#MO09 Evaluation of explicit NO_x chemistry methods in AERMOD using a new compressor station dataset

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Guideline on Air Quality Models:
Planning Ahead

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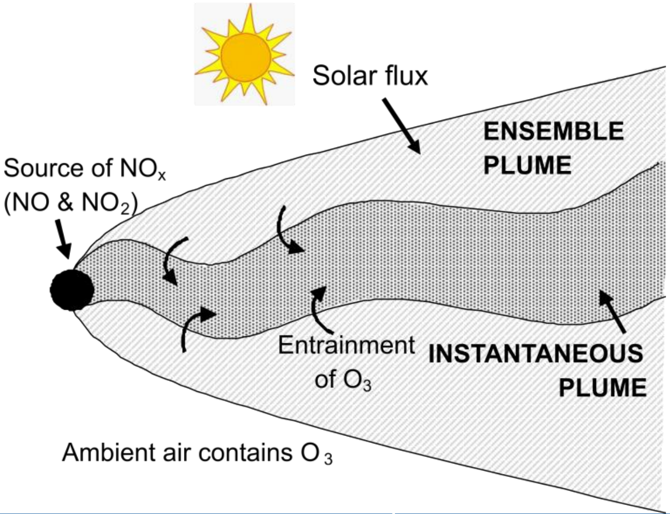
Background

- For some industrial installations, demonstrating compliance with the 1-hour NO_2 National Ambient Air Quality Standard (NAAQS) using AERMOD can be difficult.
- AERMOD Tier 3 chemistry methods, OLM (Ozone Limiting Method) and PVMRM (Plume Volume Molar Ratio Method), can predict overly conservative concentration values for some model configurations.
- A new explicit NO_x chemistry method for AERMOD 'Atmospheric Dispersion Modelling System Method' (ADMSM) has been implemented in a previous version of AERMOD. ADMSM was evaluated using available NO_2 databases (Empire Abo, Palaau, Wainwright and Prudhoe Bay)*.
- This presentation provides results of additional ADMSM assessment using a new compressor station evaluation dataset.

* Carruthers, D.J.; Stocker, J.R.; Ellis, A.; Seaton, M.D.; Smith, S.E., Evaluation of an explicit NOx chemistry method in AERMOD; Journal of the Air and Waste Management Association. 2017, 67:6, 702-712

Chemistry schemes



NO_x chemistry

'Ozone titration'

$NO + O_3 \rightarrow NO_2 + O_2$

'Photolysis'

$NO_2 + \text{sunlight} \rightarrow NO + O_3$

Fast reactions (seconds - minutes)

Item	OLM (Ozone-Limiting Method)	PVMRM (Plume Volume Molar Ratio Method)	ADMSM (ADMS Method)
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 *ensemble* plume	Limited entrainment (volume-based approach) into *instantaneous* plume	Limited entrainment (cross-sectional area-based approach) into *instantaneous* 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

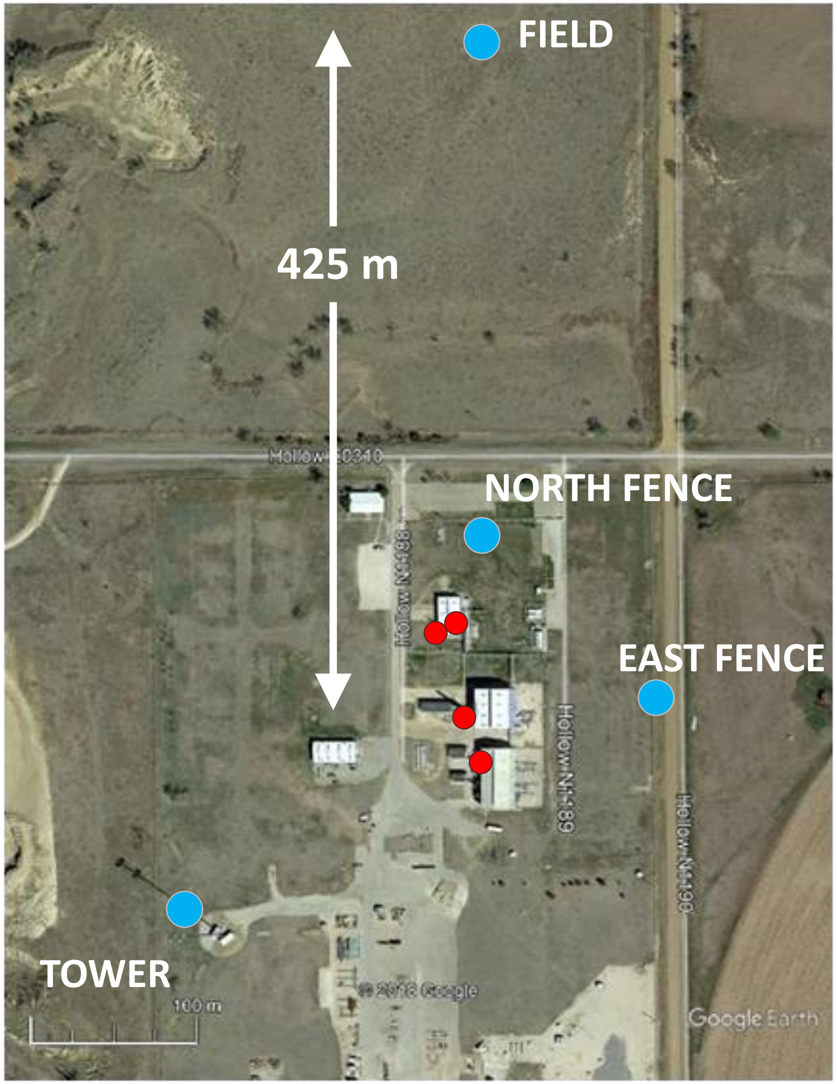
Campaign set up

13 month campaign (Dec. 2015 – Dec. 2016)

Flat, scrubby grassland

● 4 main NO_2 sources:
- 2 compressor engine stacks
- 1 boiler
- 1 emergency generator

Meteorological instruments on 30 m tower



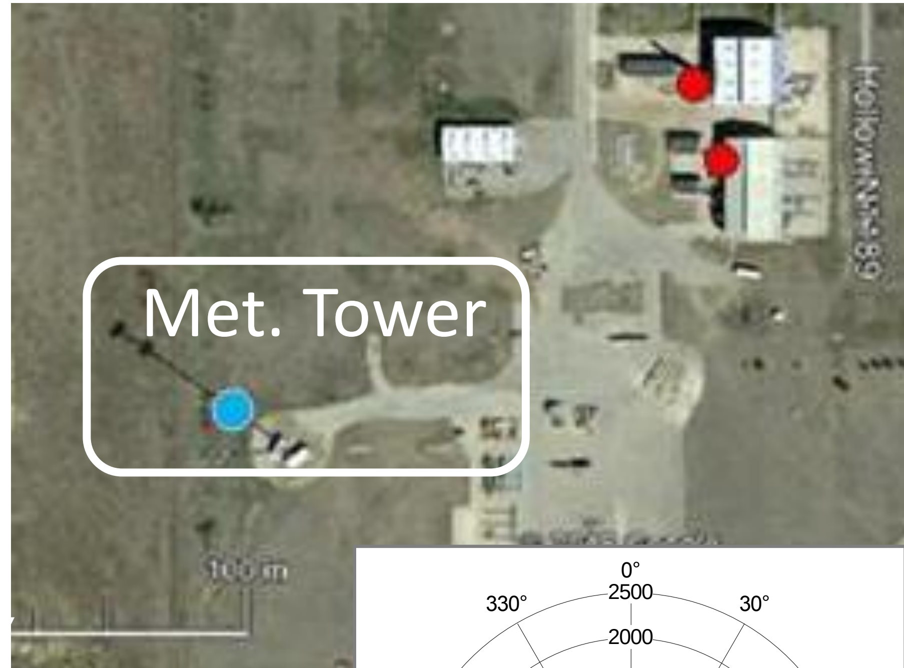
Parametric Emissions Monitoring Systems (PEMS) recorded hourly engine parameters (compressor engines only)

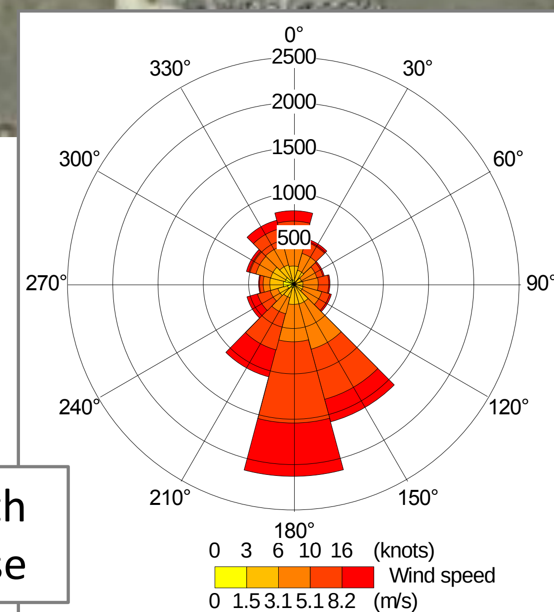
● 4 monitors:
- ‘North Fence’ and ‘Field’ in alignment with the stacks and the prevailing wind
- ‘East Fence’
- ‘Tower’

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

Meteorological data

- Recorded wind speed, wind direction, temperature, solar radiation, pressure, precipitation and humidity
- Standard deviation of the horizontal wind direction (sigma theta) derived from 1-minute wind direction data
- 2 m, 10 m and 30 m measurements
- Good quality data:
  - On-site
  - Away from significant buildings
  - Located to record prevailing conditions

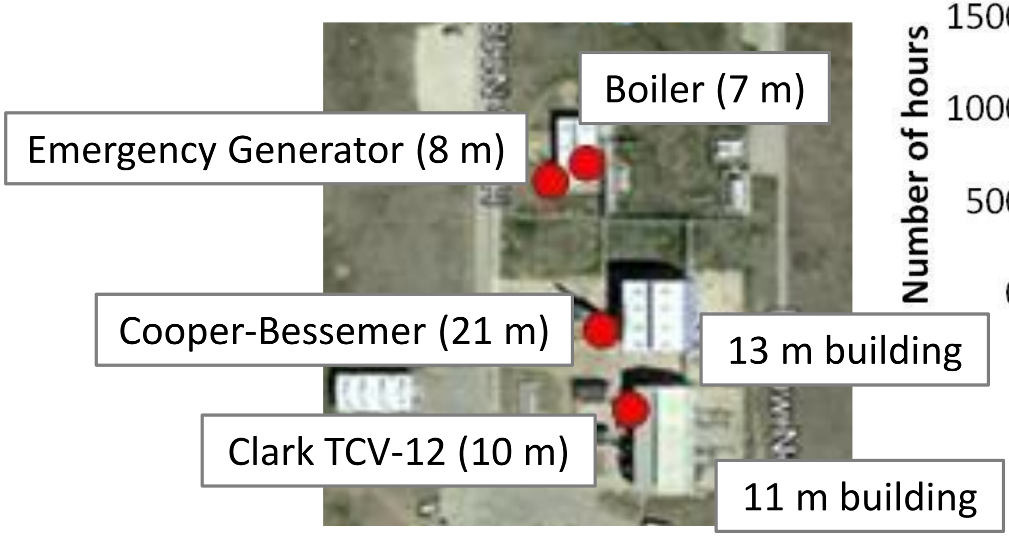


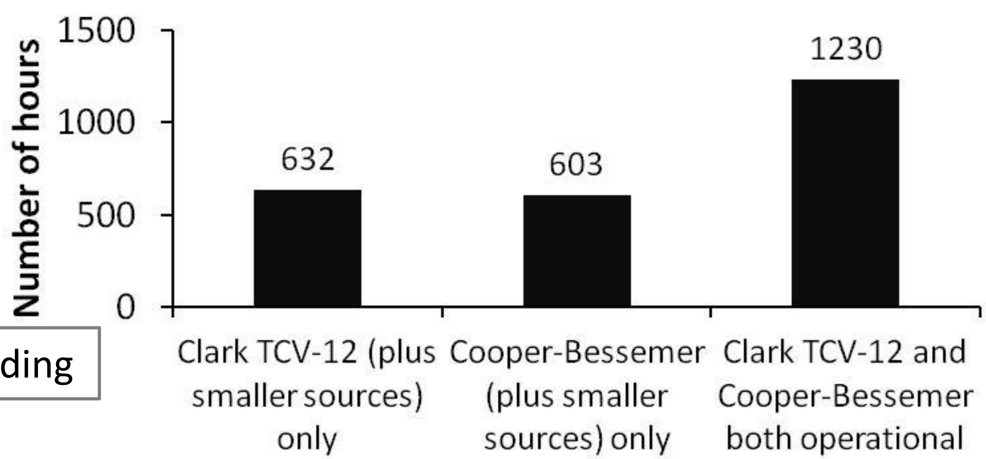


13 month wind rose

Source and emissions data

Source	No. operational hours (out of 9528)	Av. NO_x emission rate when operational (g/s)	Exit Temp. (°C)	Exit vel. (m/s)
Clark TCV-12 comp. engine	1862	12.8	316	17.4 (average)
Cooper-Bessemer comp. engine	1833	1.75	277	19.8
Boiler (with rain cap)	5134	0.062	427	10.9
Emergency generator (EG)	86	0.29	538	13.1



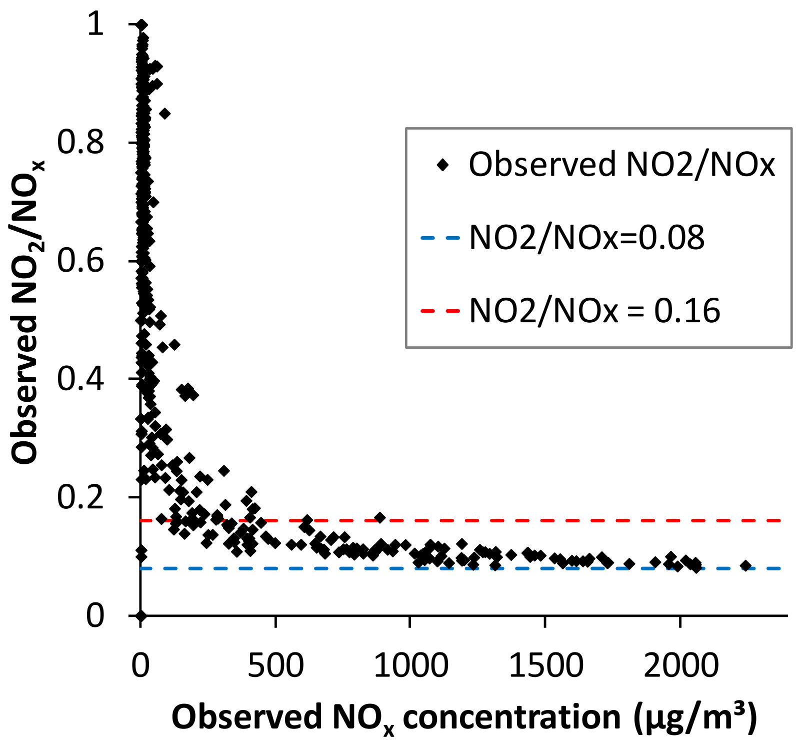


Clark TCV-12 compressor engine emissions dominate

In-stack ratios

Source	Supplied in-stack ratio	Modelled in-stack ratio
Clark TCV-12 comp. engine	0.16 (PEMS)	0.08 (ambient monitoring data)
Cooper-Bessemer comp. engine	0.3 (PEMS)	0.3 (PEMS)
Boiler	0.1	0.1
Emergency generator (EG)	0.1	0.1

- This is a scientific evaluation study - not a regulatory assessment
- Consider ambient monitoring data from the closest monitor with the highest frequency and magnitude of concentrations (North Fence)
- Filter data for when the Cooper-Bessemer is not operational
- Minimum NO_2/NO_x asymptotes to 0.08



Analysis methodology

- Analyse NO_x performance then analyse NO_2 performance:
  - Are the predictions of NO_2 consistent with NO_x? (e.g., if NO_x is overpredicted then NO_2 should also be overpredicted, and vice versa.)
  - Are the NO_2 predictions consistent with the chemistry scheme formulation?
- Consider:
  - Statistics
  - Quantile-quantile (Q-Q) plots
  - Variation of the ratio of modelled to observed NO_2 against ratio of modelled to observed NO_x*
- Analyse data where emissions are high and the wind advects from the source(s) to the monitor(s); i.e., filter by wind direction

* Smith, S.; Stocker, J.; Seaton, M.; Carruthers, D., Model inter-comparison and validation of ADMS plume chemistry schemes; International Journal of Environment and Pollution. 2017, 62(2-4), 395-406.

Statistical results: average concentrations

Tables: data paired in space and time

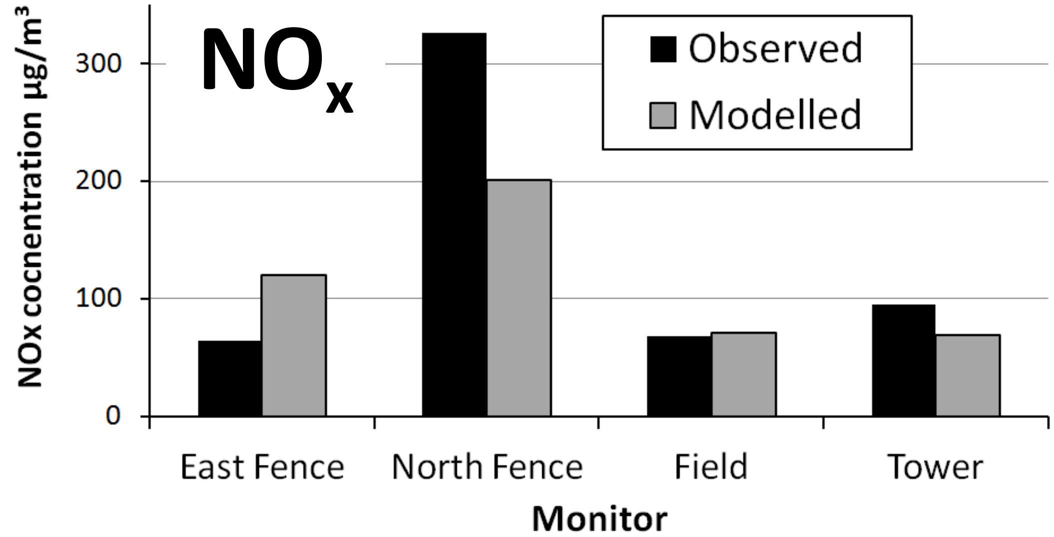
- NO_x performance

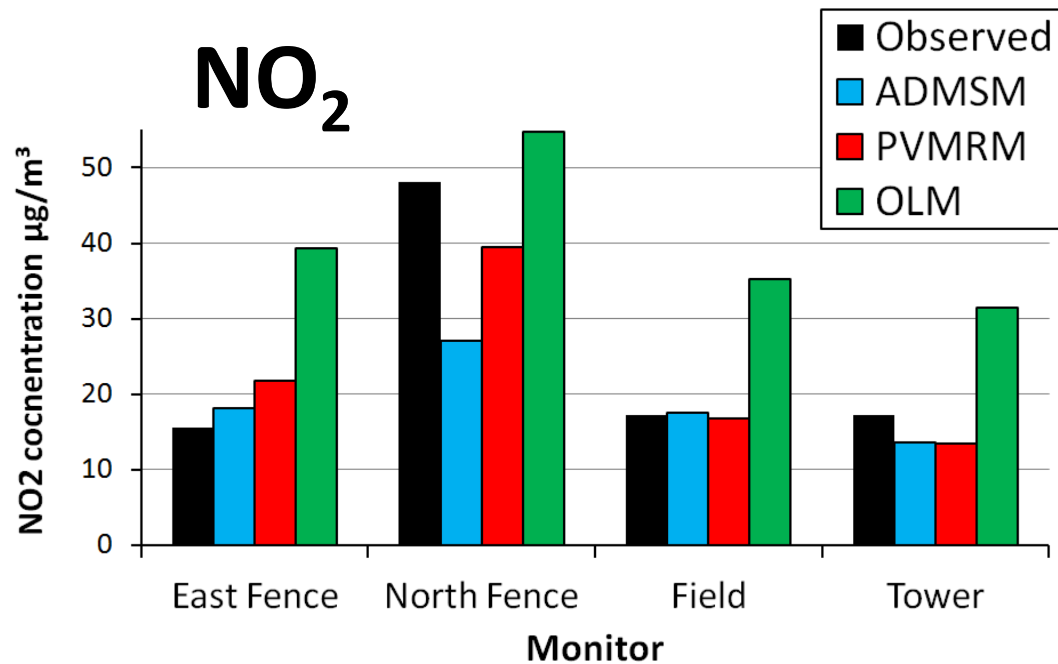
Monitor	N	R	Fac 2
East Fence	238	0.67	0.54
North Fence	**803**	0.57	0.45
Field	**576**	0.59	0.51
Tower	149	0.47	0.45

- NO_2 performance

Underline performance better than NO_x

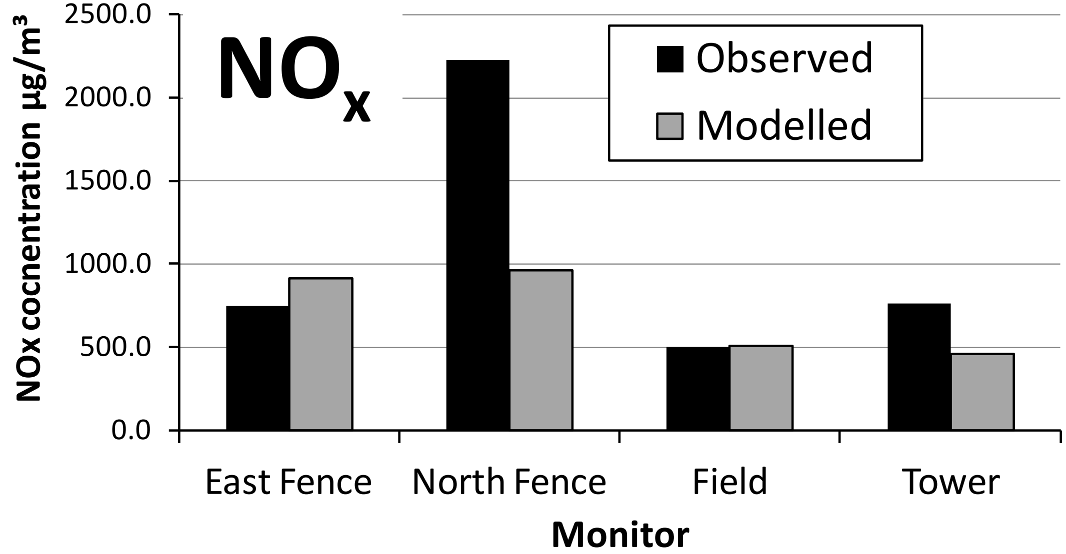
Monitor	R			Fac 2		
	ADMSM	PVMRM	OLM	ADMSM	PVMRM	OLM
East Fence	0.71	0.73	0.61	0.68	0.73	0.51
North Fence	0.57	0.39	0.50	0.57	0.54	0.53
Field	0.61	0.45	0.62	0.70	0.64	0.50
Tower	0.56	0.50	0.59	0.58	0.54	0.49



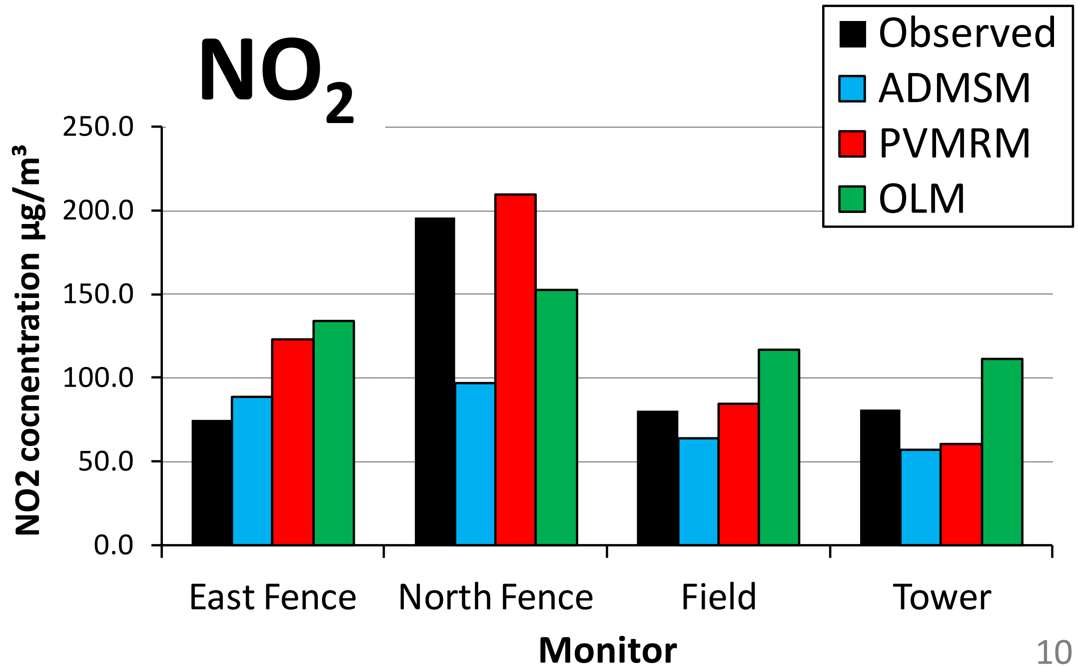


Statistical results: high concentrations

- Consider:
  - the ratio of modelled to observed mean: highest 10 values



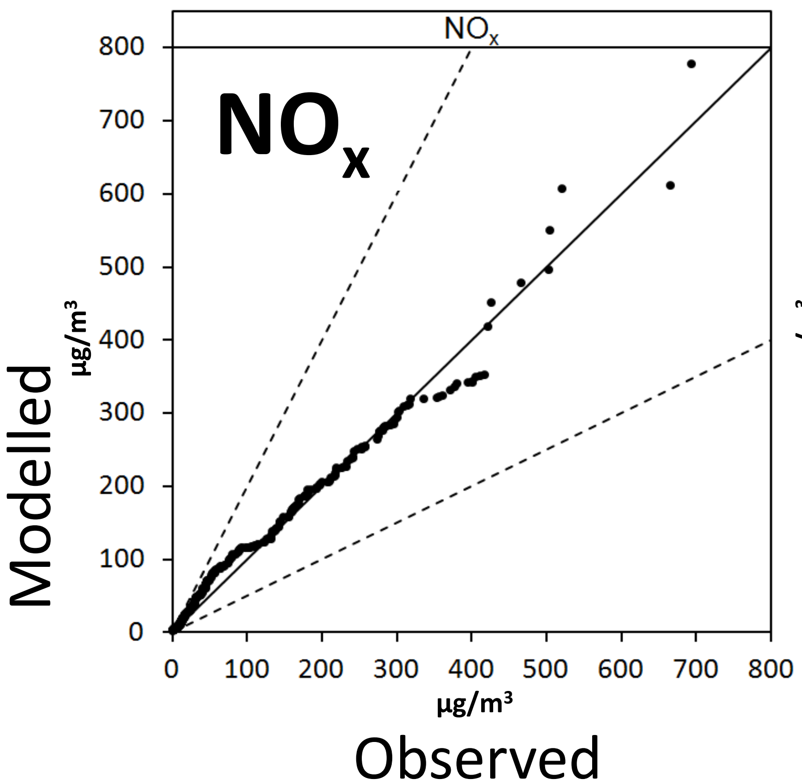
- ADMSM shows more consistency between NO_x and NO_2 concentrations than other schemes *e.g. modelled NO_x at North Fence less than half observed value, so modelled NO_2 should be significantly under-predicted*

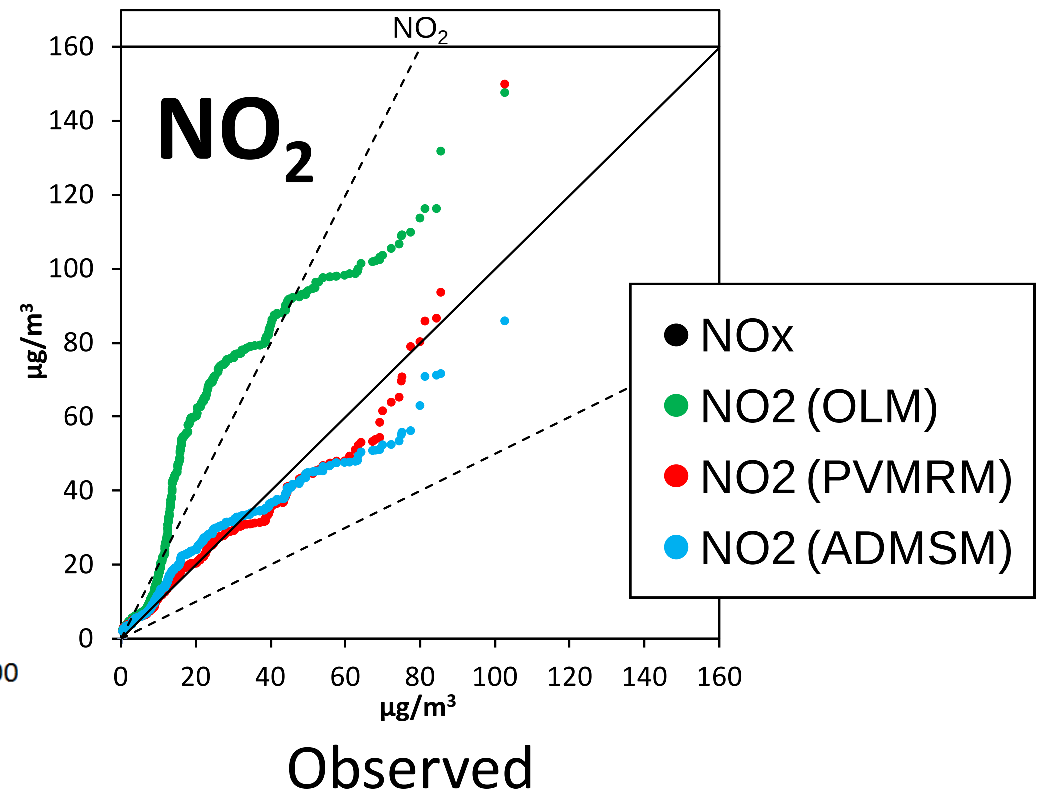


Quantile-quantile plots

Field

- Clark TCV-12 distance to monitor: 425 m
- PVMRM and ADMSM NO_2 broadly consistent with NO_x
- High NO_2 PVMRM values higher than corresponding ADMSM values

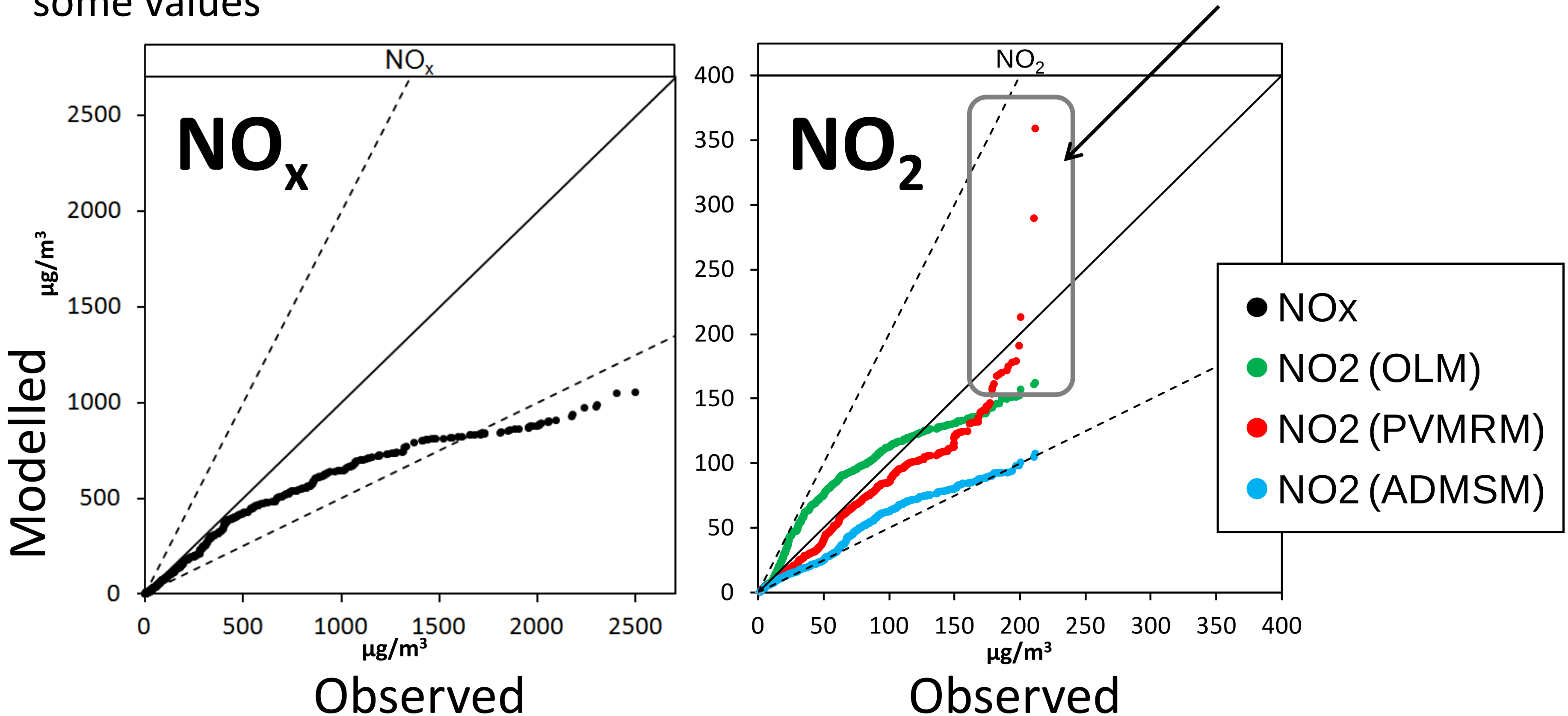




Quantile-quantile plots

North Fence

- Clark TCV-12 distance to monitor: 140 m
- ADMSM NO_2 broadly consistent with NO_x
- PVMRM NO_2 higher than corresponding NO_x and exceed OLM concentrations for some values

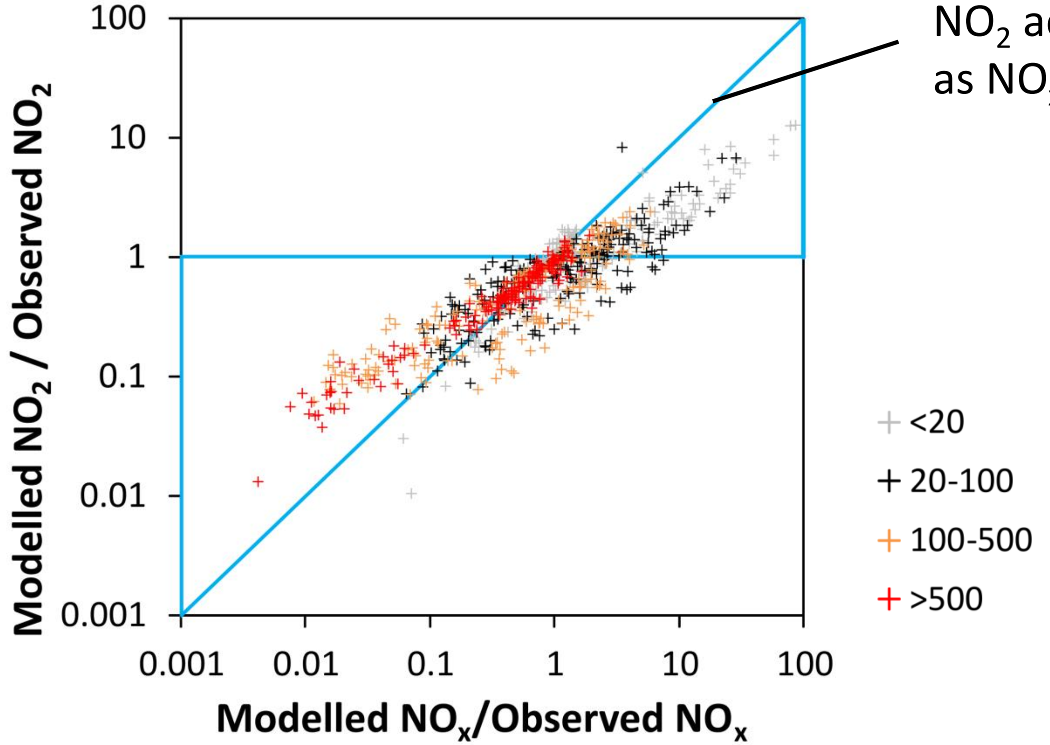


Ratio plots

- If NO_x is overpredicted then NO_2 should also be overpredicted, but not by quite so much due to the non-linearity in the chemical equations, and vice versa
- Consider **Modelled NO_2 / Observed NO_2** against **Modelled NO_x / Observed NO_x**

Overpredicted NO_2

Underpredicted NO_2



NO_2 accuracy the same as NO_x accuracy

Categorised by observed NO_x concentration (μg/m^3)

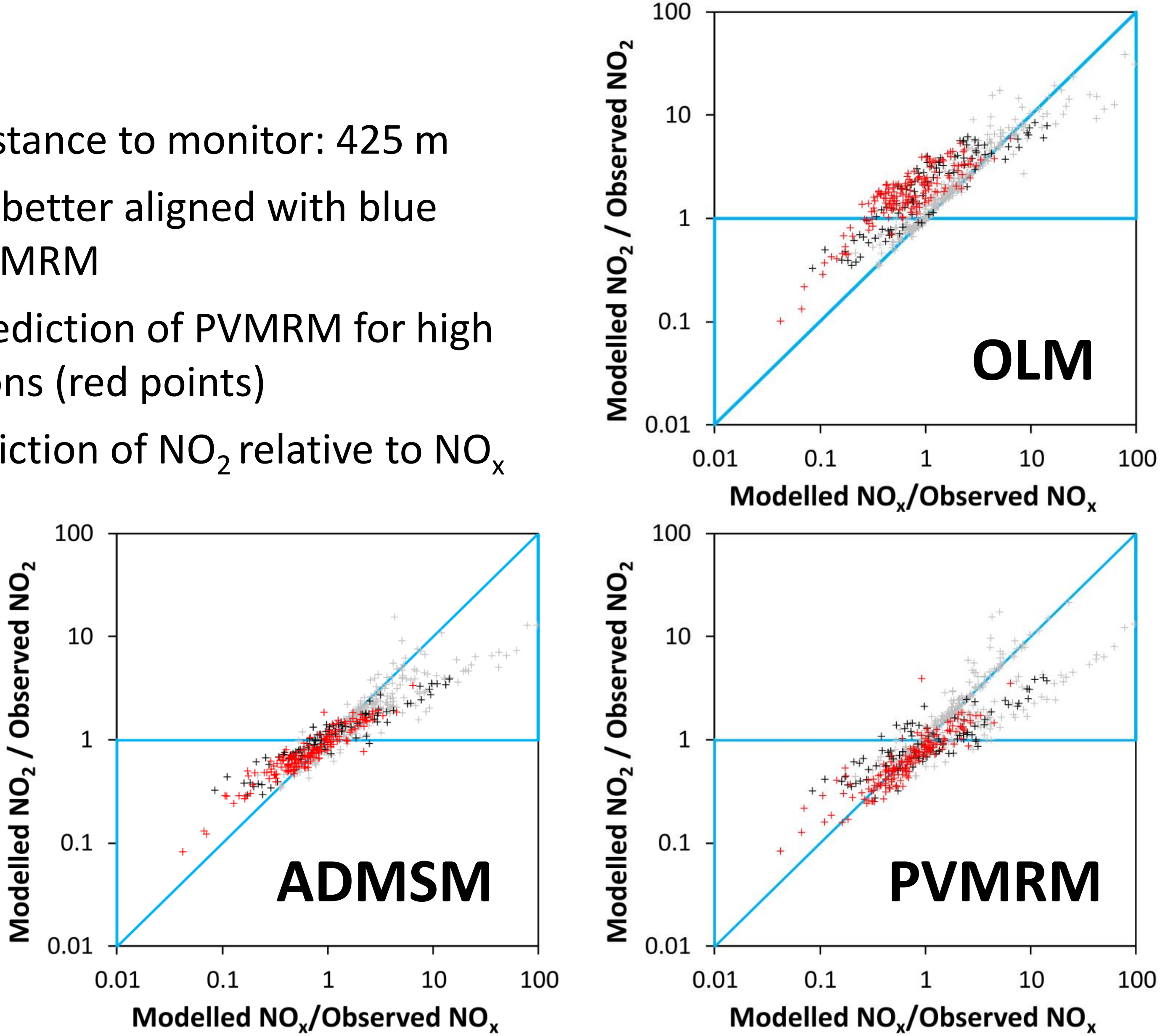
Underpredicted NO_x

Overpredicted NO_x

Ratio plots

Field

- Clark TCV-12 distance to monitor: 425 m
- ADMSM values better aligned with blue triangles than PVMRM
- Some under-prediction of PVMRM for high NO_2 concentrations (red points)
- Clear over-prediction of NO_2 relative to NO_x for OLM



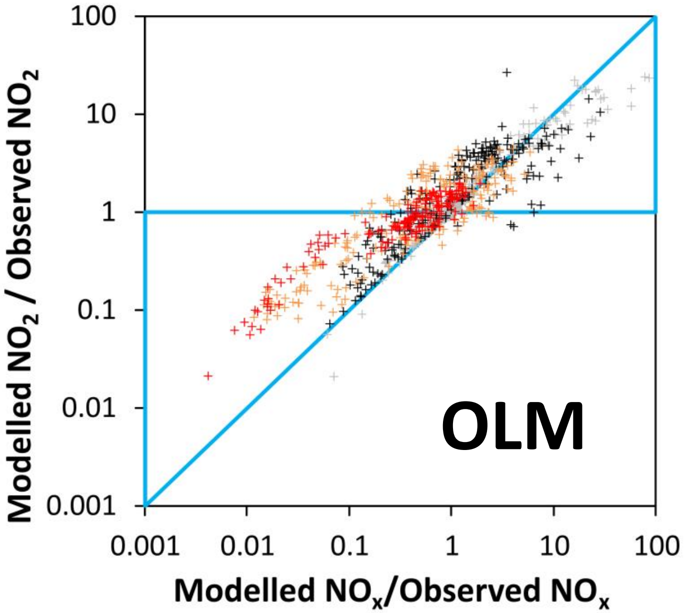
Points coloured by NO_x concentration (µg/m³)

- <20
- 20-50
- >50

Ratio plots

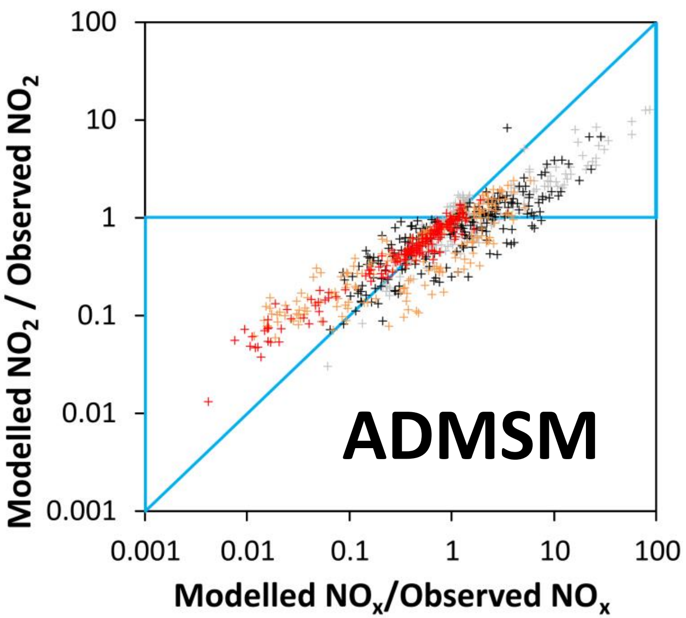
North Fence

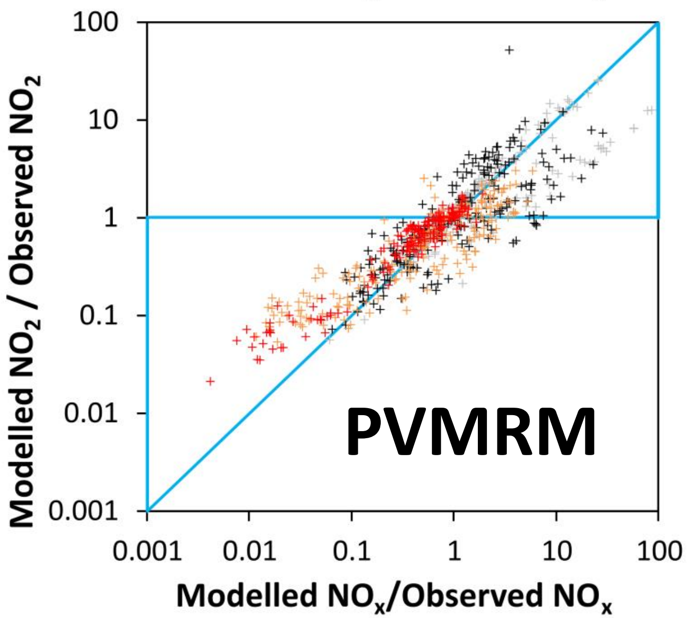
- Clark TCV-12 distance to monitor: 140 m
- ADMSM and PVMRM much better aligned in the blue triangles than OLM



Points coloured by NO_x concentration (µg/m³)

+ <20
+ 20-100
+ 100-500
+ >500





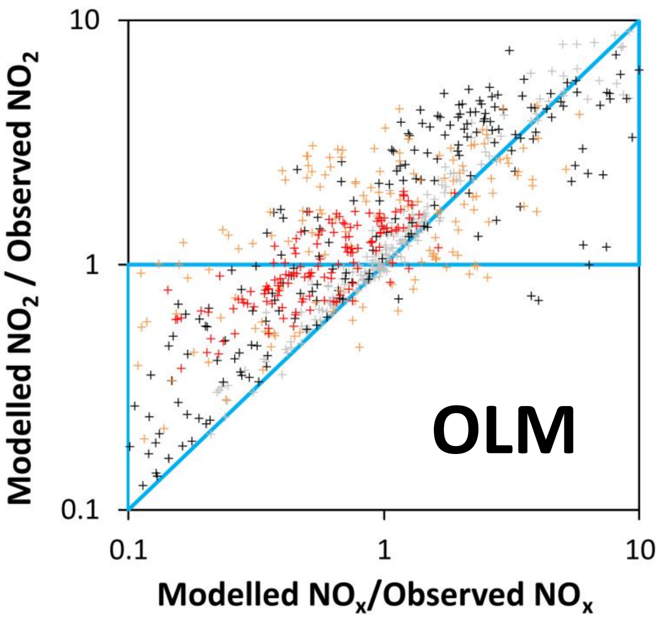
Ratio plots

North Fence

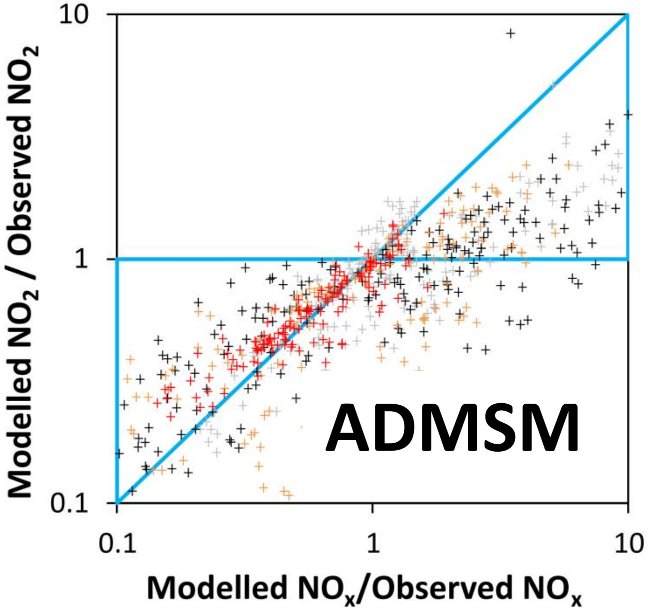
- Clark TCV-12 distance to monitor: 140 m

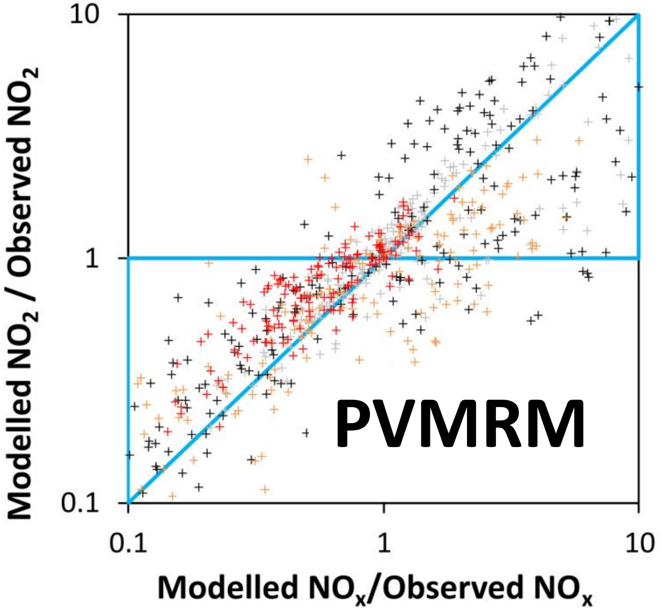
Zooming in to NO_x values within a factor of 10

- ADMSM has a tighter grouping of high concentration values (representing better R)
- PVMRM has some high NO_2 predictions that correspond to low-moderate NO_x concentrations (seen on Q-Q plot)



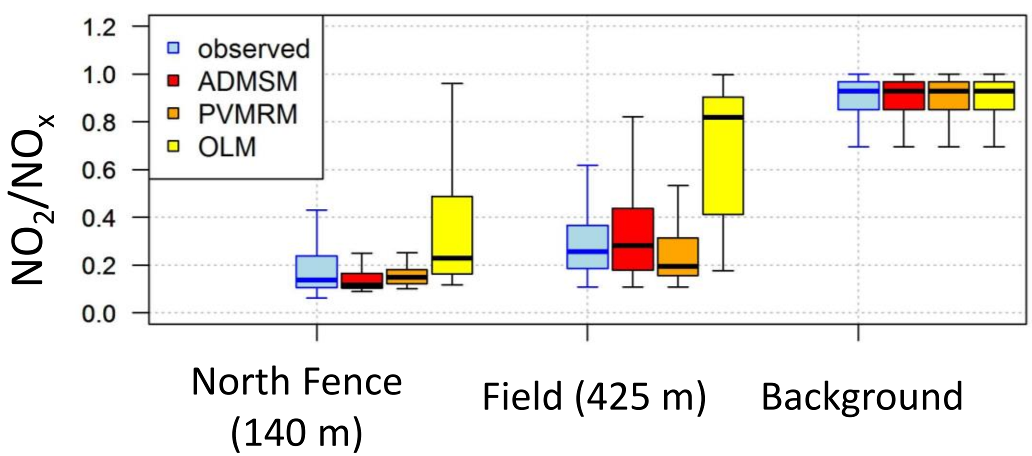
Points coloured by NO_x concentration (µg/m³)
+ <20
+ 20-100
+ 100-500
+ >500





Conclusions (1 of 2)

- Superior dataset for evaluation of NO_x chemistry schemes, with short source to monitor distances, and two monitors aligned with the prevailing wind.
- NO_x evaluation: AERMOD performs well at some monitors
- NO_2 evaluation:
  - PVMRM and ADMSM perform better than OLM; OLM overpredicts
  - PVMRM and ADMSM broadly replicate near-field NO_2/NO_x ratios
  - PVMRM predicts some high NO_2 concentrations exceeding the ‘upper bound’ OLM values – likely related to entrainment method rather than lack of explicit chemistry
  - ADMSM NO_2 statistics more consistent with NOx than PVMRM; ADMSM shows better performance in ratio plots



Conclusions (2 of 2)

Next steps

- Further chemistry scheme evaluation is planned using other new datasets
- ADMSM to be incorporated within the latest version of AERMOD

Other uses for this dataset

- Building downwash evaluation
- Sensitivity of model results to sigma-theta

Suggestion for future measurement campaigns

- More downwind monitors in the range 0.5 – 1 km and further, to evaluate performance in terms of the variation of NO_2/NO_x with distance

Co-authors and acknowledgments

Co-authors

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- David Carruthers
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Questions?

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