AERMOD Evaluations Under the 1-hour NO_2 and SO_2 NAAQS

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Outline

- Overview of AERMOD model performance evaluations conducted to support AERMOD's promulgation
- Discuss some caveats associated with interpreting model-to-monitor comparisons
- Summarize evaluations of AERMOD for the 1-hour NO_2 NAAQS, including current Tier 3 options for NO-to-NO_2 conversion in AERMOD

AERMOD Performance Evaluation

- Evaluated on total of **17 Field Study Databases**
  - 10 without Building Downwash, 7 with Downwash
  - 13 with Flat or Rolling Terrain, 4 with Complex Terrain
- Included Developmental and Independent Evaluations
  - Developmental evaluations conducted during development of model, with evaluation results informing model formulation
  - Independent evaluations conducted on separate data bases not included in developmental stage
- Included short-term and long-term studies
  - Short-term studies typically included controlled tracer releases with intensive monitoring network (e.g., Prairie Grass study on next slide)
  - Long-term studies based on SO_2 impacts from operating power plants (e.g., Lovett Power Plant study on next slide)

Field Study Examples

Prairie Grass Tracer Study

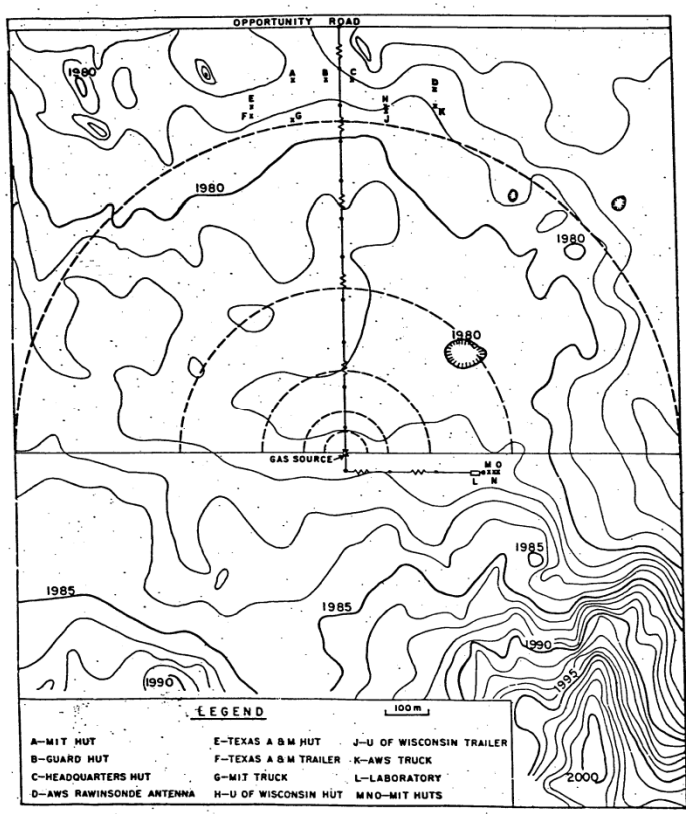


Figure 1 Layout of the Prairie Grass SO_2 Tracer Experiment

Lovett Power Plant SO_2 Study

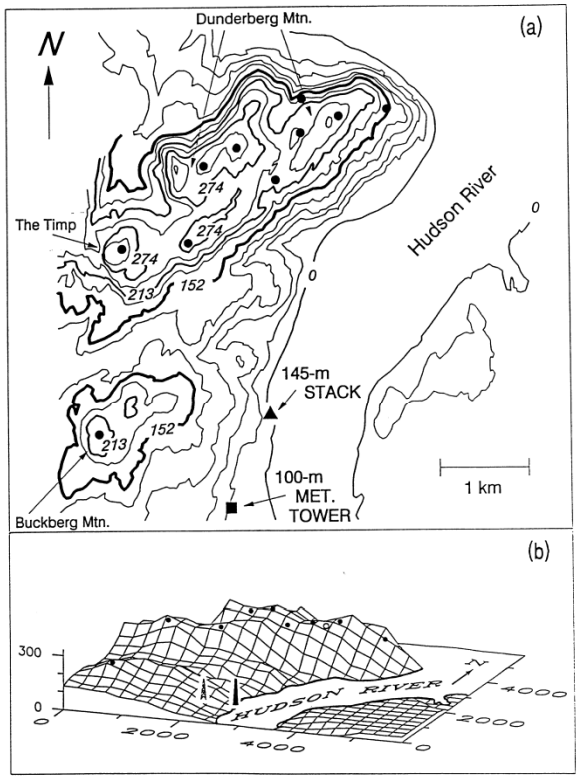


Figure 7 Depiction of the Monitoring Network Used for the Lovett Complex Terrain Model Evaluation Study

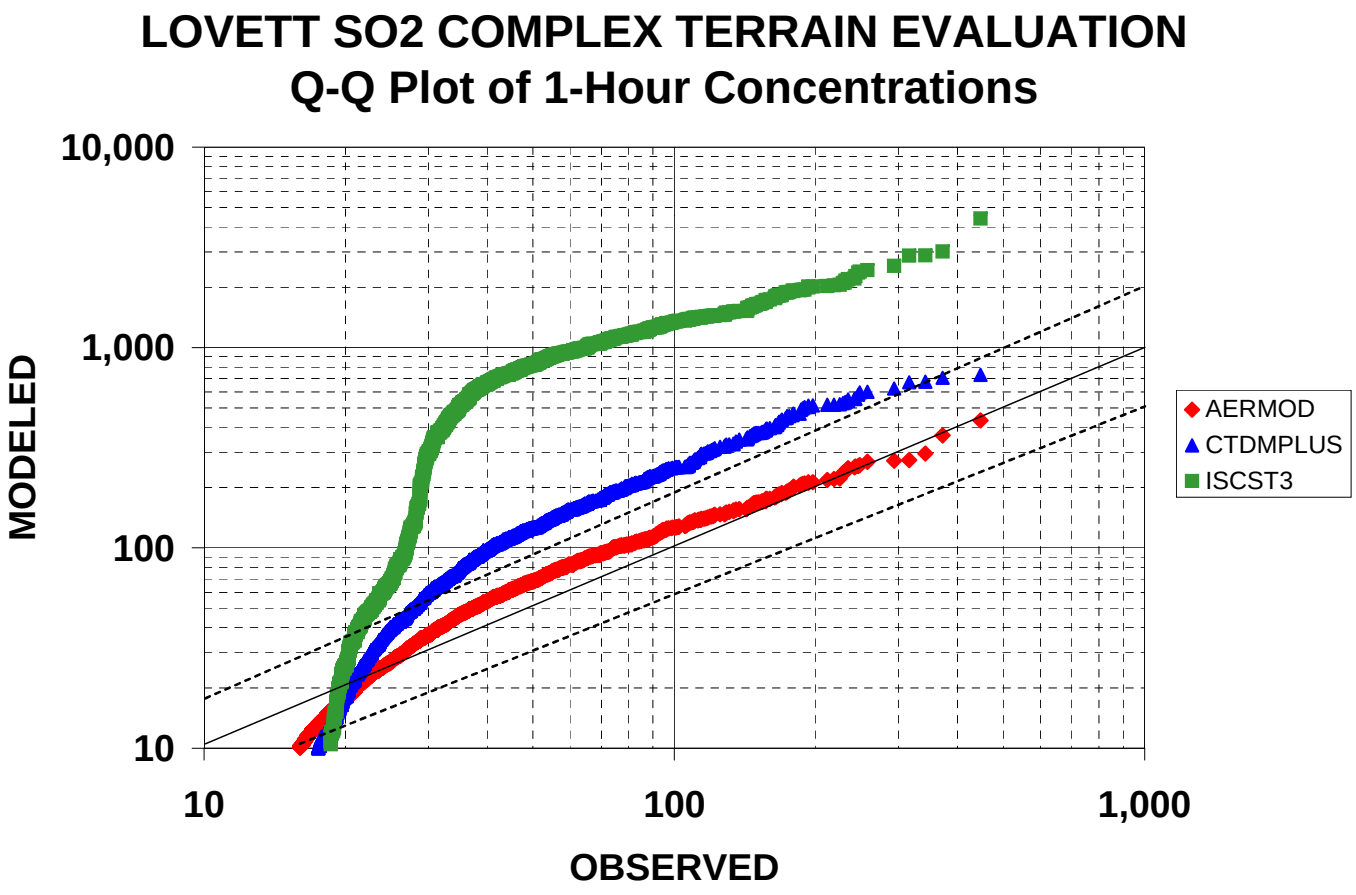
AERMOD Performance Evaluation

- Performance evaluation included a range of methods and metrics depending on the type of data available
  - Evaluation for long-term studies at operating power plants was based on EPA's Cox-Tikvart "Protocol for Determining Best Performing Model"
- AERMOD performance compared to other refined models:
  - ISCST3 for non-downwash/non-complex-terrain databases
  - CTDMPLUS for complex terrain databases
  - ISC-PRIME for downwash databases
- AERMOD consistently outperformed ISCST3, ISC-PRIME and CTDMPLUS

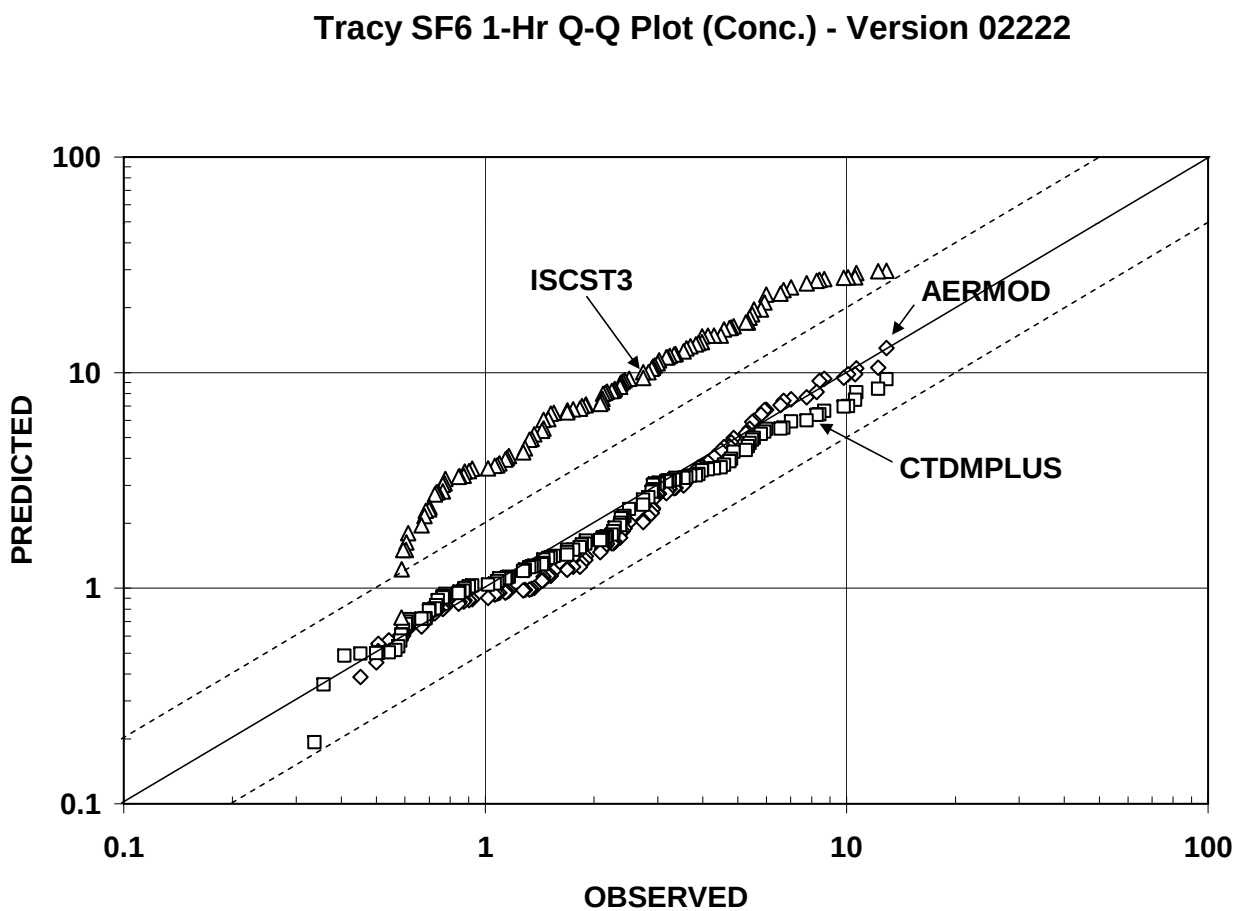
AERMOD Performance Evaluation

- The following slides document AERMOD model performance for estimating hourly concentrations from several field studies
- Results are summarized in Q-Q plots of highest ranked modeled vs. highest ranked observed concentrations, unpaired in time and space
- Solid diagonal line shows 1:1 (perfect agreement) and dashed lines show plus/minus factor of 2 agreement
- AERMOD exhibits consistently unbiased performance for estimating the distribution of peak hourly concentrations across a wide range of scenarios
- Performance of other models is included for comparison, demonstrating that model performance has significantly improved with AERMOD relative to models used in the past

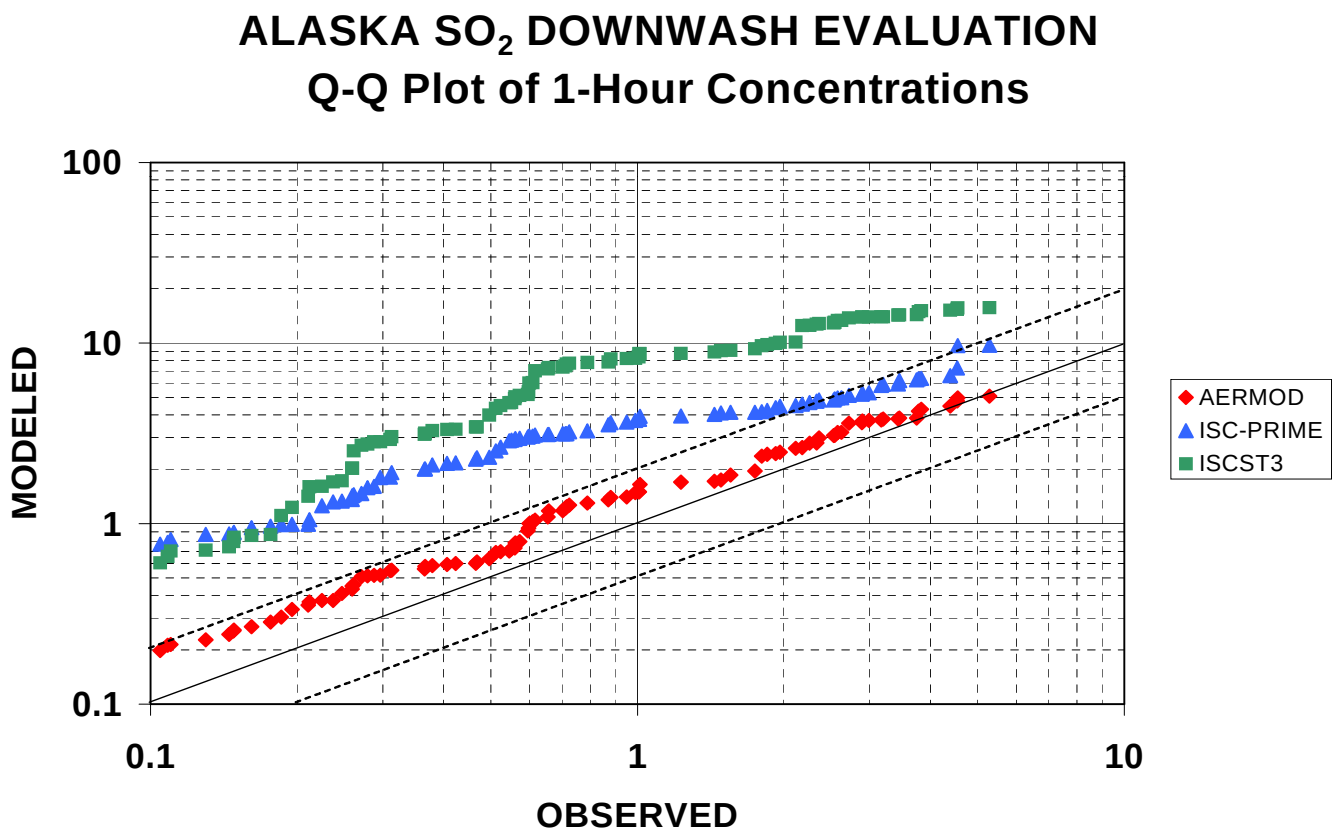
AERMOD Performance: Complex Terrain



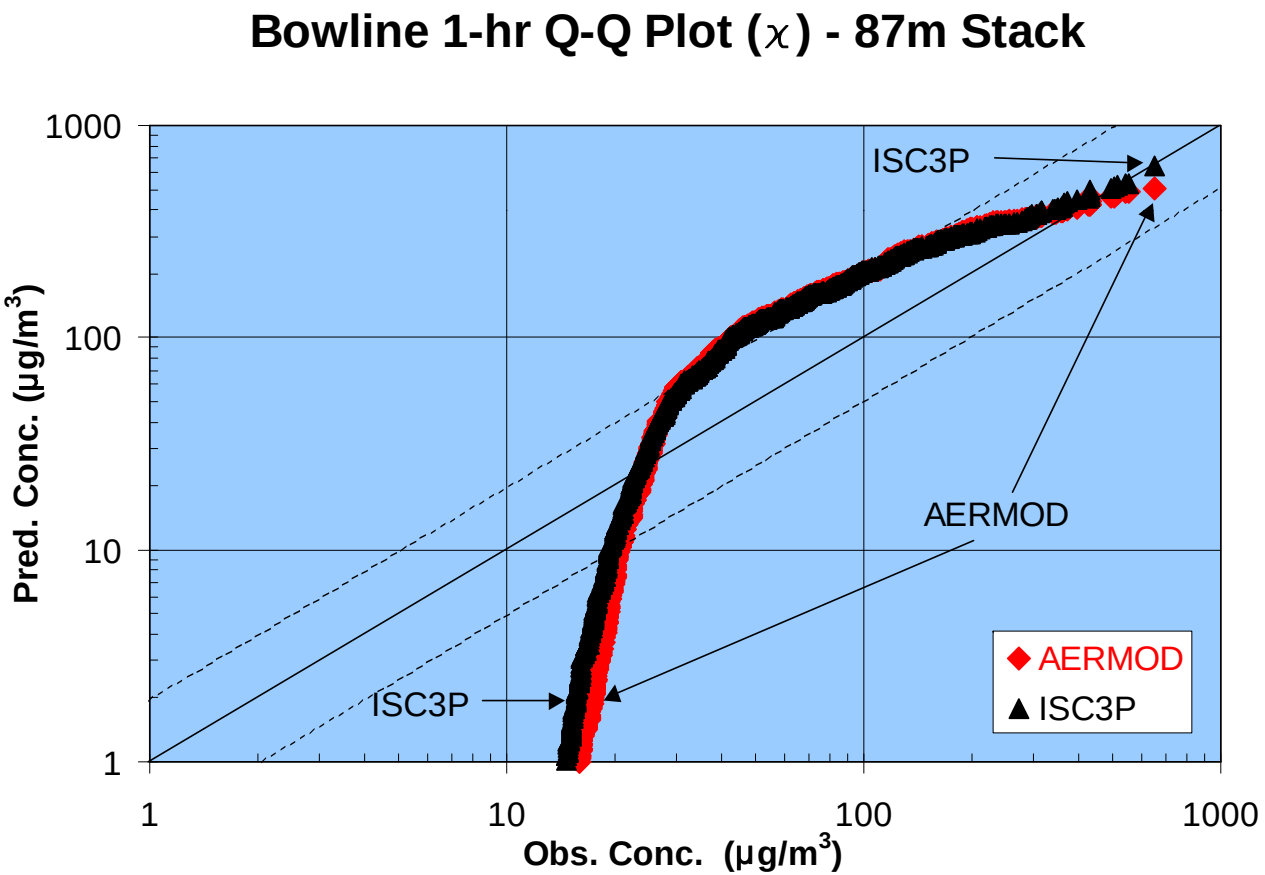
AERMOD Performance: Complex Terrain



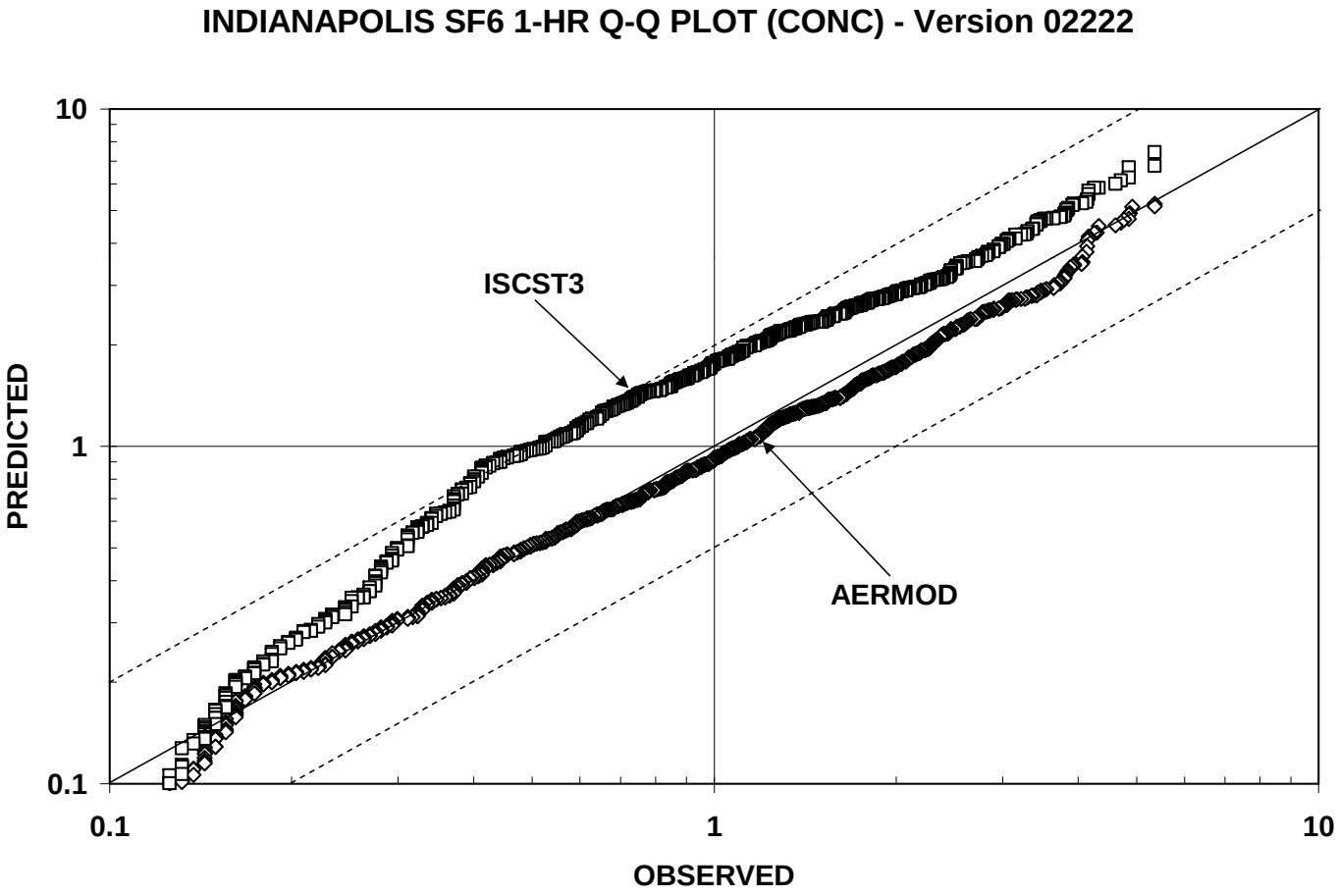
AERMOD Performance: Building Downwash



AERMOD Performance: Building Downwash



AERMOD Performance: Urban Dispersion

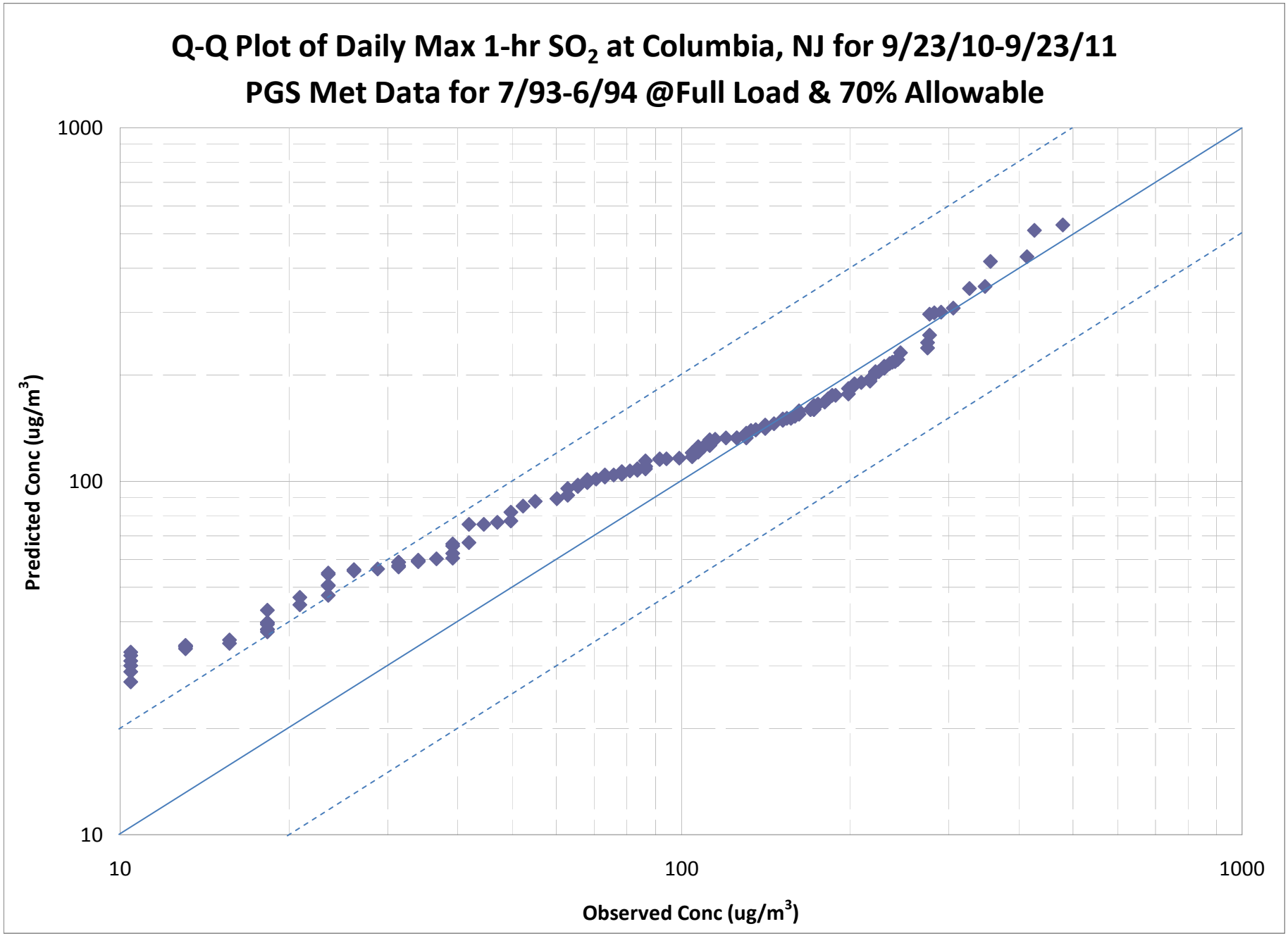


Performance Evaluation Caveats

- Model performance evaluations typically include robust site-specific meteorological data and hourly actual emissions, removing as much uncertainty or bias associated with these key model inputs as possible
- Regulatory modeling applications for PSD permits are based on maximum allowable emissions, and typically use the most representative airport meteorological data
- Model evaluation field studies also include multiple monitoring sites designed to adequately capture ambient impacts; intensive field studies typically use arcs of receptors designed to capture the full plume, minimizing the sensitivity of model-to-monitor comparisons to errors in wind direction

Performance Evaluation Caveats

- As a result of these factors, comparisons of PSD permit modeling results with observed concentrations at a single monitor are subject to misinterpretation and generally are not good indicators of model performance
- That being said, the following anecdotal case suggests that properly conducted model-to-monitor comparisons can provide useful information regarding model performance in some “real-life” situations:
  - Q-Q plot of predicted daily maximum 1-hr SO_2 values for Portland Generating Station (PGS) based on 7/92 – 6/94 met data vs. Columbia, NJ observed values for 9/23/10 – 9/23/11 using representative maximum actual emissions shows very good agreement, within 10-20% across significant portion of distribution


Q-Q Plot of Daily Max 1-hr SO_2 at Columbia, NJ for 9/23/10-9/23/11
PGS Met Data for 7/93-6/94 @Full Load & 70% Allowable
1000
100
10
Predicted Conc (ug/m^3)
10
100
1000
Observed Conc (ug/m^3)

AERMOD NO_2 Evaluation Results

- The AERMOD model incorporates two non-default options to estimate the conversion of NO emissions to ambient NO_2 based on ozone titration:

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

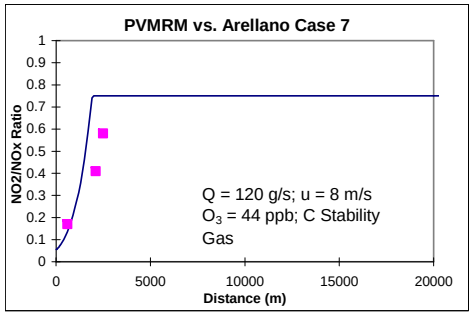
- The Plume Volume Molar Ratio Method (PVMRM) option and Ozone Limiting Method (OLM) both account for ozone titration, but PVMRM estimates the amount of titration based on the amount of O_3 in the volume of the plume (from the source to the receptor), whereas OLM estimates the conversion based on the predicted NO_x concentration

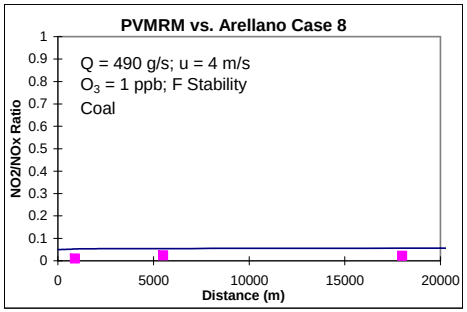
AERMOD NO_2 Evaluation Results

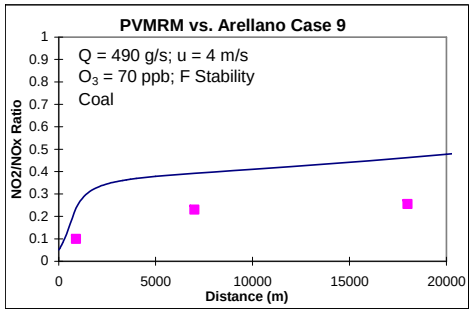
- The PVMRM option in AERMOD was evaluated against two aircraft plume studies, two long-term monitoring studies, and a large eddy simulation (LES) model
- Evaluation results show generally good agreement with observed NO_2/NO_x ratios and ambient NO_2 concentrations
- Results of aircraft studies also demonstrate importance of in-stack ratios, especially under stable conditions:
  - Initial evaluation results based on default in-stack NO_2/NO_x ratio of 0.1, which may be conservative for EGUs;
  - Revised evaluations based on 0.05 in-stack NO_2/NO_x ratio more typical for EGUs shows better agreement with observations

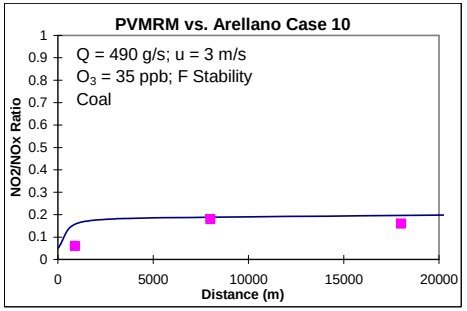
AERMOD-PVMRM vs. Aircraft Data
Examples of Paired NO2/NOX Ratios

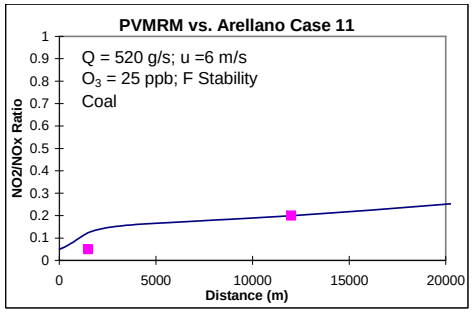
NO_2/NO_x Ratio Predictions
AERMOD-PVMRM Model Predictions vs. Arellano Aircraft Data

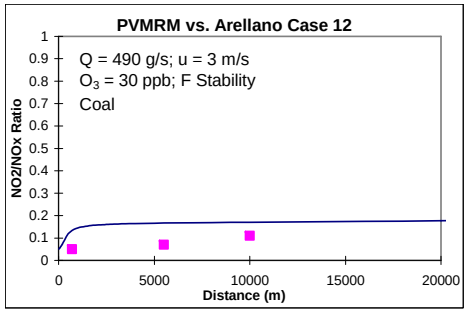




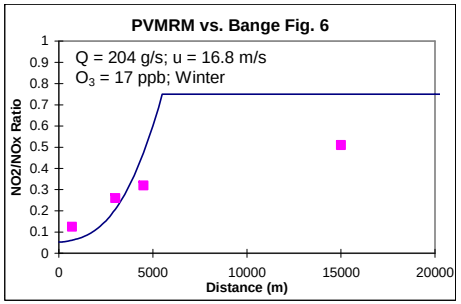


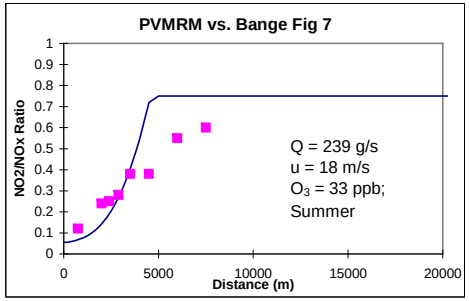


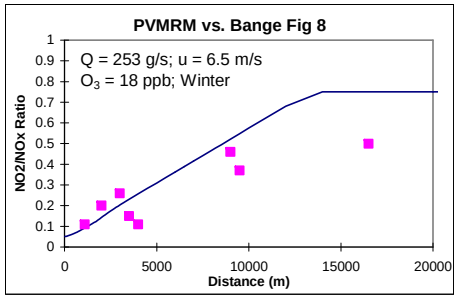


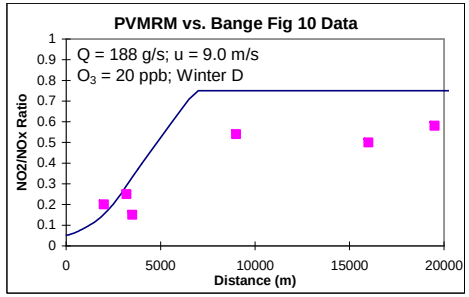


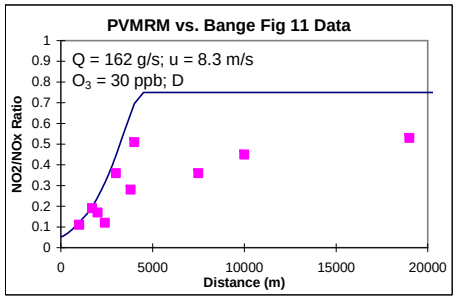
NO_2/NO_x Ratio Predictions
AERMOD-PVMRM Model Predictions vs. Bange Aircraft Data

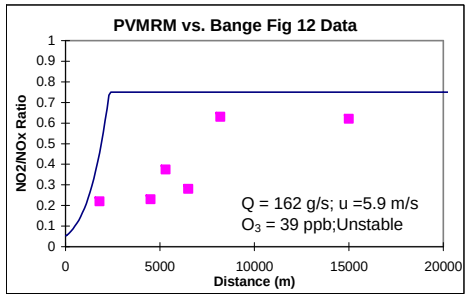












PVMRM Meas.

PVMRM Meas.

AERMOD NO_2 Evaluation Results

- Two long-term field studies were used in evaluation of PVMRM for ISCST model for annual the NO_2 NAAQS:
  - Empire Abo, NM, including two ambient NO_2 monitors; and
  - Palaau, HI, including one ambient NO_2 monitor
- These studies have been updated to evaluate the PVMRM option in AERMOD, to incorporate the OLM option, with and without OLMGROUP ALL (OLMGRP), and to evaluate 1-hour NO_2 impacts
- Preliminary results indicate generally good performance for PVMRM and OLMGRP for the North monitor at Empire Abo and at Palaau, with some overprediction for the South monitor at Empire Abo
- Significant overprediction is shown for the OLM option (without OLMGROUP ALL) and for FULL conversion, supporting the recommendation to use OLMGROUP ALL whenever OLM is used

Long-term Monitoring Studies
1-hr NO_2 Robust Highest Concentrations

	Observed	PVMRM	OLMGRP	OLM	FULL
New Mexico Abo North Monitor RHC	117.87	116.26	108.38	444.87	449.24
New Mexico Abo South Monitor RHC	70.10	218.98	104.81	440.96	454.68
Hawaii Palaau Monitor RHC	95.42	101.57	113.18	368.57	480.38
Geometric Mean Pred/Obs RHC	---	1.486	1.177	4.510	4.993

Figure A-1. AERMOD Model Evaluation - New Mexico North Monitor - Hourly NO2 Q-Q Plot

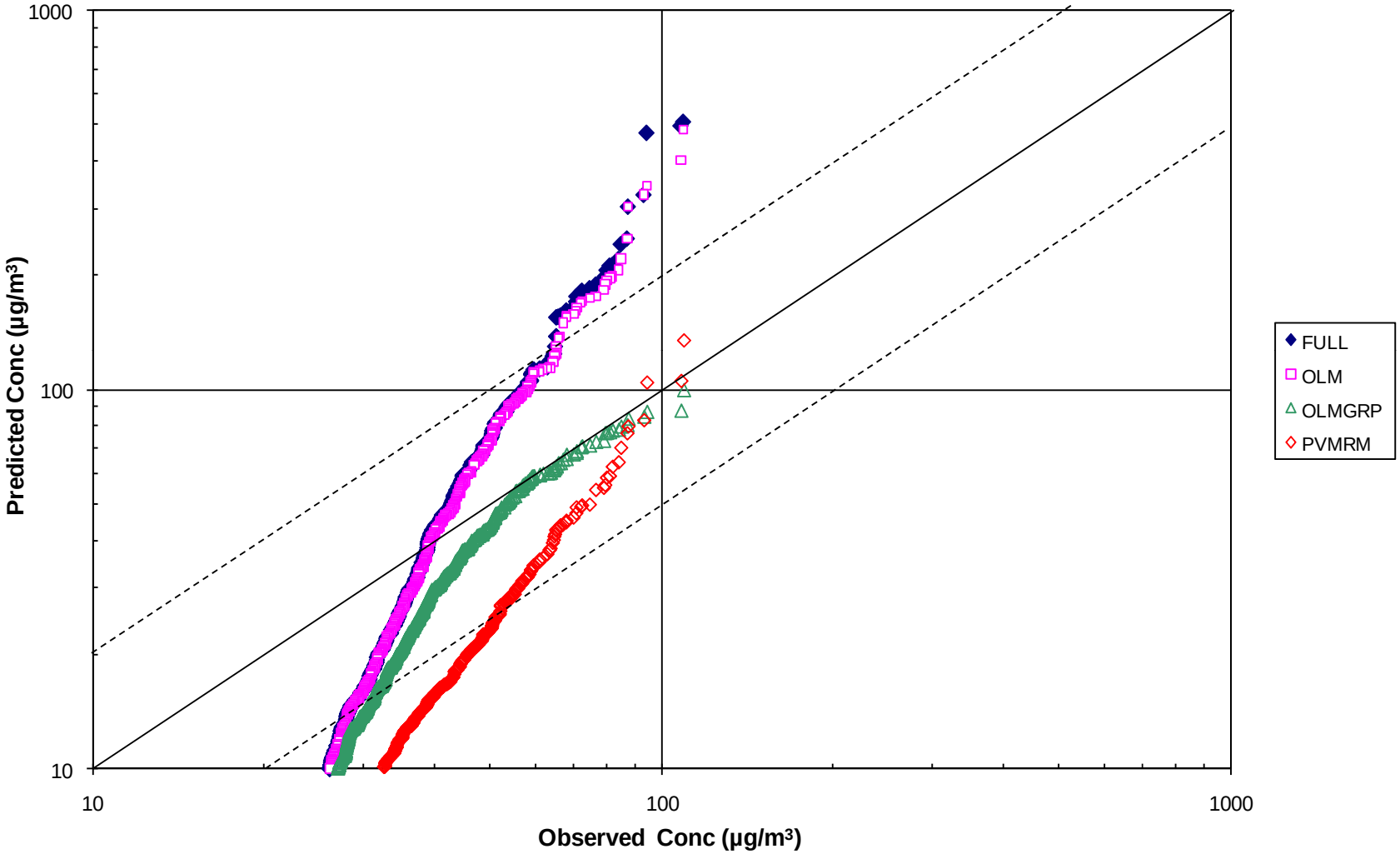


Figure A-2. AERMOD Model Evaluation - New Mexico South Monitor - Hourly NO2 Q-Q Plot

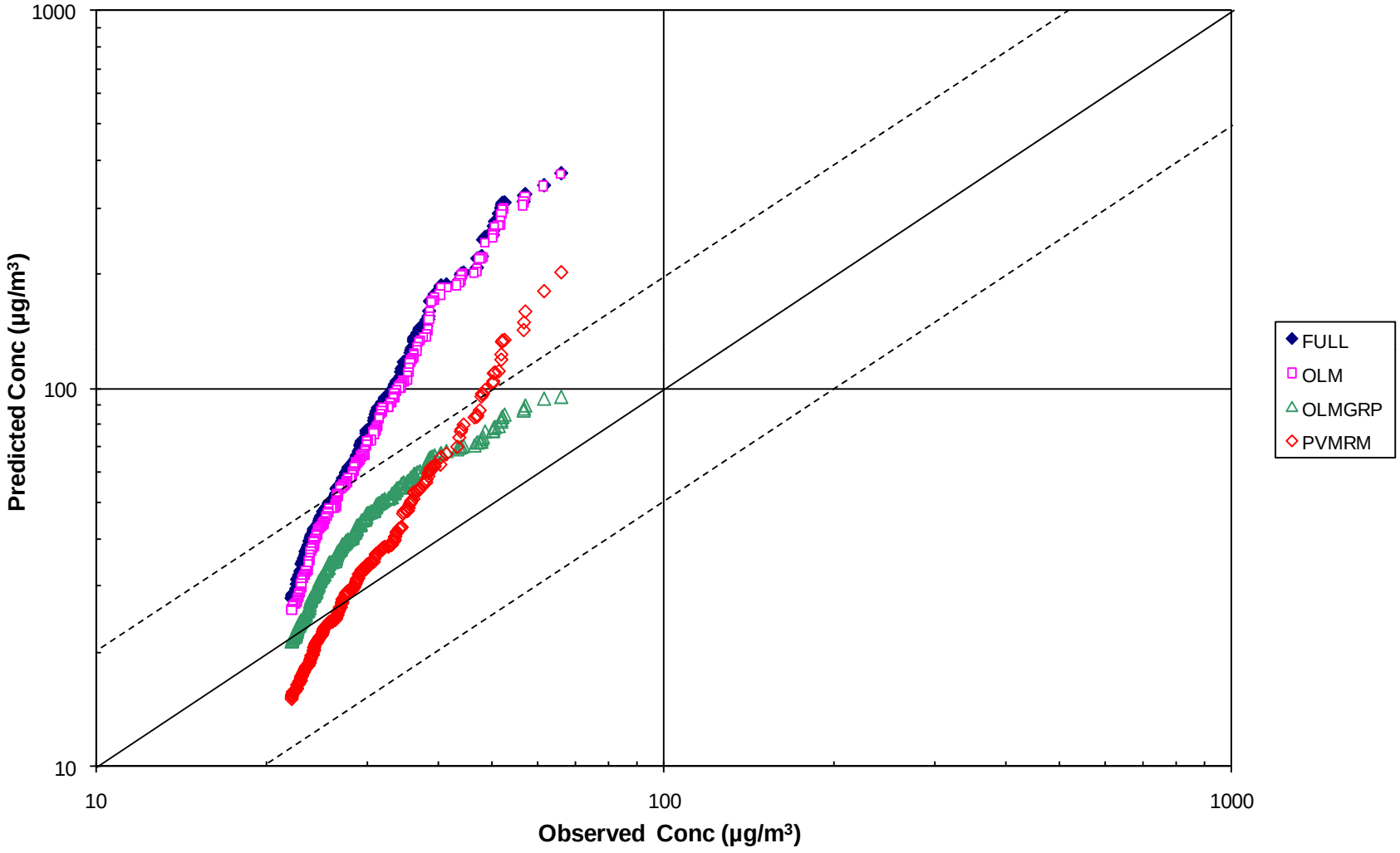
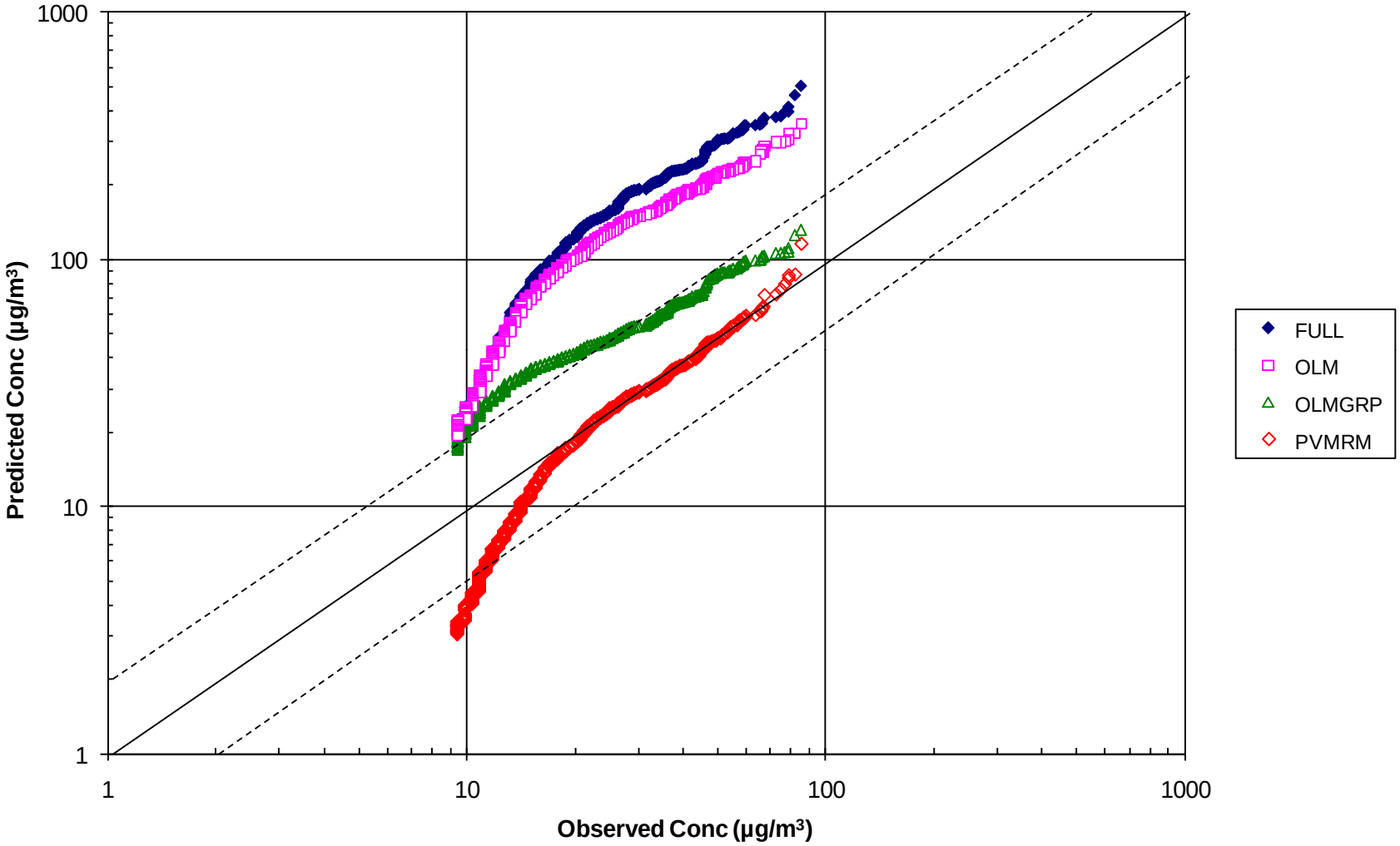


Figure A-3. AERMOD Model Evaluation - Palaau, HI - Hourly NO2 Q-Q Plot

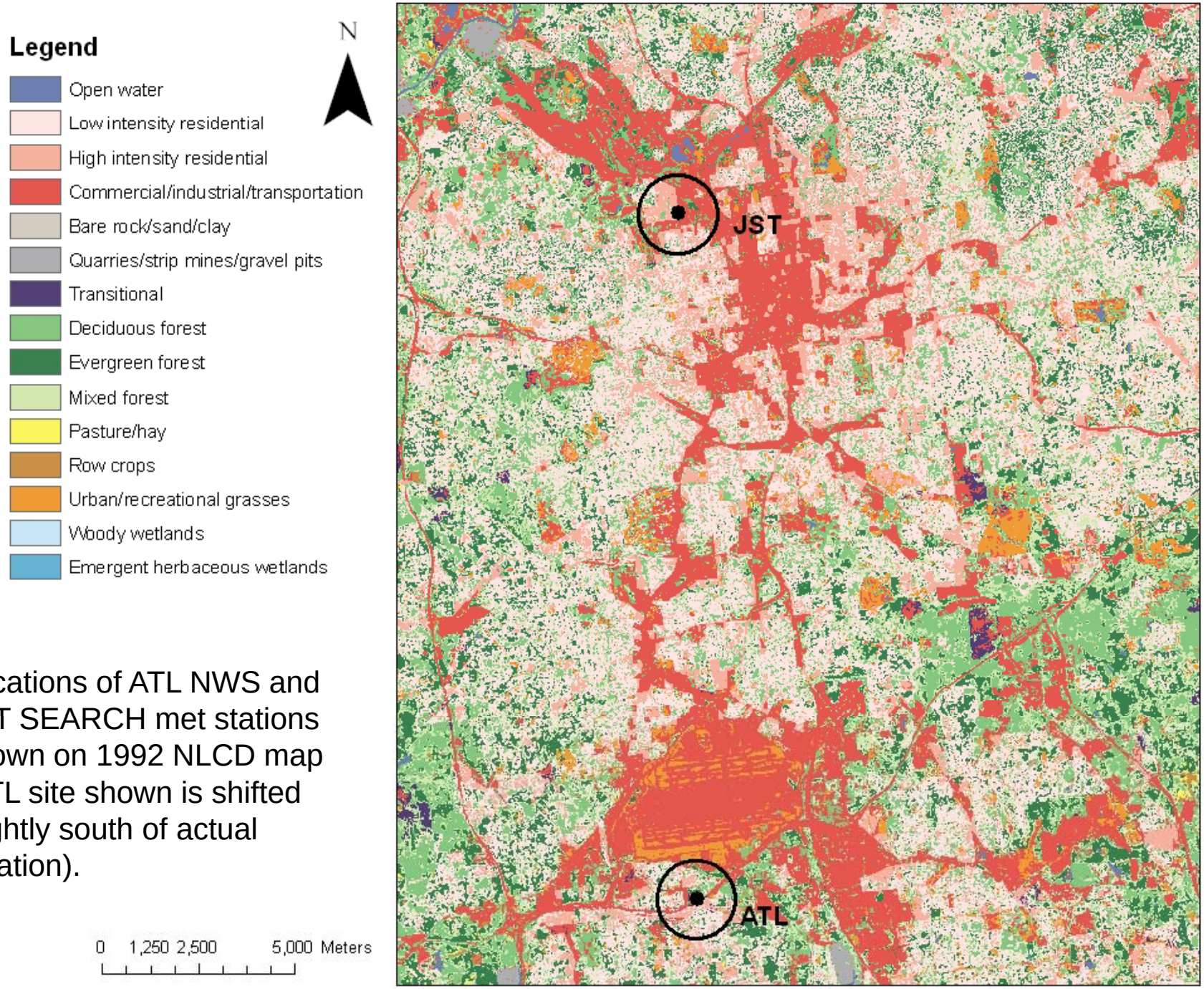


Example from NO_2 NAAQS Review

- AERMOD was applied for the Risk and Exposure Assessment (REA) for the Atlanta area in support of recent NO_2 NAAQS review, focused on hourly impacts
- Majority of NO_2 impacts attributed to mobile sources
- Initial model-to-monitor comparisons showed AERMOD concentrations significantly exceeding monitored NO_2 concentrations at 3 Atlanta monitors
- Initial assessment by contractor was that low surface roughness used to process airport data was not representative of roughness typical of source locations, and suggestion was to re-process airport data with 1m roughness

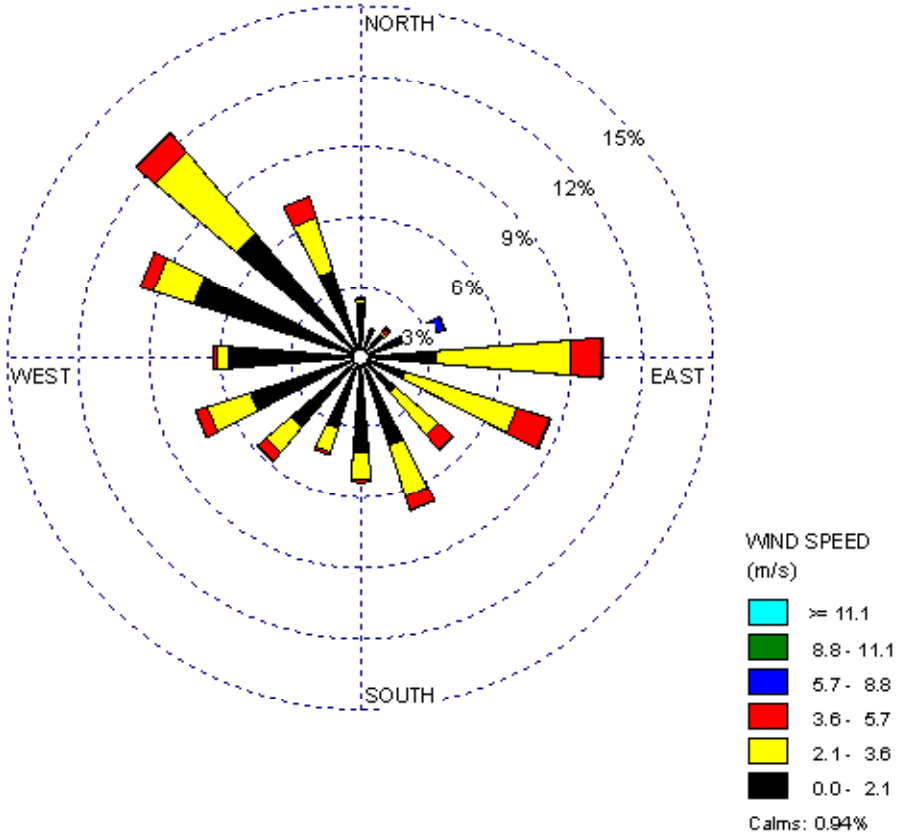
Example from NO_2 NAAQS Review

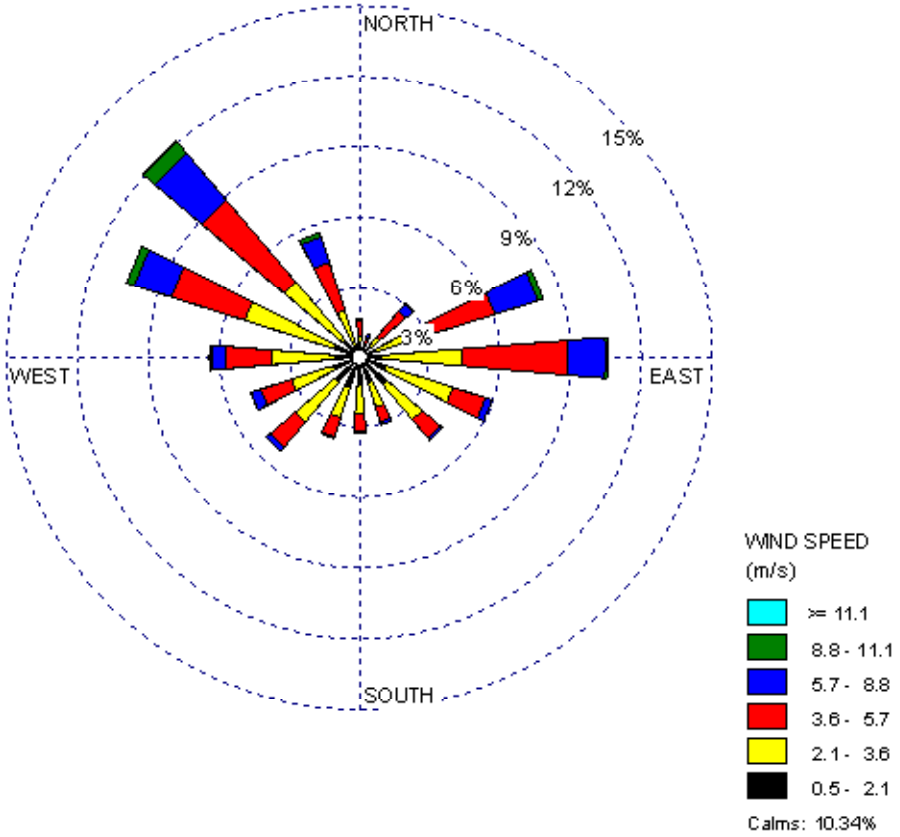
- Based on a broader assessment, recommendations were made to:
  - Acquire and process SEARCH met data as more representative of surface characteristics for mobile source emissions across the area;
  - Apply OLMGROUP ALL option for OLM;
  - Modify source characteristics for mobile source emissions to better account for vehicle induced turbulence; and
  - Adjust met inputs to address urban morning transition issue (later addressed in version 11059 of AERMOD)
- Next slides show time-series comparisons of hourly NO_2 "before" and "after" these adjustments to modeling analysis. Use of OLMGROUP ALL was one of the key factors in the improved model performance.
  - "Before" slide shows ambient NO_2 in blue, initial AERMOD results in black, and AERMOD results with SEARCH met data in red;
  - "After" slide shows ambient NO_2 in blue and final AERMOD results in black.



Locations of ATL NWS and JST SEARCH met stations shown on 1992 NLCD map (ATL site shown is shifted slightly south of actual location).

Wind Rose Comparison for SEARCH and ATL-NWS Data for 2002



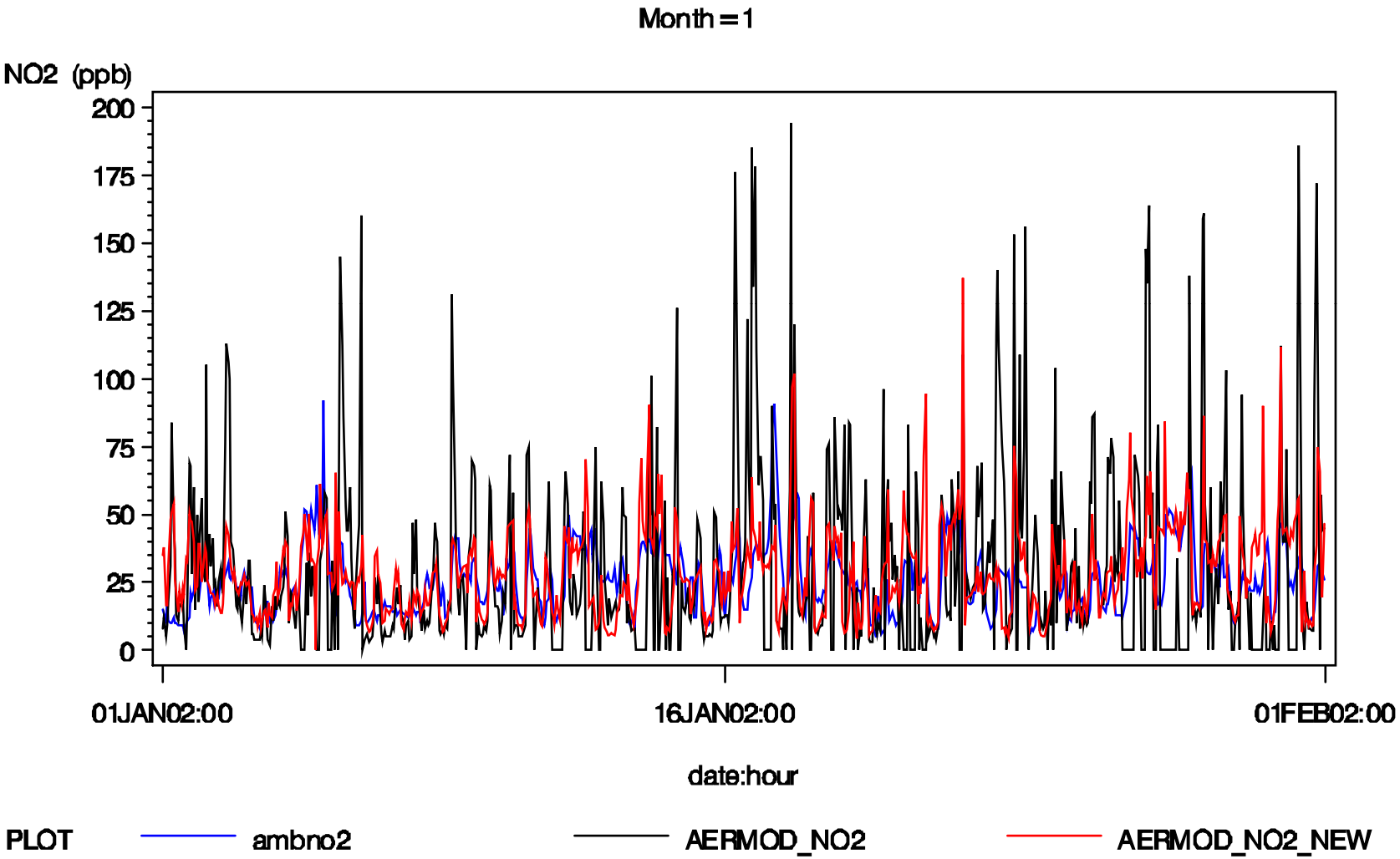


JST
82 calms

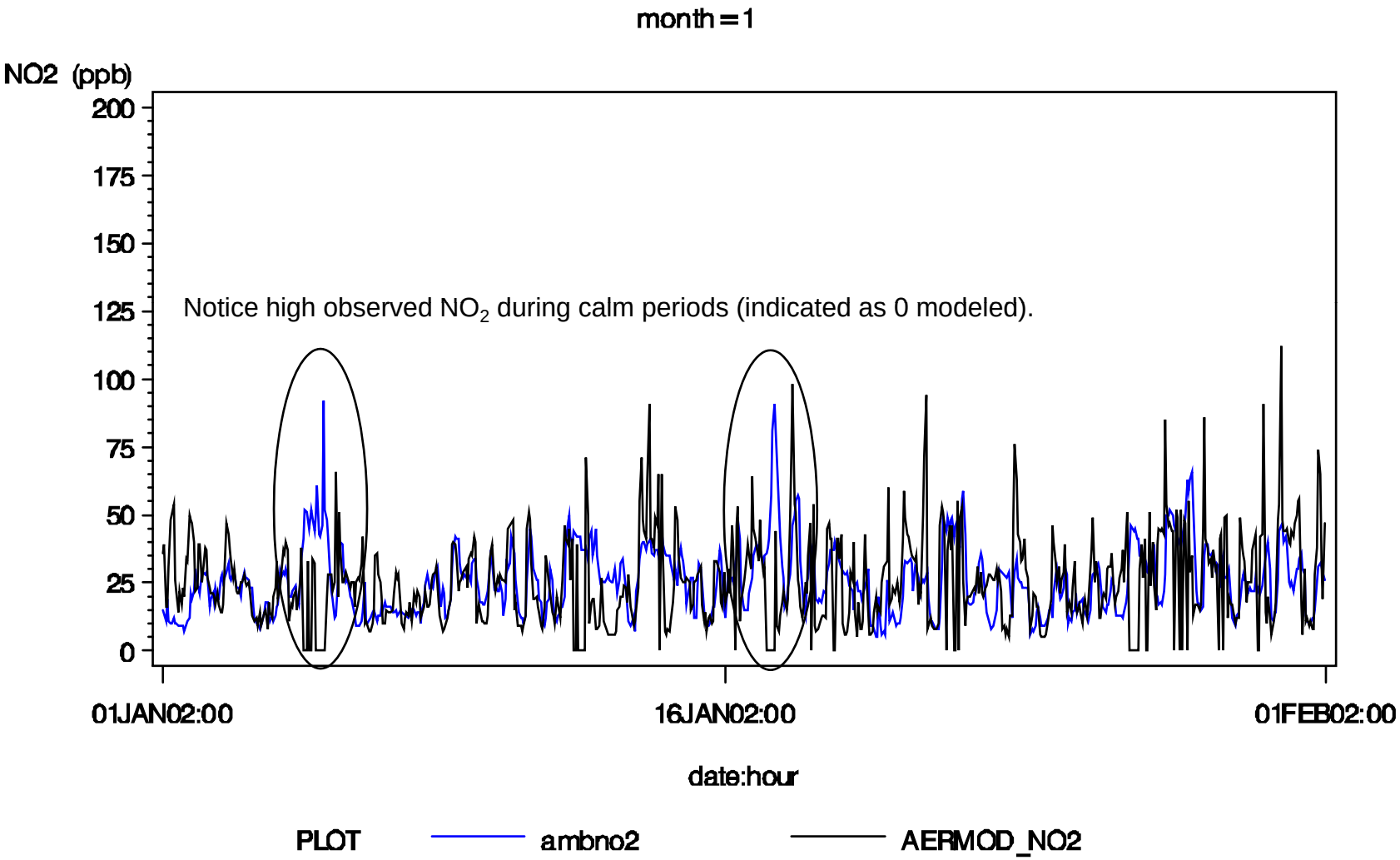
2002

ATL
856 calms

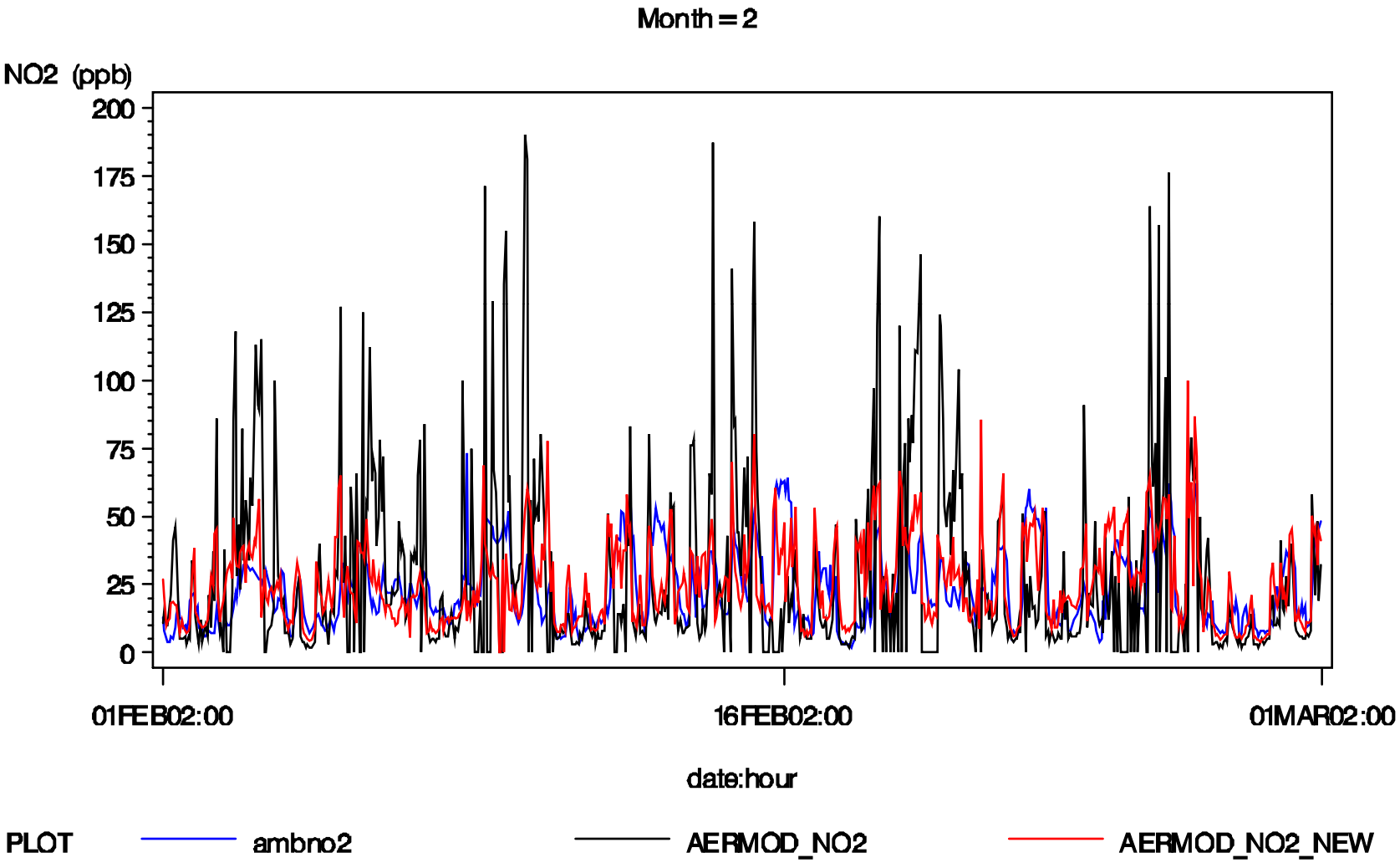
Model-to-Monitor Comparison - Before



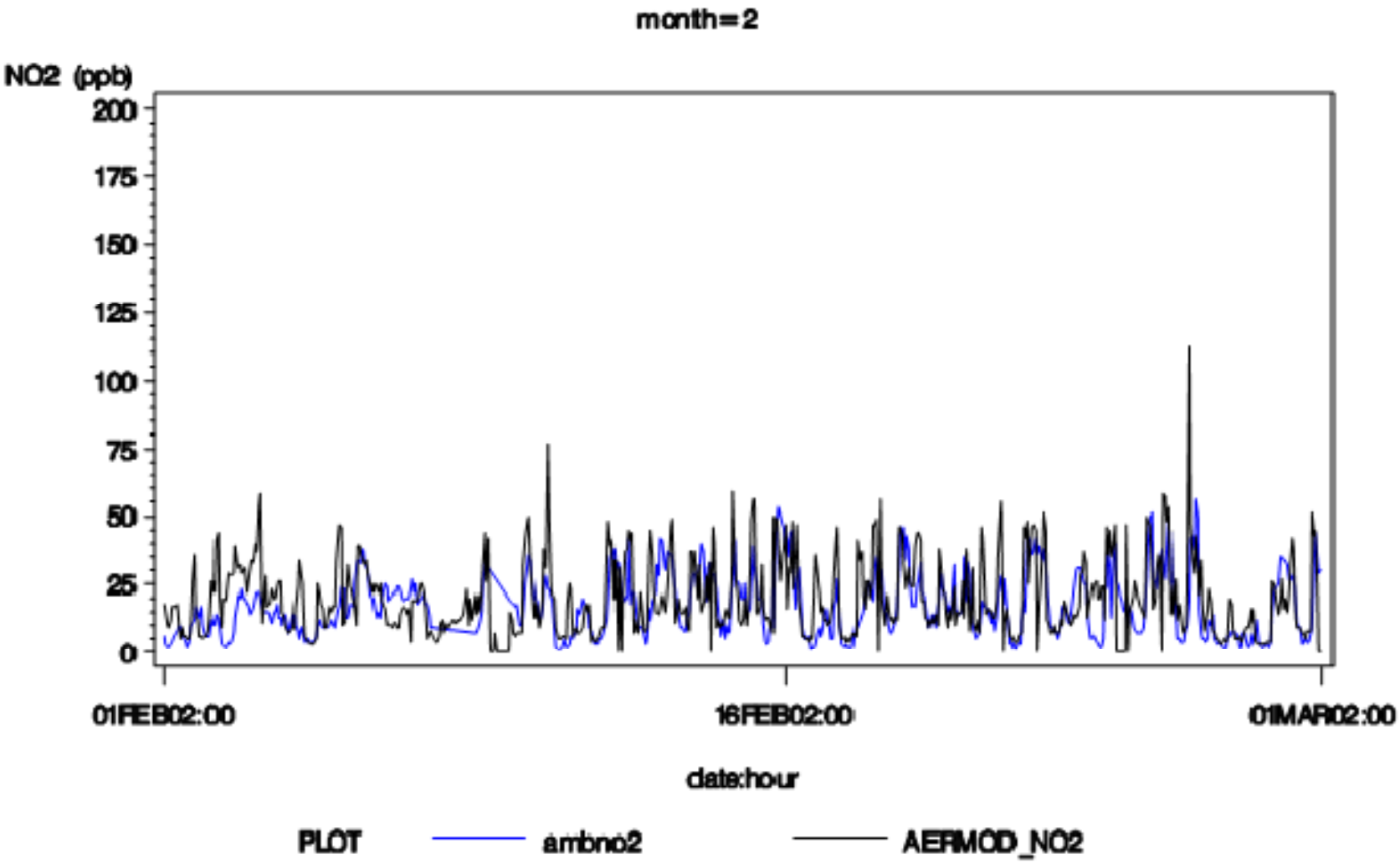
Model-to-Monitor Comparison - After



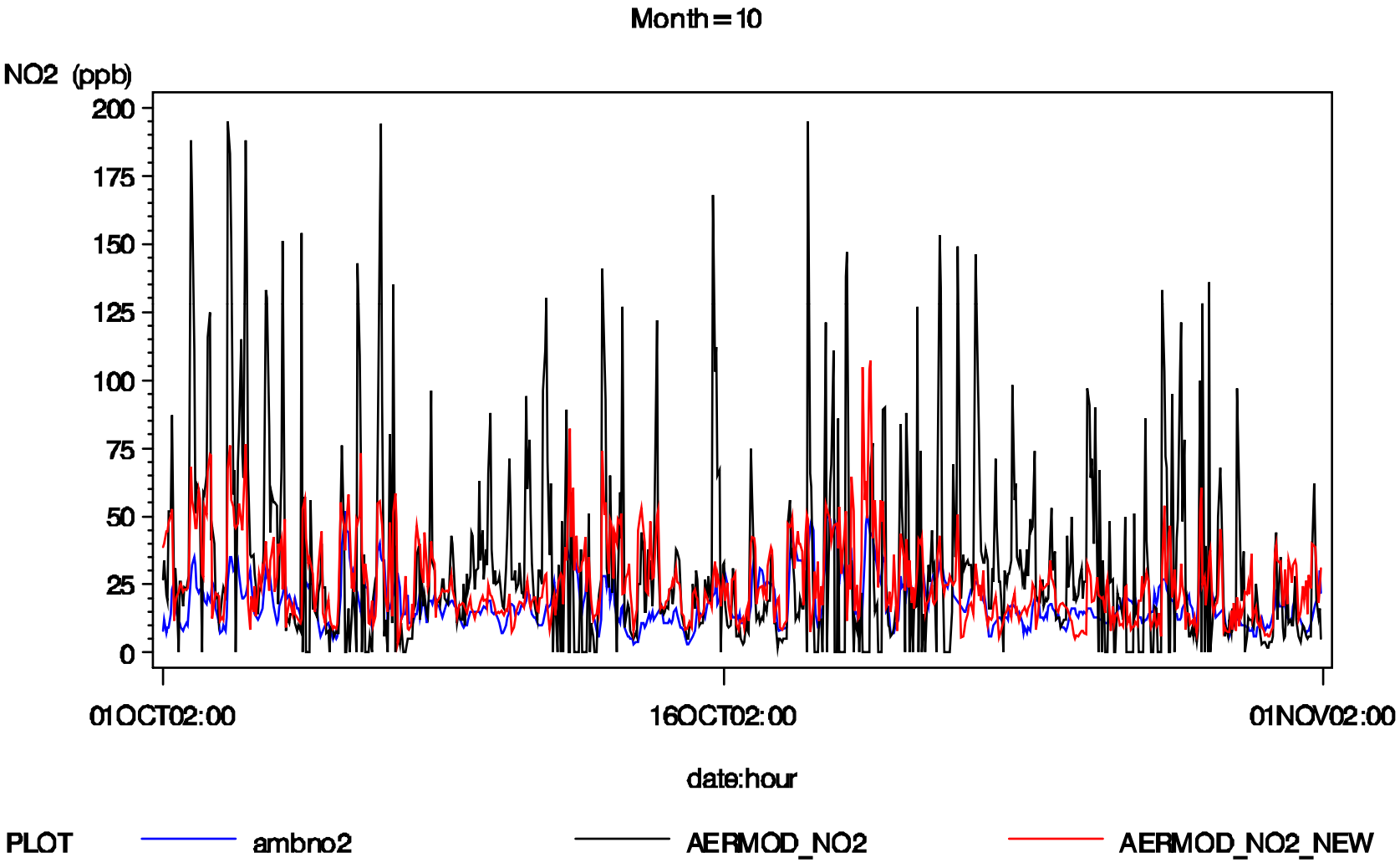
Model-to-Monitor Comparison - Before



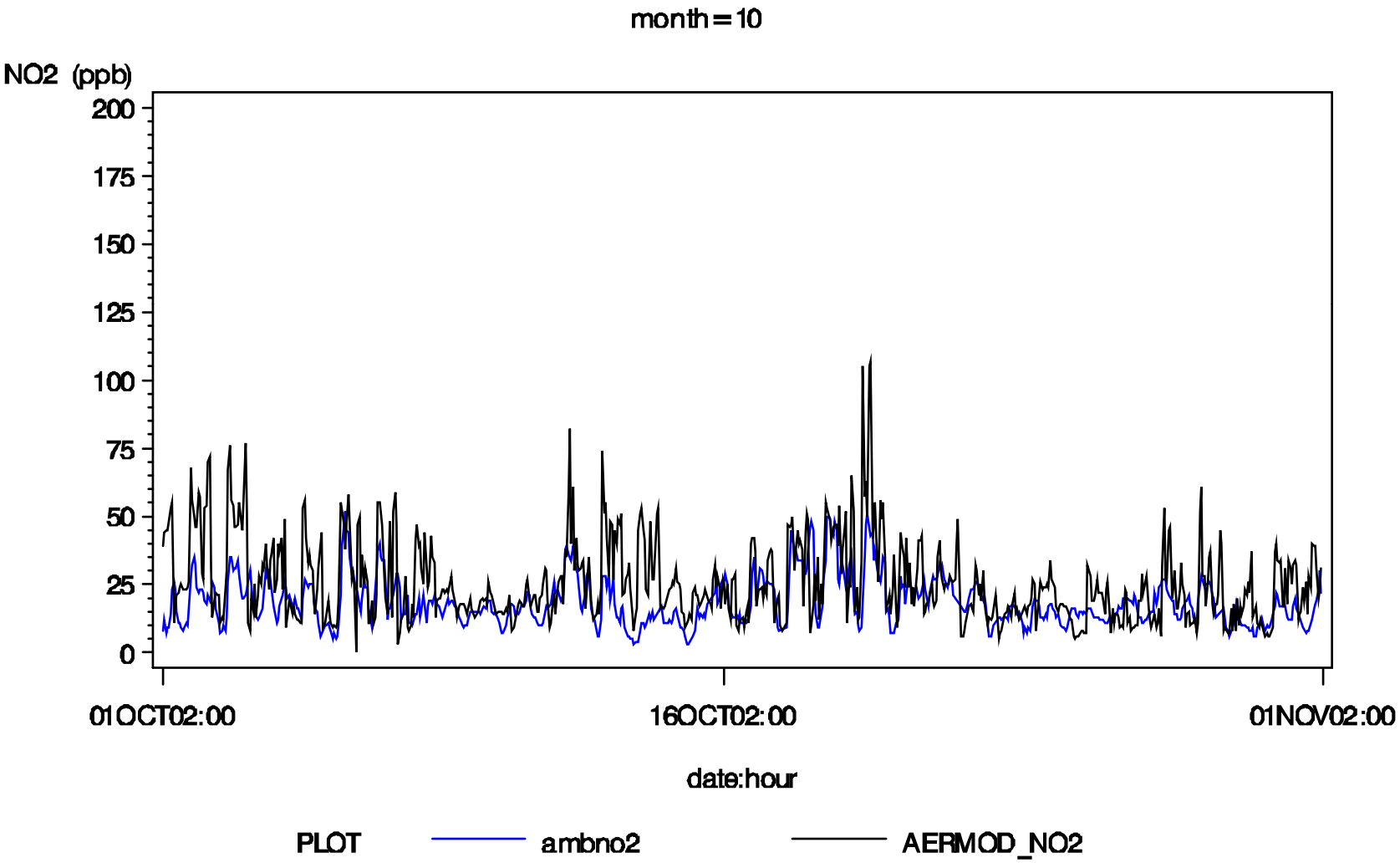
Model-to-Monitor Comparisons - After



Model-to-Monitor Comparisons - Before



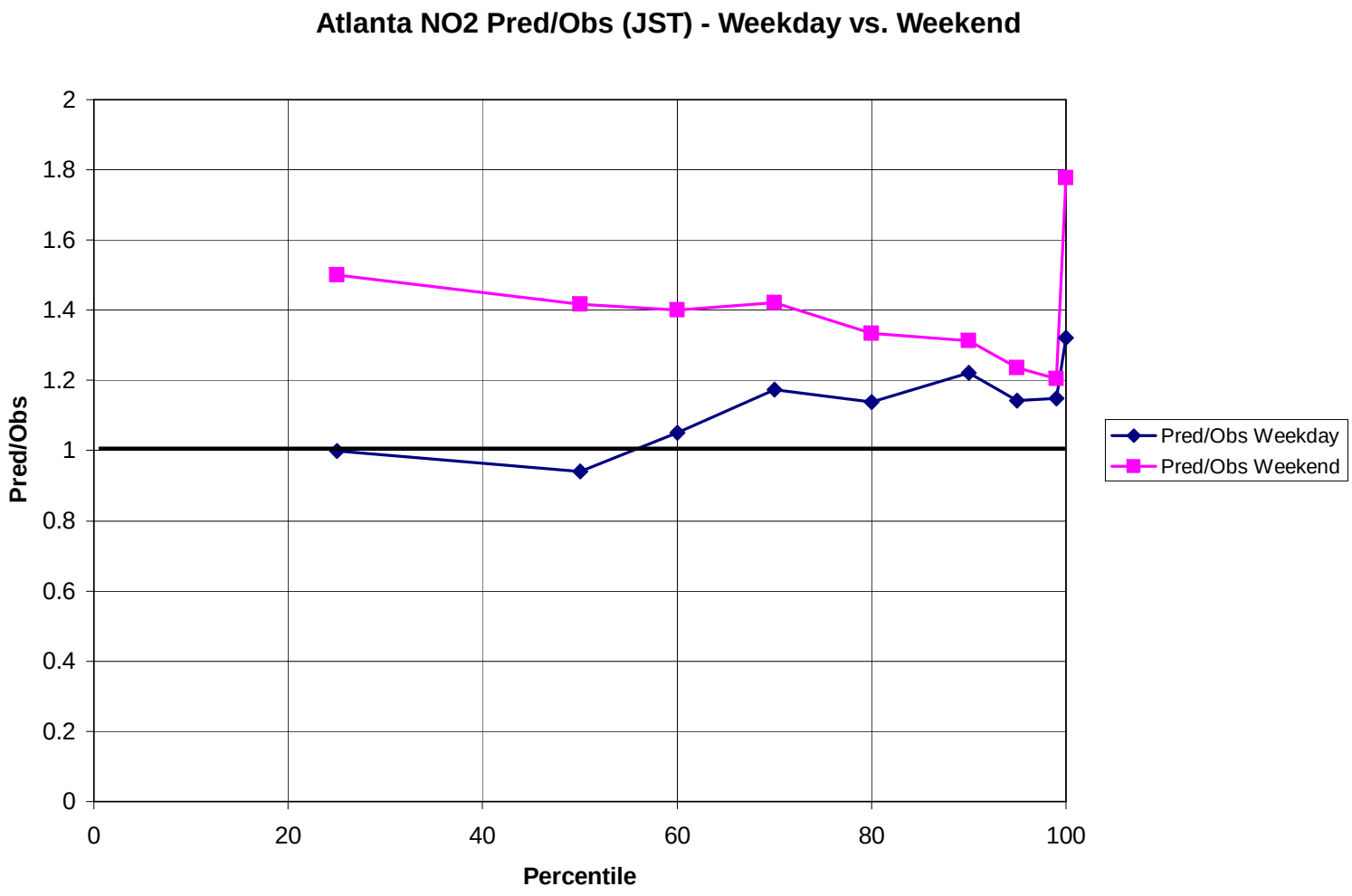
Model-to-Monitor Comparisons - After



Example from NO_2 NAAQS Review

- Mobile source emissions input to AERMOD for the Atlanta NO_2 REA were varied by season and hour-of-day, but did not include a day-of-week component
- Next slide compares the average Pred/Obs ratio of 1-hr NO_2 concentrations by percentile rank for the JST SEARCH monitor for weekdays vs. weekends
- Results show better agreement for weekdays than weekends, with some overestimation for weekends, suggesting that overall model performance may have been improved somewhat if day-of-week dependence of emissions were included

Average Pred/Obs 1-hr NO2 Concentrations by Percentile Rank for JST Monitor – Weekday vs. Weekend



Additional AERMOD NO_2 Evaluation Results

- Recent comments by API on the Empire Abo, NM field study for NO_2 suggest some scavenging of O_3 occurring at the downwind monitor
- Following slides compare evaluation results for Empire Abo based on use of O_3 from upwind vs. downwind monitor
- Revised results show slightly higher ambient NO_2 concentrations based on use of O_3 from upwind monitor, suggesting that some O_3 scavenging may be affecting results

Figure A-1. AERMOD Model Evaluation - NM N Monitor w/S-O3 - Hourly NO2 Q-Q Plot

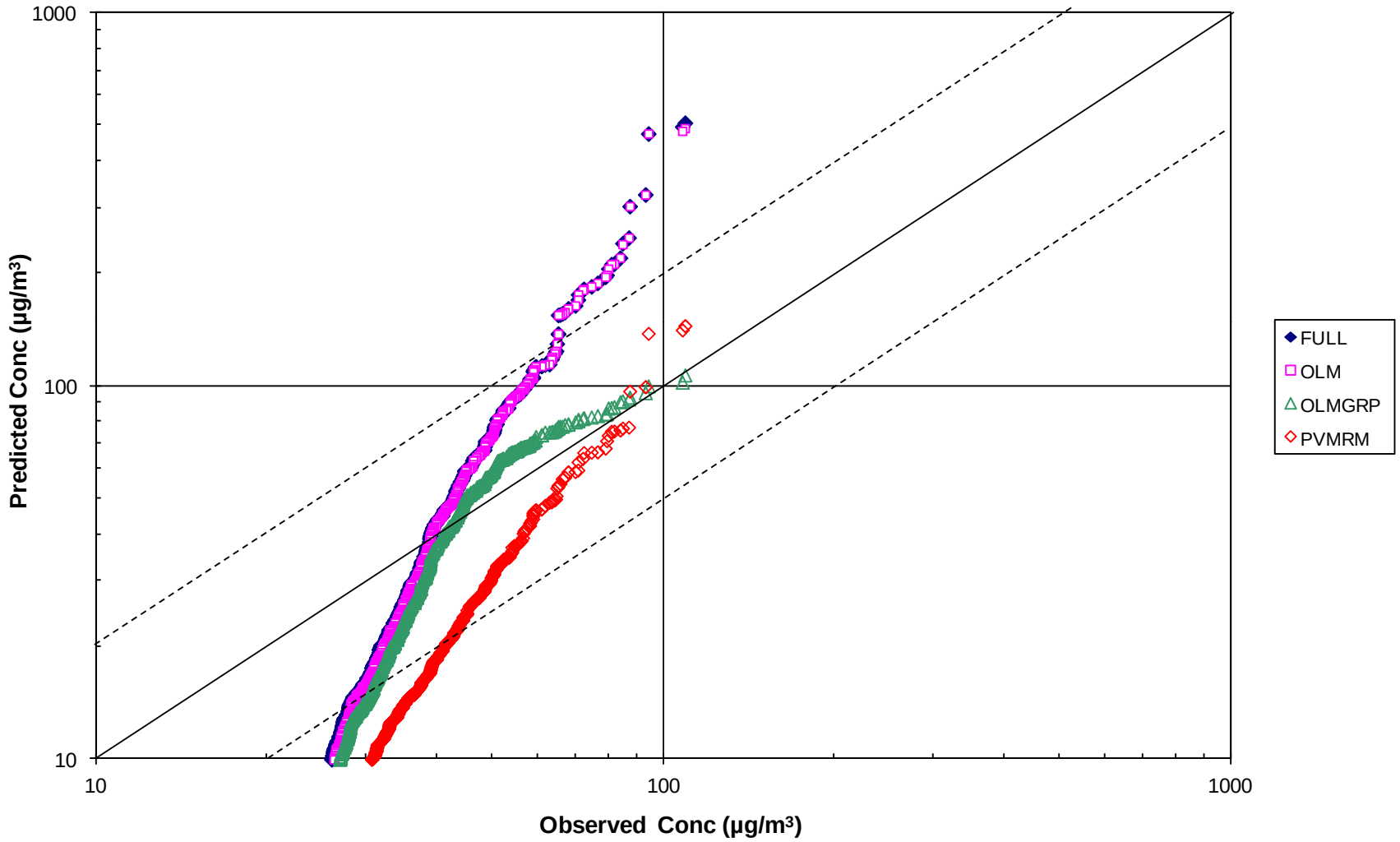


Figure A-1. AERMOD Model Evaluation - New Mexico North Monitor - Hourly NO2 Q-Q Plot

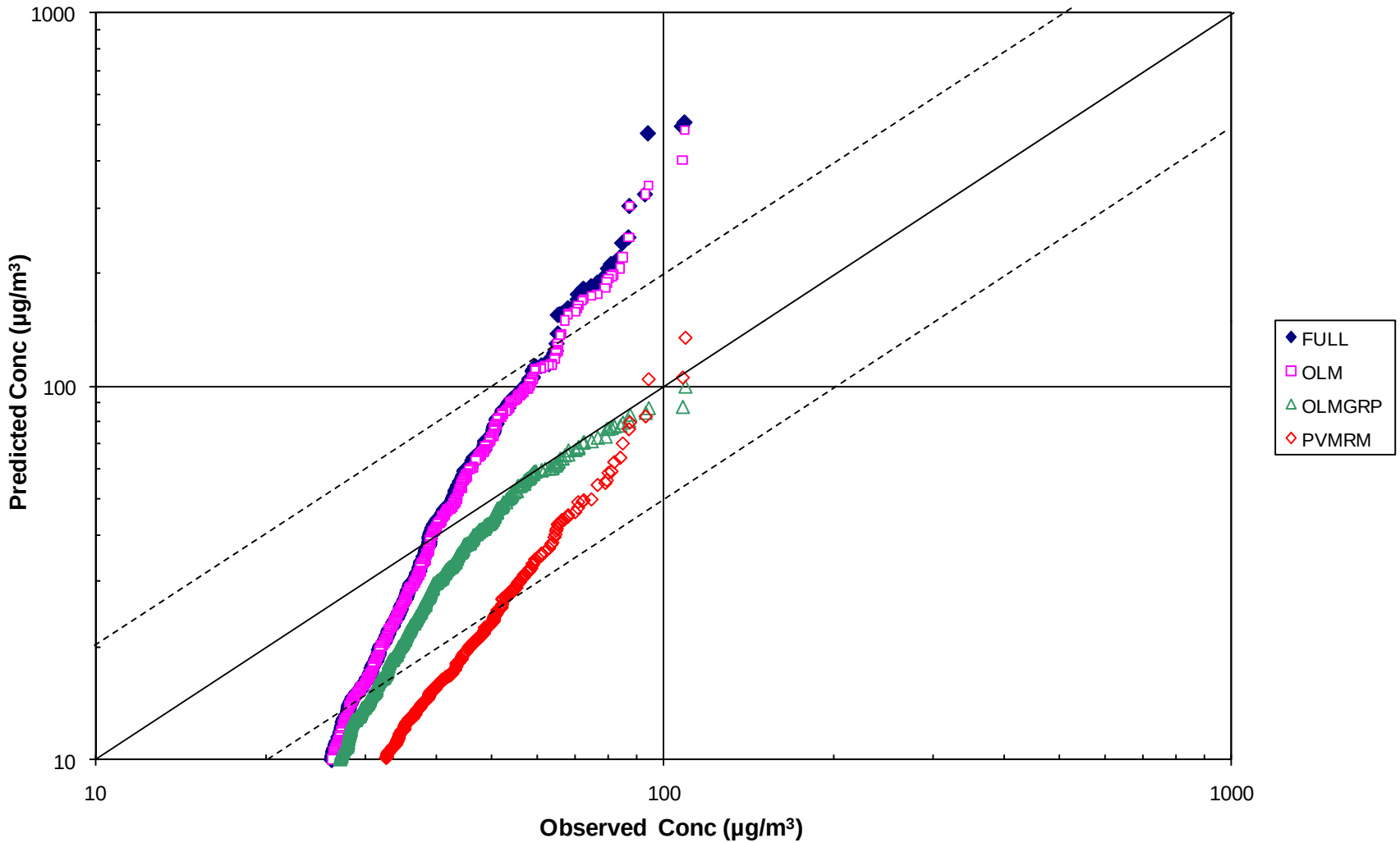


Figure A-2. AERMOD Model Evaluation - NM S Monitor w/N-O3 - Hourly NO2 Q-Q Plot

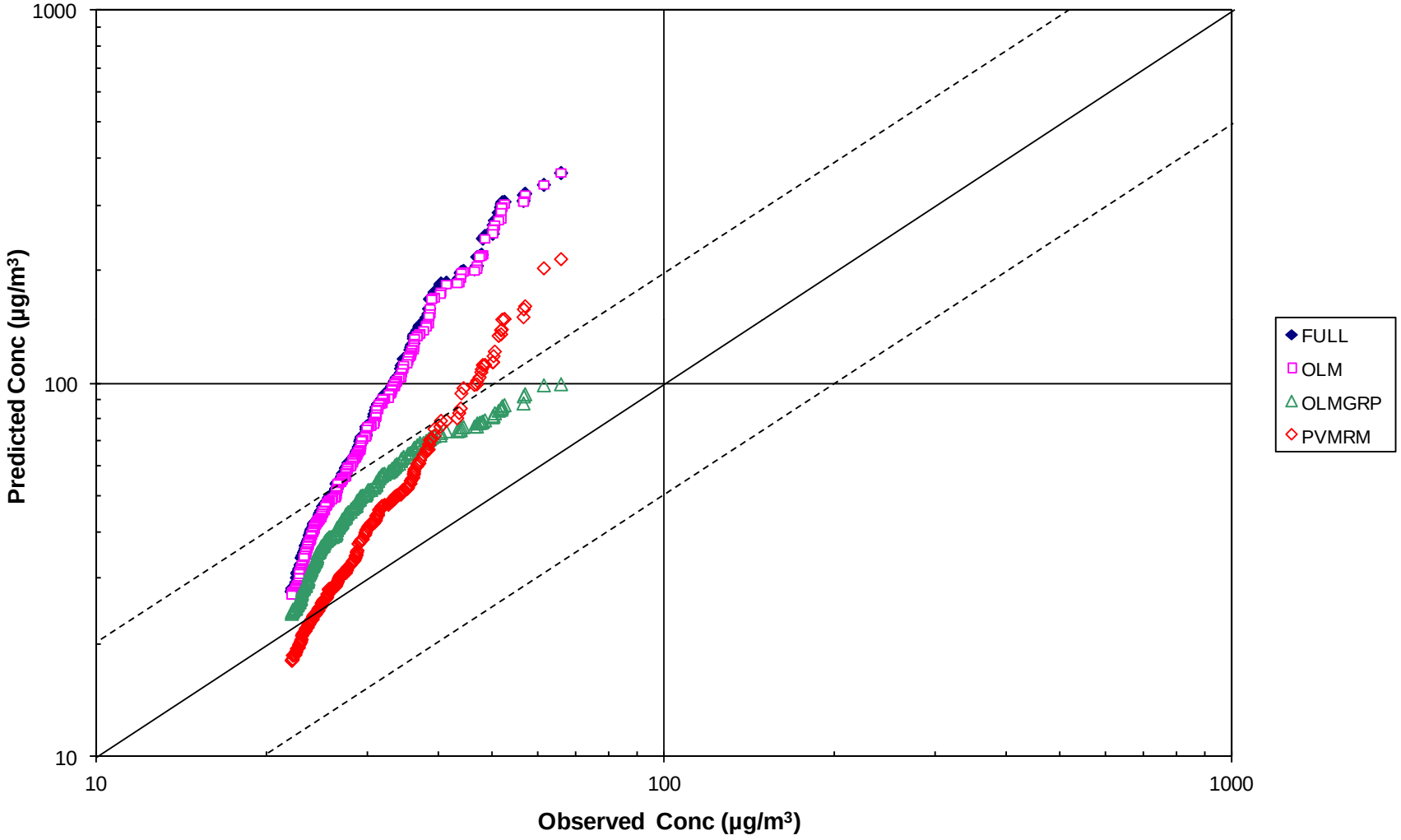
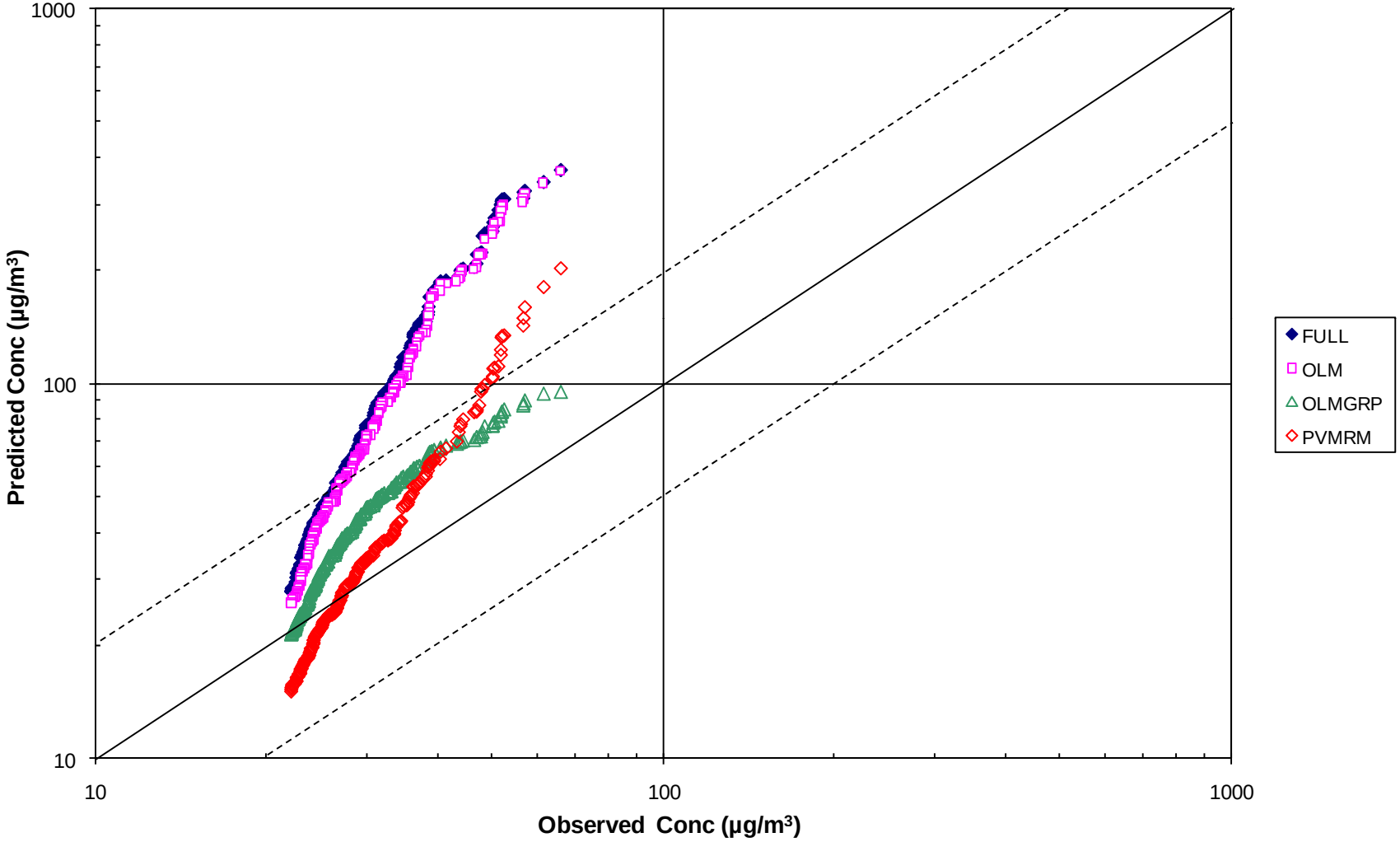


Figure A-2. AERMOD Model Evaluation - New Mexico South Monitor - Hourly NO2 Q-Q Plot

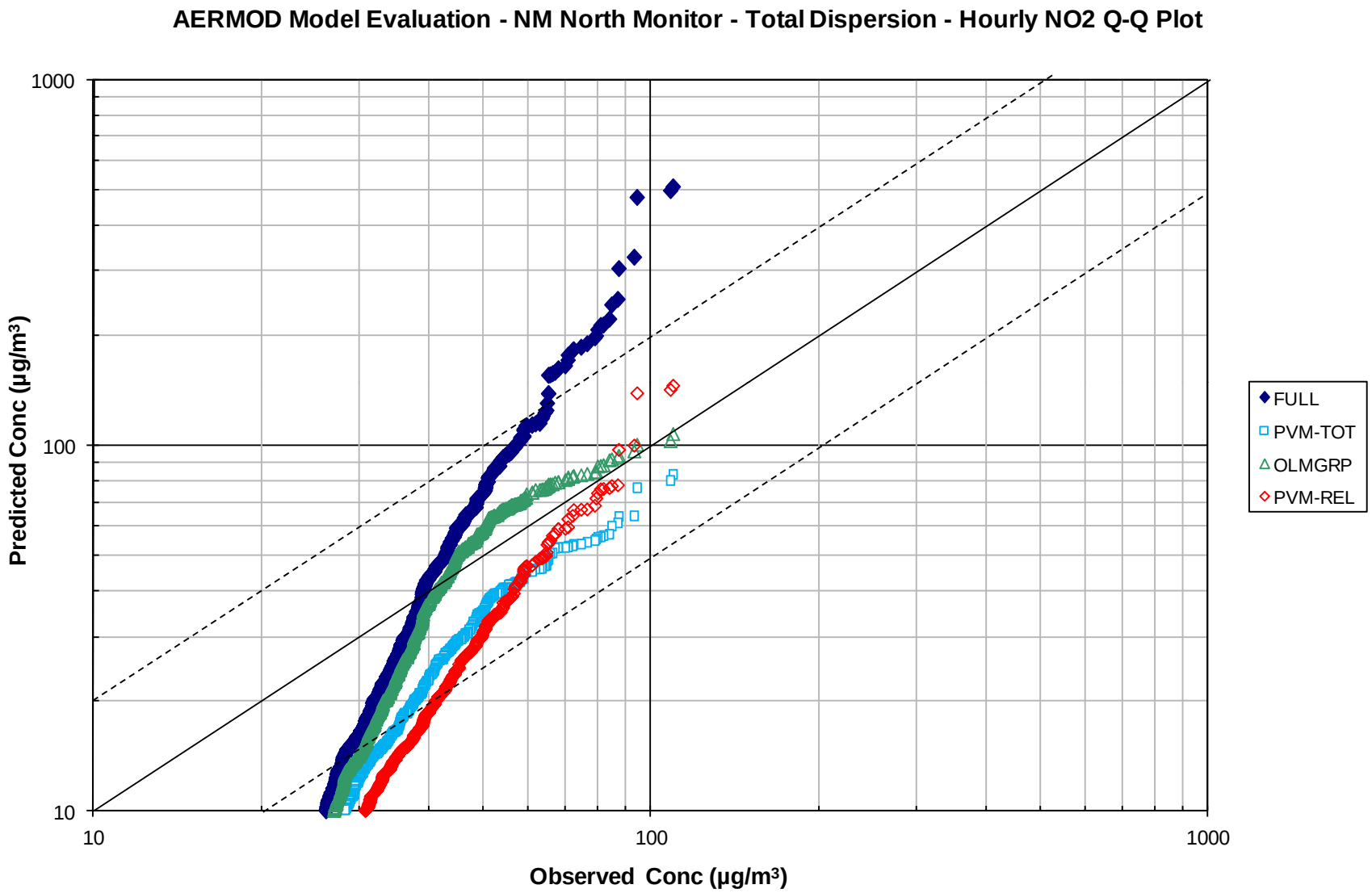


Additional AERMOD NO_2 Evaluation Results (cont.)

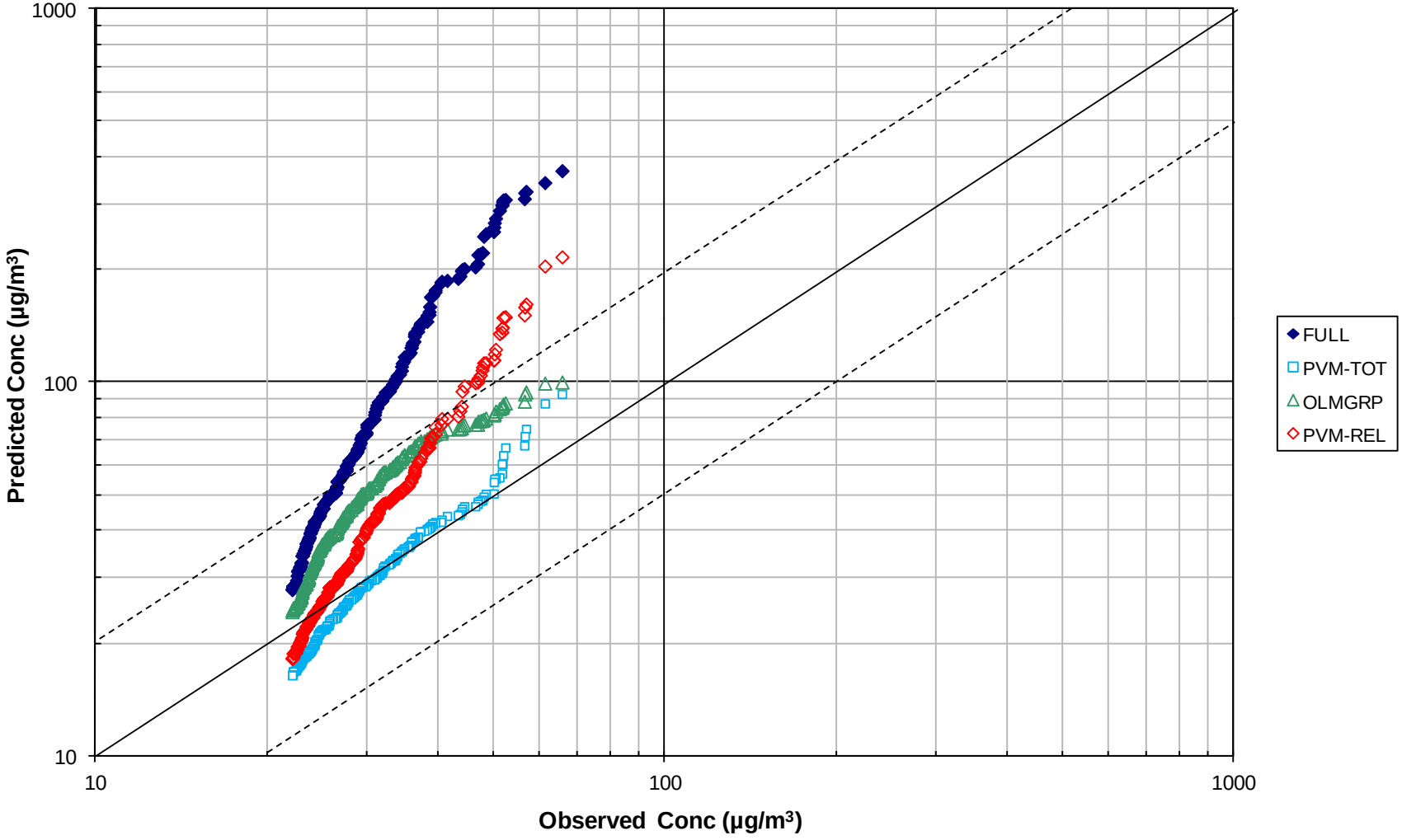
- The PVMRM option implemented in AERMOD uses relative (instantaneous) dispersion coefficients to estimate the plume volume, rather than total (time-averaged) dispersion coefficients, which were used in PVMRM for the ISCST model
- Relative dispersion coefficients are more appropriate for determining the volume of the plume for purposes of O_3 titration, but the number of standard deviations used to compute plume volume differs depending on whether relative or total dispersion coefficients are used:
  - Original PVMRM option for ISCST used 1.282 standard deviations (n_z) to estimate plume volume based on total dispersion coefficients as the "best fit"
  - AERMOD PVMRM option currently uses 4.0 standard deviations to estimate plume volume based on relative dispersion coefficients (accounts for nearly 100% of plume)
  - API has commented on the appropriateness of using $n_z = 4.0$ in AERMOD

Additional AERMOD NO_2 Evaluation Results (cont.)

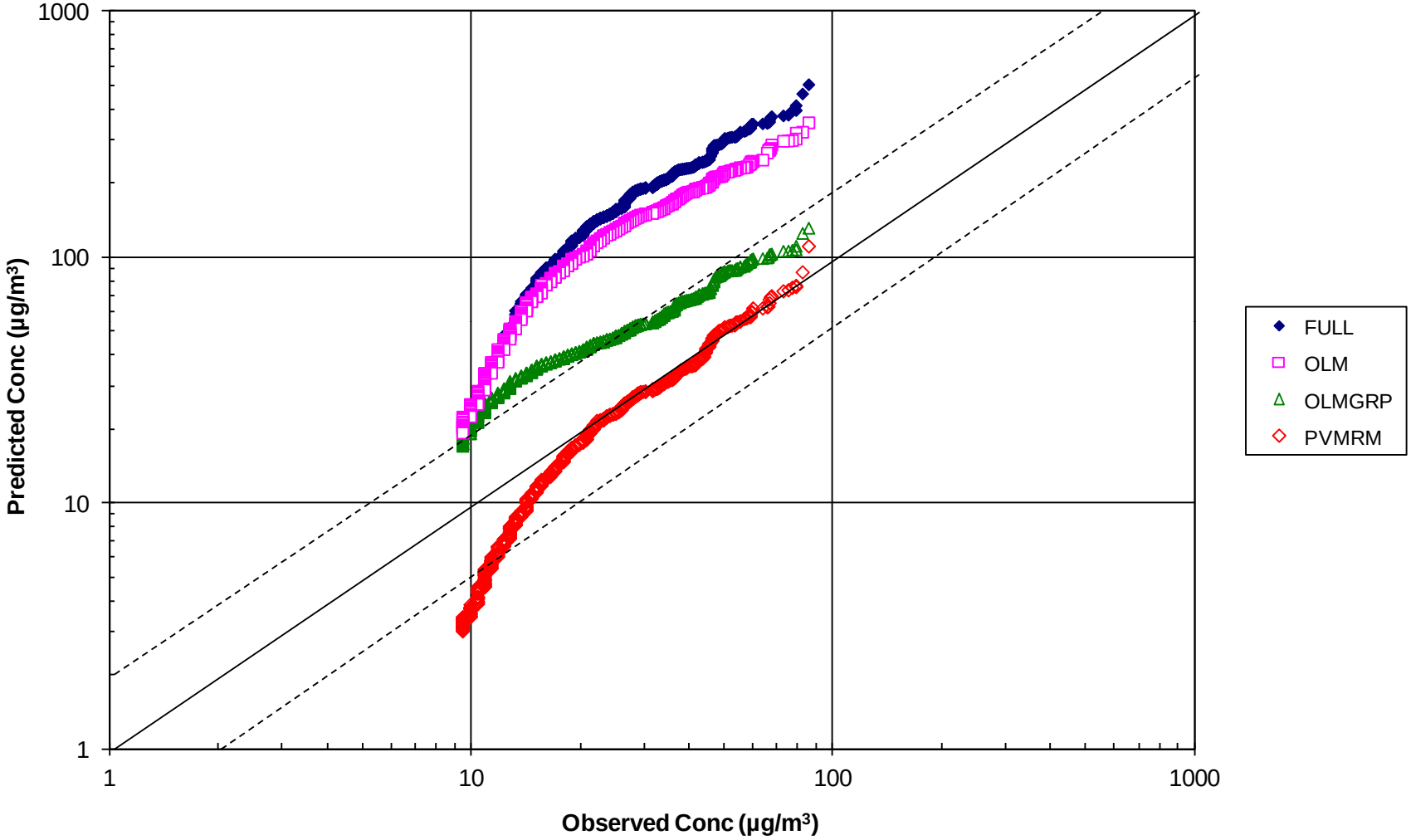
- Preliminary evaluations are presented below based on use of total dispersion coefficients for PVMRM option in AERMOD with $n_z = 1.282$, comparable to the approach used with PVMRM option for ISCST
- Results for Empire Abo are based on use of O_3 from upwind monitor
- Modeled concentrations are reduced for all three monitors based on use of total dispersion as compared to current version using relative dispersion:
  - Results for NM North Monitor shift from 20% overprediction to 30% underprediction
  - Results for NM South Monitor shift from 250% overprediction to 30% overprediction
  - Results for Palaau, HI, show slight improvement, from 6.5% overprediction to 3% overprediction
  - Geometric mean of Pred/Obs RHC ratios improved from 1.65 to 0.98


AERMOD Model Evaluation - NM North Monitor - Total Dispersion - Hourly NO2 Q-Q Plot
1000
100
10
10
100
1000
Predicted Conc (µg/m³)
Observed Conc (µg/m³)
FULL
PVM-TOT
OLMGRP
PVM-REL

AERMOD Model Evaluation - NM South Monitor - Total Dispersion - Hourly NO2 Q-Q Plot



AERMOD Model - Palaau, HI - Total Dispersion - Hourly NO_2 Q-Q Plot



Preliminary Results for AERMOD PVMRM with Total Dispersion and n_z = 1.282

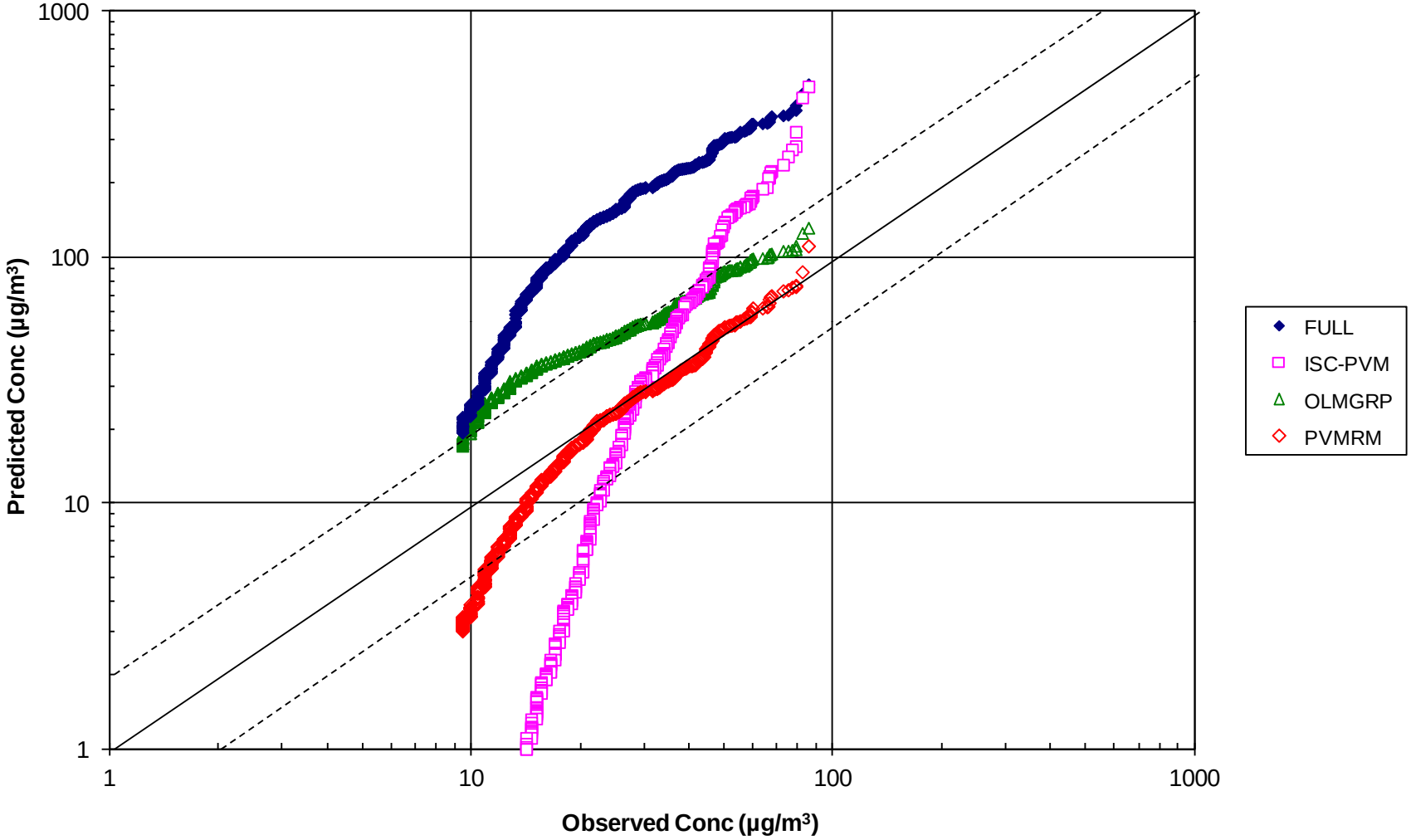
1-hour NO_2 Robust Highest Concentrations (µg/m^3)
Using O_3 Data from Upwind Monitor for New Mexico

	Observed	PVMRM	PVM-Total	OLMGRP	OLM	FULL
New Mexico Abo North Monitor RHC	117.87	141.10	80.79	110.38	444.69	449.24
New Mexico Abo South Monitor RHC	70.10	246.92	92.70	107.61	449.79	454.68
Hawaii Palaau Monitor RHC	95.42	101.57	98.28	131.18	368.57	480.38
Geometric Mean Pred/Obs RHC	---	1.650	0.977	1.255	4.539	4.993

Comparison with ISCST-PVMRM NO_2 Evaluation Results

- For comparison, the following slide shows a Q-Q plot of 1-hour NO_2 results for Palaau, HI, for AERMOD-PVMRM and ISCST-PVMRM, based on total dispersion to define plume volume for both models
- The 1-hour NO_2 RHC for ISCST-PVMRM overpredicts the observed 1-hour RHC by about 320%, compared to a 3% overprediction bias for AERMOD
- Although limited to a single monitor from a single field study, these results suggest that improvements in the dispersion algorithms in AERMOD as compared to ISCST3 may contribute significantly to the model's ability to estimate 1-hour NO_2 ambient concentrations

AERMOD - Palaau, HI - Total Disp - With ISCST-PVMRM - Hourly NO_2 Q-Q Plot



Summary

- AERMOD model performance has been extensively evaluated and shown to provide generally unbiased estimates of 1-hr SO_2 concentrations across a wide range of scenarios
- Existing Tier 3 options in AERMOD for modeling 1-hr NO_2 impacts also show generally good results, but the amount of field study data is very limited and the quality of the available data is less than ideal
- Preliminary evaluation results based on the use of total dispersion to calculate the plume volume for the PVMRM option in AERMOD are encouraging, but further tests are needed and the preliminary implementation significantly degrades model runtime