United States Environmental Protection Agency

Technical Support Document (TSD) for Adoption of the Generic Reaction Set Method (GRSM) as a Regulatory Non-Default Tier-3 NO_2 Screening Option

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Technical Support Document (TSD) for Adoption of the Generic Reaction Set Method (GRSM) as a Regulatory Non-Default Tier-3 NO_2 Screening Option

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Preface

This technical support document (TSD) provides a review of the GRSM NO_2 option model performance and implementation in AERMOD version 23132. The TSD presents and summarizes GRSM model performance based on four NO_2 model evaluation databases used to determine appropriate application of NO_2 screening options as part of the regulatory default version of AERMOD. The purpose of this TSD is to support adoption of GRSM as a new regulatory non-default Tier 3 NO_2 screening option in AERMOD.

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1. Introduction

The proposed revisions to Appendix W to CFR 40 Part 51—*Guideline on Air Quality Models* (*Guideline*), includes a new version of AERMOD (23132)[1]. This new version of AERMOD includes a proposed regulatory non-default Tier 3 NO_2 screening option, i.e., the Generic Set Reaction Method (GRSM; (Carruthers, Stocker, Ellis, Seaton, & Smith, 2017); (Stocker, et al., 2023)). This TSD reviews the scientific merit, implementation of the GRSM formulation, and summarizes selected model evaluations to support the application of GRSM as a Tier 3 NO_2 screening option for use as part of the proposed regulatory version of AERMOD.

2. Background

The chemistry, regulatory status, and performance evaluations of all existing AERMOD NO_2 screening options are discussed in the U.S. EPA TSD for NO_2-Related AERMOD Options and Modifications (U.S. EPA, 2015, December). This TSD will discuss the chemistry, proposed regulatory status, and model behavior and performance of GRSM. Following the 2015 TSD, selected graphical and statistical (U.S. EPA, 1992) comparisons between GRSM and other NO_2 regulatory options are presented.

2.1 The 3-Tiered Approach for AERMOD NO_2 Modeling Demonstrations

Section 4.2.3.4 of Appendix W details a 3-tiered approach for evaluating the modeled impacts of NO_X emission sources. These tiers assume increasing levels of conservatism (i.e., conservation of air quality as a resource for protecting public health) in the assessment of hourly and annual average NO_2 impacts from point, volume, and area sources for the purposes of supporting the PSD program, SIP planning, and transportation general conformity. The 3-tiered approach addresses the co-emissions of NO and NO_2 and the subsequent conversion of NO to NO_2 in the atmosphere. The tiered levels include:

- Tier 1 – assuming that all emitted NO is converted to NO_2 (full conversion),
- Tier 2 – using the Ambient Ratio Method 2 (ARM2), which applies an assumed equilibrium ratio of NO_2 to NO_X, based on analysis of and correlation with nationwide hourly observed ambient conditions (Podrez, 2015), and
- Tier 3 – applying the Ozone Limiting Method (OLM; (Cole & Summerhays, 1979)) and Plume Volume Molar Ratio (PVMRM; (Hanrahan, P.L., 1999a and 1999b)) screening options based on site-specific hourly ozone data and source-specific NO_2 to NO_X in-stack ratios.

As discussed in section 4.2.3.4(e), regulatory application of Tier 3 screening options shall occur in consultation with the EPA Regional Office and appropriate reviewing authority.

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[1] For more information on the proposed revisions to Appendix W and updates to AERMOD, please reference: https://www.epa.gov/scram/2023-appendix-w-proposed-rule

3. Current Regulatory Status and Features of GRSM

As part of the 2023 proposed revisions to the Guideline, the EPA is proposing to include the GRSM as a regulatory non-default Tier 3 NO_2 screening option in AERMOD version 23132.

Following peer-reviewed publication (Carruthers, Stocker, Ellis, Seaton, & Smith, 2017), GRSM was added to AERMOD as an alpha option in version 21112 and later updated to a beta option in version 22112. The GRSM option is proposed to be adopted as a beta option in AERMOD version 23132, and later advanced to a full regulatory NO_2 screening option upon release of the 2024 version of AERMOD.

The primary motivation behind the formulation and development of the GRSM NO_2 screening option is to address photolytic conversion of NO_2 to NO and to address the time-of-travel necessary for NO_X plumes to disperse and convert the NO portion of the plume to NO_2 via titration and entrainment of ambient ozone. The current regulatory non-default Tier 3 NO_2 screening options, PVMRM and OLM, do not address or provide for treatment of these photolysis and time-of-travel mechanisms, and have been shown to over-predict for some source characterizations and model configurations at project source ambient air boundaries and within the first 1-3 km. (Stocker, et al., 2023) and as presented in this TSD.

4. GRSM Implementation in AERMOD

The functionality of the GRSM code implementation in AERMOD is similar to that of the PVMRM and OLM schemes, with exception to some additional input requirements necessary for treatment of the reverse NO_2 photolysis reaction during daytime hours. Modeled source inputs for GRSM require NO_2/NO_X in-stack ratios, with similar assumptions as applied to PVMRM and OLM pursuant to section 4.2.3.4 of the *Guideline*. Ambient model inputs for GRSM require hourly ozone concentrations taken from an appropriately representative monitoring station or selection of monitoring stations for varying upwind sector concentrations. GRSM also requires hourly NO_X concentration inputs to resolve the daytime photolysis of NO_2 reaction in equilibrium with ozone titration conversion of the NO portion of the NO_X plume. Hourly NO_X and NO_2 concentrations input to AERMOD when using the GRSM method can also vary by upwind sector concentration, as appropriate. Background NO_2 concentrations are accounted for in the GRSM daytime equilibrium NO_2 concentration estimates based on the chemical reaction balance between ozone entrainment and NO titration, photolysis of NO_2 to NO, and ambient background NO_2 participation in titration and photolysis reactions. Nighttime NO_2 estimates from GRSM are based on ozone entrainment and titration of available NO in the NO_X plume, and by default, AERMOD sets nighttime ozone concentrations to 40 parts per billion (ppb) unless the NOMINO3 model option is specified. Note that all hourly ozone and NO_X ambient inputs to GRSM must coincide with the hourly meteorological data records for the period of the modeling analysis (i.e., minimum of 1-year for on-site data, 3 years of prognostic data, and 5 years of airport data (i.e., meteorological data collected by either the National Weather Service (NWS) or the Federal Aviation Administration (FAA), typically at airport locations).

Updates to the GRSM formulation in AERMOD version 22112 were completed in late 2022 to address more realistic building effects on instantaneous plume spread, accounting for multiple plume effects on entrainment of ozone, and the tendency of GRSM to over-predict in the far-field (e.g., beyond approximately 3 km for typical point source releases). Sensitivity testing and model performance evaluations of these updates to GRSM in AERMOD version 23132 have shown consistent or improved model behavior and performance. The model performance evaluations are presented and discussed in the following section.

5. Model Evaluation of GRSM

Statistical evaluation of GRSM NO_2 model performance was conducted based on four source-oriented ambient ozone and NO_2 monitoring databases assuming rural dispersion conditions. Two legacy (1993) databases reflect the ARM2, OLM, and PVMRM evaluations presented in the 2015 TSD for NO_2 modeling options (U.S. EPA, 2015, December). These legacy databases included 1-year datasets developed for a power plant located on the island of Moloka'i, Pala'au, Hawaii, and for a gas processing plant located in Artesia, New Mexico (Empire Abo). Details of the Pala'au and Empire Abo databases are discussed at length in a 2013 technical report (RTP Environmental Associates, Inc., 2013). The other two evaluation databases were developed more recently in the 2014-2016 time period and include a 1-year field study at a gas compressor station facility located near Balko, Oklahoma (Balko), and a six-week field study at an oil and gas drill rig installation located in the Denver-Julesburg Basin near Platteville, Colorado. The Balko database included ozone and NO_2 data collected at four monitoring stations from December 2015 through December 2016. Details on the development of the Balko database were published in March of 2020 (Panek, 2020) along with model observation comparisons with ARM2, PVMRM, and OLM. The Colorado database included data collected at a total of 12 monitoring locations upwind and downwind of two oil and gas well drilling pads for a five-week period October 10th through November 16th, 2014. Further details on the Colorado database are available at EPA's SCRAM website and documented in a separate TSD (Colorado Field Study Workgroup: ERM, 2020).[2] All four model evaluation databases included site-specific meteorological data collected at the site, re-processed with AERMET version 23132. Summaries of all databases and performance model evaluations are also discussed in a technical report authored by the developers of GRSM for AERMOD (Stocker, et al., 2023).

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[2] Denver-Julesburg Bason, Colorado NO2 Evaluation Database: https://gaftp.epa.gov/Air/aqmg/SCRAM/models/preferred/aermod/eval_databases/denver-julesburg.zip

As discussed previously in Section 4.3 of (RTP Environmental Associates, Inc., 2013), conversion of NO_2 and NO_X measurements in ppb to micrograms per cubic meter ($\mu g/m^3$) requires careful consideration of the actual and standard meteorological conditions as well as the separate contributing constituent components of the NO_X plume in terms of NO and NO_2 ppb by volume. Conversion of ppb to $\mu g/m^3$ from actual to standard temperature and pressure conditions generally increases measurement concentrations by approximately 10% depending on season, climatology, and elevation. Additionally, this conversion, typically based on the conventional assumption that all NO_X is NO_2 with a molecular weight of 46 grams/mole, would increase the $\mu g/m^3$ measurement estimates by 20-30% for some shorter source-receptor distances, especially between 10's to 100's of meters and possibly as far away as approximately 3 km depending on dispersion conditions. The "true" NO_X plume at these shorter distances is composed of mostly NO (e.g., 50-95% NO/NO_X by volume) and therefore, would contain less mass given the 30 g/mole molecular weight of NO, which accounts for the 20-30% conservative estimates of NO_X as NO_2 emission inputs typically used in AERMOD NO_2 demonstrations. As such, and based on the most current information on the four field datasets considered in this TSD, the NO_X as NO_2 assumption was applied to all NO_X emissions inputs, thereby introducing a conservative bias in the modeled mass emission rates. From a regulatory perspective, the performance of this conservative NO_X as NO_2 emissions assumption when compared to actual measured NO_X concentrations was considered because a regulatory modeling result would need to show some level of performance as it pertains to the Appendix W requirement that the model does not show bias to underpredict. Therefore, all input emissions assume NO_X as NO_2 (based on most current understandings of emission factors applied), and any dispersion performance indicated from NO_X modeled compared to NO_X measured assumes no change to the modeled $\mu g/m^3$ concentrations whereas measured NO_X represents the actual $\mu g/m^3$ concentrations (at standard temperature and pressure; STP) as would be the case for any regulatory modeling or monitoring demonstration. Note that AERMOD NO_X and NO_2 concentrations in $\mu g/m^3$ are calculated internally based on standard temperature and pressure (i.e., 298.15 K and 1013.25 mb). Chemistry performance was assessed in terms of modeled $\mu g/m^3$ NO_2 at STP compared to measured $\mu g/m^3$ NO_2 (after conversion from ppb to $\mu g/m^3$ at STP).

5.1 Pala'au, Hawaii NO_2 Database

The Pala'au hourly NO_2 and ozone data were collected at a monitoring station located approximately 220 meters northwest of the facility. Hourly varying ozone data was developed from the on-site monitoring data (93% complete). The annual ozone substitution value was set to the default 40 ppb for all NO_2 models. A single annual NO_X value was set to 2.5994 $\mu g/m^3$ for the model simulations using GRSM. Background NO_2 assumed 0.69838 ppb for all conversion methods. NO_X emissions were assumed to be non-varying for the entire 1993 study period, and included six diesel engines and one combustion turbine with emission rates ranging from an average of 12.6 lb/hr to a maximum of 27 lb/hr; total NO_X emissions of 88.3 lb/hr. All sources assumed NO_2/NO_X in-stack ratios of 10%. Stack heights at the power plant were relatively short, and range from 24-32 feet and were modeled assuming flat terrain. All NO_2 model outputs were based on 1-hour averages as predicted at the single monitor receptor location.

AERMOD performs well at Pala'au as indicated in the Q-Q ranked plot shown in Figure 1 where the modeled versus observed NO_X concentrations track the 1:1 line throughout the ranked distribution. As previously discussed, modeled mass emission rates assumed all NO_X was NO_2, thus, introducing a conservative emission estimate bias that could be influencing the agreement between observed and modeled NO_X concentrations. Another emissions uncertainty for Pala'au, which could inadvertently bias model-observation agreement during non-operating periods, is the non-varying emission rates assumed for the 1-year evaluation period. However, given the proximity of the monitoring station located 220 meters northwest of the power plant, and the relatively consistent distribution of the NO_X concentrations throughout the monitoring period, altogether, these factors would indicate that the power plant operated continuously at a normal demand load for the entire year. Note that no filtering of the NO_X observations was conducted (e.g., by downwind sector) to determine the final set of 7,856 model-observation pairings shown in Figure 1.

Figure 2 shows a ranked Q-Q plot of modeled versus observed NO_2 concentrations for modeling scenarios that use the proposed GRSM NO_2 Tier 3 option as well as the other Tier 2 (ARM2) and 3 (OLM, PVMRM) regulatory NO_2 options available in AERMOD. The ARM2 option performs as intended the most conservatively, whereas OLM becomes the less conservative option by comparison. PVMRM shows some slight underprediction whereas GRSM maintains a slightly conservative performance trend just above the 1:1 line for most of the ranked distribution. GRSM performs consistently compared to the other AERMOD NO_2 options, and shows no unacceptable bias to underpredict peak concentrations for the Pala'au database.

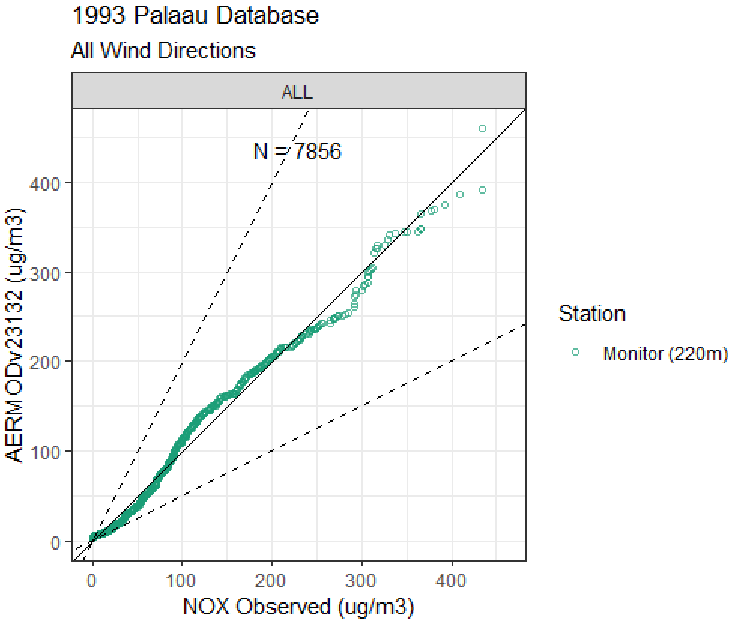

Figure 1 – Pala'au NO_X Ranked Q-Q Plot

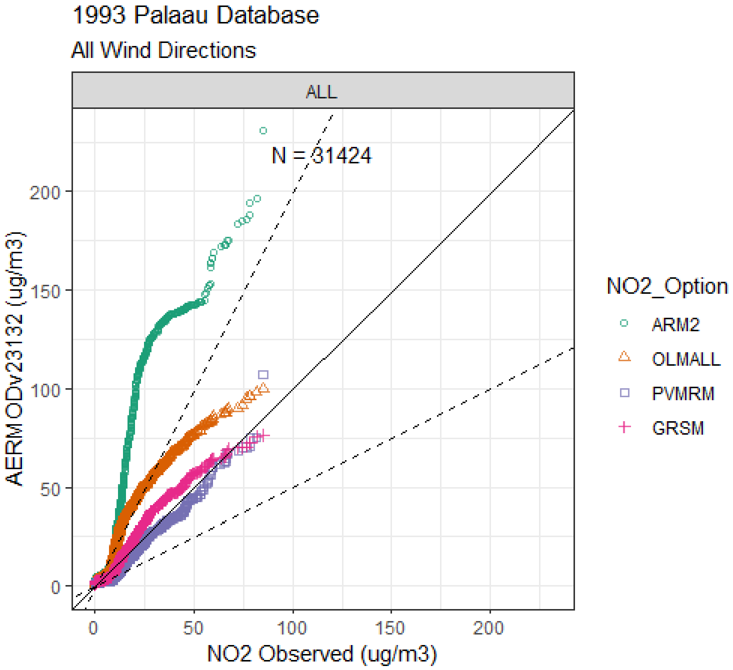

Figure 2 – Pala'au NO_2 Ranked Q-Q Plot

Table 1 shows a summary of fractional bias (FB) and robust highest concentration (RHC) model performance statistics for the NO_X and NO_2 model option scenarios evaluated for Pala'au. The FB shows decreasing conservative agreement between observations and model outputs for NO_X, ARM2, OLM, PVMRM, and GRSM model options; note that negative FB indicates a conservative bias for the option, or overprediction. The RHC ratio and RHC FB results show similar conservative hierarchy across the NO_2 option evaluations, with increasing conservatism shown for GRSM, PVMRM, OLM, ARM2, and full conversion NO_X runs.

Table 1 – Pala'au Model Performance Statistics Summary (µg/m^3)

Model Opt.	FB	RHC_Obs	RHC_Mod	RHC_ratio	RHC_FB
NO_X	-1.01763	456.5125	471.9136	1.033737	-0.03318
ARM2	-1.22483	90.9536	237.2565	2.608545	-0.89152
OLM	-1.00706	90.9536	103.8257	1.141523	-0.13217
PVMRM	-0.79509	90.9536	98.17854	1.079436	-0.0764
GRSM	-0.90174	90.9536	82.87393	0.911167	0.092962

5.2 Empire Abo, Artesia, New Mexico NO_2 Database

The Empire Abo hourly NO_2, ozone, and meteorological data were collected at two monitoring stations located approximately 1.6 km northeast (north station) and 2.4 km southeast of the facility from June 11, 1993 through June 10, 1994. Model inputs for hourly ozone and background NO_2 and NO_X were based on two wind sectors starting at 100 and 280 degrees, which AERMOD interprets as downwind or flow vector wind directions. The first sector (winds blowing towards 100-280 degrees) used upwind hourly ozone and NO_2 concentrations from the north station, while the second sector (winds blowing towards 280-100) used upwind data from the south station. Substitution values for missing hourly ozone and NO_X data were taken from season-hourly varying maximum, while NO_2 season-hourly values were developed from highest-3rd-high observed values. The highest-3rd-high was selected for NO_2 substitution values in order to reflect a median value between unreasonably high maximum NO_2 values and the 1-hour NAAQS highest-8th-high. Similar to Pala'au, NO_X emissions for Empire Abo were assumed to be non-varying for the entire study period, and included 21 combustion sources with emission rates ranging from an average of 20.2 lb/hr to a maximum of 69.4 lb/hr, and with a facility total of 423 lb/hr. All sources assumed NO_2/NO_X in-stack ratios of 20%. Stack heights at the power plant from dominant sources averaged about 30 feet and all sources were modeled assuming flat terrain. All NO_X and NO_2 model outputs were based on 1-hour averages as predicted at the north and south monitor receptor locations.

As shown in the ranked Q-Q plot in Figure 3, modeled NO_X concentrations at the north and south monitors tend to overpredict; note the north monitor shows some underprediction for the lower half of the ranked distribution. As previously mentioned, the overpredictions may be in part due to the NO_X mass emission rates that assume all NO_X has converted to the mass of NO_2. Given the 1.6 km and 2.4 km distances to the north and south monitors, respectively, this assumption may be valid for most worst-case scenarios; however, the ambient monitoring data at these stations indicates the inner quartile range of the ambient NO_2/NO_X ratios varies between 66-86%. The non-varying hourly emissions from Empire Abo dispersed over these longer distances may also play a role in overestimating NO_X concentrations. Note that pre-filtering of the NO_X observations was not conducted (e.g., by downwind sector, or other parameter) to determine the final set of 16,547 model-observation pairings shown in Figure 3.

Figures 4 and 5 show ranked Q-Q plots of modeled versus observed NO_2 concentrations at the north and south monitors, respectively, for modeling scenarios that use the proposed GRSM NO_2 Tier 3 option as well as the other Tier 2 (ARM2) and 3 (OLM, PVMRM) regulatory NO_2 screening options available in AERMOD. Similar to the results at Pala'au, the ARM2 option performs the most conservatively, whereas OLM and GRSM modeled concentrations track closely together and are more conservative than PVMRM. GRSM performs consistently compared to the other AERMOD NO_2 options, and shows no unacceptable bias to underpredict peak concentrations for the Empire Abo database.

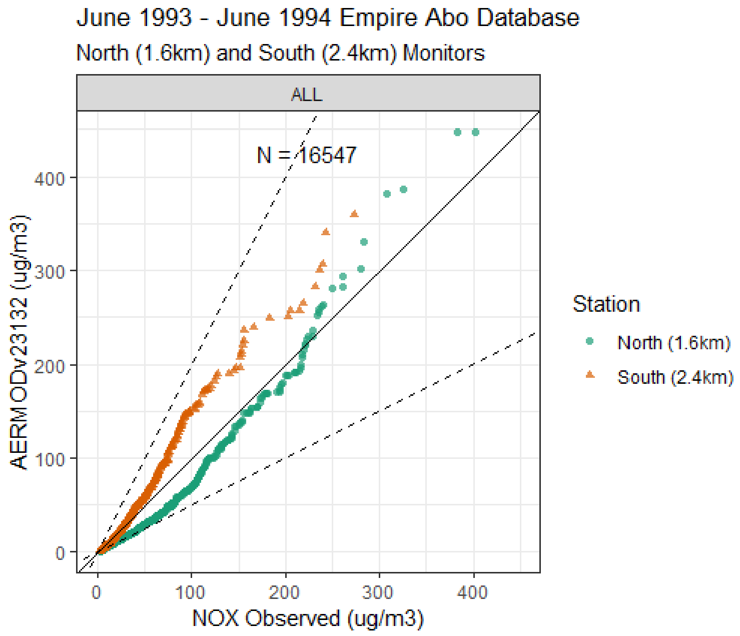

Figure 3 – Empire Abo NO_X Ranked Q-Q Plot

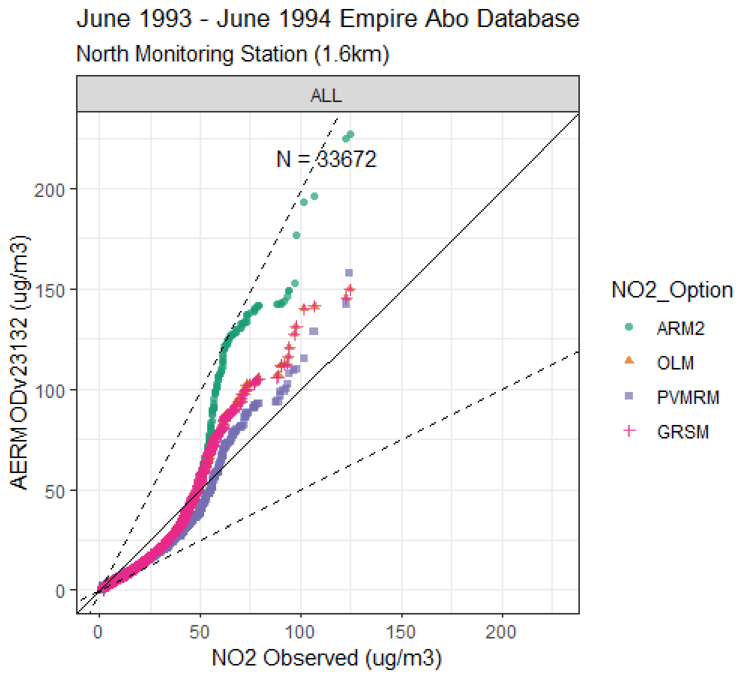

Figure 4 – Empire Abo NO_2 Ranked Q-Q Plot for the North Monitor

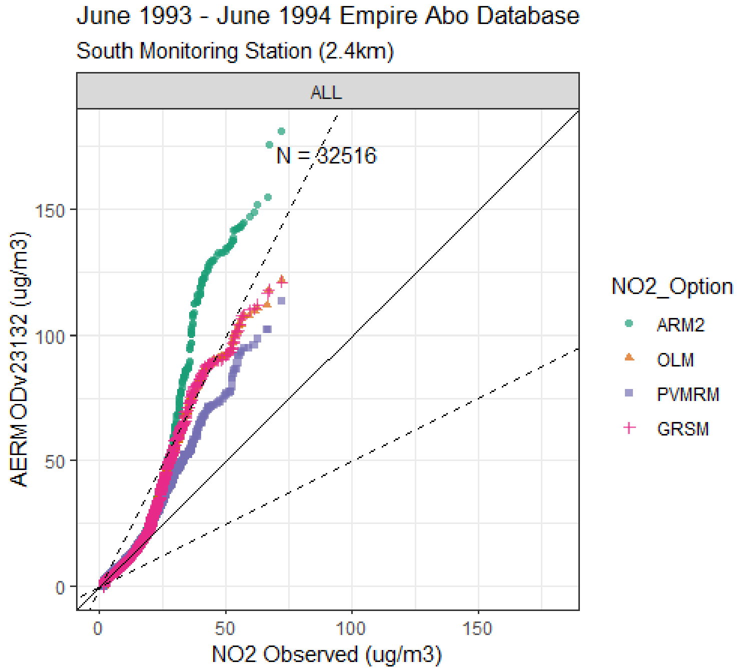

Figure 5 – Empire Abo NO_2 Ranked Q-Q Plot for the South Monitor

Table 2 shows summary model performance statistics for NO_X and NO_2 at the Empire Abo north and south monitors. The FB shows conservative agreement between observations and model outputs. The RHC ratio and RHC FB show conservative bias for the north monitor and south monitor, with the most conservatism shown for NO_X and ARM2, whereas OLM, PVMRM, and GRSM display consistent conservative bias for the north and south monitors.

Table 2 – Empire Abo Model Performance Statistics Summary (µg/m^3)

Station	Model Opt.	N	FB	RHC_Obs	RHC_Mod	RHC_ratio	RHC_FB
North (1.6km)	NO_X	8418	0.519675	356.2944	477.27	1.339538	-0.29026
	ARM2	8418	0.289203	130.2695	204.0459	1.566337	-0.44136
	OLM	8418	0.292575	130.2695	152.6254	1.171613	-0.15805
	PVMRM	8418	0.354584	130.2695	141.475	1.086018	-0.08247
	GRSM	8418	0.314298	130.2695	152.9922	1.174428	-0.16044
South (2.4km)	NO_X	8129	0.364385	323.4253	392.8127	1.214539	-0.19375
	ARM2	8129	-0.00239	72.57853	172.0086	2.369966	-0.81304
	OLM	8129	0.000409	72.57853	128.2316	1.766798	-0.55429
	PVMRM	8129	0.045474	72.57853	121.1714	1.669522	-0.5016
	GRSM	8129	0.01555	72.57853	129.4047	1.782962	-0.56268

5.3 Balko, Oklahoma NO_2 Database

The 1-year of hourly NO_2 observations records for each of the four monitoring stations were reduced by excluding values collected during hours when NO_X concentrations were below 20 ppb and when the downwind direction from the source to the monitoring receptor location was more than approximately 20-30 degrees (i.e., assuming a 40-60-degree downwind sector of influence). As such, non-missing hourly modeling results were paired in time with the reduced observations (total N pairs = 1742) to generate ranked Q-Q plots and summary statistics. In brief, the monitoring stations, distances, and downwind directions from the sources were: Field 425 m, 360 deg; North Fence (NF) 140 m, 360 deg; East Fence (EF) 101 m, 68 deg; and Tower 66 m, 246 deg. NO_X emissions at Balko were dominated by two of the large 2-stroke cycle lean-burn natural gas-fired engines with combined maximum hourly NO_X emission rates on the order of 120 lb/hr and NO_2/NO_X in-stack ratios of 10%. Relatively short stacks for these units were modeled at 10 m and 20 m, with adjacent dominant building heights at 11-13 m. For further details on the Balko field study and model configurations see (Panek, 2020).

The NO_X and NO_2 Q-Q plots shown in Figure 6 represent all model-observation data pairs from the four monitoring stations. Both NO_X, OLM, and GRSM NO_2 predictions trend below the 1:1 line at the upper end of the concentration distributions, but above the 1:2 line. ARM2 performs above the 2:1 line through the first half of the ranked distribution, converging to the 1:1 line at the upper end of the distribution. The negative bias shown in the NO_X performance suggests dispersion assumptions such as downwash and stack parameters could be refined for some monitoring locations. The negative bias in NO_X is largely driven by the model performance and higher observed NO_X impacts at the North Field (NF) monitor, which is well within the near wake zone of two adjacent end-to-end, long buildings. As shown in Figure 7, all other monitor locations show more conservative, or positive bias for NO_X.

The ranked Q-Q plot panels for NO_X and NO_2 shown in Figure 7 are presented for each monitor location. NO_X model predictions at the Field and East Fence show conservative bias with peak value data pairs falling between the 2:1 and 1:1 lines. NO_2 model predictions at these stations ranging from 175 µg/m^3 to 200 µg/m^3 show a consistent conservative hierarchy across the NO_2 options decreasing in order of the ARM2, OLM, PVMRM, and GRSM options. The NO_X predictions at the meteorological Tower monitor fall mostly along the 1:1 line; however, PVRM is the least conservative performing NO_2 option at this predominantly southwesterly, upwind location. NO_X predictions at the North Fence follow the 1:1 line with negative bias trends starting at 750 µg/m^3 and ending above the 1:2 line at about 1600 µg/m^3. The negative bias at the upper part of the distribution is most likely influenced by uncertainties in source and building downwash characterizations at what is a relative short downwind 140-meter distance from the dominant stack. The conservative hierarchy shown for NO_2 predictions at the North Fence is similar to the other monitor locations; however, the overly conservative PVMRM predictions for the last three data pairs suggest further uncertainties in instantaneous plume and building downwash formulations coded for PVMRM. GRSM does not mimic this behavior.

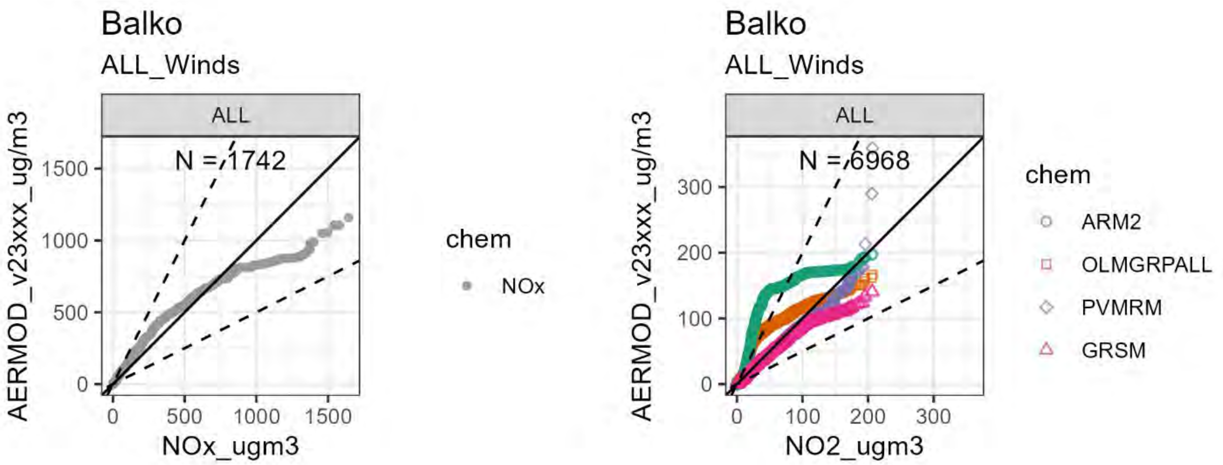

Figure 6 – Balko NO_X and NO_2 Ranked Q-Q Plot for all monitors

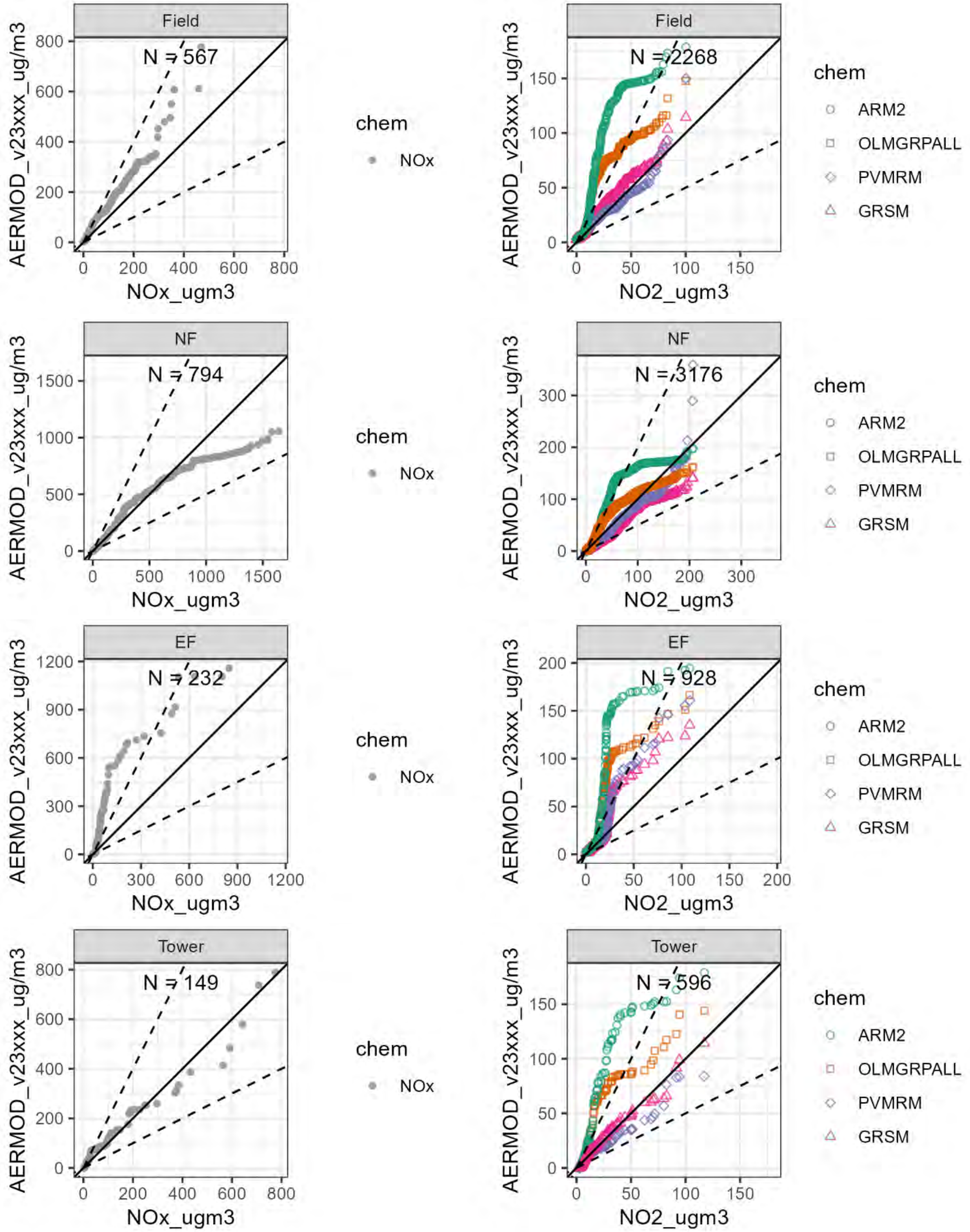

Figure 7 – Balko NO_X and NO_2 Ranked Q-Q Plot by monitor

Table 3 provides FB and RHC statistics calculated for all monitor locations and for all NO_2 model options evaluated including NO_X, ARM2, OLM, PVMRM, and GRSM. The table is sorted by model option and decreasing RHC ratio values. In all, the GRSM RHC ratio and RHC FB results indicate more consistent, logical model behavior when compared with modeled NO_X performance at the four monitors. With exception to the uncertainties discussed at the NF monitor, GRSM performance statistics show less conservative bias than the other NO_2 model options.

Table 3 – Balko Model Performance Statistics Summary (μg/m^3)

Station	Model Opt.	N	FB	RHC_Obs	RHC_Mod	RHC_ratio	RHC_FB
EF	NO_X	232	-0.30893	785.1347	1449.214	1.845816	-0.59443
Field	NO_X	567	-0.33405	481.5579	637.3523	1.323521	-0.27848
Tower	NO_X	149	0.050238	825.8741	719.8355	0.871604	0.137204
ALL	NO_X	1742	-0.13172	1884.88	1162.402	0.616698	0.474179
NF	NO_X	794	0.030388	1884.88	1069.941	0.567644	0.551599
EF	ARM2	232	-0.5797	106.2721	210.4881	1.980653	-0.65801
Tower	ARM2	149	-0.23291	121.7104	211.9201	1.741183	-0.54078
Field	ARM2	567	-0.67069	104.2684	171.3581	1.643433	-0.48682
ALL	ARM2	1742	-0.44312	220.7673	199.6457	0.904326	0.100481
NF	ARM2	794	-0.28016	220.7673	191.5234	0.867535	0.141861
EF	OLMGRPALL	232	-0.51368	106.2721	164.5996	1.548851	-0.43067
Field	OLMGRPALL	567	-0.59014	104.2684	130.0644	1.2474	-0.22017
Tower	OLMGRPALL	149	-0.16588	121.7104	137.5235	1.129924	-0.122
ALL	OLMGRPALL	1742	-0.34007	220.7673	172.0811	0.779468	0.247863
NF	OLMGRPALL	794	-0.14346	220.7673	169.5039	0.767794	0.262707
EF	PVMRM	232	-0.14628	106.2721	192.0816	1.807451	-0.57522
NF	PVMRM	794	0.17654	220.7673	269.9143	1.222619	-0.20032
ALL	PVMRM	1742	0.048435	220.7673	259.2444	1.174288	-0.16032
Field	PVMRM	567	-0.11716	104.2684	110.9297	1.063887	-0.06191
Tower	PVMRM	149	0.299099	121.7104	92.84917	0.76287	0.269028
EF	GRSM	232	-0.11145	106.2721	147.6259	1.389132	-0.32575
Field	GRSM	567	-0.26831	104.2684	105.8487	1.015156	-0.01504
Tower	GRSM	149	0.217114	121.7104	104.3644	0.857481	0.153454
ALL	GRSM	1742	0.034885	220.7673	142.8789	0.647192	0.428375
NF	GRSM	794	0.259959	220.7673	138.3798	0.626813	0.458796

5.4 Denver-Julesburg Basin, Platteville, Colorado NO_2 Database

The Colorado NO_2 database is comprised of twelve monitors deployed for roughly six weeks (October 10 – November 16, 2014) at two adjacent oil and gas drilling installations, Pads 1 and

2 outside Platteville, CO. At Pad 1, the six upwind (southeast) and six downwind (northwest) monitors were positioned around the pad on which the emission sources included a drill rig, five generators, and one small boiler. Similarly, at Pad 2, six monitors upwind and six downwind were located around the pad with the same emission sources. The monitors were re-positioned at Pad 2 on three separate occasions to capture NO_X emissions during changing wind patterns for the last three weeks of the monitoring period. Monitor locations for both Pad 1 and 2 were placed approximately 50-100 m away from the drill rig and support generators. Hourly varying NO_X emissions were modeled for the five diesel-fired support generators and standby boiler at Pads 1 and 2 during the six-week study period. NO_X hourly emission rate totals at both pads range from roughly 10 lb/hr to 20 lb/hr with stack release heights at 18 ft just at or above the 18 ft high drill rig and 30 total adjacent and nearby buildings. Non-missing hourly modeling results were paired in time with the available observations at Pads 1 and 2 (total N pairs = 1473) to generate ranked Q-Q plots and summary statistics. All five generators show relatively equal contribution to total NO_X emissions when operating at Pads 1 and 2. The standby boiler contributions to total NO_X emissions appear to be negligible. The generator operating loads varied between approximately 50-100% load throughout the study periods at Pad 1 and 2. For further details on the Colorado field study monitor locations, hourly emission rates and operating scenarios, background hourly ozone and NO_X data wind sector filtering, and other model configurations see (Colorado Field Study Workgroup: ERM, 2020). Note that there were more than a dozen small adjacent buildings located within downwash near wake zones that extend between source and monitor locations at Pads 1 and 2. Downwash effects from these collections of buildings as well as non-varying in-stack NO_2/NO_X ratios assumed for the five generators likely influence model performance biases and uncertainties for this database.

Figures 8 and 9 show ranked Q-Q plots of AERMOD versus observed NO_X and NO_2 concentrations at Pads 1 and 2, respectively. NO_X model predictions at Pad 1 compare well with observations with exception to the last three data pairs showing some underprediction. At Pad 2, roughly half of the upper distribution of NO_X predictions show negative bias trending toward the 1:2 line, suggesting AERMOD may be overestimating dispersion; however, NO_X emissions and/or NO_2/NO_X ratios inputs may be underestimated perhaps related to uncertainties in the assumed non-varying in-stack NO_2/NO_X ratios during varying genset operating loads. Uncertainties in source characterization of building downwash may also be contributing to the model estimates at both Pads 1 and 2, especially attributable to movement of monitoring equipment at three different times around Pad 2. The conservative bias hierarchy for NO_2 options at Pads 1 and 2 is similar to NO_2 option performance discussed for the other three databases with exception to PVMRM. The unreasonable conservative bias shown for PVMRM at Pads 1 and 2 as it compares to ARM2 may be related to similar model uncertainties discussed for the North Fence monitor at Balko, where enhanced downwash and entrainment effects on the ensemble plume are overestimated by PVMRM in the immediate vicinity of recirculation cavities and near wake downwash zones.

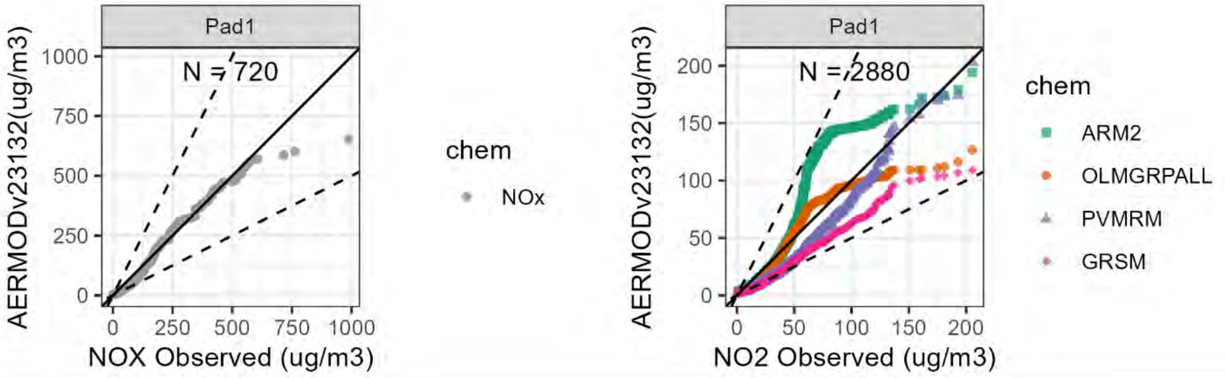

Figure 8 – Colorado NO_X and NO_2 Ranked Q-Q Plots for Pad 1

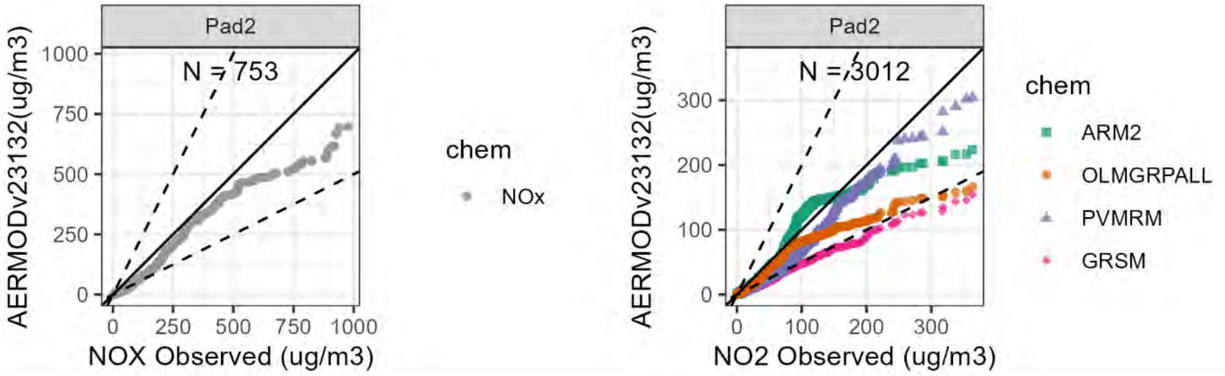

Figure 9 – Colorado NO_X and NO_2 Ranked Q-Q Plots for Pad 2

Table 4 provides summary FB and RHC statistics for all NO_2 modeled options at Pads 1, 2, and both Pads 1 and 2, sorted by model option and conservative RHC ratio. GRSM shows refined performance consistent with the ARM2 and OLM, with underpredictions most likely attributable to source characterization uncertainties. No extreme underprediction or overprediction is indicated in the RHC fractional bias values shown for GRSM at Pads 1 or 2. In general, performance for all NO_2 options seems more degraded at Pad 2 as compared to Pad 1.

Table 4 – Colorado Model Performance Statistics Summary (μg/m^3)

Pad	Model Opt.	N	FB	RHC_Obs	RHC_Mod	RHC_ratio	RHC_FB
Pad1	NO_X	720	0.315616	840.7064	734.6718	0.873874	0.134615
ALL	NO_X	1473	0.405245	1250.35	731.5125	0.585046	0.523586
Pad2	NO_X	753	0.490945	1289.554	743.2198	0.576338	0.537526
Pad1	ARM2	720	-0.02909	196.3466	185.0584	0.942509	0.059192
Pad2	ARM2	753	0.181117	388.8654	253.4506	0.65177	0.421645
ALL	ARM2	1473	0.07837	388.8343	247.755	0.637174	0.443235
Pad1	PVMRM	720	0.423036	196.3466	216.9619	1.104995	-0.09976
ALL	PVMRM	1473	0.438573	388.8343	337.1309	0.86703	0.142441
Pad2	PVMRM	753	0.45343	388.8654	335.9631	0.863957	0.145972
Pad1	OLMGRPALL	720	0.081058	196.3466	119.3968	0.608092	0.48742
Pad2	OLMGRPALL	753	0.294795	388.8654	188.1758	0.48391	0.695581
ALL	OLMGRPALL	1473	0.19032	388.8343	184.8962	0.475514	0.71092
Pad1	GRSM	720	0.525857	196.3466	121.2005	0.617279	0.473291
Pad2	GRSM	753	0.723	388.8654	180.1383	0.463241	0.733658
ALL	GRSM	1473	0.626637	388.8343	157.2032	0.404293	0.848408

6. Summary

Four NO_2 model evaluation databases were used to assess the comparative model behavior and statistical performance of GRSM. These databases represent a broad range of NO_X source characterizations, ozone and NO_X model inputs, ozone and NO_2 monitoring networks, and local and regional NO_X chemistry and meteorological environments. All database evaluations included comparisons between GRSM and all existing AERMOD Tier 1 (NO_X), Tier 2 (ARM2), and Tier 3 (OLM and PVMRM) AERMOD NO_2 regulatory screening options. Based on the ranked Q-Q plots showing NO_X and NO_2 model versus observation concentrations, and with exception to previously discussed uncertainties and degraded model performance at Pad 2 for Colorado, GRSM performs within a factor of +/- 2 range of the NO_2 observations, and thus, demonstrates no unacceptable under or over prediction biases. The statistical summaries of RHC and fractional biases for all NO_2 databases further demonstrate GRSM behaves and performs consistently in comparison with the other existing AERMOD NO_2 screening options.

References

Carruthers, D. S., Stocker, J. R., Ellis, A., Seaton, M. D., & Smith, S. E. (2017). Evaluation of an explicit NO_X chemistry method in AERMOD. *Journal of the Air & Waste Management Association*, 67:6, 702-712, DOI: 10.1080/10962247.2017.1280096.

Cole, H. S., & Summerhays, J. E. (1979). A Review of Techniques Available for Estimating Short-Term NO_2 concentrations. *J. Air Poll. Cont. Assoc., 29:8*, 812-817. doi:10.1080/00022470.1979.10470866

Colorado Field Study Workgroup: ERM, A. A.-W. (2020). *2014 Colorado Oil and Gas Drill Rig Field Study Model Evaluation Database - Technical Support Document.* Platteville.

Hanrahan, P. L. (1999a). The Plume Volume Molar Ratio Method for Determining NO_2/NO_X Ratios in Modeling - Part I: Methodology. *J. Air & Waste Manage. Assoc.*, 1324-1331.

Hanrahan, P. L. (1999b). The Plume Volume Molar Ratio Method for Determining NO_2/NO_X Ratios in Modeling - Part II: Evaluation Studies. *J. Air & Waste Manage. Assoc.*, 1332-1338.

Panek, J. A. (2020). PRCI ambient NO_2 AERMOD performance assessment and model improvement project: Modeled to observed comparison. *Journal of the Air & Waste Management Association, Vol. 70, No. 5*, 504-521.

Podrez, M. (2015). An update to the ambient ratio method for 1-h NO_2 air quality standards dispersion modeling. *Atm. Env.*, 163-170.

RTP Environmental Associates, Inc. (2013, March 3). *Ambient Ratio Method Version 2 (ARM2) for use with AERMOD for 1-hr* NO_2 *Modeling.* Retrieved from http://www.epa.gov/ttn/scram/models/aermod/ARM2_Development_and_Evaluation_Report-September_20_2013.pdf

Stocker, J. R., Seaton, M. D., Smith, S. E., O'Neill, J., Johnson, K., Jackson, R., & Carruthers, D. (2023). *Evaluation of the Generic Reaction Set Method for* NO_2 *conversion in AERMOD. The modification of AERMOD to include ADMS chemistry.* Cambridge Environmental Research Consultants (CERC) Technical Report.

U.S. EPA. (1992). *Protocol for Determining the Best Performing Model. EPA-454/R-92-025.* Research Triangle Park, NC: Office of Air Quality Planning and Standards.

U.S. EPA. (2015, December). *Technical support document (TSD) for* NO_2*-related AERMOD modifications. Publication No. EPA-454/B-15-004.* Research Triangle Park, North Carolina: Office of Air Quality Planning and Standards.

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