

NO₂ Modeling - PVMRM and OLM Evaluation using a New Data Set

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PVMRM

Plume Volume Molar Ratio Method

- Developed by Hanrahan (1999)
- Evaluated with a few limited data sets (Empire Abo, Palaau, Arellano/Bange Neth. power plant plumes)
- Assumes simplified chemistry and:
 - Initial in-stack NO/NO_x ratio
 - Instantaneous reaction (conversion of NO to NO₂) based on amount of entrained ozone at distance x
 - Originally uses ISC3 dispersion estimates, revised to use AERMOD estimates of NO_x concentration and plume spread. Uses relative dispersion estimates for ozone entrainment and reactions
 - Can simulate multiple sources

OLM

Ozone Limiting Method

- Compares the estimated $[\text{NOx}]_{\text{max}}$ and the ambient O_3 to determine which is the limiting factor to NO_2 formation
- If $\text{O}_3 > [\text{NOx}]_{\text{max}}$, then total conversion is assumed
- If $[\text{NOx}]_{\text{max}} > \text{O}_3$ the formation of NO_2 is limited by the ambient O_3

Evaluation Objectives

- Identify existing dataset that could be used to evaluate AERMOD and the PVMRM and OLM options for predicting 1-hour NO₂ concentrations
- Evaluate:
 - AERMOD predictions of NO_x
 - OLM and PVMRM predictions of NO₂/NO_x ratio
 - AERMOD/PVMRM and AERMOD/OLM predictions of NO₂ concentrations

Wainwright, AK Data Set

- Single monitoring station sited 500 m from the local power plant
- Observes NO₂, NO, and ozone concentrations, as well as meteorological variables
- 12 ½ months of observations

Wainwright, Alaska



Source Information

- Five diesel-fired generators and stacks
- Hourly operating logs, listing engine runtimes and kW output
- Stack emissions rate, exit flow and exit temperature have been interpolated from engine design capacity data
- In-stack NO_2/NO_x ratio estimated at 0.2

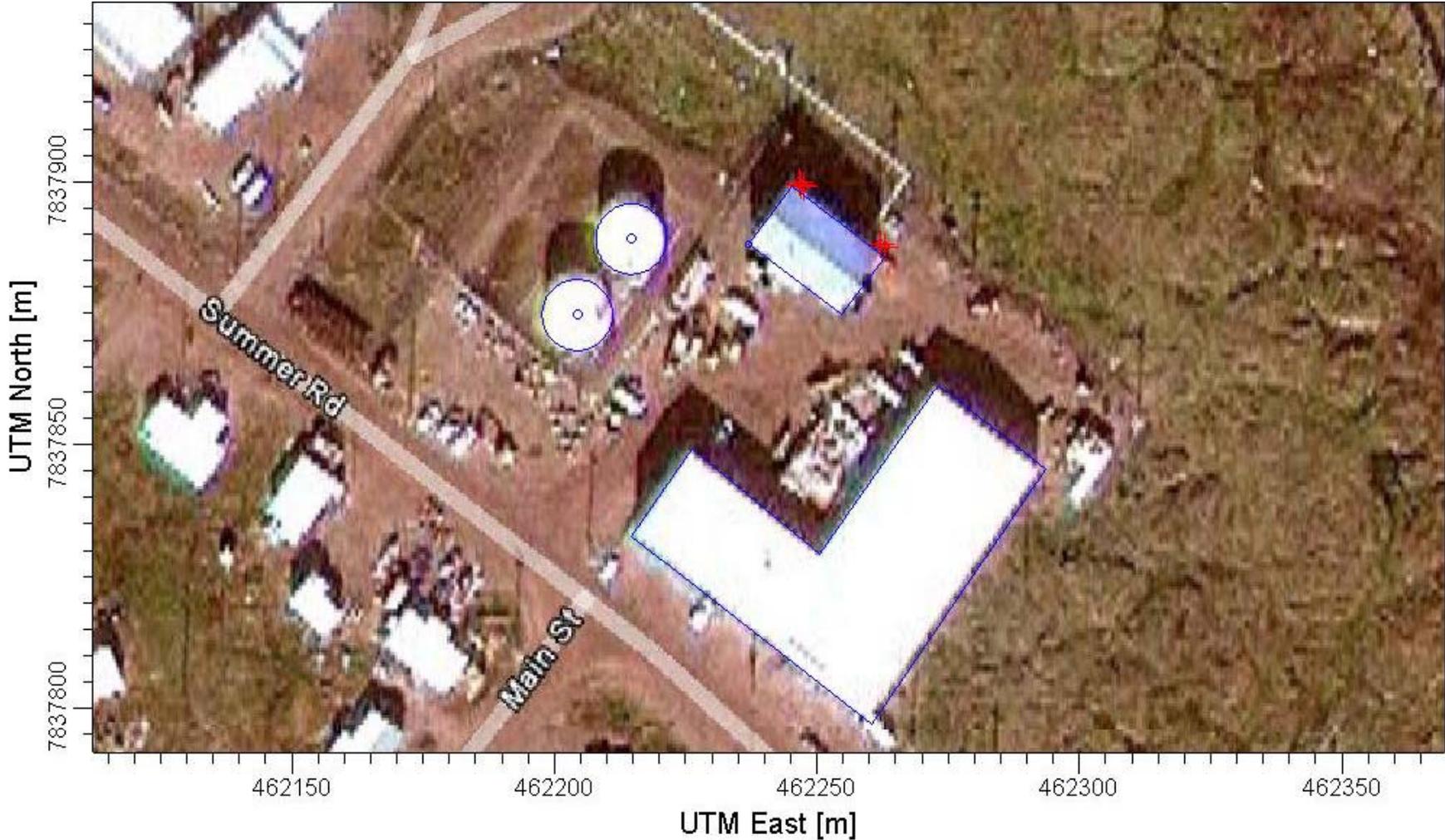
Wainwright Power Plant Building



Model Options Tested

- AERMOD version 11103 runs:
 - OLM option
 - PVMRM option
 - PVMRM algorithms, but with modified relative dispersion parameters
 - PVMRM, but with initial ambient ozone = monitored ozone plus monitored NO₂
- BPIP-Prime was run for downwash for all runs

Stacks shown in red; shop building and storage tanks shown in blue outline

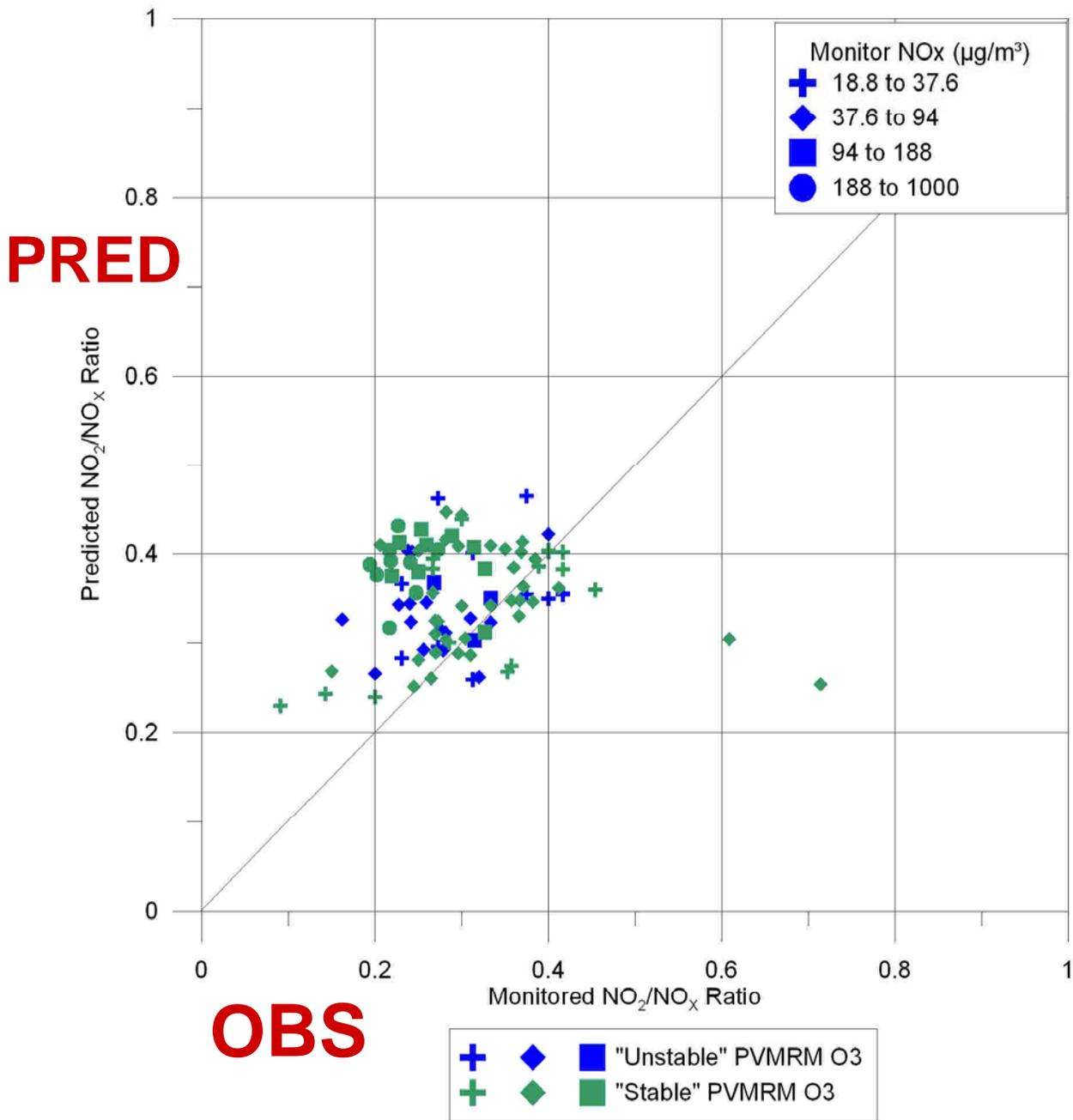


Meteorology and Land Use

- Monitoring station provided primary meteorological data; ASOS data used when monitoring station data missing
- No AERSURFACE land use data available for Wainwright, so land use values assigned manually:
 - 37° - 218° “desert shrubland”
 - 218° - 37° “water”

Evaluation Methodology

- Use hours when wind direction is blowing from power plant towards the 60° sector containing the monitor
- Paired NO₂/NO_x ratio evaluations use data with NO_x > 10 ppb
- BOOT software applied to observed and predicted NO_x and NO₂ concentrations paired in time and space
- Also list top-10 and present Q-Q plots

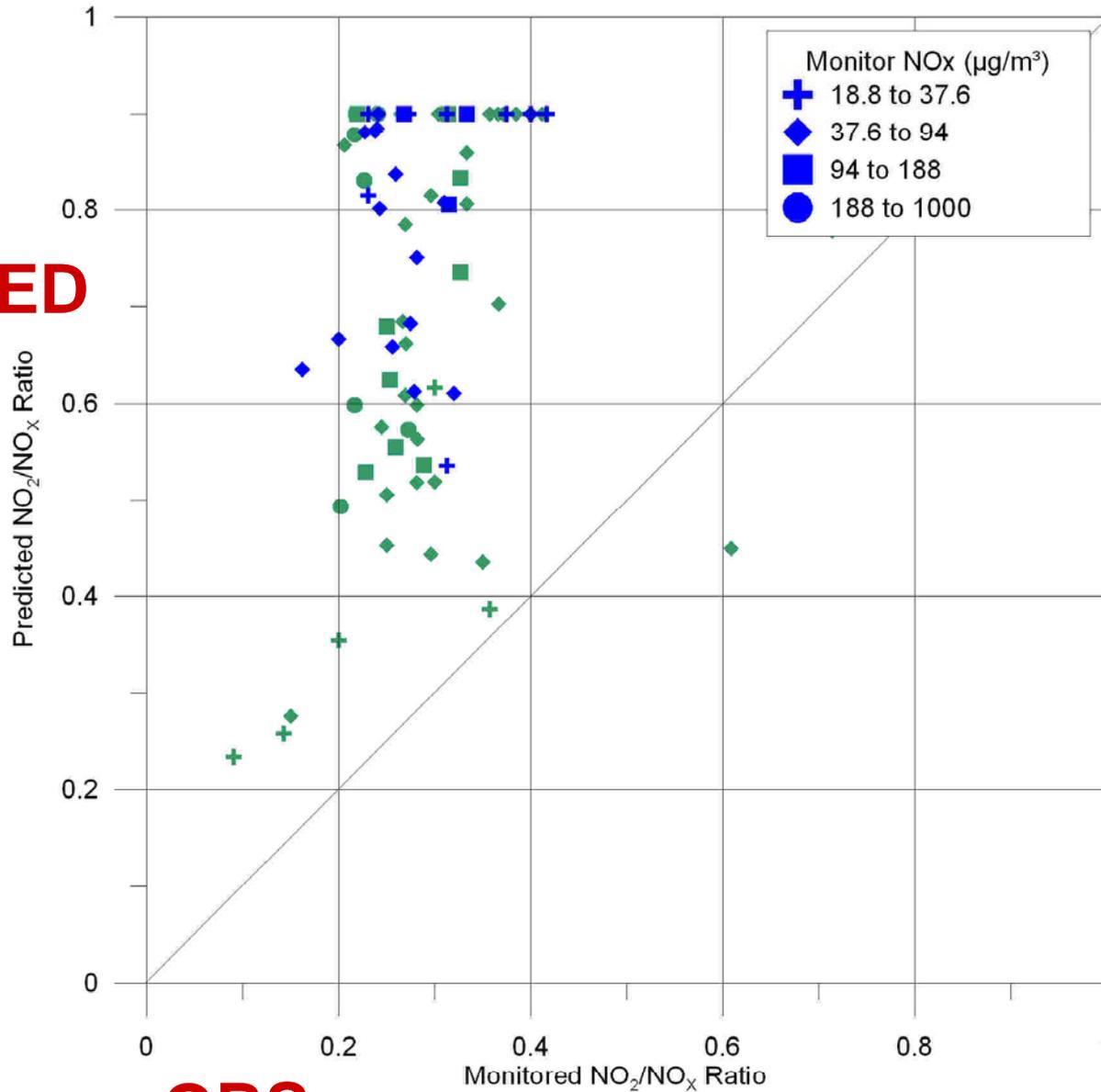


**AERMOD/
PVMRM
 NO_2/NO_x**

**Green –
Stable**

**Blue -
Unstable**

PRED



OBS



**AERMOD/
OLM
NO₂/NO_x**

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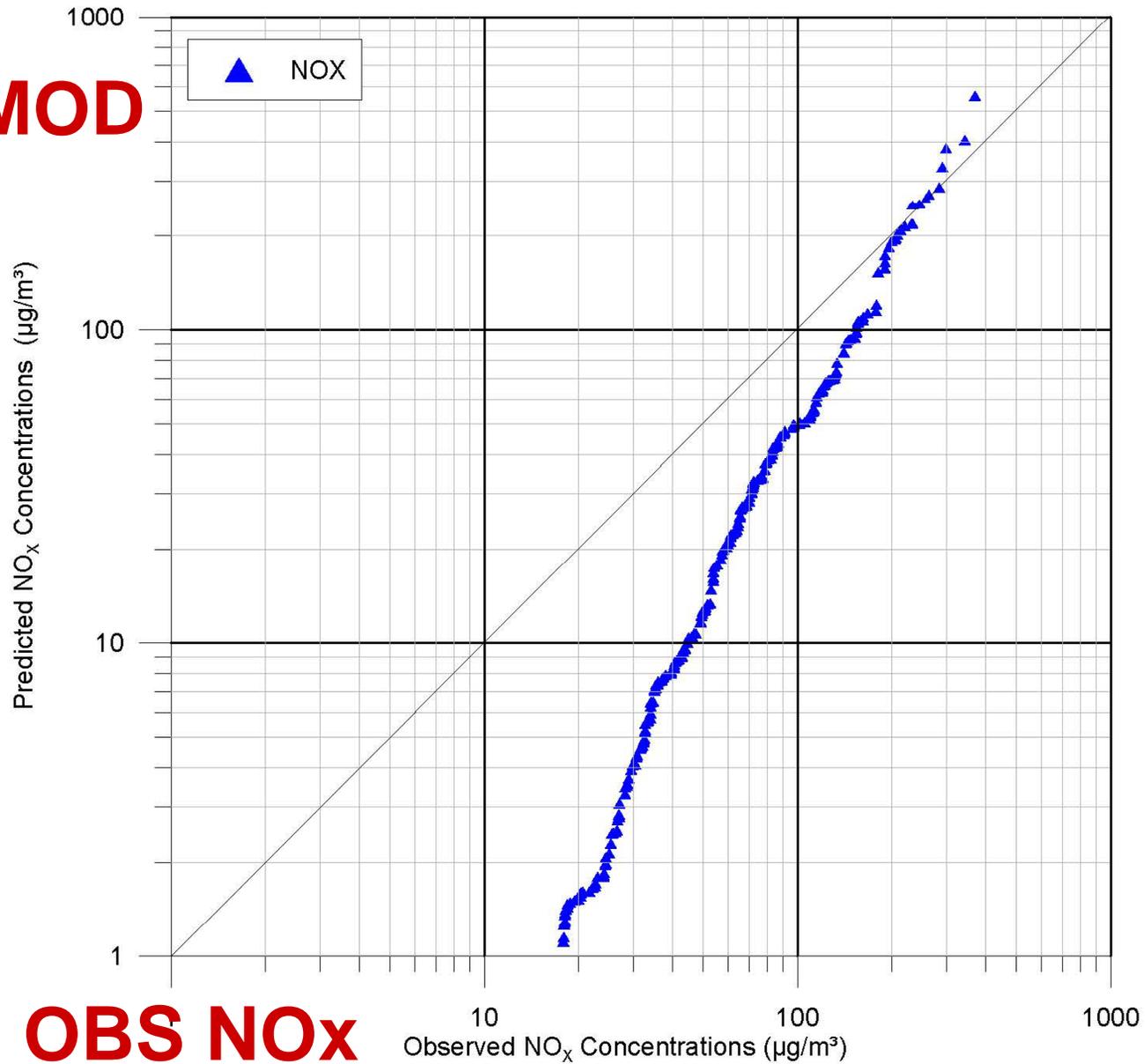
Some BOOT Results for NO₂

PERFORMANCE MEASURE	OBS	AERMOD/ OLM	AERMOD/ PVMRM
Highest NO ₂ (µg/m ³)	73	158	130
Mean	13	21	13
Fractional Mean Bias FB		-0.50	0.01*
Normalized Mean Sq Error NMSE		3.6	3.1
FAC2		0.40	0.47

* Not significantly different from 0.00 (no mean bias) at 95% confidence level

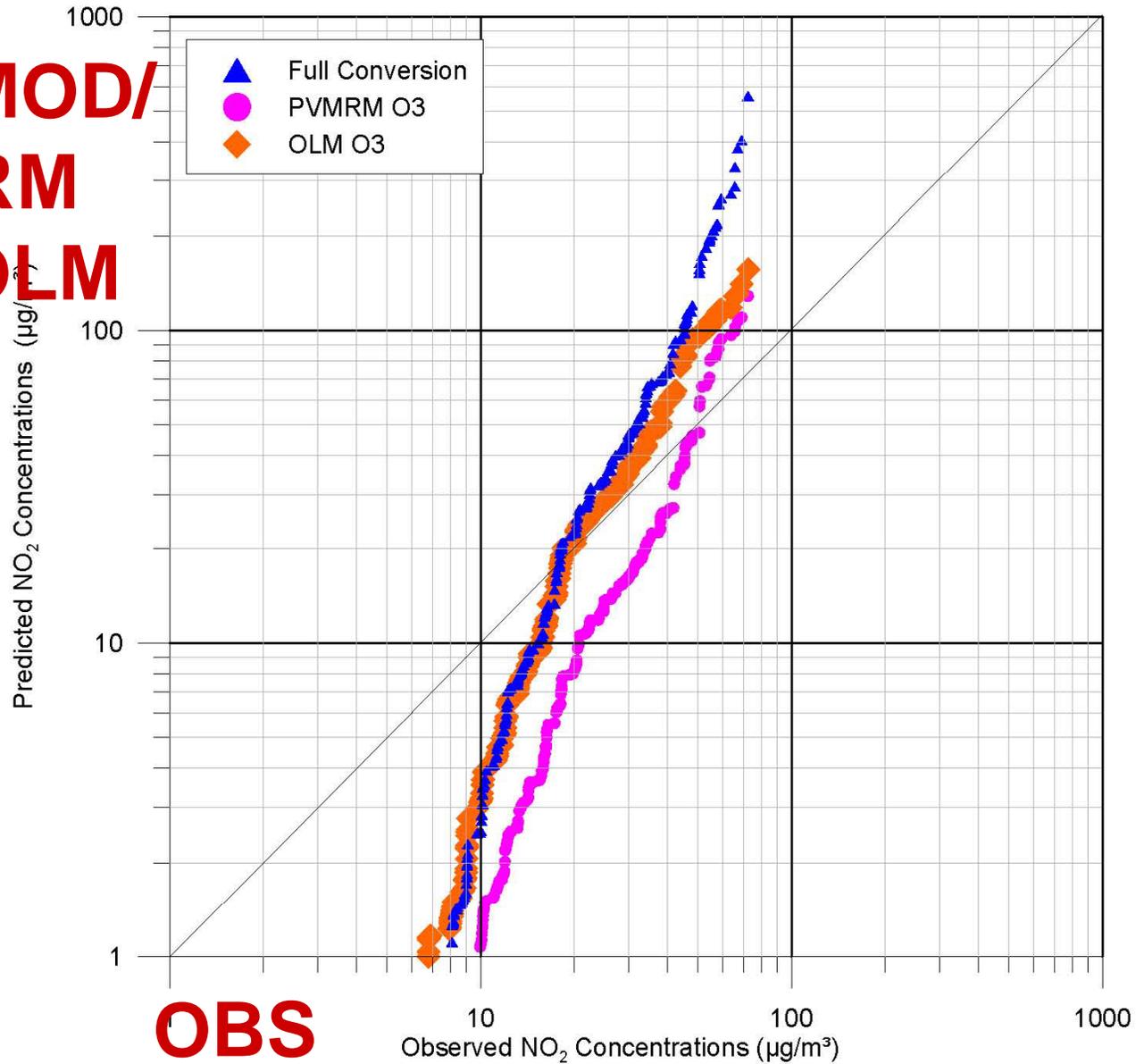
AERMOD Wainwright Model Evaluation
Hourly NO_x Q-Q Plot
"Flat Roof" Power Plant Building

**AERMOD
NO_x**



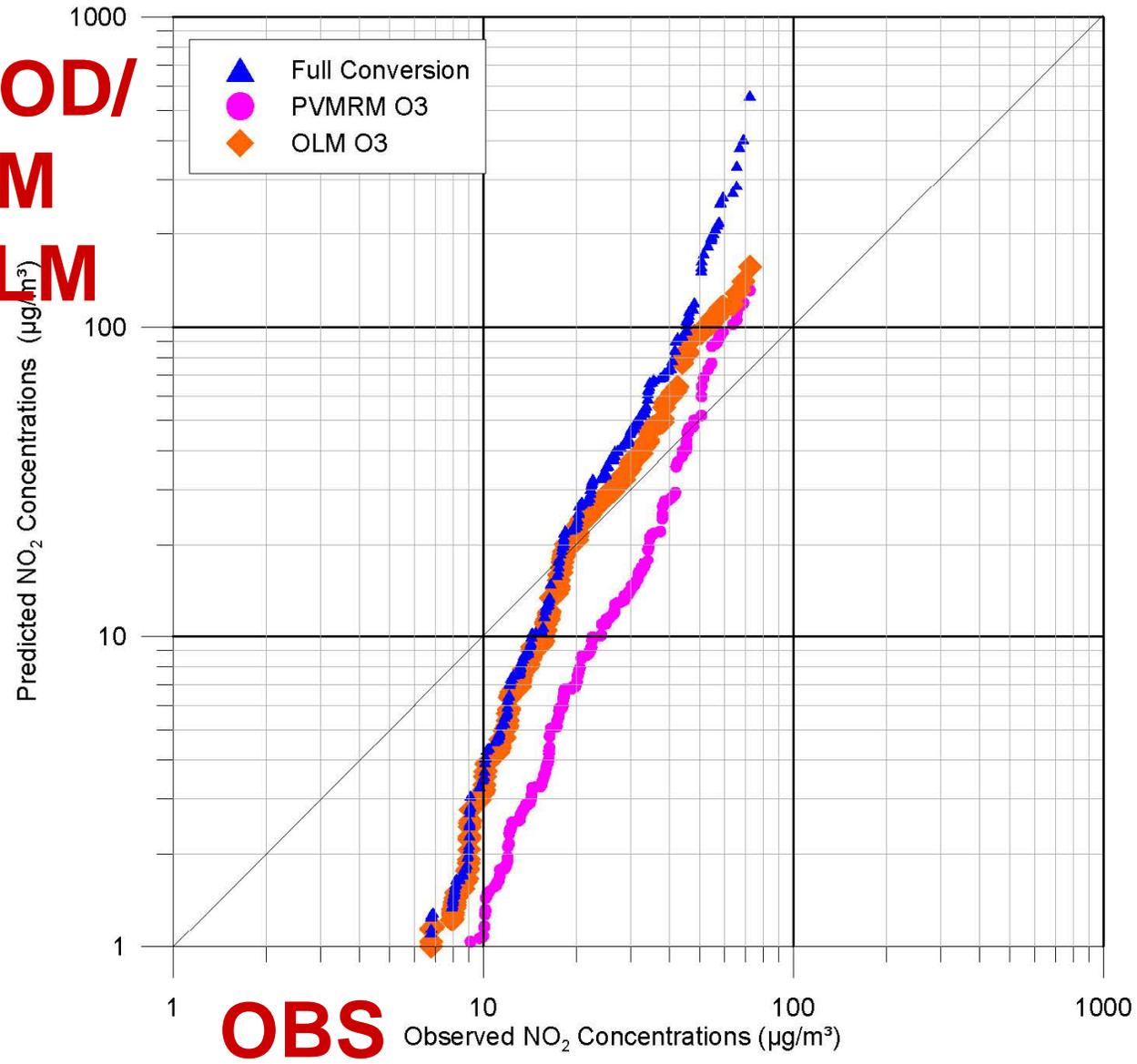
AERMOD Wainwright Model Evaluation
Hourly NO₂ Q-Q Plot
"Flat Roof" Power Plant Building
 $n_z = 4; \sigma_r = 5m$

**AERMOD/
PVMRM
and OLM**



AERMOD Wainwright Model Evaluation
Hourly NO₂ Q-Q Plot
"Flat Roof" Power Plant Building
 $n_z = 1.282$; $A=0.8$; $\sigma_r = 15m$

**AERMOD/
PVMRM
and OLM**



Key Limitations

- Hourly emissions and stack parameters were estimated using operating logs and vendor performance data
- Ambient O_3 was observed only at a single monitoring location. That O_3 may have been affected by scavenging by NO in the plume to form NO_2
- Ambient NO_x and NO_2 concentrations were relatively small

Conclusions

- PVMRM is doing well at predicting the NO_2/NO_x ratio (minimal bias, with most ratios from 0.2 to 0.4).
- OLM has a general 70 % overprediction tendency for the NO_2/NO_x ratio.
- Both AERMOD/OLM and AERMOD/PVMRM overpredict the high end NO_2 concentrations by about a factor of two (OLM by more) (But this may be caused by the fact that AERMOD overpredicts the high end NO_x concentrations).
- There was little skill (correlations) evident in both AERMOD/PVMRM or AERMOD/OLM.

This Evaluation in the Context of all PVMRM and OLM Comparisons

To be robust, many data sets should be used in a model evaluation so that a multitude of conditions, source data, etc. can be included.

This evaluation using the Wainwright data set should be considered an additional piece of information to supplement the limited number of data sets used by EPA to date to evaluate the PVMRM and OLM options in AERMOD for predicting 1-hour NO₂.

A detailed field experiment is needed.