Final Report

EVALUATION OF BIAS IN AERMOD-PVMRM

Alaska DEC Contract No. 18-9010-12

Submitted to:

Alaska Department of Environmental Conservation
Division of Air Quality
410 Willoughby Avenue, Suite 303
Juneau, Alaska 99801-1795

June 2005

MACTEC

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Prepared for

Alan E. Schuler, P.E.
Alaska Department of Environmental Conservation
Division of Air Quality
410 Willoughby Avenue, Suite 303
Juneau, Alaska 99801-1795

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Submitted by

MACTEC Federal Programs, Inc.
5001 S. Miami Blvd., Suite 300
P.O. Box 12077
Research Triangle Park, NC 27709-2077
(919) 941-0333   FAX (919) 941-0234

ACKNOWLEDGMENTS

This report of the evaluation of bias in the AERMOD-PVMRM model was prepared by Roger W. Brode of MACTEC Federal Programs, Inc., Research Triangle Park, NC, under Alaska Department of Environmental Conservation (ADEC) Contract No. 18-9010-12, with Alan E. Schuler, P.E., as the ADEC project manager.

TABLE OF CONTENTS

LIST OF FIGURES

LIST OF TABLES

1.0 INTRODUCTION

The purpose of this report is to document an analysis of the performance evaluation results for the Plume Volume Molar Ratio Method (PVMRM) option in the AERMOD dispersion model to determine if PVMRM produces biased or unbiased results. The PVMRM and OLM options for modeling the conversion of NO_x emissions to NO_2 have been incorporated into the AERMOD dispersion model. The PVMRM approach was originally developed as a post-processor for the ISCST3 model (Hanrahan, 1999a). A technical description of the implementation of PVMRM in AERMOD is provided in the Addendum to the AERMOD Model Formulation Document (Cimorelli, *et al*., 2002), and user instructions on the application of the PVMRM and OLM options in AERMOD are provided in the Addendum to the AERMOD User's Guide (EPA, 2002).

The analysis of potential bias is based on an evaluation of the performance of the AERMOD-PVMRM algorithm using data from two aircraft studies of power plant plumes, and two long-term field studies. The original evaluations of the AERMOD-PVMRM algorithms using data from the two aircraft studies were based on the default values of 0.10 for the in-stack NO_2/NO_x ratio and 0.90 for the equilibrium NO_2/NO_x ratio proposed by Hanrahan (1999a). The evaluations of the two aircraft studies presented in this report are based on more representative values of these ratios.

Section 2.0 presents the representative NO_2/NO_x ratios used in the aircraft evaluations. Section 3.0 provides a description of the evaluation databases, and Section 4.0 provides a description of the evaluation results. Section 5.0 presents a summary and conclusion of the evaluation results.

2.0 REPRESENTATIVE NO_2/NO_x RATIOS

This section documents the selection of representative values for the in-stack NO_2/NO_x ratio and the equilibrium NO_2/NO_x ratio for use in the evaluation study for the aircraft data from power plant plumes. Use of more representative and realistic values for these ratios will facilitate a more refined assessment of whether the AERMOD-PVMRM algorithm is unbiased in estimating ambient concentrations of NO_2.

The evaluations for the long-term field studies were based on the default value for the in-stack NO_2/NO_x ratio, since these studies reflected a range of source types for which the default value is considered reasonably representative. The default equilibrium NO_2/NO_x ratio was also used for the long-term field studies since the receptors were close enough to the sources for the equilibrium ratio to be relatively unimportant.

2.1 IN-STACK NO_2/NO_x RATIO

The default in-stack NO_2/NO_x ratio used in the AERMOD-PVMRM model is 0.10 or 10 percent. This value has a precedent in the Ozone Limiting Method (Cole and Summerhays, 1979), and was also used by Hanrahan (1999a) in the initial design of the PVMRM algorithm. Since the evaluation studies based on aircraft data examined in this report involved measurements from power plant plumes, a value more representative of external combustion sources was used. The U.S. EPA emission factor document, AP-42 (Compilation of Air Pollutant Emission Factors, Volume 1: Stationary Point and Area Sources, Fifth Edition), states that for external combustion sources "Generally, 95 volume % or more of NO_x present in combustion exhaust will be in the form of NO, the rest NO_2," (EPA, 1979). Arellano, et al. (1990) also states that "Initially, of all the NO_x compounds released from a large power station, 95% is NO and the rest NO_2." A review of the Arellano (1990) and Bange (1991) studies on which this reevaluation is based suggests that an in-stack NO_2/NO_x ratio of 0.05 or 5 percent was used in the refined modeling simulations presented in both papers. Furthermore, examination of the observed NO_2/NO_x ratios taken closest to the sources strongly suggests that this value is representative for these sources. Another study of power plant plumes reported by Bofinger, et al. (1986) states that "all but a small fraction [of nitrogen oxides are] in the form of nitric oxide." He further states that "The fraction of NO emitted as NO_2 appears to be in the range of 3-6%, in agreement with similar studies elsewhere." Based on all of the information reviewed, a more representative in-stack NO_2/NO_x ratio of 0.05 was used for the reevaluations of the Arellano and Bange data presented in this report.

2.2 EQUILIBRIUM NO_2/NO_x RATIO

The default equilibrium ratio of NO_2/NO_x used in the AERMOD-PVMRM model is 0.90 or 90 percent, based on the initial design of the algorithm by Hanrahan (1999). This is based on an estimate of the maximum conversion of NO to NO_2 that would occur under typical conditions, but Hanrahan suggests that "Local data may be used to refine this maximum ratio for the facility being modeled." The Ambient Ratio Method (ARM) identified in the Guideline on Air Quality Models (40 CFR Part 51, Appendix W) as a 2nd level screening analysis, uses a default ambient NO_2/NO_x ratio of 0.75, which represents a reasonably conservative value based on a review of nationwide monitoring data. Bofinger et al. (1986) states that "the plume centerline ratio of NO_2 to total oxides of nitrogen (NOx) does not exceed a value of 80% conversion for plume ages of the order of seven hours." He further states that ratios reach about 0.22 at 50 km for stable conditions, with an asymptotic value of 0.7, and ratios of about 0.55 at 50 km for unstable conditions, with an asymptotic value of 0.8. The maximum measurement distances presented in the Arellano and Bange studies are about 20 km. The model results presented in those papers, based on models that account for the photostationary state associated with equilibrium ratios, appear to reach equilibrium at ratios of about 0.6 to 0.75.

Based on all of the information reviewed, a more representative value of 0.75 or 75 percent was used for the equilibrium NO_2/NO_x ratio for the Arellano and Bange evaluations presented in this report. This value may still be somewhat conservative for these studies, based on the observed data and model results presented in the Arellano and Bange papers, and perhaps due to the location of the power plants at higher latitudes (above 50º) in the Netherlands. However, it is consistent with the default ARM ratio, and provides a more realistic value than the current PVMRM default of 0.90. Since the equilibrium ratio is typically reached well beyond the point of maximum ground-level concentration, this ratio is considered to be somewhat less important than the in-stack ratio in terms of evaluating whether AERMOD-PVMRM produces unbiased results.

3.0 DESCRIPTION OF EVALUATION DATABASES

This section includes a description of the evaluation databases used in the analysis of whether the PVMRM algorithm produces biased or unbiased results.

3.1 ARELLANO STUDY

The Arellano (1990) study included 12 cases with observed NO_2/NO_x ratios measured by aircraft from plumes associated with several power plants. Seven of the 12 cases involved neutral or unstable conditions, and the other five cases involved stable conditions (F stability). Measurements were made at distances ranging from about 500 meters to 20 kilometers downwind. The information available from the Arellano paper for each case included the plume height, wind speed at plume height, PG stability class, NO_x emission rate, flow rate, fuel type, and ozone concentration. Since ozone concentrations were available from within the plume, no minimum ozone value was applied for the stable cases for the evaluation.

Basic stack information needed to run the model was not available, including stack height, stack diameter, exit velocity and exit temperature. In order to run AERMOD-PVMRM for these cases, estimates of the necessary stack parameters and meteorological conditions were made based on the information provided in the paper and assumptions about the typical physical characteristics of power plant stacks. The meteorological conditions and stack parameters used in the Arellano evaluation are presented in Table 3.1. Since the model results are somewhat sensitive to the assumptions made, the results should be interpreted with some extra caution. However, the consistency of the evaluation results across a range of conditions suggests that the assumptions are reasonable.

Table 3.1. Meteorology and Source Characteristics Used for Arellano Evaluation

Case No.	Stability Class	Plume Ht. WS (m/s)	Plume Height (m)	Ozone Conc. (ppb)	NO_x Emission Rate (g/s)	Stack Height (m)	Exit Temp. (K)	Exit Velocity (m/s)	Stack Diam. (m)
1	B	4	380	10	500	100	400	20	5
2	D	10	215	15	200	200	400	15	3
3	C	7	520	38	200	200	500	15	3
4	D	11	295	51	200	200	450	15	3
5	D	20	450	32	500	300	450	15	5
6	D	10	485	38	560	200	400	36	5
7	C	8	400	44	120	250	400	15	6
8	F	4	575	1	490	200	400	20	6
9	F	4	510	70	490	200	400	20	6
10	F	3	552	35	490	200	400	20	6
11	F	6	475	25	520	200	400	20	6
12	F	3	602	30	490	200	400	20	6

3.2 BANGE STUDY

The Bange (1991) study included observed NO_2/NO_x ratios for six cases. As with the Arellano database, the evaluation of AERMOD-PVMRM on the Bange aircraft data required some assumptions regarding the stack parameters and meteorological conditions. In this case, the information available included the emission rate, wind speed at plume height, ozone concentration, some indication of season and/or stability class, and a range of surface roughness lengths. A similar process was used to estimate stack parameters and meteorological conditions for input to AERMOD-PVMRM. However, since the plume height and flow rate were not provided for the Bange data, the uncertainty regarding the stack parameters and meteorology used in the AERMOD-PVMRM evaluation is somewhat greater than for the Arellano evaluation. The meteorological conditions and stack parameters used in the Bange evaluation are presented in Table 3.2.

Table 3.2. Meteorology and Source Characteristics Used for Bange Evaluation

Figure (Case) No.	Season/ Stability	Plume Ht. WS (m/s)	Ozone Conc. (ppb)	NO_x Emission Rate (g/s)	Stack Height (m)	Exit Temp. (K)	Exit Velocity (m/s)	Stack Diam. (m)
6	Winter[1]	16.8	17	204	100	440	15	4
7	Summer[1]	18	33	239	100	440	15	4
8	Winter[1]	6.5	18	253	100	440	15	4
10	Winter/ Neutral	9	20	188	100	440	15	4
11	Spring/ Autumn/ Neutral	8.3	30	163	100	440	15	4
12	Spring/ Autumn/ Unstable	5.9	39	163	100	440	15	4

[1] Stability undefined, assumed to be near neutral/daytime.

3.3 NEW MEXICO - EMPIRE ABO GAS

One of the long-term databases used in the initial evaluation of AERMOD-PVMRM was the Empire Abo Gas plant located in southeastern New Mexico. The New Mexico database included a full year (June 11, 1993 – June 10, 1994) of ozone, NO_x, and NO_2 monitoring for the north monitor, located about 1.6 km north of the plant, and for the south monitor, located about 2.5 km south of the plant. Site-specific meteorological measurements were also collected during the field study. The meteorological and ambient monitoring data were collected in accordance with PSD monitoring guidance. The Empire Abo Gas plant consists of 15 compressor engines, five boilers, two heaters, a sulfur recovery unit flare, an inlet flare, an acid gas flare, and a diesel fire pump. Given the number of NO_x sources included in the database and the lack of a single dominant emission source, this database provides a good test of the plume merging component of the PVMRM algorithm.

The building data were processed through the BPIPPRM program to provide the direction-specific building dimensions needed by the PRIME downwash algorithm in AERMOD. The site-specific meteorological data, including 10m wind speed, wind direction, sigma-theta and ambient temperature, and solar radiation, were processed through the AERMET meteorological processor to provide the meteorological data needed by AERMOD. The AERMOD model was run using the flat terrain option, consistent with the local topography.

3.4 HAWAII - PALAAU GENERATING STATION

The second long-term database was from the Palaau Generating Station located on the island of Molokai in Hawaii. The Palaau database included a full year (January 1, 1993 – December 31, 1993) of ozone, NO_x, and NO_2 monitored data for a single monitor located about 220m northwest of the station. As with the New Mexico database, site-specific meteorological measurements were also collected during the field study, and the monitoring data were collected in accordance with PSD monitoring guidance. The Palaau station consists of four diesel-engine generators and an oil-fired combustion turbine, which provides another test for the plume merging component of the PVMRM algorithm. The Palaau data were also run using the flat terrain, consistent with local topography, and the BPIPPRM and AERMET processors were used to process the building and meteorological data, respectively.

4.0 DESCRIPTION OF EVALUATION RESULTS

The results of the AERMOD-PVMRM evaluation are presented in this section. The focus of the evaluation is on how well the PVMRM algorithm predicts the NO_2/NO_x ratios. Given the limited number of cases available, both from the aircraft studies (consisting of 18 cases) and the long-term field studies (consisting of three receptors), the focus of the evaluation is on simple statistical comparisons in a weight of evidence approach to determine whether the evaluation results indicate any bias in the performance of the AERMOD-PVMRM model.

4.1 ARELLANO AND BANGE AIRCRAFT STUDIES

The evaluation results for the Arellano and Bange studies are based on paired values of the observed and predicted NO_2/NO_x ratios. The use of paired values provides a more rigorous standard than is commonly used in evaluating the performance of regulatory dispersion models, which are normally based on unpaired comparisons of the peak of the predicted and observed concentration distributions.

Figure 4.1 presents the paired results for the twelve cases included in the Arellano studies. Given the uncertainties regarding the source characteristics discussed in Section 3.1, the overall results for AERMOD-PVMRM NO_2/NO_x ratios match the measured ratios very well within the first several kilometers of the source, where the ground-level maximum is likely to occur for neutral and unstable conditions. The paired results for Bange for all six cases are presented in Figure 4.2, which also shows generally good agreement between predicted and observed NO_2/NO_x ratios within the first several kilometers of the source. Figure 4.3 shows a scatter plot of predicted vs. observed NO_2/NO_x ratios paired in space for the observation closest to the maximum modeled ground-level concentration for the twelve Arellano cases. The results taken nearest the maximum ground-level concentration show generally good correlation, with all cases within a factor of three, and all but one case within about a factor of two. Figure 4.4 shows the paired Bange results for the observation closest to the maximum modeled ground-level concentration. As with the Arellano results, Figure 4.4 shows good correlation between the predicted and observed NO_2/NO_x ratios, with all but one case within a factor of 1.5.

Both the Arellano and Bange papers included results of reactive plume models that incorporated more refined chemistry algorithms than are included in the PVMRM algorithm. In the case of the Arellano paper, the model is referred to as the chemically reactive plume model (CRPM). The Bange paper included comparisons between a dynamic model and a photostationary model, and also between models based on instantaneous dispersion parameters and based on total dispersion. The paired results for the CRPM model from the Arellano study for the observations closest to the maximum ground-level concentrations are presented in Figure 4.5, and the results of the more refined dynamical model with instantaneous dispersion parameters from the Bange study are presented in Figure 4.6. The CRPM model shows a few cases with predicted/observed ratios of greater than 3, and the overall results appear to be somewhat less correlated with observations than the PVMRM results. The results of the dynamic model from the Bange study show good agreement between predicted and observed NO_2/NO_x ratios, with no evident bias. The results for the dynamic model presented in the Bange paper show much better comparison between predicted and observed NO_2/NO_x ratios for the model based on instantaneous dispersion parameter compared to the use of total dispersion. The good performance of the dynamic model may also have benefited from the fact that the instantaneous plume dimensions used in the model were derived from the aircraft data collected during the study. Note that the PVMRM algorithm as implemented in AERMOD utilizes relative (instantaneous) dispersion coefficients to define the plume volume.

Table 4.1 provides a summary of statistical comparisons for the Arellano results for the AERMOD-PVMRM model compared to the CRPM model. Table 4.2 provides a summary of statistical comparisons for the Bange results for the AERMOD-PVMRM model compared to the dynamic model presented in the Bange paper. All of the statistical measures presented in these tables are based on the observed vs. predicted NO_2/NO_x ratios nearest the maximum modeled ground-level concentration, except for the percent of cases within a factor of two which is based on all data points.

Table 4.1. Statistical Comparison Results for Arellano Data

Statistical Measure	PVMRM Results	CRPM Model Results
Average Predicted/Observed NO_2/NO_x Ratio	1.514	1.971
Correlation Coefficient	0.916	0.631
Linear Regression Best-fit Slope	1.045	0.421
Linear Regression Best-fit Intercept	0.065	0.180
Average Fractional Bias	0.337	0.341
Average Absolute Fractional Bias	0.374	0.524
Normalized Mean Square Error (NMSE)	0.172	0.315
Root Mean Square Error (RMSE)	0.108	0.139
Fraction within a factor of 2 (all cases)	61.1 %	69.4 %

Table 4.2. Statistical Comparison Results for Bange Data

Statistical Measure	PVMRM Results	Dynamic Model Results
Average Predicted/Observed NO_2/NO_x Ratio	1.379	0.966
Correlation Coefficient	0.768	0.756
Linear Regression Best-fit Slope	0.898	0.478
Linear Regression Best-fit Intercept	0.153	0.160
Average Fractional Bias	0.288	-0.052
Average Absolute Fractional Bias	0.288	0.187
Normalized Mean Square Error (NMSE)	0.141	0.057
Root Mean Square Error (RMSE)	0.155	0.082
Fraction within a factor of 2 (all cases)	80.0 %	97.8 %

For the Arellano study, the AERMOD-PVMRM results show overall better performance than the CRPM model, and show generally good agreement between predicted and observed NO_2/NO_x ratios. The average ratio of predicted to observed values for PVMRM is 1.514 compared to an average ratio for CRPM of 1.971. The PVMRM results also show much better correlation between the predicted and observed ratios, with a correlation coefficient of 0.916, compared to 0.631 for CRPM. Both models show over 60 percent of the cases with predicted NO_2/NO_x ratios within a factor of two of the observed ratios.

The PVMRM statistical results for Bange are similar to the PVMRM results for Arellano, with an average predicted/observed ratio of 1.379, a correlation coefficient of 0.768, and 80 percent of the cases within a factor of two. The statistical results for the dynamic model presented in the Bange report show better overall performance than PVMRM, with an average predicted/observed ratio of 0.966, an average fractional bias of -0.052, and almost 98 percent of cases within a factor of two. The only statistical measure where the dynamic model does not perform as well as PVMRM is correlation coefficient (0.756) and the slope of the best-fit line (0.478). The linear regression results may not be very significant for the Bange data since there were only six data points included in the study.

4.2 NEW MEXICO AND PALAAU FIELD STUDIES

Table 4.3 presents the results for the two long-term field studies, including the North and South monitors at the New Mexico facility and the single monitor at the Palaau facility. The results are based on the ratio of the predicted/observed average NO_2/NO_x ratio for all cases with a NO_x concentration of 20 ppb or higher. This comparison is the most meaningful result for the long-term studies since the PVMRM algorithm is intended for use in evaluating compliance with the annual NO_2 National Ambient Air Quality Standard (NAAQS) and Prevention of Significant Deterioration (PSD) increment. Table 4.3 also shows the number of cases included for each monitor. The results for the South monitor at New Mexico and the Palaau monitor are clearly unbiased, with predicted/observed ratios of 1.06 and 1.09, respectively. The predicted/observed ratio for the North monitor at New Mexico is 0.70. The average of the three ratios is 0.96, which indicates unbiased performance.

Table 4.3. Results for New Mexico and Palaau Long-term Field Studies

Location	Monitored NO_2/NO_x	Predicted NO_2/NO_x	Predicted/ Observed	Number of Cases > 20ppb
New Mexico Abo North Monitor	0.562	0.391	0.70	772
New Mexico Abo South Monitor	0.465	0.493	1.06	262
Hawaii Palaau Monitor	0.138	0.150	1.09	672

NO_2/NO_x Ratio Predictions

AERMOD-PVMRM Model Predictions vs. Arellano Aircraft Data

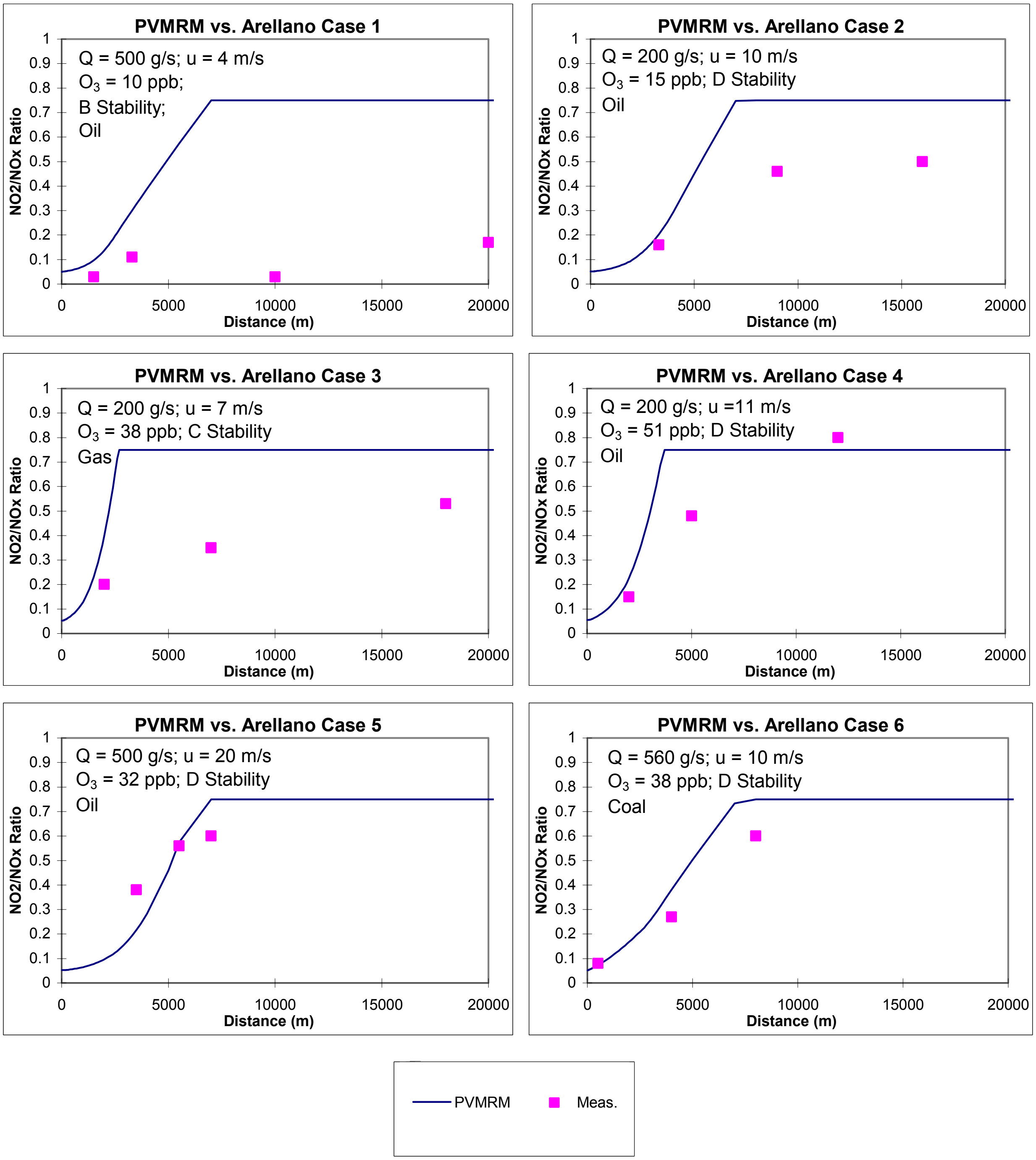

Figure 4.1a. Paired PVMRM and Observed NO_2/NO_x Ratios for Arellano Study

NO_2/NO_x Ratio Predictions

AERMOD-PVMRM Model Predictions vs. Arellano Aircraft Data

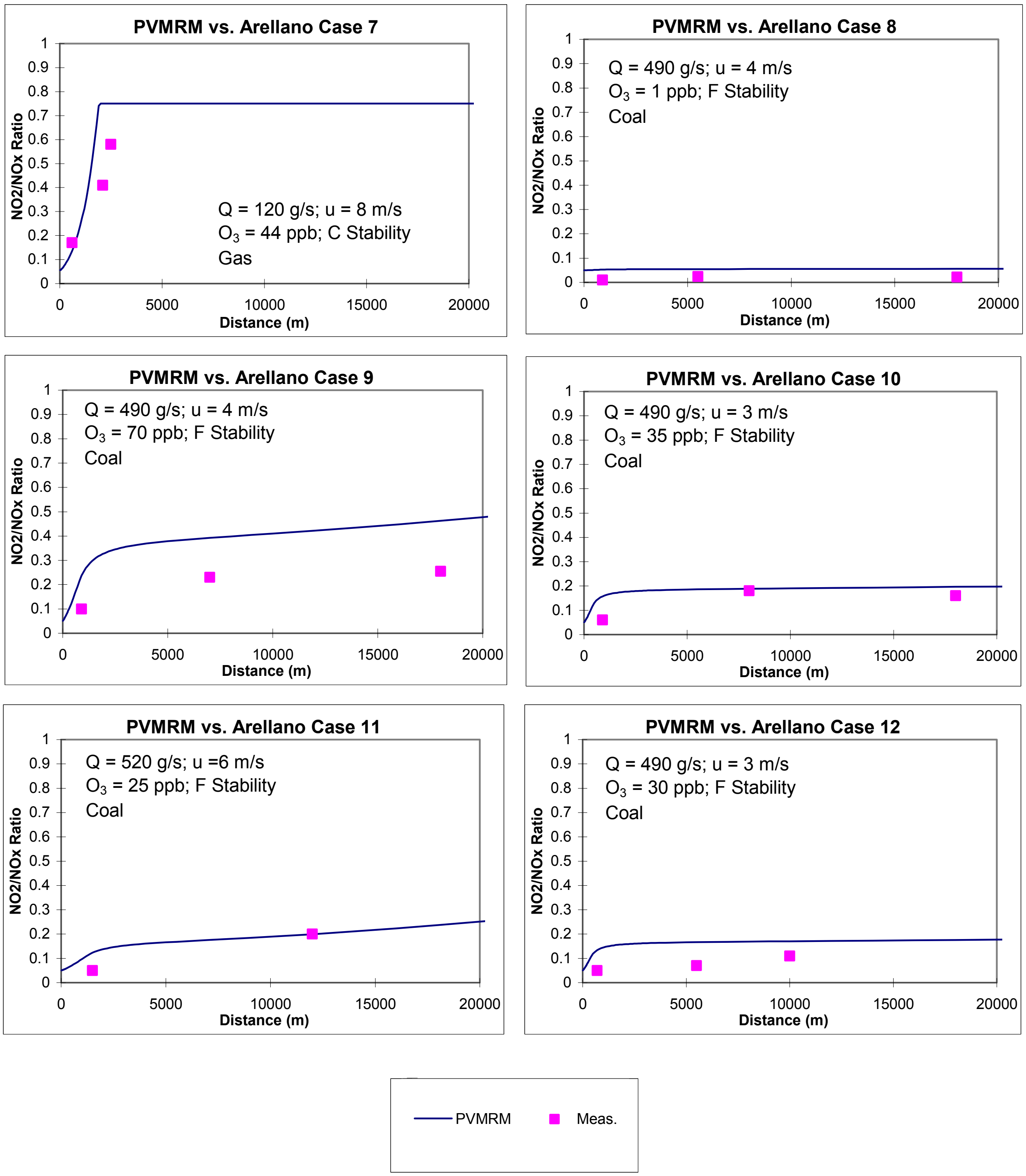

Figure 4.1b. Paired PVMRM and Observed NO_2/NO_x Ratios for Arellano Study

NO_2/NO_x Ratio Predictions

AERMOD-PVMRM Model Predictions vs. Bange Aircraft Data

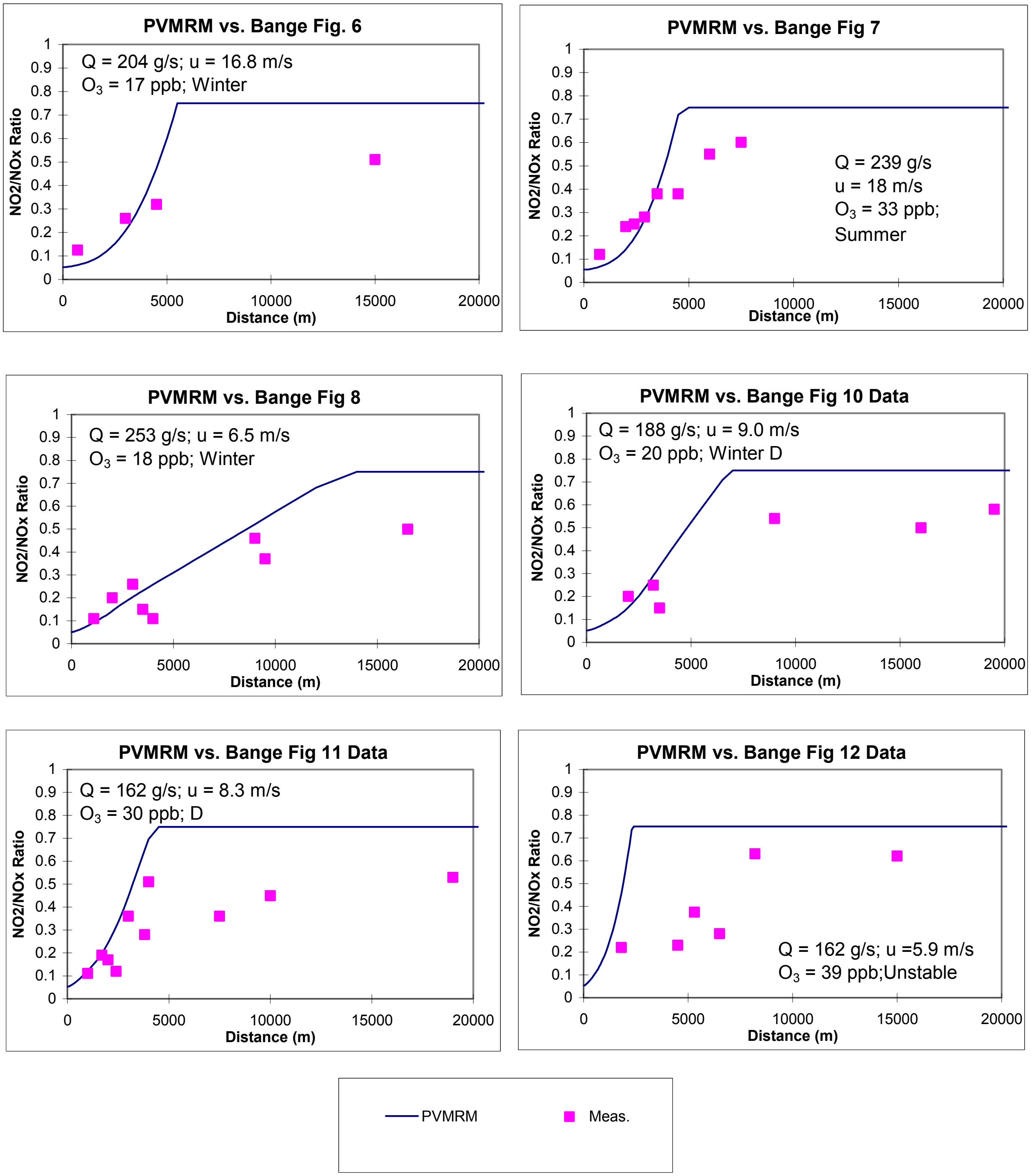

Figure 4.2. Paired PVMRM and Observed NO_2/NO_x Ratios for Bange Study

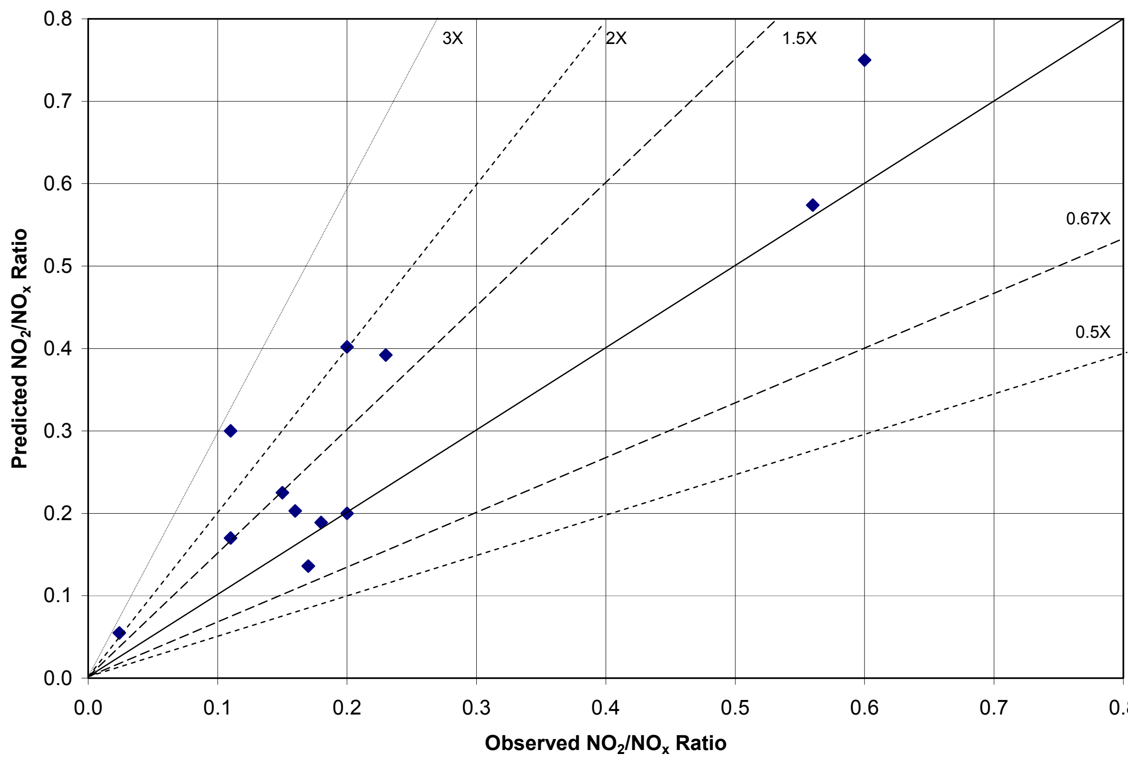

Figure 4.3. Paired PVMRM Predicted and Observed NO_2/NO_x Ratios for Arellano Study for Observations Closest to Maximum Modeled Ground-level Concentration

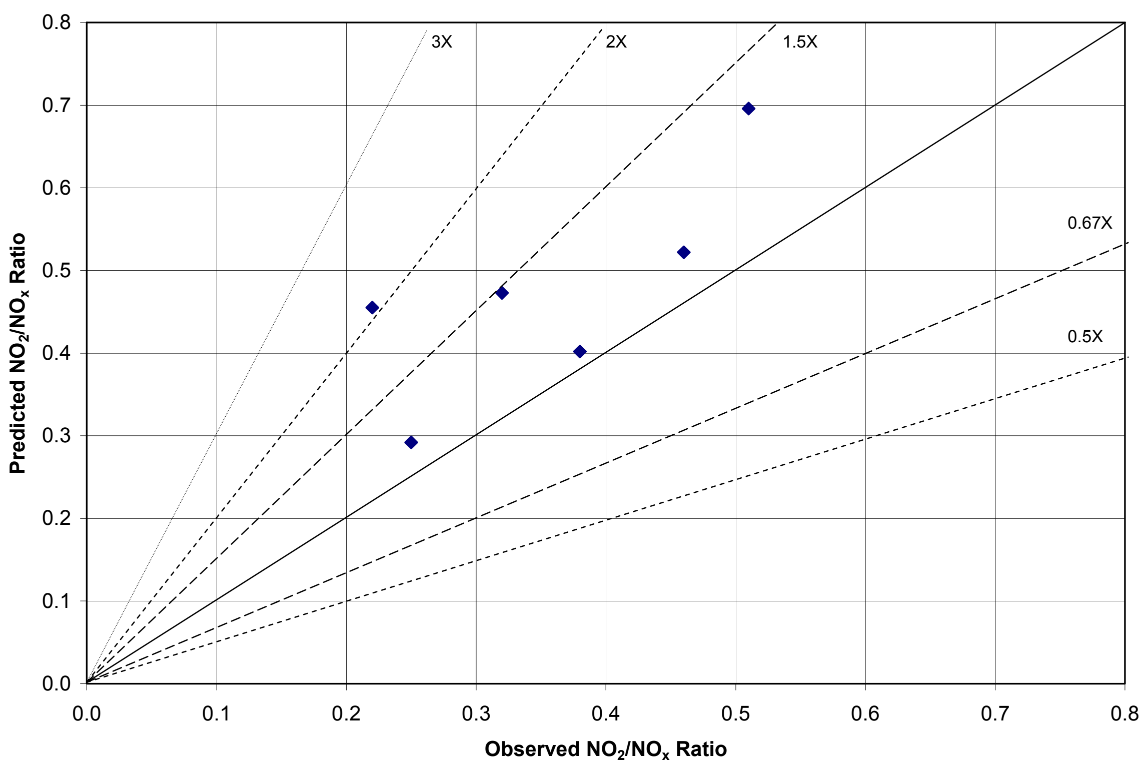

Figure 4.4. Paired PVMRM Predicted and Observed NO_2/NO_x Ratios for Bange Study for Observations Closest to Maximum Modeled Ground-level Concentration

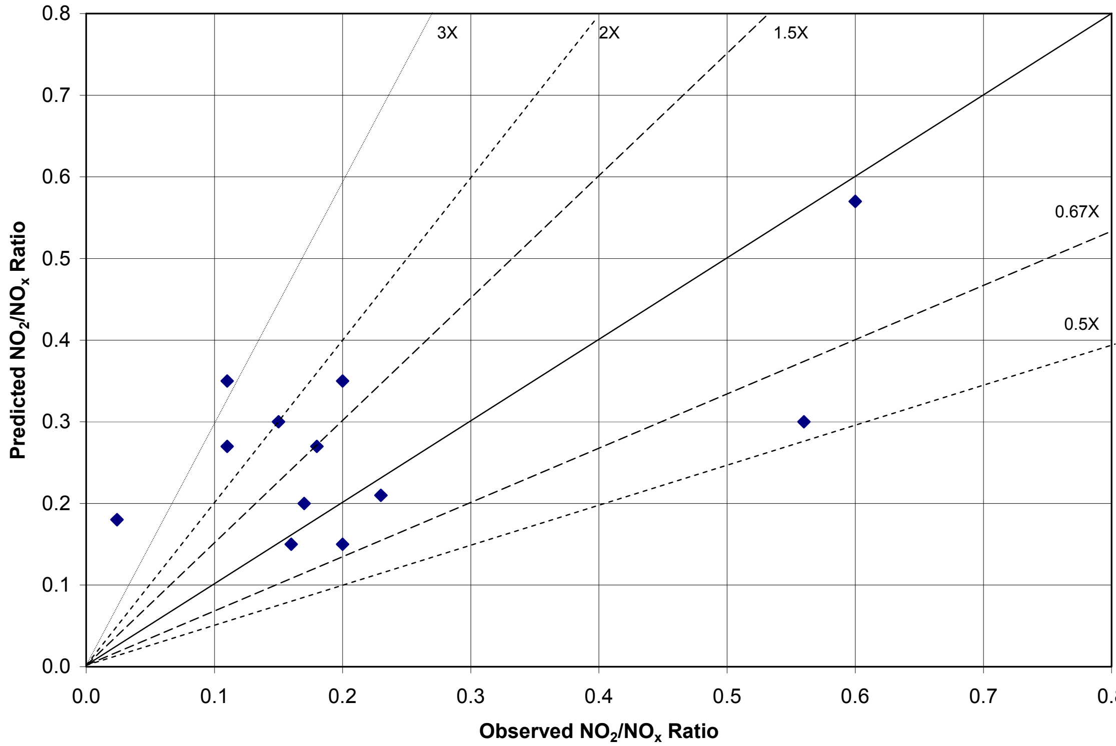

Figure 4.5. Paired CRPM Predicted and Observed NO_2/NO_x Ratios for Arellano Study for Observations Closest to Maximum Modeled Ground-level Concentration

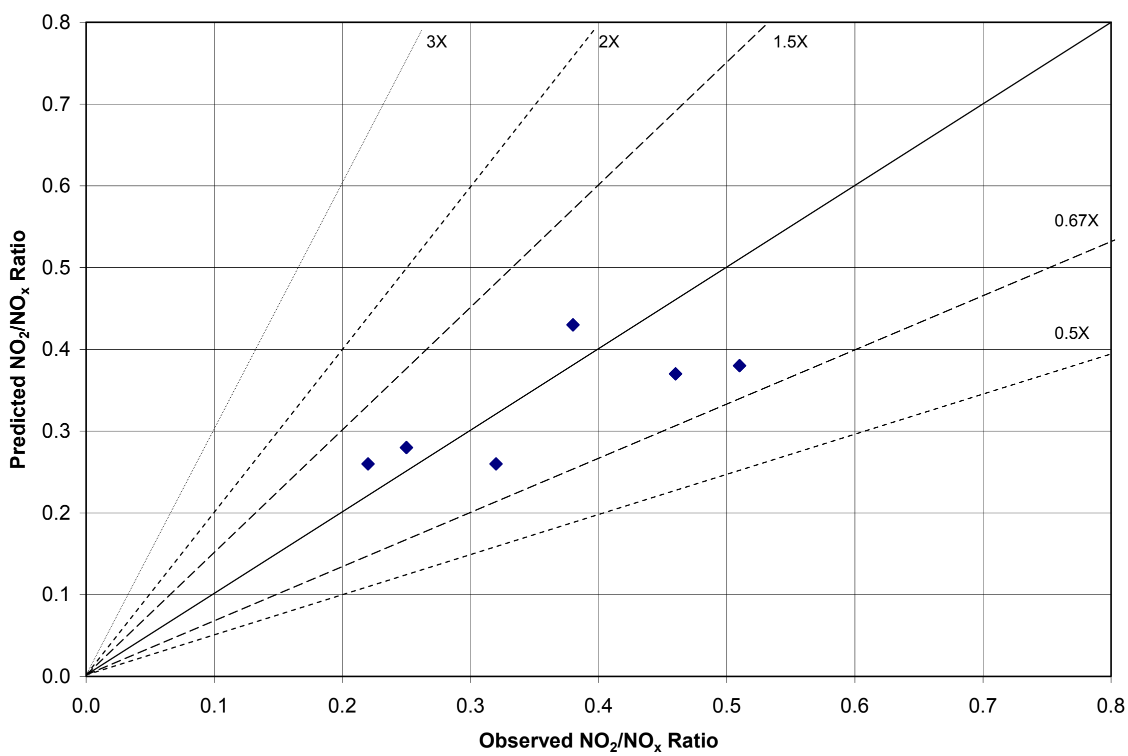

Figure 4.6. Paired Dynamic Model Predicted and Observed NO_2/NO_x Ratios for Bange Study for Observations Closest to Maximum Modeled Ground-level Concentration

5.0 SUMMARY AND CONCLUSIONS

This report presents results of an analysis of evaluation results to determine whether the AERMOD-PVMRM algorithm produces biased or unbiased estimates of the NO_2/NO_x ratio. Evaluation results from two aircraft studies and two long-term field studies were examined, as well as comparisons between AERMOD-PVMRM and other refined chemically reactive plume models. Comparisons between predicted and observed NO_2/NO_x ratios were based on results paired in time and space, providing a more rigorous assessment than is commonly used in evaluating the performance of air dispersion models. While there does not appear to be a clear and objective criterion established by EPA for determining whether a model is biased or unbiased, a general "rule of thumb" that is commonly used as a benchmark in judging the performance of air dispersion models is agreement with observations within a factor of two.

Given the relatively small number of samples available, including a total of 18 aircraft cases, and three receptors with long-term field data, a number of statistical comparisons were made between the predicted and observed NO_2/NO_x ratio in a weight of evidence assessment of potential bias. In all cases, the average ratio between predicted and observed NO_2/NO_x ratios showed agreement within a factor of two, and in most cases within about a factor of 1.5. The fraction of cases (based on all observations) within a factor of two exceeded 60 percent for both aircraft studies. The AERMOD-PVMRM algorithm in AERMOD also performed well compared to other models with more refined chemistry algorithms for the two aircraft studies.

Based on all of the data available, the AERMOD-PVMRM algorithm is judged to provide unbiased estimates of the NO_2/NO_x ratio based on criteria that are comparable to, or more rigorous than, evaluations performed for other dispersion models that are judged to be refined, implying unbiased performance.

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