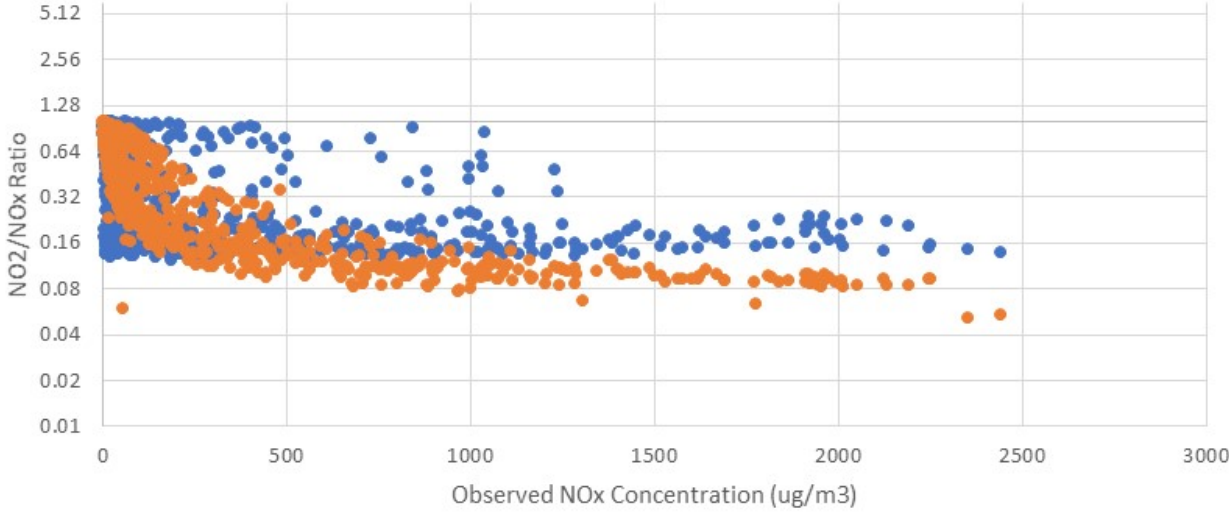
● PVMRM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



PVMRM + TTRM

North Fence Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

● TTRM-PVMRM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)

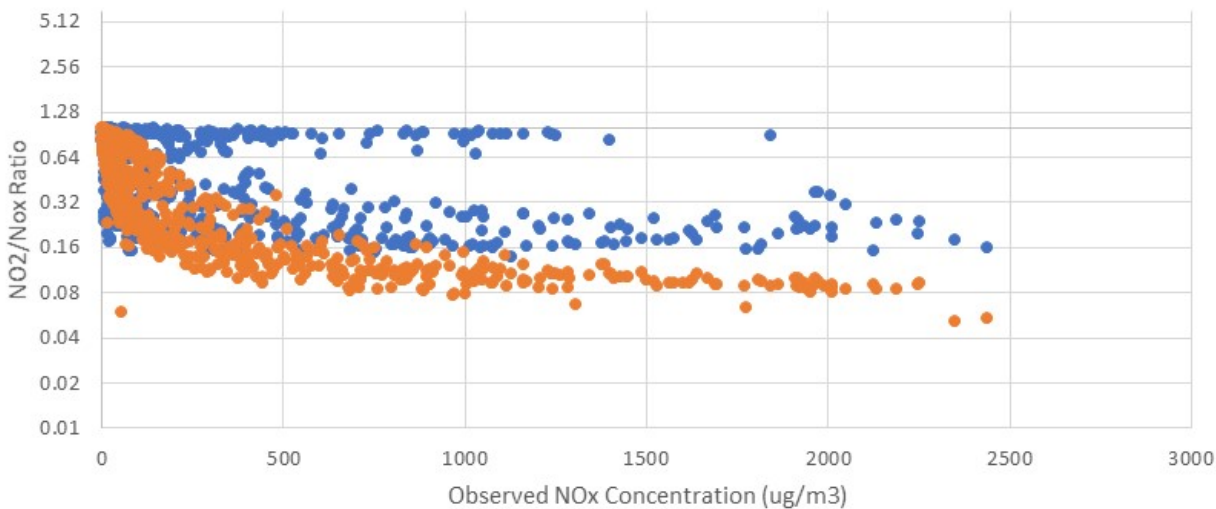


North Fence: NO₂/NO_x Ratio vs. NO_x for OLM and OLM + TTRM

OLM

North Fence Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

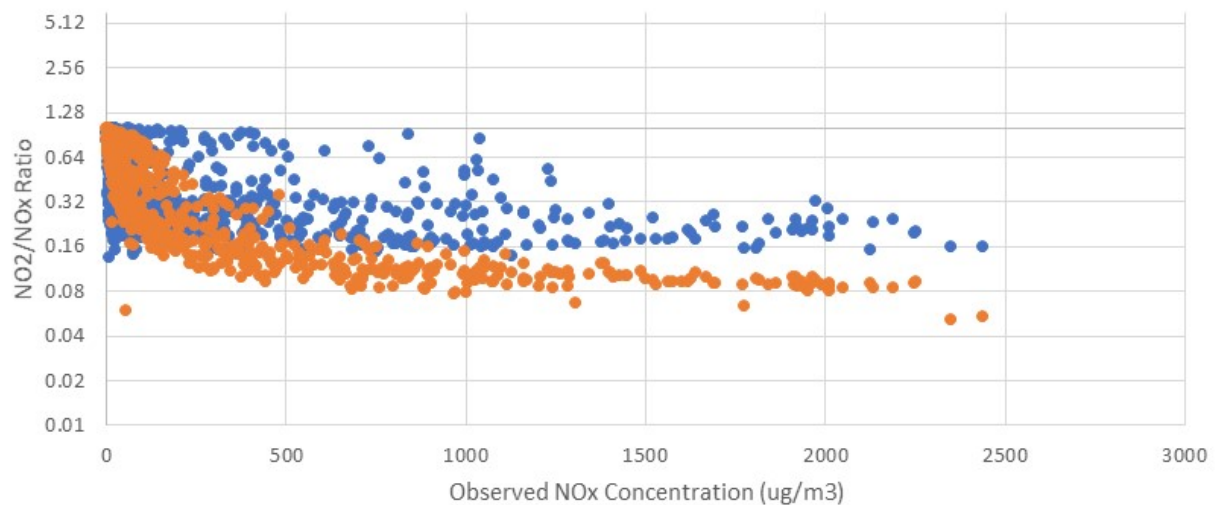
● OLM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



OLM + TTRM

North Fence Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

● TTRM-OLM NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)

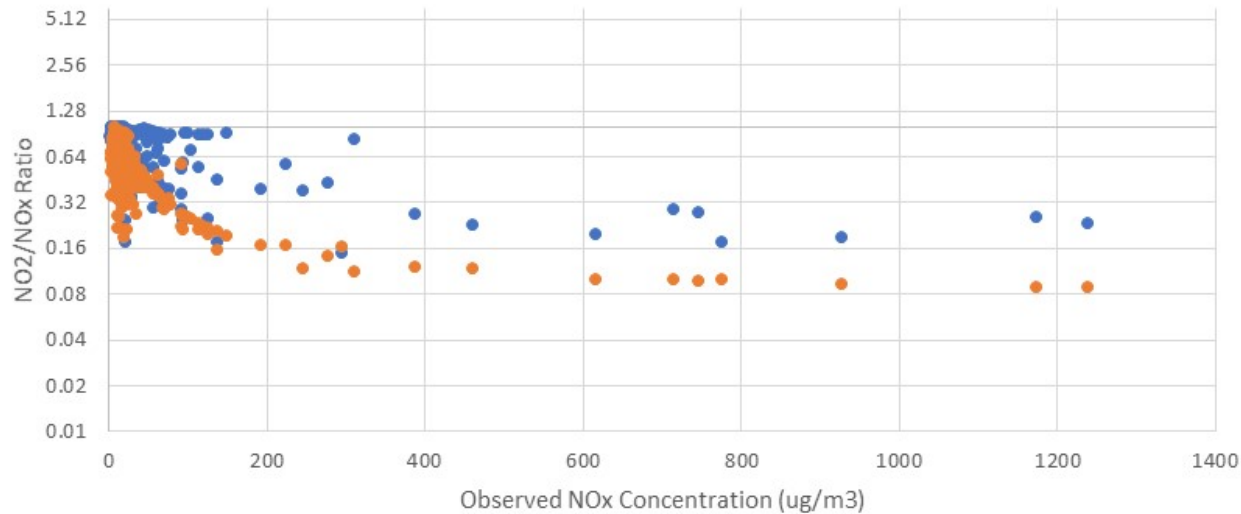


East Fence: NO₂/NO_x Ratio vs. NO_x for ARM2 and ARM2 + TTRM

ARM2

East Fence Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, $\sigma\theta$)

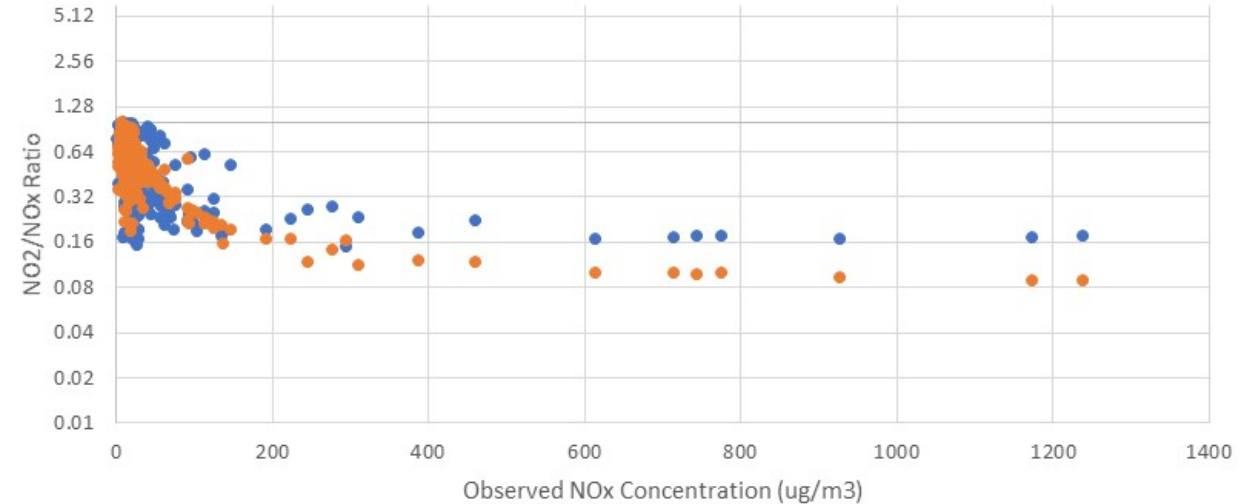
● ARM2 NO₂/NO_x ($\mu\text{g}/\text{m}^3$) ● Obs NO₂/NO_x ($\mu\text{g}/\text{m}^3$)



ARM2 + TTRM

East Fence Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, $\sigma\theta$)

● TTRM-ARM2 NO₂/NO_x ($\mu\text{g}/\text{m}^3$) ● Obs NO₂/NO_x ($\mu\text{g}/\text{m}^3$)

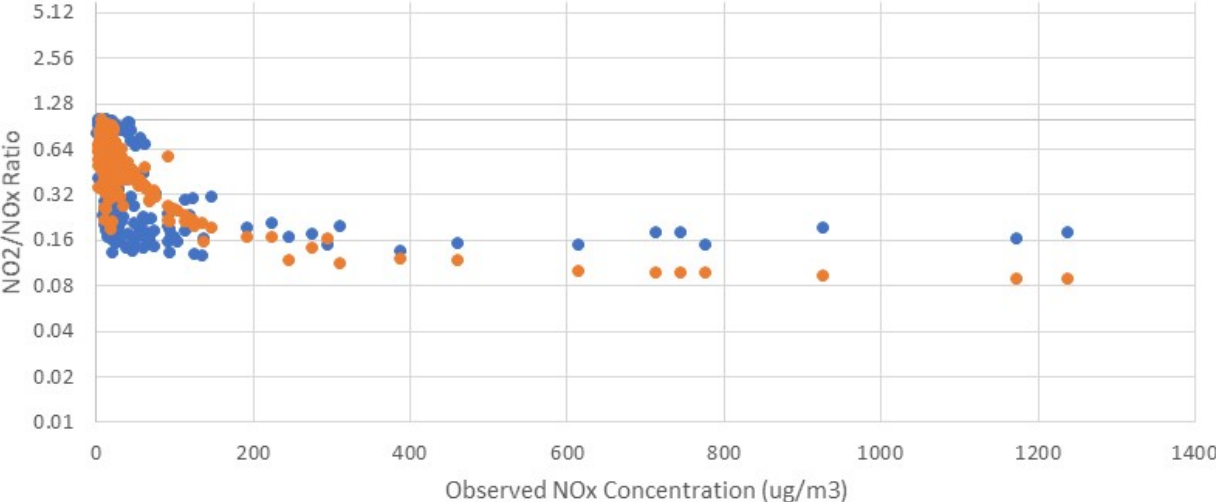


East Fence: NO₂/NO_x Ratio vs. NO_x for PVMRM and PVMRM + TTRM

PVMRM

East Fence Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

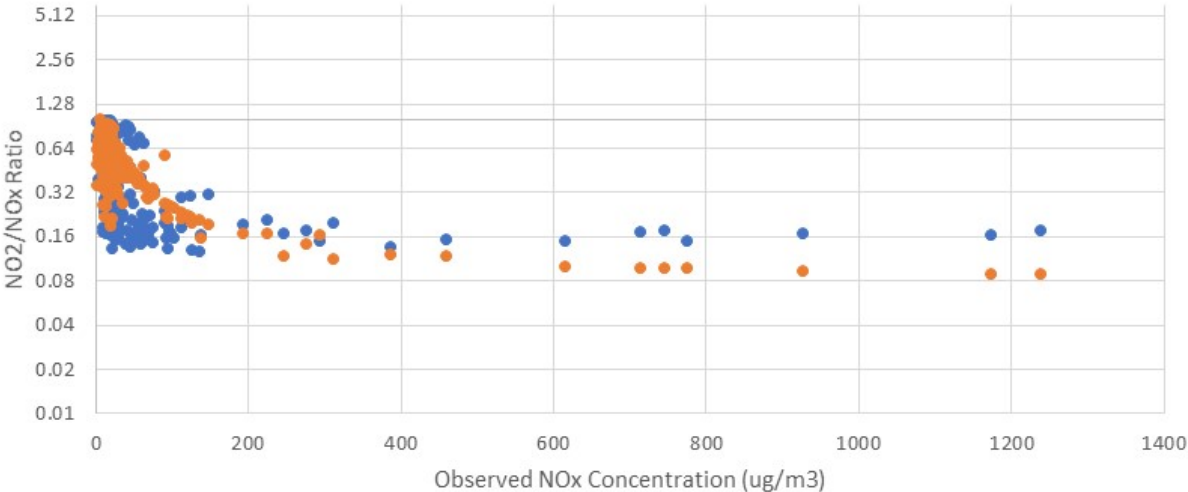
- PVMRM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)



PVMRM + TTRM

East Fence Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

- TTRM-PVMRM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)

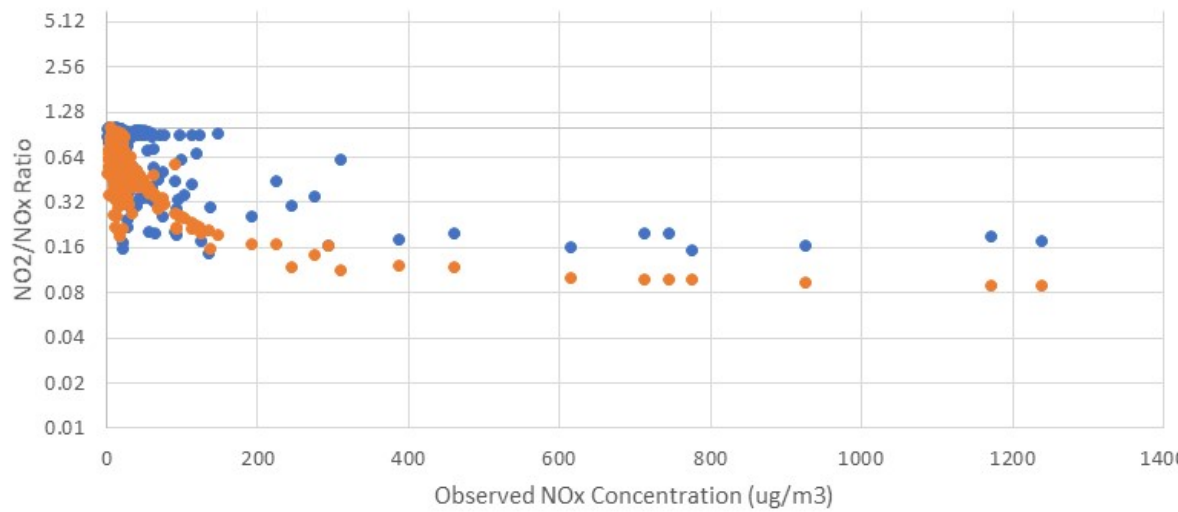


East Fence: NO₂/NO_x Ratio vs. NO_x for OLM and OLM + TTRM

OLM

East Fence Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

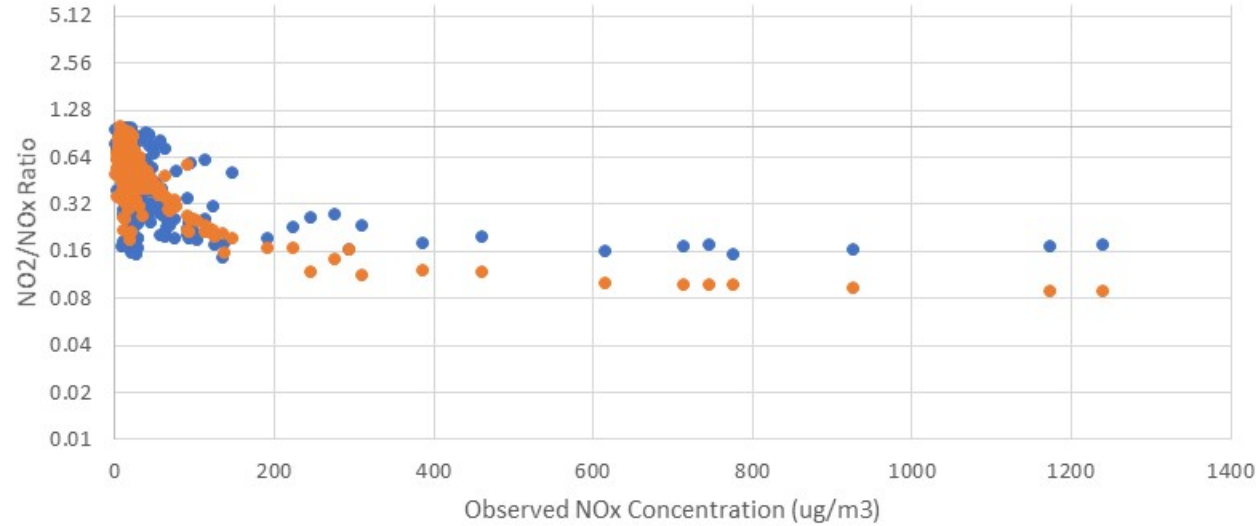
- OLM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)



OLM + TTRM

East Fence Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

- TTRM-OLM NO₂/NO_x (μg/m³)
- Obs NO₂/NO_x (μg/m³)

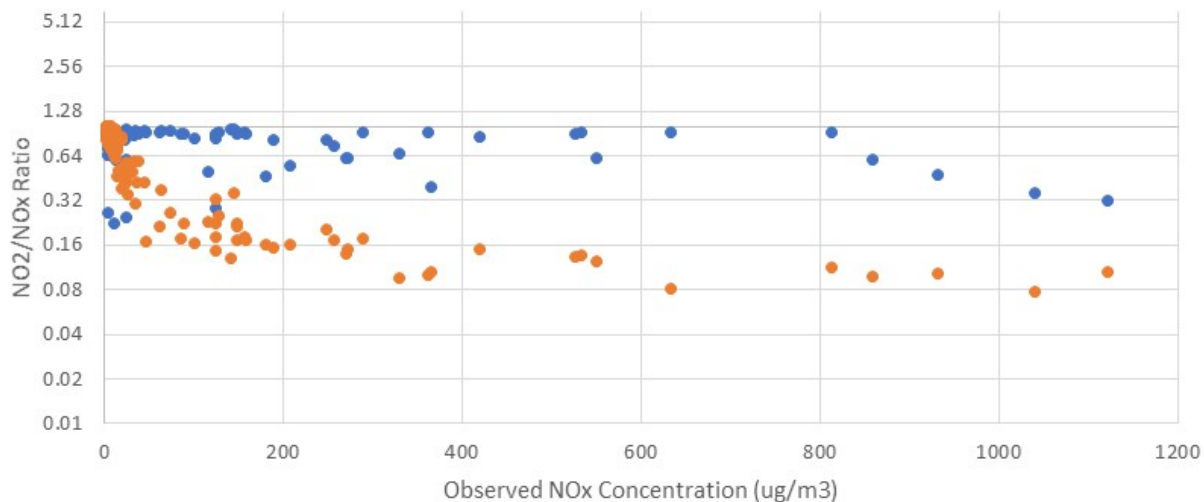


Tower: NO₂/NO_x Ratio vs. NO_x for ARM2 and ARM2 + TTRM

ARM2

Tower Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, $\sigma\theta$)

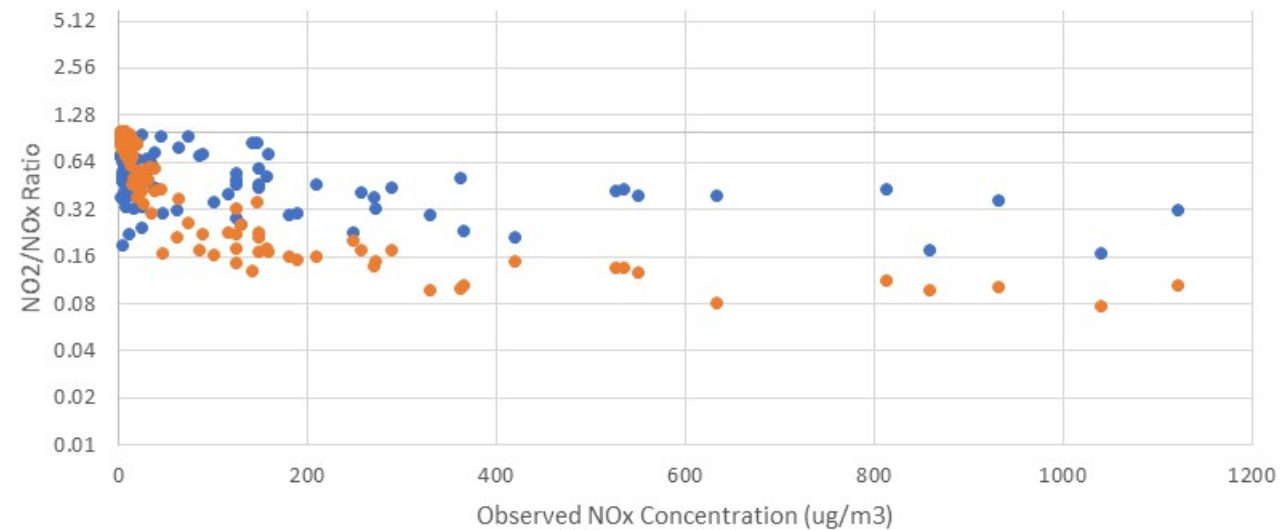
● ARM2 NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)



ARM2 + TTRM

Tower Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, $\sigma\theta$)

● TTRM-ARM2 NO₂/NO_x (μg/m³) ● Obs NO₂/NO_x (μg/m³)

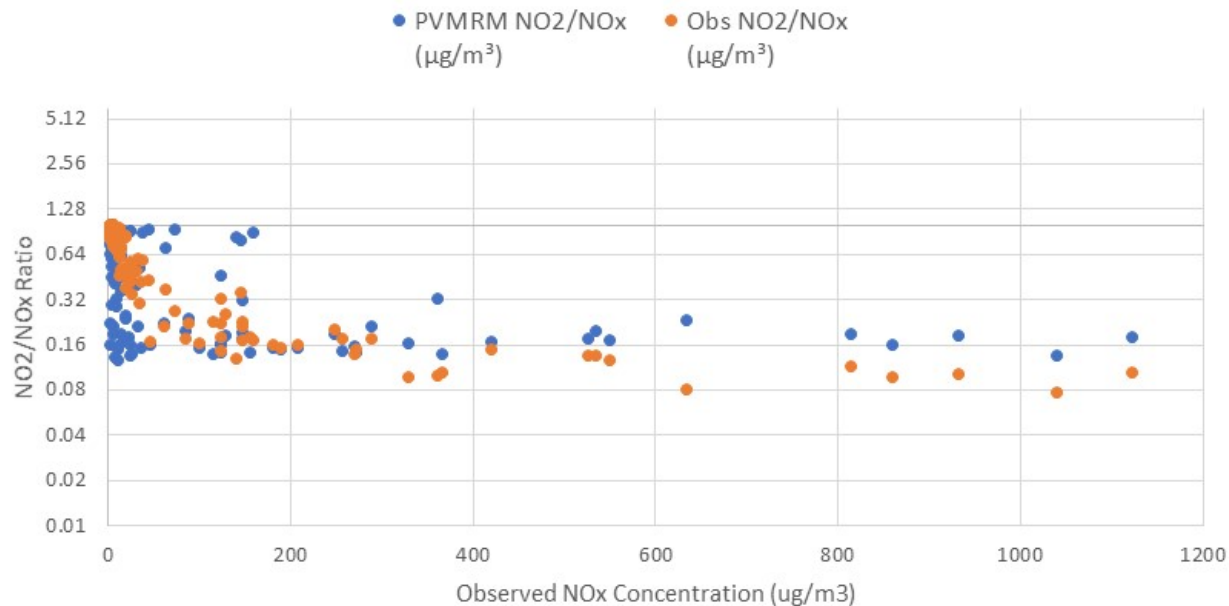


Tower: NO₂/NO_x Ratio vs. NO_x for PVMRM and PVMRM + TTRM

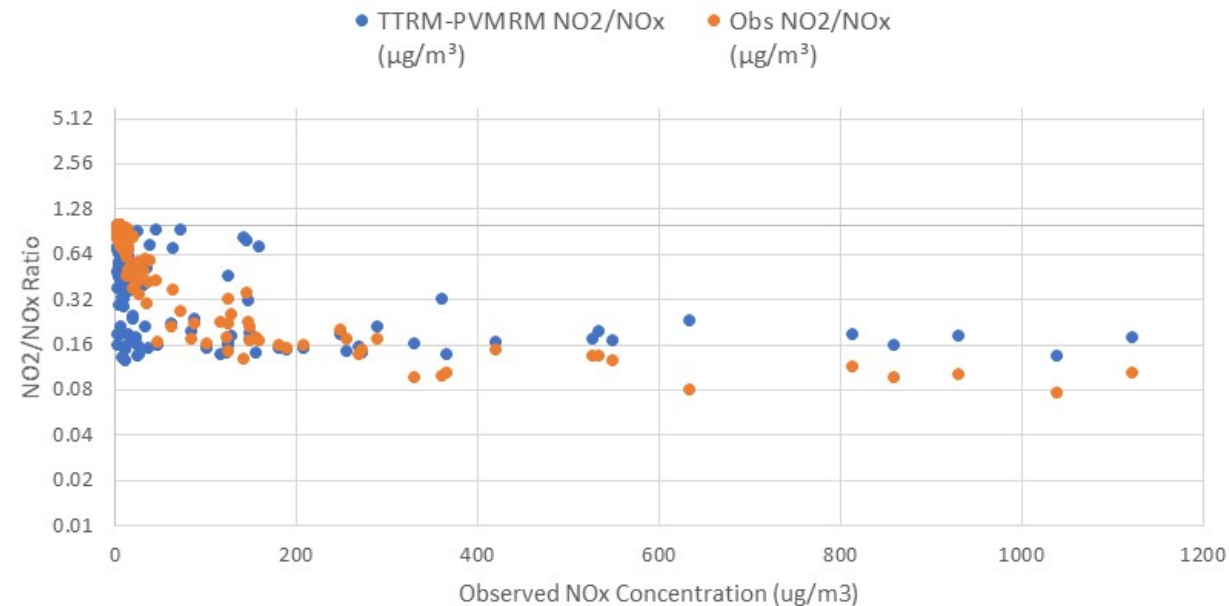
PVMRM

PVMRM + TTRM

Tower Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)



Tower Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, σθ)

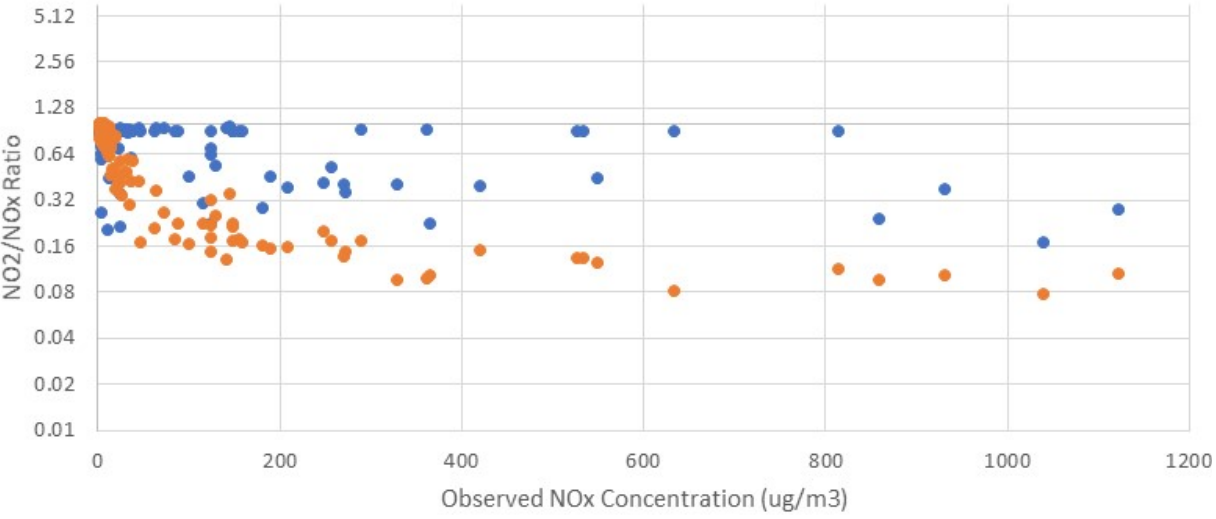


Tower: NO₂/NO_x Ratio vs. NO_x for OLM and OLM + TTRM

OLM

Tower Ratio of Predicted & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, $\sigma\theta$)

● OLM NO₂/NO_x ($\mu\text{g}/\text{m}^3$) ● Obs NO₂/NO_x ($\mu\text{g}/\text{m}^3$)



OLM + TTRM

North Field Ratio of Predicted w/ TTRM & Observed NO₂/NO_x Ratio vs. Observed NO_x (Bulk RI, $\sigma\theta$)

● TTRM-OLM NO₂/NO_x ($\mu\text{g}/\text{m}^3$) ● Obs NO₂/NO_x ($\mu\text{g}/\text{m}^3$)

