Technical Support Document

EPA Region 6's Review of TCEQ's Alternative Model Request of AERMOD with Highly Bouyant Plume Treatment (HBP)

(HBP TSD)

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1. Overview of TCEQ Alternative Model Request

In October 2020, Texas Commission on Environmental Quality (TCEQ) and Vistra initiated discussions with Environmental Protection Agency (EPA) Region 6 on potentially developing an alternative model request for AERMOD with a modification to how AERMOD treats plumes that penetrate the boundary layer and when the penetrated plume mixes back into the mixed layer. EPA Region 6; EPA Office of Air Quality, Planning and Standards (OAQPS) Air Quality Modeling Group representatives; TCEQ and their consultant Ramboll; and Vistra and their consultant AECOM had several calls and reviewed preliminary information in development of what TCEQ should develop to support a submission up through July 2021. TCEQ submitted a letter dated May 24, 2021 from Ms. Tonya Baer (TCEQ Director of the Office of Air) to Mr. David Garcia (Air and Radiation Division Director) of EPA Region 6 requesting approval of an alternative model request for use of the American Meteorological Society/EPA Regulatory Model (AERMOD) with Highly Buoyant Plume (HBP) code modifications in the Rusk-Panola 2010 1-Hour SO_2 NAAQS attainment demonstration. EPA and TCEQ continued to have discussions on the necessary information to support the determination and TCEQ continued to submit information from May through August 2021 to EPA in support of the alternative model request. EPA Region 6 has included TCEQ's attainment demonstration SIP Appendix M that includes TCEQ's alternative model request for AERMOD-HBP and AERMOD-HBP documentation as Appendix A to this TSD.

40 CFR Part 51.112(a)(1) states that all applications of air quality modeling shall be based on the applicable models specified in 40 Code of Federal Regulations (CFR) Part 51, Appendix W – Guideline on Air Quality Models (hereafter "App. W"). However, 51.112(a)(2) also provides that on a case-by-case basis, a modification or substitution of an air quality model may be used following written approval. In addition, the use of a modified or substituted model is subject to notice and opportunity for public comment. App. W, Sections 4.2.2 and 4.2.2.1 and Appendix A of App. W, identifies AERMOD as EPA's preferred model for development of a 1-hour SO_2 attainment demonstration SIP. TCEQ's alternative model request was made in accordance with App. W, Section 3.2.2(b)(2). TCEQ asked for EPA Region 6's review and approval of an alternative model that includes a model formulation with alternate treatment of penetrated plume included coded into AERMOD (AERMOD-HBP). TCEQ and EPA Region 6 continued to have discussions through August 2021 to obtain the information EPA Region 6 needed to review the alternative model request. A formal alternative model evaluation protocol was never finalized and approved by EPA Region 6. However, a draft protocol was developed that EPA reviewed and provided comment back to TCEQ, and TCEQ provided a revised protocol dated July 29, 2021 (Appendix B to this TSD).

The approval of an alternative model is outlined in App. W, Section 3.2. Section 3.2.2(a) specifies that the determination of acceptability of an alternative model is a Regional Office responsibility with concurrence from the Model Clearinghouse (MCH) and that an alternative model may be used subject to Regional Office approval based on the Section 3.2.2 requirements. Section 3.2.2(b) states the alternative model shall be evaluated from both a theoretical and performance perspective before regulatory use and outlines the three separate conditions where an alternative model may be approved.

Relevant portions of App. W governing the evaluation and approval of an alternative model include:

- App. W 3.2.2(b) “An alternative model shall be evaluated from both a theoretical and a performance perspective before it is selected for use. There are three separate conditions under which such a model may be approved for use:[1]”
- App. W 3.2.2(b)(2) (Condition 2) “If a statistical performance evaluation has been conducted using measured air quality data and the results of that evaluation indicate the alternative model performs better for the given application than a comparable model in appendix A”
- App. W 3.2.2(d) “For condition (2) in paragraph (b) of this subsection [above], established statistical performance evaluation procedures and techniques[2] for determining the acceptability of a model for an individual case based on superior performance should be followed, as appropriate. Preparation and implementation of an evaluation protocol that is acceptable to both control agencies and regulated industry is an important element in such an evaluation.”
- App. W 3.2.2(e) “Finally, for condition (3) in paragraph (b) of this subsection, an alternative model or technique may be approved for use provided that:
    - i. The model or technique has received a scientific peer review;
    - ii. The model or technique can be demonstrated to be applicable to the problem on a theoretical basis;
    - iii. The databases which are necessary to perform the analysis are available and adequate;
    - iv. Appropriate performance evaluations of the model or technique have shown that the model or technique is not inappropriately biased for regulatory application [3]; and
    - v. A protocol on methods and procedures to be followed has been established.”

While not specifically cross-referenced, App. W 3.2.2(e) sets forth five conditions that must be satisfied for alternative model approval under Condition 2 of 3.2.2(b)(2) by providing a framework on how to address the requirements of App. W 3.2.2 and on how to perform an analysis from both a theoretical and performance perspective. The fact that each alternative

[1] The other 2 conditions discussed in App. W 3.2.2.(b)(1) and b(3) do not apply in this situation as the applicant has asked for approval in accordance with App. W 3.2.2(b)(2).

[2] Endnotes 28 and 29 “28. ASTM D6589: Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance. (2010). 29. U.S. Environmental Protection Agency, 1992. Protocol for Determining the Best Performing Model. Publication No. EPA–454/R–92–025. Office of Air Quality Planning and Standards, Research Triangle Park, NC. (NTIS No. PB 93– 226082).”

[3] Footnote a “For PSD and other applications that use the model results in an absolute sense, the model should not be biased toward underestimates. Alternatively, for ozone and PM2.5 SIP attainment demonstrations and other applications that use the model results in a relative sense, the model should not be biased toward overestimates.”

model request is unique augments the importance of developing a model evaluation package in accordance with App. W 3.2.2(d) that both EPA Region 6 and TCEQ determine to be acceptable.

Through the discussions from October 2020 through August 2021 a list of information that would need to be provided to EPA Region 6 in support of the alternative model request was developed. TCEQ provided a modeling protocol for alternative model approval based on these requests that is dated July 29, 2021. Since there is only one near field monitor (Martin Creek) EPA Region 6 recommended including the Longview airport monitor (19 km from Martin Lake) when performing any model evaluation.

Among the items that TCEQ provided to EPA Region 6 in support of the alternative model request were:

1 Formulation of AERMOD-HBP documentation detailing the nature of the alleged overprediction tendency of regulatory version of AERMOD, including peer reviewed published information. Technical documentation of how proposed algorithm changes (with revised AERMOD modules incorporating HBP changes) will address alleged problems. (see Sections 2 and 3 of this document for discussion and evaluation)
2 Modeling with AERMOD 21112 regulatory version and AERMOD-HBP for performing evaluation with Martin Creek and Longview Airport monitoring data.
3 For 3.2.2.(b)(2) - Comparisons of AERMOD-regulatory version vs. AERMOD-HBP vs. monitored data at the monitoring sites (three years for Martin Creek and five years at Longview). This analysis should include several statistical evaluations including Cox-Tikvart (CT); hourly time series of for all hours and daily maximum concentrations; and an evaluation of the top percentile rankings including the 1st through 10th high days, 95th and 90th percentile days; and Scatter/Quantile-Quantile (Q-Q) plots. Analysis included CT done several ways (each monitor separately and also grouped) for each year individually and also for the combined years.
4 Documentation and evaluation of AERMOD modules model code changes implementing HBP.
5 Updated MPE based on new stack locations identified in July 2021.
6 Documentation of other field data sites with penetrated plume overprediction issues to help demonstrate that this is a potential problem given the limited local monitoring data around the Martin Lake facility. AECOM provided information of other USA sites such as Labadie (Missouri) and Baldwin (Illinois) where the regulatory version of AERMOD allegedly appears to overpredict due to the penetrated plume issue.

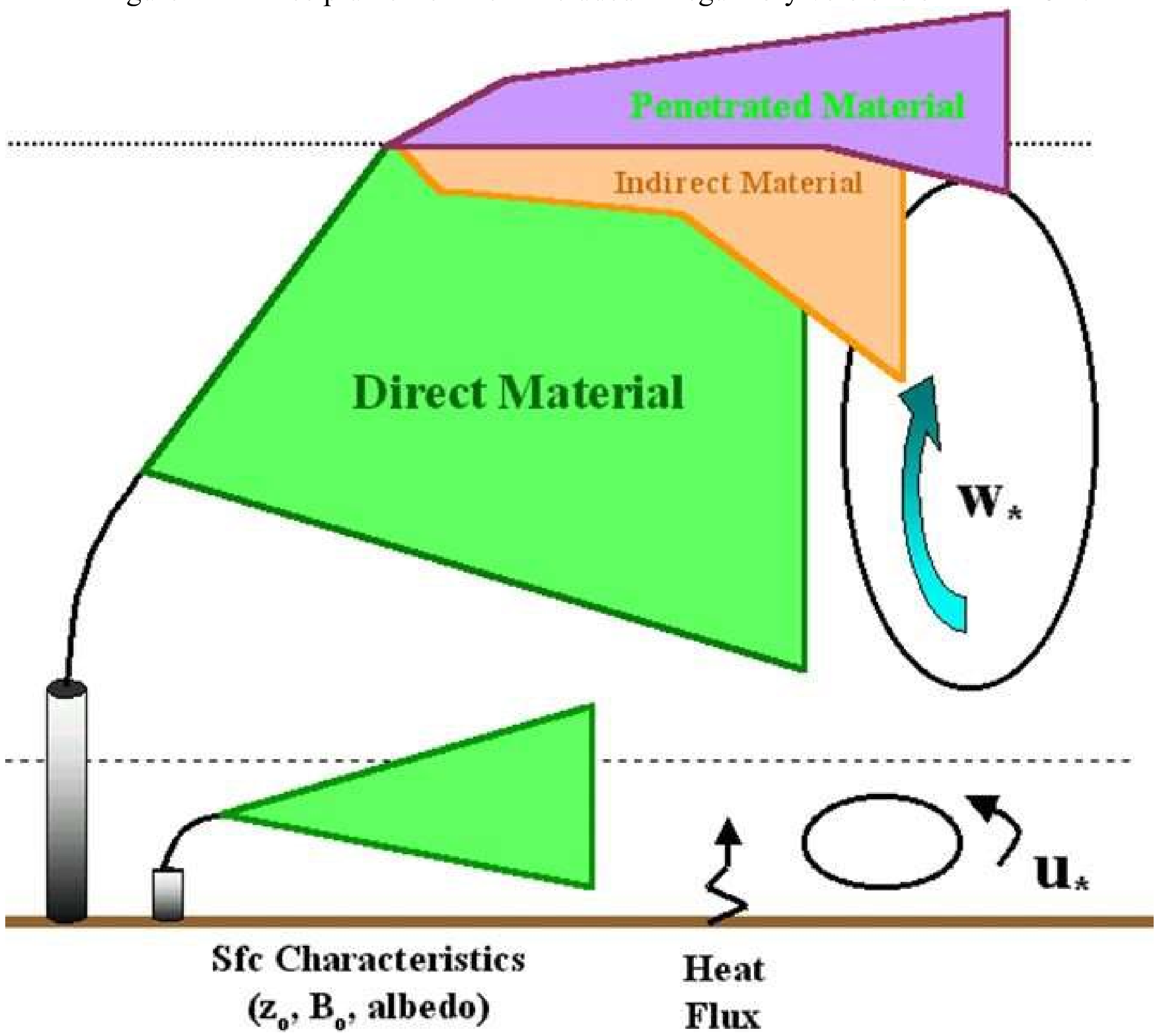
The following sections of this TSD provide EPA Region 6's evaluation of these elements of TCEQ's AERMOD-HBP alternative model submittal. TCEQ proposed and submitted a 1-hour SO_2 attainment demonstration SIP for the Rusk-Panola nonattainment area using AERMOD-HBP without EPA Region 6's prior approval of AERMOD-HBP as TCEQ indicated they did not have time to obtain EPA Region 6's approval of the alternative model due to SIP deadlines. EPA Region 6's review and approval of AERMOD-HBP alternative model is necessary to be able to review TCEQ's 1-hour SO2 attainment demonstration for Rusk/Panola SIP.

Vistra's contractor AECOM provided materials supporting the HBP alternative model request of TCEQ in May 2021 that TCEQ included in their alternative model request of EPA Region 6. During EPA Region 6's review there were some questions and a concern that some of the material was copyrighted and/or not released by the author for public circulation, and EPA Region 6 reached out to AECOM for further documentation. AECOM provided an updated document May 1st, 2024 to EPA Region 6 that included updated theory discussion, more details on the HBP formulation in AERMOD, and more details on the changes in the different AERMOD modules.

2. HBP Theory Review

In convective conditions, the regulatory version of AERMOD has a 3-plume treatment for stack emissions: direct, indirect and penetrated components. The direct and indirect plumes remain within the mixed/convective layer. The penetrated plume (purple portion in Figure 2.1 replicated from AECOM 2021) is the portion of the plume that is sufficiently buoyant to break through the elevated inversion into the stable layer aloft which has less vertical mixing than the mixed/convective layer.

Figure 2-1 Three plume treatment included in regulatory versions of AERMOD.[4]



AECOM and TCEQ provided that some observations of the behavior of the penetrated plume (such as from the EPRI Bull Run 1982 field study) indicate that the penetrated plume material

[4] From AECOM's "Discussion of Penetrated Plume Treatment in AERMOD – Recommended Highly Buoyant Plume Improvements" Robert Paine, Carlos Szembek, and Christopher Warren, AECOM; May 19, 2021

mostly stays aloft until the rising convective mixing height intercepts part of the buoyant plume aloft, causing it to fumigate to the ground. Prior to the time of fumigation, the likelihood of elevated ground-level concentrations from a penetrated plume is low. EPA's formulation in AERMOD does account for penetrated plume but the assertion by AECOM and TCEQ is EPA's formulation prematurely mixes the penetrated plume back into the convective layer resulting in penetrated plume impacts adding to the receptors on the ground in its predictions prematurely, and repeats this behavior for hours leading up to the actual interception of the penetrated plume by the rising convective mixed layer. AECOM and TCEQ provided information indicating this behavior has been observed by investigators associated with field studies where the model is found to overpredict ground-level concentration events due to the penetrated plume component, and make those predictions too early in the day. AECOM and TCEQ assert that part of the problem in AERMOD's formulation is it is assuming more vertical mixing resulting in more vertical spread of the penetrated plume in the stable layer aloft than actually occurs, and this results in premature and more frequent mixing down of penetrated plume into the convective layer.

2.1. **Specific Concern of how Penetrated Plumes are Currently Implementated in AERMOD and May Bias Impacts in Modeling of Martin Lake facility**

AECOM raises that the key area of concern is the parameterization of the penetrated plume's vertical spreading through the calculation of "effective" dispersion parameters. AERMOD's formulation computes vertically-integrated values between the plume centerline and the receptor at the ground (such as the variance of the vertical wind speed, or sigma-w), even for the penetrated plume component. AECOM indicates that this calculation could substantially overstate the vertical plume growth, since direct observations in a few field studies of the actual penetrated plume behavior shows it is not escaping from the stable layer aloft, while AERMOD presumes that the plume spreads to the ground. AECOM indicates that for cases where the vertical integration involves a significant depth within the convective boundary layer, the plume spreading will be overestimated because the values of sigma-w in the convective boundary layer can be an order of magnitude higher than those in the stable layer aloft and that the plume spreading for the penetrated plume all the way to the ground is only appropriate for the hour when the convective mixing height rises to overtake the plume. AECOM concludes that the current implementation in AERMOD should be viewed as a formulation "bug" that should be corrected. In this case-specific alternative model review, EPA Region 6 is only focusing on whether the phenomena identified by AECOM may be occurring specifically in modeling of Martin Lake emissions and impacting modeled ground level concentrations.

AECOM asserts the central issue for the penetrated plume handling in AERMOD is that the computation of sigma-z (used to determine the plume's bottom edge) is a function of the stability in the layer occupied by the plume. AECOM continues that the penetrated plume is in a stable layer above the mixing height, but the AERMOD formulation assumes a neutral layer for computing the penetrated plume sigma-z, which substantially and incorrectly increases the sigma-z value and this formulation, according to the AERMOD model formulation document,[5] and assumes that the penetrated plume mixes into the CBL and thus encounters a non-stable layer for the portion of the plume that reaches the ground. AECOM indicates that this assumption is only correct if the mixing height rises fast enough to capture at least a portion of the penetrated plume by the end of the current hour, according to Weil et al. 1997 and otherwise, AECOM indicates that this assumption is incorrect as evidenced by the direct observations of the actual penetrated plume behavior not mixing down from the stable layer aloft while the CBL remains below the plume.

AECOM indicates that the computation of the effective turbulence values for the penetrated plume should be limited to the plume height level until the mixed layer rises to overtake the plume and mix it to the ground and that this altered treatment would mix the penetrated plume to the ground starting at the hour during which the convective mixing height starts below the plume level and then intercepts at least a portion of the penetrated plume. AECOM indicates that this solution would help to minimize the early onsite bias that currently exists in AERMOD and be more aligned with actual observation and plume behavior. Again, in this case-specific alternative model review, EPA Region 6 is only focusing on whether the phenomena may be occurring specifically in modeling of Martin Lake emissions and impacting modeled ground level concentrations. EPA's review of AERMOD code and changes to the regulatory version of AERMOD has to be done by EPA's OAQPS in Research Triangle Park, North Carolina in accordance with their procedures for review and modification of the regulatory version of AERMOD. This review is limited to case-specific review of the AERMOD-HBP model used by TCEQ for modeling in the 1- hour SO_2 attainment demonstration SIP for Rusk/Panola nonattainment area.

AECOM conducted modeling of the Martin Lake facility using actual emissions (2018-2020) and 2018-2020 meteorology and they indicated that the model overestimates the 3-year design value at the Martin Creek monitoring site by approximately 30%. AECOM used AERMOD's MODEL and METEOR debug files and another tool "DISTANCE DEBUG" to diagnose if the AERMOD regulatory version's treatment of penetrated plumes was potentially responsible for overestimations on certain days. AECOM provided a Table (replicated below as Table 2.1-1) of the top 10 daily maxima modeled values that indicates that penetrated plume was a factor for all three of the Martin Lake boiler stacks except for one stack on one hour.

[5] EPA, 2019. AERMOD Model Formulation and Evaluation Document. Available at https://gaftp.epa.gov/Air/aqmg/SCRAM/models/preferred/aermod/aermod_mfed.pdf.

Table 2.1-1 AECOM Table 1: Excerpts of DISTANCE-DEBUG Output for Top 10 Daily Maxima AERMOD Default Impacts at Martin Lake Creek Monitor

Daily Maxima RANK	YYMMDDHH	TOTAL Conc. (µg/m³)	u* (m/s)	w* (m/s)	OBULEN (m)	Z_{mech} (m)	Z_{conv} (m)	SFC Z_0 (m)	Source ID	Actual Emissions (g/s)	Ts (K)	Vs (m/s)	Final Plume Height (FPH) (m)	Distance to FPH (m)	WDIR @ FPH (deg.)	Effective Wind Speed (m/s)	Plume Type	Meander Fraction	Partial Penetration Fraction	Effective Sigma V (m/s)	Effective Sigma W (m/s)	Hourly Conc. (µg/m³)
1	18090609	666.1	0.14	0.74	-5.2	130	285	0.032	S1	*875.4*	*360.2*	*33.7*	445.5	924.9	77	1.9	PEN	0.177	1.000	0.51	0.36	210.3
									S2	*824.3*	*347.7*	*29.8*	419.3	924.9	77	1.8	PEN	0.179	0.969	0.51	0.38	218.9
									S3	*972.8*	*363.1*	*32.4*	445.6	924.9	77	1.9	PEN	0.177	1.000	0.51	0.36	221.8
2	20032213	619.2	0.14	0.67	-7.3	125	322	0.025	S1	*0.3*	*306.4*	*2.3*	238.8	307.6	80	2.0	IND	0.147	0.075	0.48	0.42	0.1
									S2	*1097.6*	*361.7*	*31.8*	418.9	1227.1	80	2.0	PEN	0.141	0.769	0.48	0.38	321.8
									S3	*920.6*	*347.7*	*29.1*	405.6	1227.1	80	2.0	PEN	0.142	0.714	0.48	0.38	282.2
3	18022211	604.5	0.20	0.49	-42.1	213	259	0.02	S1	*728.1*	*345.5*	*33.1*	324.5	1656.1	82	3.5	PEN	0.052	0.779	0.48	0.31	184.2
									S2	*866.0*	*362.0*	*33.4*	332.1	1791.4	82	3.5	PEN	0.052	0.820	0.48	0.31	221.8
									S3	*701.7*	*358.3*	*34.9*	332.4	1795.8	82	3.5	PEN	0.052	0.821	0.48	0.31	183.5
4	18101910	585.8	0.13	0.43	-11.9	117	186	0.027	S1	*507.0*	*361.2*	*28.8*	348.7	965.2	77	1.9	PEN	0.094	1.000	0.35	0.15	167.0
									S2	*585.2*	*348.1*	*27.2*	334.1	965.2	77	1.9	PEN	0.095	1.000	0.35	0.17	227.6
									S3	*469.4*	*346.8*	*26.9*	332.1	965.2	77	1.9	PEN	0.095	1.000	0.35	0.17	176.2
5	18123011	572.2	0.13	0.45	-19.3	114	317	0.02	S1	*946.6*	*346.2*	*32.4*	378.2	1692.4	74	2.1	PEN	0.082	0.609	0.37	0.28	233.2
									S2	*555.1*	*347.8*	*20.5*	362.6	1420.6	74	2.1	PEN	0.083	0.506	0.37	0.28	126.6
									S3	*998.6*	*343.3*	*31.9*	376.1	1657.1	74	2.1	PEN	0.082	0.596	0.37	0.28	197.5
6	18061907	479.6	0.22	0.64	-29.6	244	303	0.032	S1	*715.5*	*362.0*	*34.8*	397.9	1703.9	82	3.5	PEN	0.066	0.802	0.56	0.38	132.3
									S2	*935.4*	*366.3*	*31.8*	395.8	1676.4	82	3.5	PEN	0.067	0.794	0.56	0.39	182.7
									S3	*746.3*	*359.4*	*33.7*	394.6	1660.9	82	3.5	PEN	0.067	0.789	0.56	0.39	149.5
7	18102210	468.3	0.16	0.77	-5.9	154	266	0.027	S1	*599.3*	*351.6*	*27.2*	363.2	957.5	85	2.2	PEN	0.150	0.904	0.55	0.42	171.9
									S2	*449.5*	*347.5*	*25.5*	357.4	957.5	85	2.2	PEN	0.151	0.882	0.55	0.42	138.0
									S3	*459.0*	*345.4*	*27.2*	359.1	957.5	85	2.2	PEN	0.151	0.888	0.548	0.42	143.4
8	20100910	464.8	0.23	0.74	-25.7	258	365	0.027	S1	*913.8*	*349.0*	*28.3*	435.0	1470.9	82	3.7	PEN	0.071	0.572	0.61	0.46	146.8
									S2	*1068.4*	*368.0*	*33.7*	456.6	1737.6	82	3.7	PEN	0.070	0.669	0.61	0.45	154.1
									S3	*930.1*	*357.5*	*29.5*	442.8	1568.0	82	3.7	PEN	0.071	0.610	0.61	0.46	149.0
9	18012711	459.7	0.10	0.54	-4.3	77	260	0.02	S1	*791.3*	*346.6*	*31.5*	438.6	867.8	75	1.4	PEN	0.172	1.000	0.37	0.23	262.4
									S2	*694.5*	*361.9*	*33.9*	465.9	867.8	75	1.4	PEN	0.171	1.000	0.37	0.19	182.3
									S3	*0.0*	--	--	<---	Source is not emitting this hour								
10	20031613	451.9	0.12	0.68	-4.3	117	360	0.025	S1	*544.1*	*357.1*	*31.5*	434.8	1051.4	80	1.5	PEN	0.215	0.603	0.46	0.40	156.4
									S2	*625.8*	*367.8*	*33.2*	442.9	1051.4	80	1.5	PEN	0.215	0.641	0.46	0.39	174.9
									S3	*364.2*	*355.7*	*28.2*	428.9	1051.4	80	1.5	PEN	0.216	0.574	0.46	0.40	105.6

AECOM also provided analysis of two specific days that were modeled that seemed to be overestimations due to penetrated plume treatment: hour 11 on June 3, 2019 and hour 11 on June 29, 2019.

For the hour ending 11 on June 3, 2019, AERMOD reported a penetrated plume at final heights for the three Martin Lake units averaging about 587 m, while the convective mixing height was 485 m (representing the value at the midpoint of the hour). For the following hour, the convective mixing height rose to about 658 m and as a result, the mixing height at the end of hour 11 was still below the three Martin Lake units' plume centerlines at about 572 m. AERMOD assigned sigma-z values of about 228 – 242 m, resulting in a layer for effective parameters reaching well into the convective mixed layer, down to a level of about 107 m above the ground. AECOM's Figure 8 replicated in Figure 2.1-1 shows a plot of the sigma-w profile and the effective turbulence calculations in AERMOD. The sigma-w (green line) is the AERMOD internally calculated sigma-w extracted from the METEOR debug file.

The local value of sigma-w at the penetrated plume centerline shown in Figure 2.1-1, AERMOD-Simulated Sigma-w as a Function of Height for June 3, 2019, Hour Ending 11, is about 0.30 m/s. However, the internal AERMOD calculations of the effective sigma-w value created an average sigma-w value of more than twice the centerline value (about 0.63 m/s) in a layer between the plume centerline at ~590 m down to ~105 m. This mixing was applied to the entire mass of the penetrated plume, even though most of it remained above the mixing height even at the end of the hour. The result was an AERMOD prediction at the monitoring site of 244.0 µg/m3, almost twice the observed value of 123.3 µg/m3.

For the hour ending 11 on June 29, 2019, AERMOD reported a penetrated plume at final heights for the three Martin Lake units averaging about 390 m, while the convective mixing height was 296 m (representing the value at the midpoint of the hour). For the following hour, the convective mixing height rose only 10 m to 306 m (well under the plume centerline); hence the mixing height at the end of hour 11 was still below the three units' plume centerlines at about 301 m. AERMOD assigned large sigma-z values of about 125 m, resulting in a layer for effective parameters reaching well into the convective mixed layer, down to a level of about 120 m above the ground. AECOM's Figure 9 replicated in Figure 2.1-2, AERMOD-Simulated Sigma-w as a Function of Height for June 29, 2019, Hour Ending 11, shows a plot of the sigma-w profile and the effective turbulence calculations in AERMOD.

Figure 2.1-1 (AECOM Figure 8: AERMOD Simulated Sigma w as a Function of Height for June 3, 2019, Hour Ending 11)

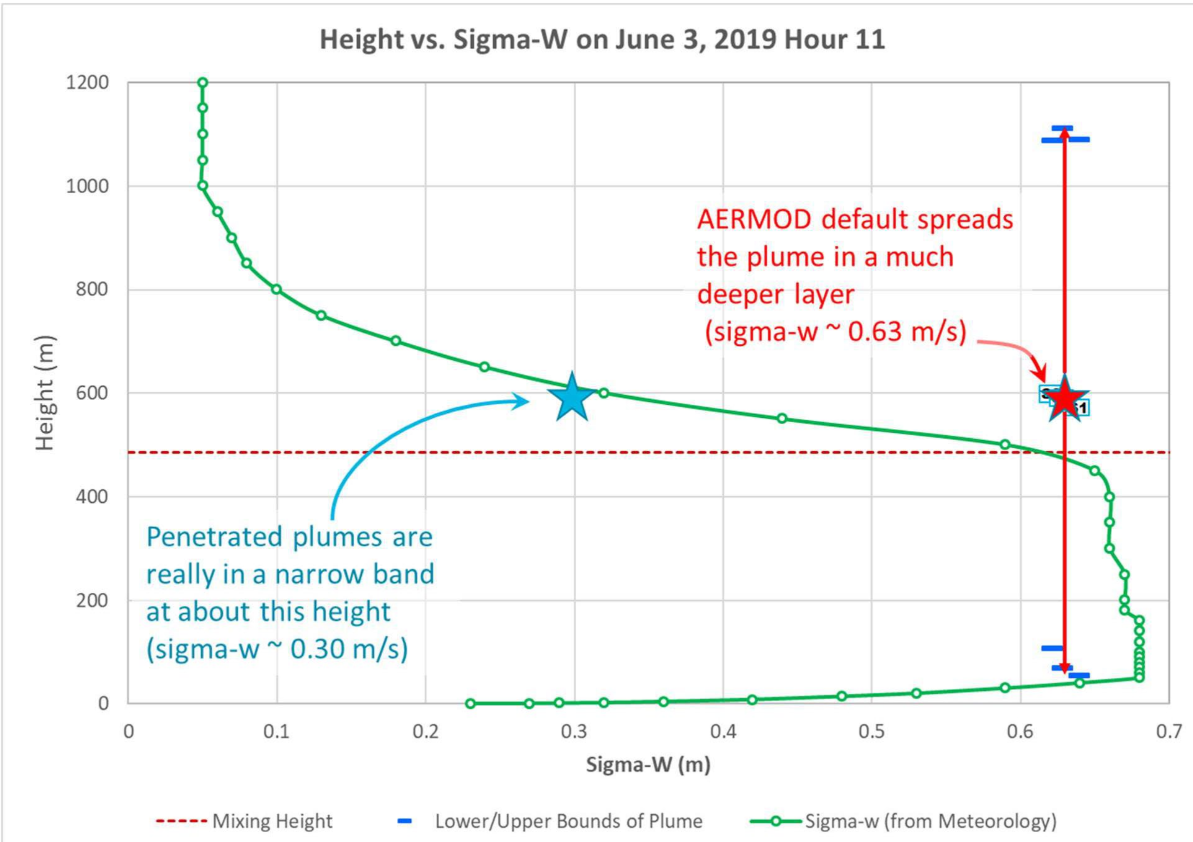
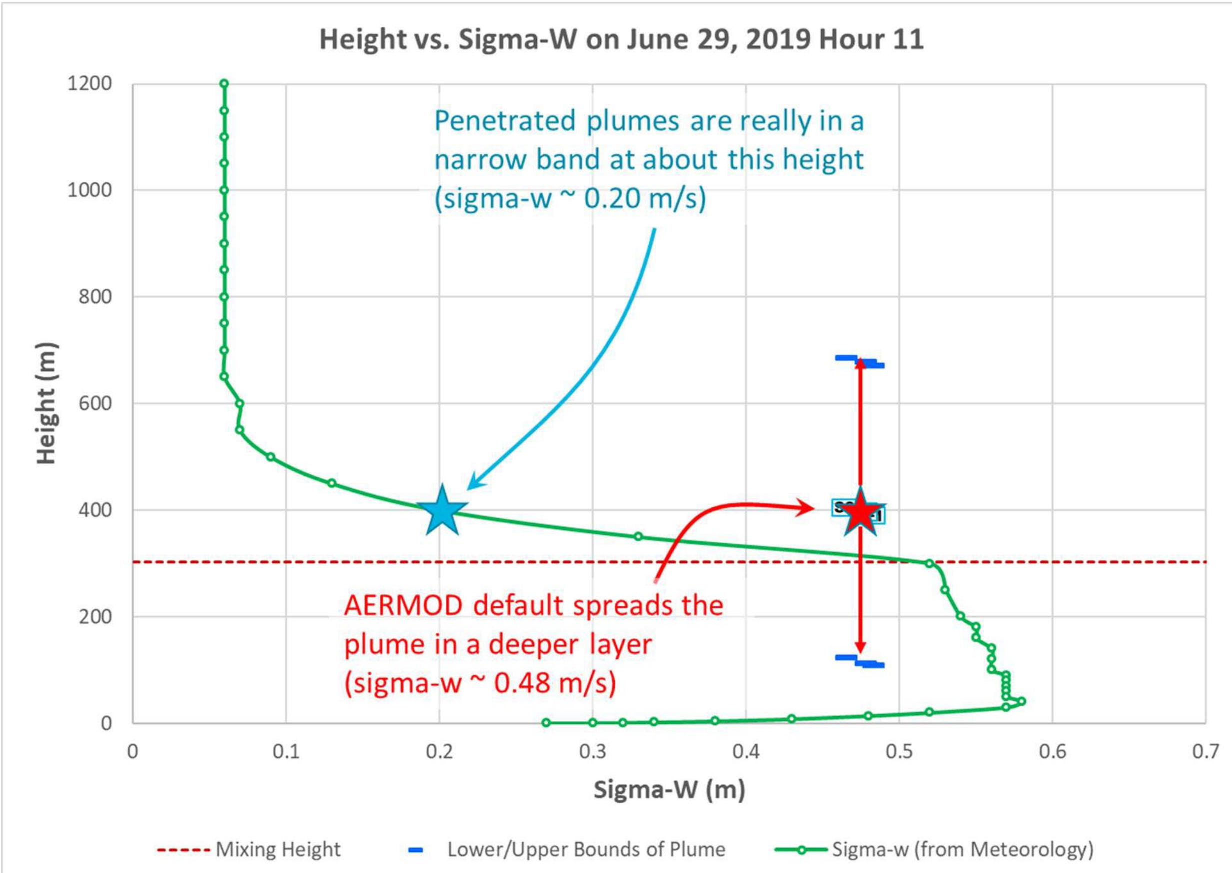


Figure 2.1-2 (AECOM Figure 9: AERMOD Simulated Sigma w as a Function of Height for June 3, 2019, Hour Ending 11)



The plot in Figure 2.1-2 shows that the local value of sigma-w at the penetrated plume centerline is about 0.20 m/s. However, the internal AERMOD calculations of the effective sigma-w value created an average sigma-w value of 2.4 times the centerline value (about 0.48 m/s) in a layer between the plume centerline at ~395 m down to ~115 m. This mixing was applied to the entire mass of the penetrated plume, although most of it remained above the mixing height at the end of the hour. The result was an AERMOD prediction at the monitoring site of 485.8 µg/m3, above any single hour's measurement at the monitor over the 3-year period.

In these cases it seems the key issue is the deep vertical layer over which the effective vertical mixing parameters, especially sigma-w, are calculated. The overly deep vertical layer extends the averaging well into the convective mixed layer, resulting in an exaggerated large plume depth and an associated high impact at the ground.

The issues raised here seem to support that in this site specific analysis of modeling for Rusk Panola Attainment Demonstration SIP sometimes AERMOD's treatment of penetrated plume may be causing a mix down and elevated ground concentrations prematurely and resulting in higher concentrations being modeled. This supports that AERMOD's treatment of penetrated plumes may be an issue in this specific case as is discussed in App. W 3.2.2(e)(ii).

AECOM also provided information related to other field studies at Labadie Energy Center (Labadie) and Baldwin Power Plant (Baldwin), and information from Dr. Ken Rayner of the Western Australia Departement of Environmental Conservation in relation to the Collie Airshed where SO_2 impacts at a key monitor. AECOM asserts that these three investigations also support that AERMOD's penetrated plume treatment is resulting in overestimation of concentrations compared to monitored values. We note that TCEQ did not evaluate AERMOD-HBP at these sites but did provide information provided by AECOM. Since TCEQ's Alternative model request is a case-specific request for the area around Martin Lake facility, we did not review or factor these into our analysis of TCEQ's Alternative model request.

2.2. AECOM's proposed HBP changes to AERMOD to address penetrated plume concerns

AECOM has been working on a potential model code change to address the treatment of penetrated plumes and when and how they are reentrained into the convective mix layer. AECOM's revised approach involves a check on the convective mixing height for the current hour as well as the next hour to determine how the effective dispersion parameters for the penetrated plume should be computed. If the average of the current and the next hour's convective mixing height (each value represents the half-hour mark, so the average is roughly at the end of the current hour) is below the bottom of the penetrated plume final height, then the contribution of the penetrated plume mass is assumed to be zero. The "bottom" of the penetrated plume is 2.15 sigma-z's below the plume centerline height, where the concentration drops to 10% of that at the plume centerline (with a Gaussian distribution assumed). If the mixing height at the end of the current hour is above the top of the penetrated plume, then the full mass of the plume is assumed to reach the ground. For convective mixing heights in between the bottom and top of the penetrated plume, a fraction of the plume mass computed with the Gaussian distribution is assumed to reach the ground (the fraction is 0.5 at the penetrated plume centerline).

AECOM has proposed code change to AERMOD for modeling at the Martin Lake facility to address the penetrated plume issue (an approach initially referred to as "HIPMOD" and now referenced as "HBP" for modifications particularly important for "highly buoyant plume").[6] This revised approach involves a check on the convective mixing height for the

[6] The name "HIPMOD" is derived from Dr. Weil's "Highly-buoyant Plume MODel" designation for this treatment, from his November 4th, 2019 report to the Western Australia Department of Environmental Conservation: "A New Dispersion Model for Highly-Buoyant Plumes in the Convective Boundary Layer" (included as Appendix C to this TSD). We note that AECOM and TCEQ included an earlier January 2019 Draft Version 4 (Weil 2019 PD V4)of this report as Attachment 3 in TCEQ's Attachment 1 to their SIP). Although his report involves additional aspects of plume dispersion in the convective boundary layer, the HIPMOD (HBP) application for AERMOD that TCEQ provided deals only with the interaction of the penetrated plume as currently coded in AERMOD version 21112 with the convective mixing layer, as described in AECOM's 2021 document. Dr. Weil and AECOM provided an updated

current hour as well as the next hour to determine how much of the penetrated plume has been captured by the convective boundary layer (CBL) by the end of the current hour.

The amount of the penetrated plume mass that is allowed to mix to the ground in the HBP modifications depends upon the result of this calculation. There are three possible outcomes.

> Case 1: No penetrated plume impact. If the average of the current and the next hour's convective mixing height (each value represents the half-hour mark,[7] so the average is roughly at the end of the current hour) is below the bottom of the penetrated plume final height, then no portion of the penetrated plume is assumed to mix into the convective boundary layer. In this situation, the contribution of the penetrated plume mass at the receptor is assumed to be zero. The "bottom" of the penetrated plume is 2.15 sigma-z's below the plume centerline height, where the concentration drops to 10% of that at the plume centerline (with a Gaussian distribution assumed).

> Case 2: Full penetrated plume impact. If the mixing height at the end of the current hour is above the top of the penetrated plume, then the full mass of the plume is assumed to reach the ground, and the current AERMOD formulation is used for that hour.

> Case 3: Partial penetrated plume impact. For convective mixing heights (by the end of the current hour) that are in between the bottom and top of the penetrated plume, a fraction of the plume mass, computed using a vertical Gaussian distribution, is assumed to reach the ground using the current AERMOD formulation. For example, the captured fraction is 0.5 if the mixing height at the end of the current hour is exactly at the penetrated plume centerline. If the mixing height at the end of the hour is below (or above) the penetrated plume centerline height, then less (or more) than half of the mass of the penetrated plume will be mixed to the ground.

The approach implemented in the HBP modifications generally only affects AERMOD during the typical period of the late morning through early afternoon when the convective mixing height rises into the layer containing penetrated plume(s); at all other hours, AERMOD-HBP calculations don't typically change AERMOD's concentration calculations run with default options. EPA Region 6 did an analysis of hour of day change due to HBP modifications in Section 5.6 to verify.

EPA Region 6 notes that the 1997 Weil, J.C et al reference for the theory of the penetrated plume treatment is based on a peer reviewed journal article, which meets one of the criteria of an alternative model {40 CFR Part 51 App. W 3.2.2(e)(i)}.

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version 10 of this report but Dr. Weil asked that it not be publically circulated online, so the version 4 and version 10 of the report are available for viewing at EPA Region 6 office.

[7] The Weil et al. (1997) paper states on page 988 that "Penetrated source material is assumed to be mixed into the CBL [convective boundary layer] only when the growing, time-dependent CBL height > Zi, where Zi is the average mixed layer depth over the hour and is representative of the midpoint of the hour." This journal is copyrighted and available for review at EPA Region 6 office.

2.3. **Other References Provided**

Weil, J.C., Corio, L.A., and Brower, R.P., August 1997. A PDF Dispersion Model for Buoyant Plumes in the Convective Boundary Layer. Published in Journal of Applied Meteorology Volume 36.

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Paine, R., Szembek, C., Warren, C., May 19, 2021. Discussion of Penetrated Plume Treatment in AERMOD – Recommended Highly Buoyant Plume (HBP) Improvements.

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Moore, G .E., Milich, L .B., Liu, M. K., 1988: Plume Behaviors Observed Using Lidar and SF_6 Tracer at a Flat and Hilly Site. Atmospheric Environment Vol. 22, No. 8, pp. 1673-1688

3. AERMOD Code Changes Review

TCEQ had its consultant Ramboll document and review the code changes made in Fortran code modules using the regulatory version of AERMOD version 21112 as the starting code to generate AERMOD-HBP (v21112) in the document "Comparison of AERMOD & AERMOD-HBP Fortran Code"; July 29, 2021. (Appendix D to this TSD). In addition to Ramboll's documentation, EPA Region 6 requested additional clarification from AECOM (Vistra's contractor) in March 2024. AECOM provided additional documentation to EPA Region 6 on May 1st 2024 that included further documentation of code changes to the different modules of AERMOD.[8]

Ramboll evaluated the AERMOD-HBP variant model based on the regulatory version of AERMOD v21112 and filename prefix was "amhbp21112" for the AERMOD-HBP executable. Ramboll noted that the code changes supplied by AECOM do not implement all of Weil (1997) nor Weil (2019 PD V4) and Weil (2019). Both papers present results, but TCEQ and AECOM indicated the code for Weil's HIPMOD is not publicly available nor nor did they consider it in the current assessment. The AECOM code implements some ideas briefly discussed by Weil (1997, 2019 PD V4, and 2019). For additional information on these specific modules and changes see pages 17 and 18 and Appendix 3 of AECOM's May 1st 2024 report to EPA Region 6. There are five AERMOD related Fortran files that contain changes made by AECOM for the proposed HBP treatment:

- aermod_HBP.f
- calc1_HBP.f
- iblval_HBP.f
- metext_HBP.f
- modules_HBP.f

In Ramboll's review they noted that where AERMOD regulatory code was changed, the original code was kept as a comment field in the code.

EPA Region 6 has reviewed Ramboll's report of the different code changes in each of the five Fortran modules and also reviewed the "***_HBP.f" modules with the AERMOD v.21112 regulatory Fortran modules and confirmed the code changes that Ramboll documented.

3.1 Differences between "modules_HBP.f" and "aermod_HBP.f" and regulatory versions

Changes made in "aermod_HBP.f" and "modules.f" were to add variable declarations and storing of additional output information for use in other modules. These changes only allow storing of additional information and do not change any calculations.

[8] Email from Christopher Warren of AECOM to Erik Snyder of EPA Region 6 received May 1st 2024 with two attachments: "HBP_Formulation_Documentation_FINAL_01MAY24_w_Attachments.pdf" and "Spreadsheet_calculation_for_PPFN_examples-01MAY24.xlsx"

Specifically, “modules.f” was modified to add variables of ‘ZICONVN’ and ‘ZIMECHN’ which are the values of convective mixing height, mechanical mixing height for the next hour after the current hour and ‘PPFN’ which is the portion of the penetrated plume below the mixing height which corresponds with Equation 32 in Weil, et al., (1997).

“aermod_HBP.f” includes declarations of added variables necessary to save the next hour’s mixing height for EVENT and MAXDCONT processing. Specifically, there are two changes in the subroutine ALLRESULT, which allocates the array to store the convective and mechanical mixing heights. There is also a change in the subroutine MAXD_METEXT which sets the value of the local versions of convective and mechanical mixing height to the values stored in the allocatable arrays.

In essence, the changes in both of these modules are only setting arrays for being able to store additional information needed for other AERMOD HBP Fortran modules.

3.2 Differences between “metext_HBP.f” and regulatory “metext.f”

There are three differences in this code which is designed to read the meteorological files. Two of the changes allow for reading of the next hour’s value for the convective mixing height (stored in ZICONVN) and the mechanical mixing height (stored in ZIMECHN). The third difference is the storing of values of the convective and mechanical mixing heights in the previously declared and allocated “global” arrays.

In essence, these changes are only reading and storing additional information to be used in other AERMOD HBP Fortran modules.

3.3 Differences between “ibval_HBP.f” and regulatory “iblval.f”

There are four additions to subroutine “ibval_HBP.f”, with no lines of AERMOD commented out. The first declares some new variables used to store the values from the next hour: ZIN is the next hour’s ZI (selected mixing height), and ZIAVG is the average of this hour’s and next hour’s ZI. HTOP and HBOT are the top and bottom of the plume, respectively. HTOPDIF is the difference between top of the plume and the average mixing height (ZIAVG). PPWID is the width of plume at 2.15 × sigma-z, where the concentration falls to 10% of its centerline value. These are the key parameters to the differences between regulatory AERMOD and AERMOD-HBP.

The next change selects the next hour’s convective and mechanical mixing heights the same way the current hour’s convective and mechanical mixing heights were selected in AERMOD. For stable conditions, the mechanical mixing height is selected to be used for the remaining calculations. For unstable conditions, the maximum value of ZICONVN and ZIMECHN is selected. In AERMOD, all sunlight hours are assumed to be unstable (convective), and nighttime hours are assumed to be stable.

The code then calculates the average between this hour's selected mixing height (ZI) and the next hour's selected mixing height (ZIN) and stores that value in ZIAVG. Code changes:

```
"C  ******************************* added code --
kja C ** determine next hour mix height ZIN from
mechan
                                                                         eights
           IF(ZICONVN .GT. 0.0D0 .AND. ZIMECHN .GT. 0.0D00) THEN
             ZIN = MAX(ZICONVN,ZIMECHN)
           ELSEIF( ZICONVN .LT. 0.0D0 .AND. ZIMECHN .GT. 0.0D0) THEN
             ZIN = ZIMECHN
           ELSEIF( ZICONVN .GT. 0.0D0 .AND. ZIMECHN .LT. 0.0D0) THEN
             ZIN = ZICONVN
           ELSE
             ZIN = ZI
           END IF
C ** Calculate average height between hours
           ZIAVG = (ZI+ZIN)/2.0D0
           IF(DEBUG) THEN
            WRITE(DBGUNT,6019) ZICONVN, ZIMECHN, ZIN,ZIAVG, HE3
6019       FORMAT(1X,'CONVN= ',F10.2,' MECHN= ',F10.2,' ZIN= ',F10.2,
     &      'ZIAVG= ',F10.2,'HE3= ',F10.2)
           END IF
C  ******************************* added code end -kja"
```

The last difference in this file calculates PPFN, the penetrated plume factor, that is the key difference between AERMOD and AERMOD-HBP:

```
"C  **************************************************  added code --
kja C  ** how much of penetrated plume still above ZIAVG
C  ** assuming gaussian entrainment factor
             HTOP = HE3 + 2.15D0*SZ3  ! top of plume
             HBOT = MAX(HE3 - 2.15D0*SZ3,ZRT)  ! Bottom of plume
C ** width of plume to 2.15 sigma-z - where conc. falls to 10% of centerline
              PPWID = HTOP - HBOT

C ** difference between top of plume and ZIAVG mixing height
             HTOPDIF = HTOP - ZIAVG

             IF (HTOPDIF .GT. 0.0D0) THEN  ! top of plume > mixing ht
C ** PPFN should be between 0 - 1
               IF(HTOPDIF .LT. PPWID) THEN ! mixing ht within plume
                 IF(ZIAVG .LE. HE3) THEN

C ** PPFN from 0 to 0.5 - amount of penetrated plume
entrained C ** lower half of plume
              PPFN = 0.5D0*ERF((ZIAVG-HBOT)/SZ3/DSQRT(2.0D0)) ELSE

C ** PPFN from 0.5 to 1.0 - amount of penetrated plume
entrained C ** more than half of plume entrained
              PPFN = 0.5D0*(1.0D0 +

     &                    ERF((ZIAVG-HE3)/SZ3/DSQRT(2.0D0)))
                ENDIF
               ELSE
C ** whole penetrated plume is still above average mixing
height C ** no contribution from penetrated plume
             PPFN = 0.0D0 ENDIF

             ELSE
C ** whole penetrated plume below below ZIAVG
              PPFN = 1.0D0 END IF

C **************************************************** added code end -kja"
```

The variables are declared as double precision, so the constants (numbers) must be written using exponential notation (normally, 1.0 is written as 1.E0) using the special character "D" to indicate a constant with double precision (i.e., 1.0 is written as 1.D0). This assures no loss of precision due to arithmetic involving constants.

3.4 Differences between "calc1_HBP.f" and "regulatory calc1.f"

There are only two (2) lines changed in subroutine CPLUME() in this Fortran file. The original block:

```
             If  (PPF .LT. 1.0D0) THEN
                 COUT = (QTK * (1.0D0-PPF) / UEFFD) * (FSUBYD*FSUBZD ) +
 &                    (QTK * (1.0D0-PPF) / UEFFN) * ( FSUBYN*FSUBZN ) +
 &                    (QTK * PPF / UEFF3) * ( FSUBY3*FSUBZ3 )
          ELSE
               COUT = (QTK * PPF / UEFF3) * ( FSUBY3*FSUBZ3 ) D
            END IF
```

was changed to:

```
              IF (PPF .LT. 1.0D0) THEN
C  ************************************* modified code  --kja
                 COUT = (QTK * (1.0D0-PPF) / UEFFD) * ( FSUBYD*FSUBZD )
     + &                   (QTK * (1.0D0-PPF) / UEFFN) * ( FSUBYN*FSUBZN
     ) +
     &                   (QTK * PPF*PPFN / UEFF3) * ( FSUBY3*FSUBZ3 )
C    &                   (QTK * PPF / UEFF3) * ( FSUBY3*FSUBZ3 )

              ELSE
                 COUT = (QTK * PPF*PPFN / UEFF3) * ( FSUBY3*FSUBZ3 )
C                COUT = (QTK * PPF / UEFF3) * ( FSUBY3*FSUBZ3 )
C  ************************************* modified code end --kja
              END IF
```

The two key changes are highlighted in green text, with the original line that was "commented out" highlighted in red text and left below the new version of the line.

PPF is the penetrated plume fraction as defined in AERMOD, while PPFN is the penetrated plume fraction calculated using the average of this hour's mixing height and next hour's mixing height and calculated in subroutine IBLVAL in file "IBVAL_HBP.f."

This corresponds to multiplying the term (1-fp) in Equation 66 of the AERMOD Model Formulation and Evaluation Document (MFED) by an extra term PPFN. That equation calculates the contribution to the predicted concentration at a receptor (xr, yr, z) due to the penetrated plume component. The Gaussian equation for the concentration from the penetrated plume (Cp), in both the lateral (xr and yr) and vertical directions (where z is either zr for the horizontal plume state or zp for the terrain-following state)

$$C_p\{x_r, y_r, z\} = \frac{Q\left(1-f_p\right)}{\sqrt{2\pi}\,\tilde{u}\,\sigma_{zp}} F_y \cdot \sum_{m=-\infty}^{\infty}\left[\exp\left(-\frac{\left(z-h_{ep}+2mz_{ieff}\right)^2}{2\sigma_{zp}^2}\right)+\exp\left(-\frac{\left(z+h_{ep}+2mz_{ieff}\right)^2}{2\sigma_{zp}^2}\right)\right]$$

Where Q is the source emission rate, f_p is the penetrated plume fraction, $\tilde{u}$ is the effective wind speed, σ_{zp} is the total dispersion for the penetrated source, F_y is the total horizontal distribution function (with meander), m is the image source (Weil et al., 1997), h_{ep} is the penetrated source plume height (at centerline) above stack base and z_{ieff} is the height of the upper reflecting surface in a stable layer.

AECOM indicates that a deficiency of AERMOD in its treatment of the penetrated plume model is the assumption of a steady-state scenario that does not consider the rate of growth of the convective boundary layer (CBL) during a given hour. As noted below, a recommended approach from Weil et al. (1997) to address the CBL growth by the end of each hour for the penetrated plume dispersion formulation has been implemented into the Highly Buoyant Plume (HBP) modifications to AERMOD.

As noted by Weil et al., (1997), the dispersion of a penetrated plume is an unsteady process, but it is implemented as a steady process in AERMOD due to the inherent limitations of steady-state models. The current AERMOD formulation for the vertical dispersion of the penetrated plume is based upon Eqn. 83 in the AERMOD MFD:

$$\sigma_{zes} = \frac{\tilde{\sigma}_{wT}\, t}{\left[1 + \frac{\tilde{\sigma}_{wT}\, t}{2}\left(\frac{1}{0.36 h_{es}} + \frac{N}{0.27 \tilde{\sigma}_{wT}}\right)\right]^{1/2}},$$

Where σ_{zes} is the elevated portion of the ambient dispersion for the stable plume, the effective value of σ_{wT} is the total vertical turbulence, h_{es} is the plume release height, and N is the stable Brunt-Vaisala frequency. However, for the penetrated plume, AERMOD currently (and inappropriately in some cases) assigns a zero value to N, corresponding to a value in the CBL, implying the assumption that the convective mixing height grows to intercept the entire penetrated plume by the end of the hour. However, in many cases, only a fraction of the penetrated plume mass has been entrained into the CBL by the end of the hour, but AERMOD does not currently check for this entrainment. Paine et al. (2019) suggest a modification that limits the AERMOD calculation for the penetrated plume contribution to the ground-level concentration to the extent to which the growing mixed layer $z_i(t)$ has intercepted the penetrated plume, which effectively adopts the fumigation onset as the dispersion trigger.

Weil et al. (1997) in its Eqn. 31 and 32 provide a formulation for the fraction of the plume mass assigned to the penetrated plume portion that has been intercepted by the CBL:

$$f_p = (1 - f)\frac{f_t f_q}{f_d}. \quad (31)$$

Here, $1 - f$ is the fraction of the source material that is in the penetrated plume, f_d (~0.6) is the fraction of the w PDF comprised by downdrafts, f_t (=0.5) is the fraction of the hourly period over which the penetrated source contributes to the GLCs, and f_q is the fraction of the penetrated plume that is captured by the growing CBL during the second half of the hour.

The f_q is given by

$$f_q = \min\left(\frac{z_{i2} - h_l}{h_u - h_l}, 1\right), \quad (32)$$

where $z_{i2} = z_i$ ($t' = 30$ min) is the CBL height at the end of the hour, and h_l and h_u are the lower and upper heights of the penetrated plume (see Fig. 3).

In this formulation, the full penetrated plume mass fraction is (1-f), defined by f_p in the AERMOD formulation. The remaining terms in Eqn. 31 from Weil et al. (1997) are f_q times 0.5/0.67[9], or rounded up to f_q (also referred to as "f_α" in the HBP implementation. Weil et al. assign fq in their Eqn. 32 to an interpolation of the fractional height of the penetrated plume mass within the CBL. As noted below, the HBP formulation improves upon this interpolation by interpolating the Gaussian plume mass within the CBL with the use of the erf function.

The Highly Buoyant Plume (HBP) option, described in detail by Warren et al. (2022), addresses the limitations of AERMOD for handling the penetrated plume's contribution to ground-level concentrations by checking on the convective mixing height for the current hour (assigned to the midpoint of the hour) as well as the next hour to determine how much of the penetrated plume has been captured by the convective boundary layer by the end of the current hour. An average mixing height ($\bar{z_i}$) based on the averaged current and next hour mixing heights is used as a measure of the mixing height at the end of the hour. If three key conditions are met (unstable atmospheric conditions, stack height lower than the mixing height and $f_p > 0$), an entrainment adjustment factor (f_α) is calculated that scales down fp to mitigate the late morning overpredictions. If these key conditions are met, HBP considers three cases based on the height of the averaged mixing layer with respect to the bottom and top of the penetrated plume (hbot and htop, respectively):

1. IF $\bar{z_i} < h_{bot}$ → $f_\alpha = 0$;
2. IF $\bar{z_i} > h_{top}$ → $f_\alpha = 1$;
3. ELSE → $0 < f_\alpha < 1$

[9] In the explanation of the equation 31 in Weil et al (1997), this fraction is derived from the solution of the vertical velocity PDF where approximately 60% of the PDF is comprised of downdrafts (f_d) and during which 50% of the hourly period (f_t) the penetrated plume contributes to the ground level concentration (GLC).

For the third case, fα can be obtained by integrating equation 1 over all possible heights yielding a piecewise solution based on the position of the averaged mixing height within the penetrated plume:

$$f_\alpha = \frac{1}{2}\operatorname{erf}\left(\frac{z_i - h_{bot}}{\sqrt{2}\sigma_{zp}}\right) \qquad \text{for } h_{bot} < \bar{z_i} < h_{ep}$$

$$f_\alpha = \frac{1}{2}\left[1 + \operatorname{erf}\left(\frac{z_i - h_{ep}}{\sqrt{2}\sigma_{zp}}\right)\right] \qquad \text{for } h_{ep} < \bar{z_i} < h_{top}$$

where erf is the error function. The error function is used to evaluate the area under the curve of the integrated equation 1 to obtain a percentage of the mass entrained within the averaged mixed layer.[10]

With f_α calculated, the contributions from the entrained penetrated plume (Cpα) can be determined:

$$C_{p\alpha}\{x_r, y_r, z_r\} = f_\alpha C_p$$

Finally, the total concentration in the CBL (CC) can be evaluated:

$$C_c\{x_r, y_r, z_r\} = C_d\{x_r, y_r, z_r\} + C_r\{x_r, y_r, z_r\} + C_{p\alpha}\{x_r, y_r, z_r\}$$

where C_d and C_r are the contributions from the direct and indirect sources, respectively. Note that the entrainment adjustment factor is only used to adjust the penetrated plume and does not affect the direct or indirect components of the plume.

3.5 Conclusions

Ramboll documented the code changes between the 24 May 2021 version of AERMOD-HBP variant and regulatory version of AERMOD v21112. Three of the five changed Fortran files differ only in ways to facilitate the reading of the "next" hour's mixing height, with all but one of the other changes used to store the "next" hour's mixing heights for use with EVENT and MAXDCONT processing (AERMOD options).

Subroutine IBLVAL (in file iblval.f), which calculates effective parameters for the inhomogeneous boundary layer (IBL), is where the key changes have been made to calculate an additional fraction of the penetrated plume (PPFN). PPFN is applied in subroutine CPLUME (in file calc.f) which calculates the contribution to the concentration due to the plume components.

[10] In Weil et al. (1997), Eq. 32 provides a linear equation for defining the entrainment adjustment factor. However, by integrating the Gaussian penetrated plume equation and using the error function, a more refined solution can be determined based on a Gaussian bell-shaped cross section of mass rather than a step-function uniform cross section (i.e., "top hat" shape) for which the linear fα is a solution.

Direct comparison between the equations expressed in the AERMOD-HBP Fortran code and equations given in either Weil et al. (1997) or Weil (2019 PD V4 and 2019) is not clear, despite the reference to the discussion on page 988 of Weil et al. (1997) given in Paine et al. (2020). Neither Weil (1997) nor Weil (2019 PD V4 and 2019) mentions reading the next hour's mixing heights and averaging with the current hour's mixing height, nor explicitly lists the equations implemented in subroutine IBLVAL in the file iblval_HBP.f.

The formulation of AERMOD's predecessor model, the Industrial Source Complex model (ISC3) assumed that if the center of the plume was above the mixed layer height, the ground-level concentrations would be zero (EPA 1995, page 1-32). It seems likely that the original formulation of AERMOD (averaging dispersion characteristics over the full plume, essentially applying characteristics from below the mixed layer to dispersion characteristics above the mixed layer) was an attempt to refine ISC3's simple formulation. The penetrated plume treatment in the AERMOD-HBP code attempts to refine this assumption further, to apply the highly dispersive characteristics of the mixed layer to only the portion of the plume below the mixed layer height by adjusting the amount of penetrated plume that is subject to calculations of impacts on receptors.

The following analysis of these changes in the following sections and whether the AERMOD-HBP performs better than AERMOD is limited to the specific Martin Lake site and for this time period for this review of an alternative model.

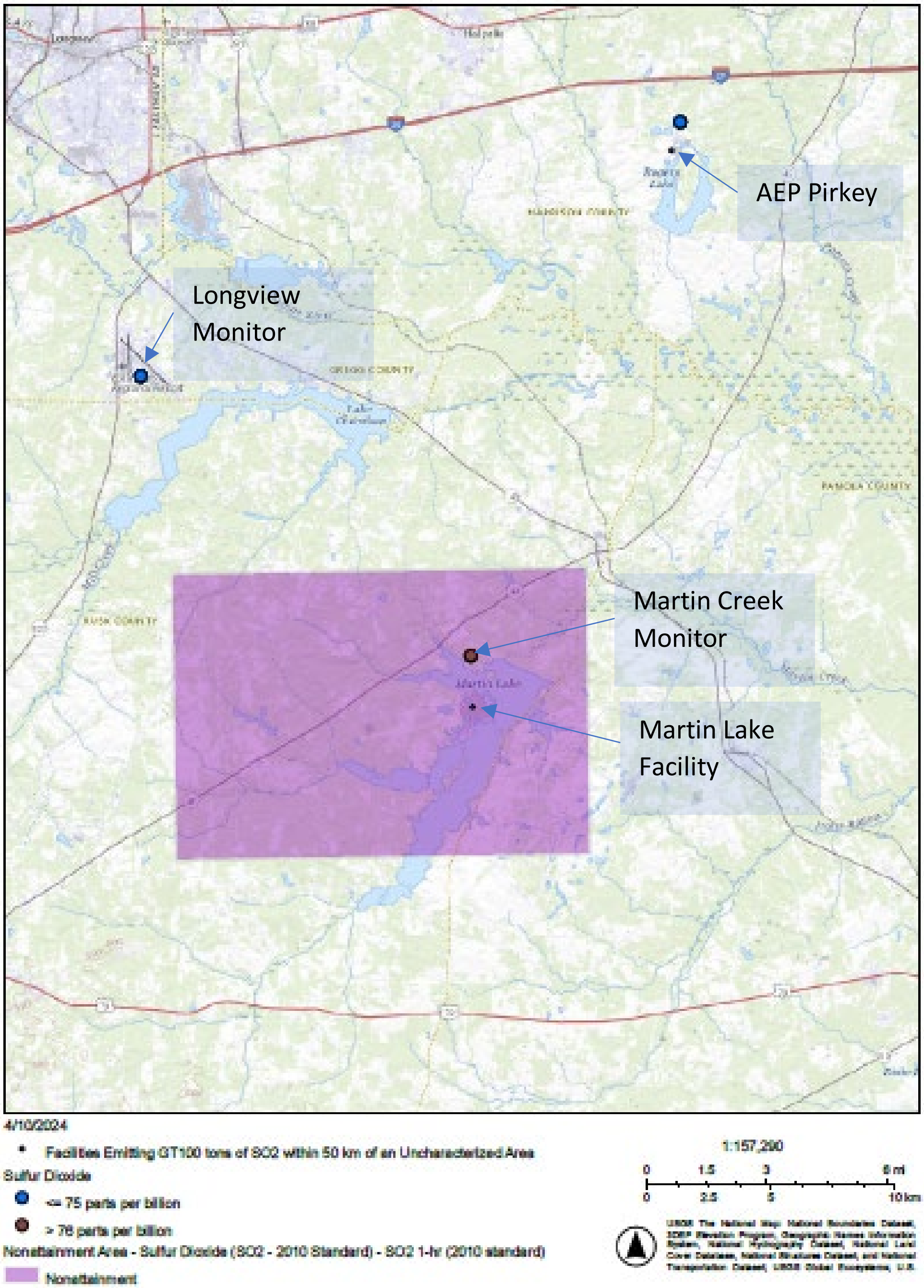
In Attachment 4 to AECOM's May 1st 2024 documentation submittal to EPA Region 6, AECOM provided clarifying information including some flow charts for these modifications and how the code works with each of the three cases (Case 1- No contribution of penetrated plume, Case 2 – All of the penetrated plume is available to contribute to ground level concentrations, Case 3 – Partial contribution of pentrated plume to ground level concentrations) including some example situations for each of these cases.

4. AERMOD setup and modeling datasets used for Model Evaluation

4.1 AERMOD modeling setup and datasets

For this alternative model equest there are two monitors in the area that EPA Region 6 and TCEQ agreed to utilize to evaluate the regulatory version of AERMOD (v21112 at the time) and the proposed alternative model AERMOD-HBP. The Martin Creek monitor (approximately 2 km from Martin Lake's main boiler stacks) started monitoring in late 2017 and had three complete years of data (2018-2020) at the tirme AECOM and TCEQ were preparing this alternative model request in 2021. Since only one near-field monitor was available for three years, EPA Region 6 and TCEQ agreed that the analysis should also compare modeled values with observed values at the Longview Airport monitor (approximately 19 km away from Martin Lake's main boiler stacks) that has been operating for much longer and the evaluation should use the most recent five years of observations available at the time (2016-2020).

Figure 4.1-1 Location of Martin Lake Generating facility, and Longview and Martin Creek SO2 monitors



Modeling for this analysis used surface meteorology data collected from the National Weather Service (NWS) station located at the Longview Airport, the SO_2 monitor located near the Longview airport and NWS upper air data from the Shreveport, Louisiana Regional Airport station. Meteorological data was processed with AERMINUTE and AERMET. AERSURFACE was used to develop surface characteristics for the Longview Airport NWS site. Meteorological processing was completed pursuant to EPA Region 6's recommendations and no issues were discovered in EPA Region 6's review.

For emissions, TCEQ's and AECOM's modeling used varying hourly emission rates and stack parameters (temperature and velocity) for the 2016 through 2020 timeframe as provided by Vistra. The data does include substituted data following the missing data procedures in the 40 CFR Part 75 requirements. The spreadsheet "2021-07-20 Martin Lake Substitute SO_2 Data.xlsx" included in materials VISTRA provided provides a list of the dates/times that have substituted data. TCEQ did not make any changes to this data provided by Vistra.

For comparison of regulatory version of AERMOD with AERMOD-HBP, TCEQ located receptors at the Martin Creek and Longview SO_2 monitoring sites. TCEQ also proposed to place a microgrid of additional receptors radially around the Longview and Martin Creek monitors to try to account for potential uncertainties in replicating spatiotemporal patterns and allow for more in-depth analysis using a +/- 2 degree arc downwind from the Martin Lake Generating facilty to each monitor. TCEQ sited that accuracy in wind measurement can vary by +/- 2 degrees as the reasoning for choosing the value used for determining the width (radius) of the microgrid around each monitor.

TCEQ proposed using the following spacing of receptors for each monitor (See Figure 4.1-2)

- Longview
    - 30 degree spacing for radius of 20 m;
    - 24 degree spacing for radius of 60 m; and
    - 15 degree spacing for radii of 150 m, 250 m, and 500 m.
- Martin Creek
    - 30 degree spacing for radius of 20 m; and
    - 15 degree spacing for radius of 60 m.

Figure 4.1-2 TCEQ's proposed Microgrid centered on Longview (left) and Martin Creek (right) monitors.

EPA Region 6 reviewed the approach of using a microgrid for evaluation of model performance in the context of alternative model review and found that this approach did not comport with EPA's guidance on model evaluations (EPA 1992 Model Evaluation Guidance).[11] EPA Region 6 had a concern that this could result in a potential bias compared to the standard model performance approach of using a receptor at the monitor with observations and would not be comparable with the selection of model performance evaluation metrics and values used in either screening or refined Cox-Tikvart analyses of EPA's guidance and in other model evaluations that EPA has performed and/or reviewed.

TCEQ also did some diagnostic modeling on a larger receptor grid that consisted of a 25.5 km by 24.5 km rectangular area centered around Martin Lake's S1 source with three nested receptor grids. The innermost grid spans 0 to 3 km from the center point, encompassing Martin Lake, with 50 m spacing between receptors. The middle-nested grid extends from 3 km to 9 km, with 100 m spacing between receptors. Receptors in the outermost grid, which covers the rest of the domain, have 500 m spacing. Figure 4.1-3 shows the larger receptor grid that covers the entire nonattainment area.

Receptors within the property owned and controlled by Vistra and considered non-ambient were removed from the grid. The non-ambient areas were determined based on discussions between Vistra, TCEQ, and EPA Region 6. Receptors were added with 25 m spacing along the non-ambient air boundary lines and along the section of public road within Vistra's property. Figure 4.1-4 shows a map of the receptor placement that shows the non-ambient Vistra property boundary. An additional receptor has been placed at the location of the Martin Creek monitor.

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[11] 1. Environmental Protection Agency, 1992. Protocol for Determining the Best Performing Model (EPA-454/R-92-025). U.S. Environmental Protection Agency, Research Triangle Park, NC.

Receptor heights were processed using the AERMAP terrain processor (Version 18081) with elevation data from the National Elevation Dataset (NED), developed by the United States Geological Survey (USGS). The same receptor grids were used in model runs with both AERMOD and AERMOD-HBP.

Figure 4.1-3 Larger modeling grid covering the 2010 Rusk-Panola Nonattainment Area.

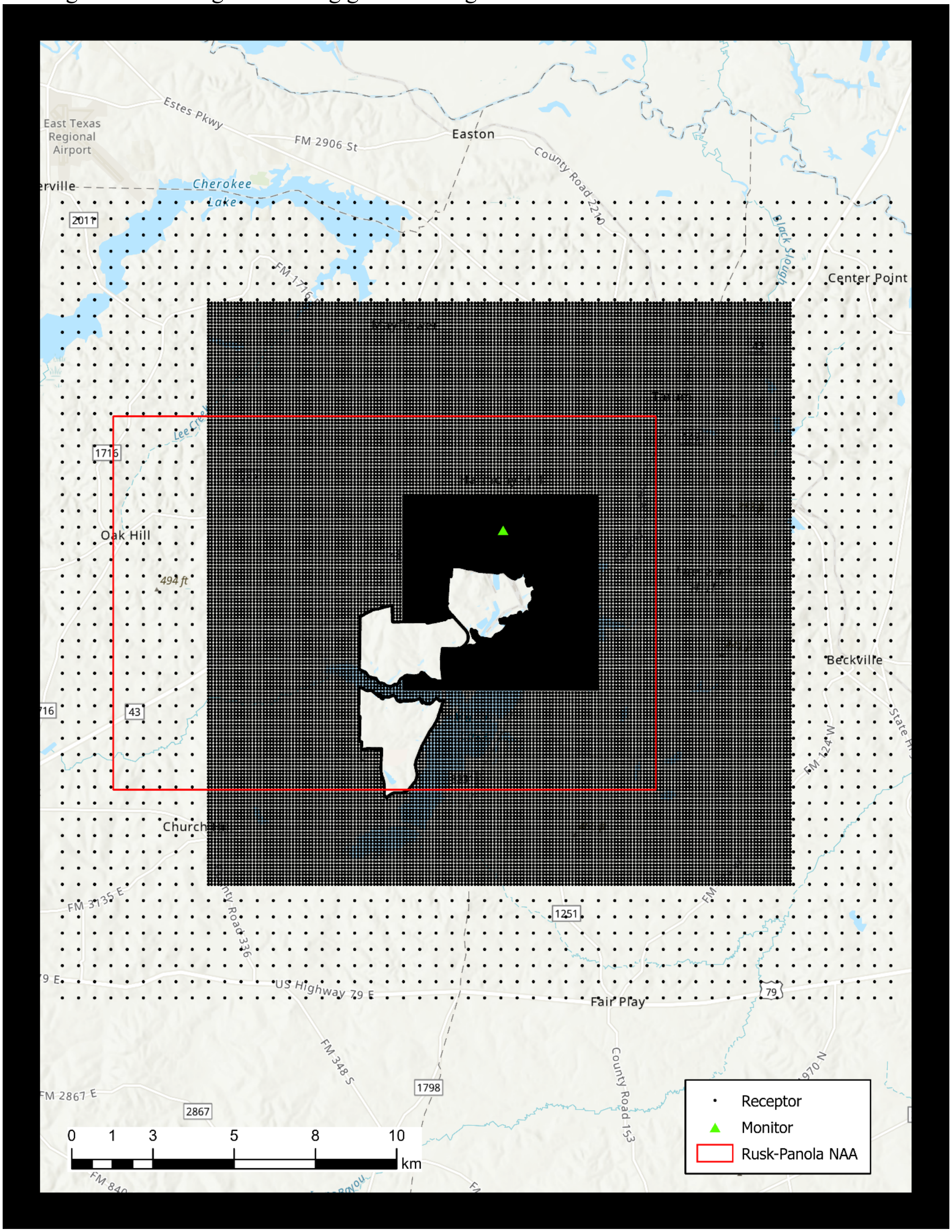


Figure 4.1-4 Map of Receptor Placement Around Non-Ambient Boundary

TCEQ's modeling also evaluated on-site structures and building downwash effects using BPIPPRM.

Vistra reviewed buildings and stack locations in July 2021 and provided TCEQ with updated locations. TCEQ provided some updated modeling results indicating the maximum did not significantly change. They provided the modeled concentrations at the Martin Creek and Longview monitors for the different model runs and the largest variation in DV was 0.69 ppb (133.535 ppb vs.134.228 ppb) at the Martin Creek monitor and 0.137 ppb (45.4368 vs. 45.2998 ppb) at Longview monitor.[12] TCEQ did not redo the full modeling evaluation since they felt these differences were relatively small compared to the modeled values. EPA Region 6 did modify the stack locations, redid the BPIPPRM analysis and reran much of the key model comparison analysis to verify the evaluation was not significantly impacted by the error in stack locations. We discuss our results in Section 5 with TCEQ's results where appropriate.

[12] TCEQ file "mpe-runs_orig_loc2.diff.xlsx"

5. Alternative Model Evaluation (AERMOD-HBP) vs. Regulatory Version of AERMOD

Model evaluation under App. W, Section 3.2.2(b) requires that a statistical performance evaluation is conducted using measured air quality data and that the results of that evaluation indicate the alternative model performs better for the given application than a comparable model in appendix A. EPA's primary guidance for performing an evaluation of differing models was included in EPA's 1992 Protocol for Determining the Best Performing Model.[13] This guidance prescribes a statistical test procedure commonly referred to as the Cox-Tikvart method that includes a screening component and a refined analysis for determing the best performing model.

While AERMOD and AERMOD-HBP share much of the same formulation, there are times when the difference in treatment of penetratred plume results in different concentrations. Dispersion in AERMOD-HBP is treated differently than AERMOD when the convective boundary layer begins to intersect the penetrated plume. Therefore, concentrations only differ for those hours where the mixed layer height is between the bottom of the plume and the center of the plume. Both models are expected to produce identical results during stable (night-time) conditions; for hours when the entire plume is above the mixed layer (i.e., when the mixed layer height is shallow, early in the morning); and for those hours where the mixed layer height exceeds the plume height (i.e., when mixed layer is high, late in the day).

To identify and help assess the differences between the two models TCEQ and EPA generated a number of different analyses including (for each year and for some multiple years combined): Q-Q plots, daily and hourly time series trends in concentrations, plots for 90^{th} and 95^{th} percentile concentrations and plots of the 10 highest observed and modeled daily maximum values. To further understand model performance across the distribution of observed and modeled values unpaired in time, Q-Q plots that compare ranked hourly concentrations were generated for the Longview and Martin Creek monitors by year with extra high concentration data points. Time series of observations, AERMOD modeled values, and AERMOD-HBP modeled values were generated for the hourly 1-Hour SO_2 values and also the Daily maximum 1-Hour SO_2 values for each year modeled.

Plots were also generated that compared observed and modeled (AERMOD and AERMOD-HBP) concentrations over the date of the nth percentile observed values as well as modeled concentrations during nth-percentile days. The daily concentration trends were compared based on the statistic (e.g. 95th percentile daily max value) in addition to presenting comparisons paired in time.

As steady state models with a 1-hour timesteps, AERMOD and AERMOD-HBP modeled concentrations are not expected to always match nearly or exactly with monitored concentrations when paired in both space and time but are expected to perform well in a

[13] Environmental Protection Agency, 1992. Protocol for Determining the Best Performing Model (EPA-454/R-92-025). U.S. Environmental Protection Agency, Research Triangle Park, NC.

statistical assessment replicating the statistical distribution of observed concentrations of datasets, especially on the values around the NAAQS.

As described in App. W, Section 3.2.2(d), for alternate model evaluations, established statistical performance evaluation procedures should be used. The Cox-Tikvart protocol method (EPA, 1992) has been used extensively for evaluating models. For the AERMOD-HBP evaluation, EPA used the Cox-Tikvart method to compare the model performance of AERMOD and AERMOD-HBP at the Martin Creek and Longview monitors.

5.1 Cox-Tikvart Screening Test

As an initial screening step, the fractional bias of the average and standard deviation is used as a metric. For each monitoring station (Longview and Martin Creek) the SO_2 concentrations were sorted by year and then by averaging period. From this data, the 25 highest observed concentrations, unpaired in space or time, are used to calculate a mean and standard deviation. The same procedure is applied to the predicted concentrations obtained from the air dispersion models AERMOD and AERMOD-HBP, using the highest value over the receptor sets for each hour. Using these top 25 values, the fractional bias of the average and of the standard deviation are determined for each model for 1-hour, 3-hour, and 24-hour averages. Fractional bias is calculated using Equation 5-1:

EQUATION 5-1

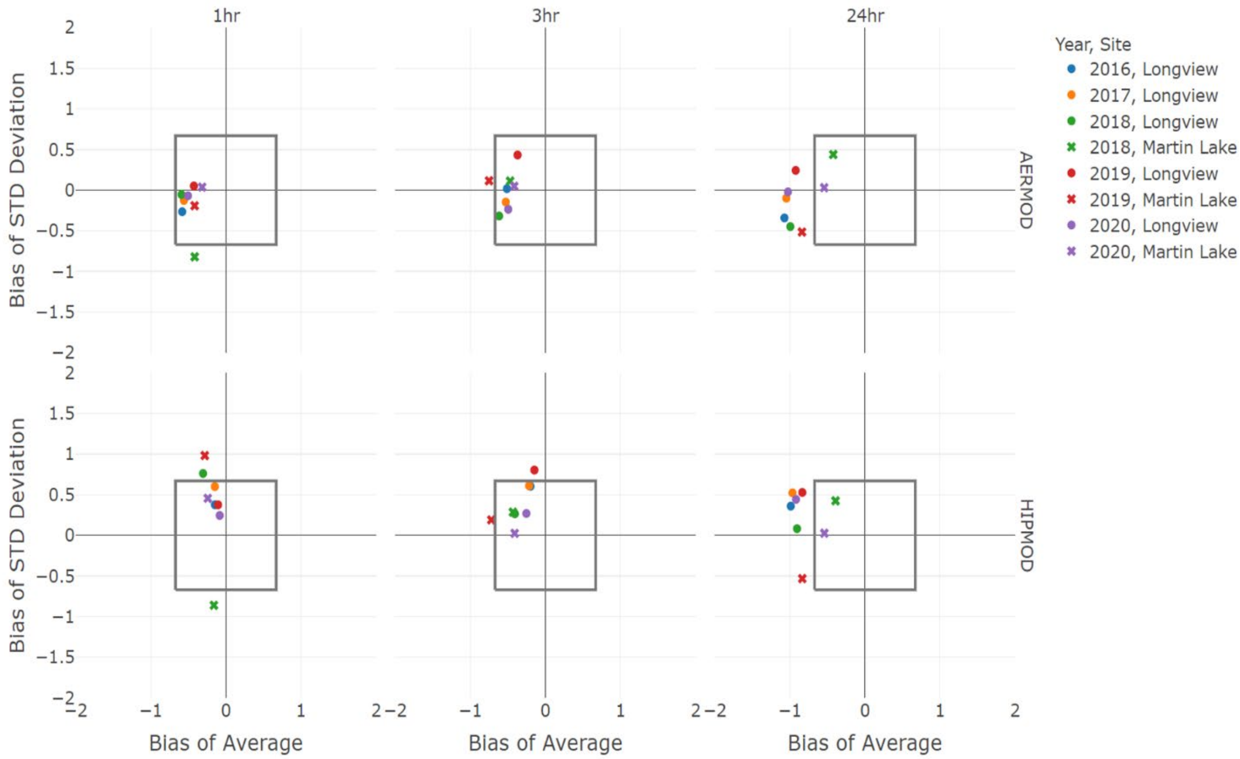
$$FB = 2 \cdot \frac{(Mean_{OBS} - Mean_{PRD})}{(Mean_{OBS} + Mean_{PRD})} \qquad (1)$$

It is important to note that the above equation will result in a negative bias when the model overpredicts and a positive bias when the model underpredicts. A positively biased standard deviation indicates that there is less variance in the top 25 predicted values compared to observations.

Fractional biases were calculated for 1-hour, 3-hour, and 24-hour averaged concentrations. If fractional biases for most periods, years, and sites are within 0.67 (equivalent to a factor of 2), the model demonstrates adequate performance to proceed to more in-depth analyses.

TCEQ's screening results were plotted as individual years for each monitor (2016-2020 for Longview Monitor and 2018-2020 for Martin Creek monitor). We replicated TCEQ's breakdown by doing each year separately for each monitor as that provided more details on how HBP was resulting in different changes yearly. See Figure 5.1-1. In general this showed that AERMOD-HBP shifted the 1-hour standard deviation to a higher value but also decreased the amount of 1-hour negative bias. For the 1-hour, the eight unique combinations of year and monitor pairs resulted in an increase of one to three of the 8 pairs outside the box goal range of the two metrics. For the 3-hour metric, AERMOD-HBP had similar shift of the standard deviation to a higher value, bias was improved most years to be less negative, and a shift from one year and monitor pairing to two year and monitor pairings was slightly outside the box goal. For the 24-hr metric, AERMOD-HBP had similar shift of standard deviation to a higher value, bias was improved most years to be less negative, and a shift from one year and monitor pairing to two year and monitor pairings was slightly outside the box goal.

Figure 5.1-1 TCEQ's individual year Cox-Tikvart screening analysis values for each monitor.



EPA Region 6 remodeled with corrected stack locations for Martin Lake and redid the Cox-Tikvart screening analysis. See Table 5.1-1 for EPA Region 6's detailed results. EPA Region 6 looked at the data three ways: Longview monitor with five years combined 2016-2020 by itself, Longview and Martin Creek for 2018-2020, and Martin Creek monitor by itself (2018-2020). In general AERMOD-HBP performance was similar when looking at Longview and Martin Creek monitors combined, and also Martin Creek by itself resulted in same results because the Martin Creek high values are much larger than Longview's high values. Overall for these two sets of 2018-2020 data, AERMOD-HBP improves or slightly improves the mean bias for all three hour bins (1-hour, 3-hour, and 24-hour) and improved standard deviation bias for 1-hour and 3-hour with slight degrade for 24-hour. For the Longview only dataset, AERMOD-HBP improved Mean Bias for all 3 averaging times; Standard Deviation Bias was mixed with improvement in 3-hour and 24-hour with an increase for the 1-hour averaging time.

Table 5.1-1 EPA Region 6 Cox-Tikvart Screening Analysis Results.

Longview (2016-2020)			
SCENARIO	AVG Time	Mean Bias	Std. Dev. Bias
DEFAULT	1-HOUR	-0.369574	0.01896
DEFAULT	3-HOUR	-0.379951	-0.77451
DEFAULT	24-HOUR	-0.680218	-0.166682
HBP	1-HOUR	-0.000713	0.513465
HBP	3-HOUR	-0.081869	-0.196924
HBP	24-HOUR	-0.541713	0.498258
Longview-Martin Creek (2018-2020)			
SCENARIO	AVG Time	Mean Bias	Std. Dev. Bias
DEFAULT	1-HOUR	-0.29508	-0.358
DEFAULT	3-HOUR	-0.31633	0.025752
DEFAULT	24-HOUR	-0.4048	-0.02223
HBP	1-HOUR	-0.1261	-0.19769
HBP	3-HOUR	-0.28933	0.001269
HBP	24-HOUR	-0.39618	-0.058222
Martin Creek (2018-2020)			
SCENARIO	AVG Time	Mean Bias	Std. Dev. Bias
DEFAULT	1-HOUR	-0.29508	-0.358
DEFAULT	3-HOUR	-0.31633	0.025752
DEFAULT	24-HOUR	-0.4048	-0.02223
HBP	1-HOUR	-0.1261	-0.19769
HBP	3-HOUR	-0.28933	0.001269
HBP	24-HOUR	-0.39618	-0.058222

Overall these values remained in the +/- 0.67 range in EPA's Cox-Tikvart screening so this metric is met and indicates a full Cox-Tikvart analysis should be completed.

5.2 Cox-Tikvart

Since AERMOD-HBP compared to AERMOD passed the screening test, AERMOD-HBP was subjected to a more comprehensive Cox-Tikvart protocol statistical comparison. The performance of AERMOD-HBP was compared with the performance of the regulatory version of AERMOD using a composite statistical measure that combines the performance of the scientific component (1-hour averages) and the operational component (3-hour and 24-hour averages).

The scientific component assesses the 1-hr averages during 6 specific meteorological conditions. The meteorological conditions are unique combinations of unstable (class A, B, C), neutral (class D), or stable (class E, F) conditions and wind speeds above or below 3 m/s. The 50th percentile of observed wind speeds is just over 3 m/s, so this cut-off value sorts the data approximately in half.

The Golder (1972) nomogram method was used to convert AERMET's Monin-Obukhov length and roughness length to stability class, using Fortran code taken from the Mesoscale Model Interface Program (MMIF7).

The robust highest concentration (RHC) is a comparison of modeled and observed concentrations at the upper end of a frequency distribution and is calculated using Equation 5-2 where n=26, cn is the nth highest concentration, and $\bar{c}$ is the average of the (n-1) highest concentrations.

EQUATION 5-2

:

$$RHC = c_n + (\bar{c} - c_n) ln\left(\frac{3n-1}{2}\right) \qquad (2)$$

For each meteorological condition, the RHC is calculated for both the observed and modeled dataset and the fractional bias (FB) as well as absolute fractional bias (AFB) between the modeled and measured RHC using Equation 5-3 and Equation 5-4, respectively.

EQUATIONS 5-3 and 5-4

$$AFB = \left|2 \cdot \frac{(RHC_{measured} - RHC_{modeled})}{(RHC_{measured} + RHC_{modeled})}\right| \qquad (4)$$

$$FB = 2 \cdot \frac{(RHC_{measured} - RHC_{modeled})}{(RHC_{measured} + RHC_{modeled})} \qquad (3)$$

The operational component evaluates the peak 3-hour and 24-hour averages independent of meteorology or spatial location. The absolute fractional bias between measured and modeled RHC is calculated in a similar manner except that the data is grouped into 3-hour and 24-hour averages, respectively.

A composite performance metric (CPM) combines the 1-hr, 3-hr, and 24-hr absolute fractional biases in RHC for both the scientific and operational components, as shown in Equation 5-5. Where AFB(i,j) is the absolute fractional bias for each meteorological condition and each station, AFB(3) is the absolute fractional bias for 3-hour averages, and AFB(24) is the absolute fractional bias for 24-hour averages.

EQUATION 5-5

$$CPM = \frac{(\, average(AFB(i,j) + AFB(3) + AFB(24))}{3} \qquad (5)$$

The CPM is lowest when there is a good agreement between measured and modeled RHC values. Comparing the magnitudes of the CPM values from different models using the same observational data allows for relative comparisons of the model performance of each dispersion model.

To improve the robustness of data used for model comparison, a statistical technique known as bootstrapping was used to generate a probability distribution of outcomes. The bootstrap method resamples the available data into three-day blocks. These blocks are grouped by season (regardless of year), then sampled with replacement until a full season of data is created. After 1,000 iterations of this process, the standard deviation of generated runs is used as the standard error for model comparison. TCEQ's Python script used to run the bootstrap analysis is available upon request.

To highlight differences between models and to determine which model performs better, the Model Comparison Measure (MCM) is used. This is simply the difference in CPM between two models, as described by Equation 5-6.

EQUATION 5-6

$$MCM = CPM(a) - CPM(b) \qquad (6)$$

A positive MCM indicates better performance from model b than model a, and vice-versa.

TCEQ performed the Cox-Tikvart full analysis using three different methods for receptor(s) to compare with monitored values:

1. Standard Methodology - One modeled receptor placed at the location of the monitor, with concentrations from both sites pooled.
2. Single Receptor - One modeled receptor placed at the location of the monitor, with concentrations from each site treated separately.
3. TCEQ also provided a 2° Microgrid approach for modeled value to compare with monitored value – max hourly concentrations from a microgrid of modeled receptors centered on the monitor, with concentrations from each site treated separately.

Option 1 is consistent with the standard Cox-Tikvart methodology (EPA, 1992). EPA Region 6 asked for the Option 2 approach as well since one monitor is 2 km away and one monitor is 19 km away from Martin Lake. EPA Region 6 did not use the 2° Microgrid approach in our evaluation as we have concerns that it changes the statistical pattern of the data being used to compare with a single monitored value and deviates from EPA's guidance on comparing models (including EPA's 1992 Model Comparison Guidance) without a full evaluation of what impacts TCEQ's microgrid approach may have on the underlying metrics and guidance on what values are appropriate cutpoints that EPA's current model comparison guidance is based on using a single receptor modeled at the monitor to compare with the observation at a monitor, and, therefore, EPA is concluding the Microgrid approach is not appropriate for this evaluation.

Since the RHC is calculated using the top 25 values and concentrations at a receptor 2 km downwind will generally be much higher than those at 19 km, if sites are pooled, RHC values will be dominated by near-field concentrations. Evaluating each site independently does provide additional insight into HBP's model performance at a range of distances.

TCEQ provided Fractional Bias and Absolute Fractional Bias (Figures 5.2-1 and 5.2-2 respectively) using the standard method at both monitors and AERMOD-HBP resulted in closer to zero fractional bias, especially for 1-hour and for the CPM compared to AERMOD. The absolute fractional bias also was reduced for the 1-hour, and similar for 3-hour and 24-hour and the resultant CPM was lower, so AERMOD-HBP performed better than AERMOD, especially for the 1-hour.

Figure 5.2-1 TCEQ's Fractional Bias Standard Methodol

ogy (both Martin Creek and Longview monitor data with receptor at monitor sites).

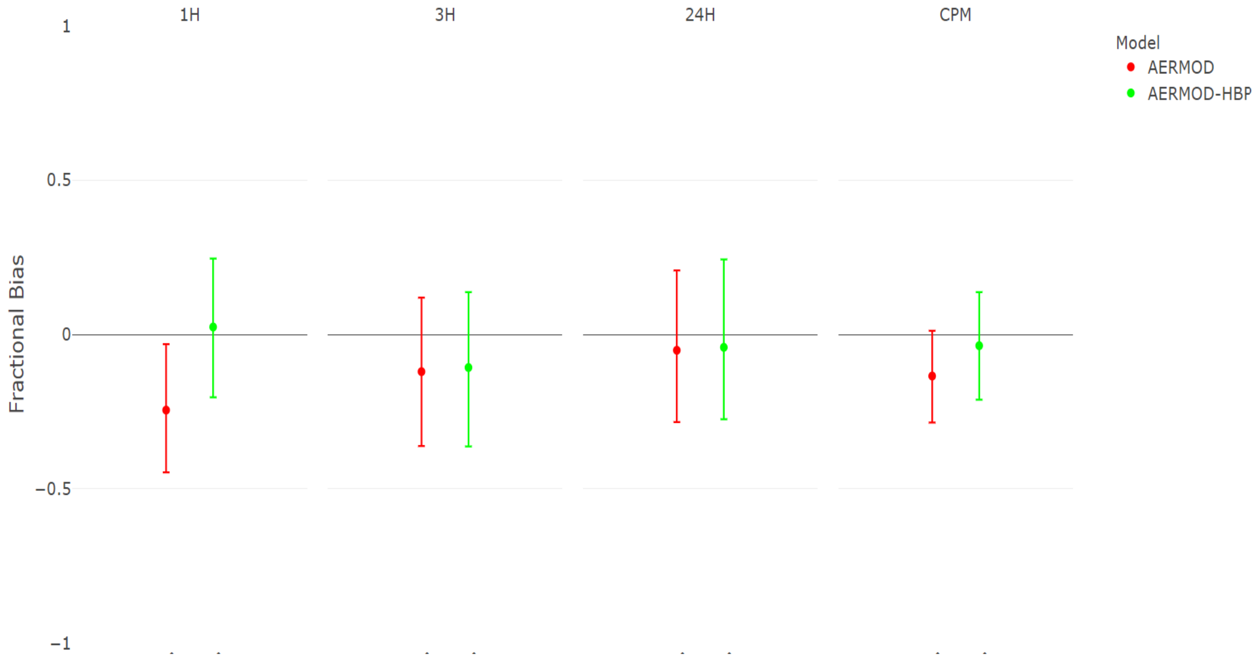


Figure 5.2-2 TCEQ's Absolute Fractional Bias Standard Methodology (both Martin Creek and Longview monitor data with receptor at monitor sites).

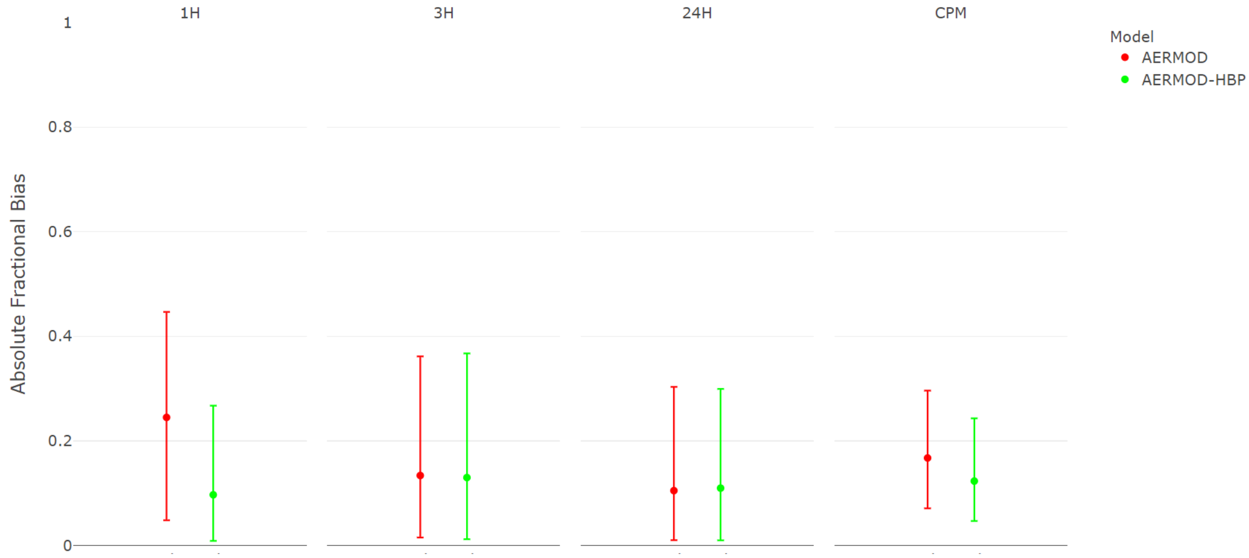


Figure 5.2-3 TCEQ's Model Comparison Standard Methodology (both Martin Creek and Longview monitor data with receptor at monitor sites)

- Model Comparison Measures

MCM (AERMOD - AERMOD-HBP)	BEST PERFORMING MODEL
0.04	AERMOD-HBP

- Composite Performance Summary

AVERAGING PERIOD	ABSOLUTE FRACTIONAL BIAS		DIFFERENCE (D)	STD ERROR (S)	RATIO (D/S)
	AERMOD	AERMOD-HBP			
1HR	0.24	0.10	0.15	0.08	1.81
3HR	0.13	0.13	0.004	0.11	0.04
24HR	0.10	0.11	-0.006	0.09	-0.06
CPM	0.17	0.12	0.04	0.06	0.68

Figure 5.2-3 includes TCEQ's MCM, absolute fractional bias for each averaging period and CPM value (each period weighted evenly), the difference, standard error, and ratio. Of note is the improvement in 1-hour absolute fractional bias and the 1-hour ratio which both stand out as showing AERMOD-HBP performs better than AERMOD. We also evaluated the information that TCEQ provided looking at each monitor individually in comparison with EPA Region 6's Cox-Tikvart analysis of EPA Region 6's modeling. We note that for the CPM ratio it is 0.68 and ratios within ± 1.7 is typically not considered to be statiscally significant, but the 1-hour Ratio is 1.81 which is statistically significant and of interest since the modeling is for the 1-hour standard.

Figures 5.2-4 and 5.2-5 include the fractional bias and absolute fractional bias on a monitor specific basis for the Longview and Martin Creek monitors. Figure 5.2-4 indicates that AERMOD-HBP improves the fractional bias at Longview for the 3-hour, 24-hour, and CPM and changes the fractional bias from negative to a higher positive value in the absolute value. For Martin Creek AERMOD-HBP improves 1-hour, 3-hour, and CPM fractional bias while 24-hour fractional bias is similar. Figure 5.2-5 indicates that AERMOD-HBP's absolute fractional bias is better for the 3-hour, 24-hour, and CPM, but slightly worse for the 1-hour for Longivew. It also indicates that AERMOD-HBP's absolute fractional bias is better for 1-hour and CPM but similar for 3-hour and 24-hour at Martin Creek. Figure 5.2-6 indcates that AERMOD-HBP is the better performing model based on the MCM's for Longview and Martin Creek.

Figure 5.2-4 TCEQ Fractional Bias Monitor Specific – Single Receptor

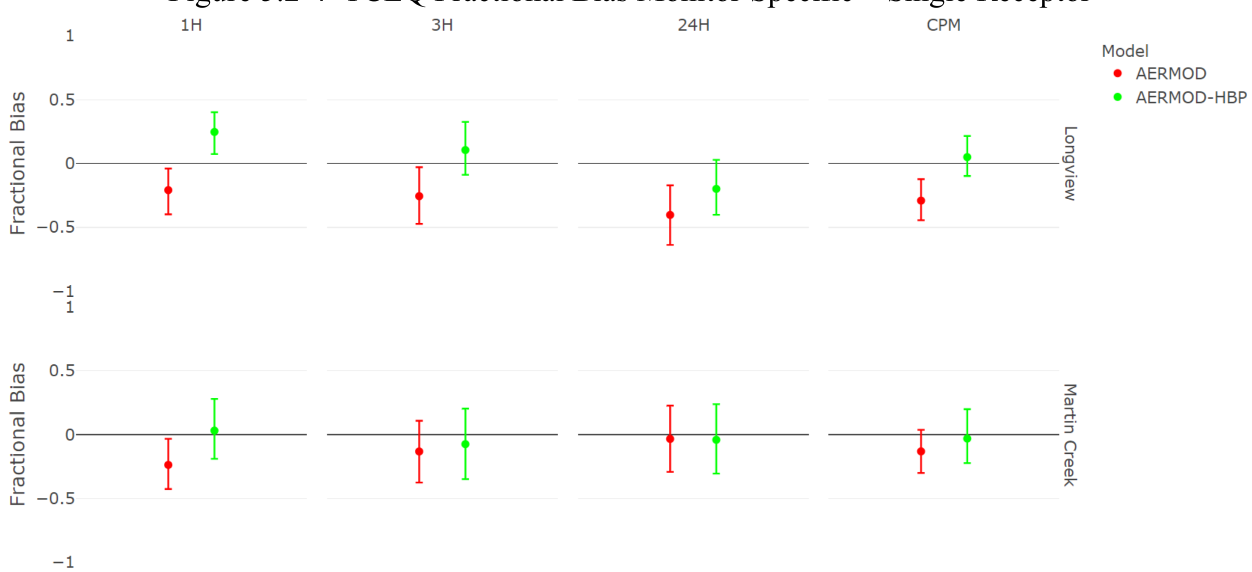


Figure 5.2-5 TCEQ Absolute Fractional Bias Monitor Specific – Single Receptor

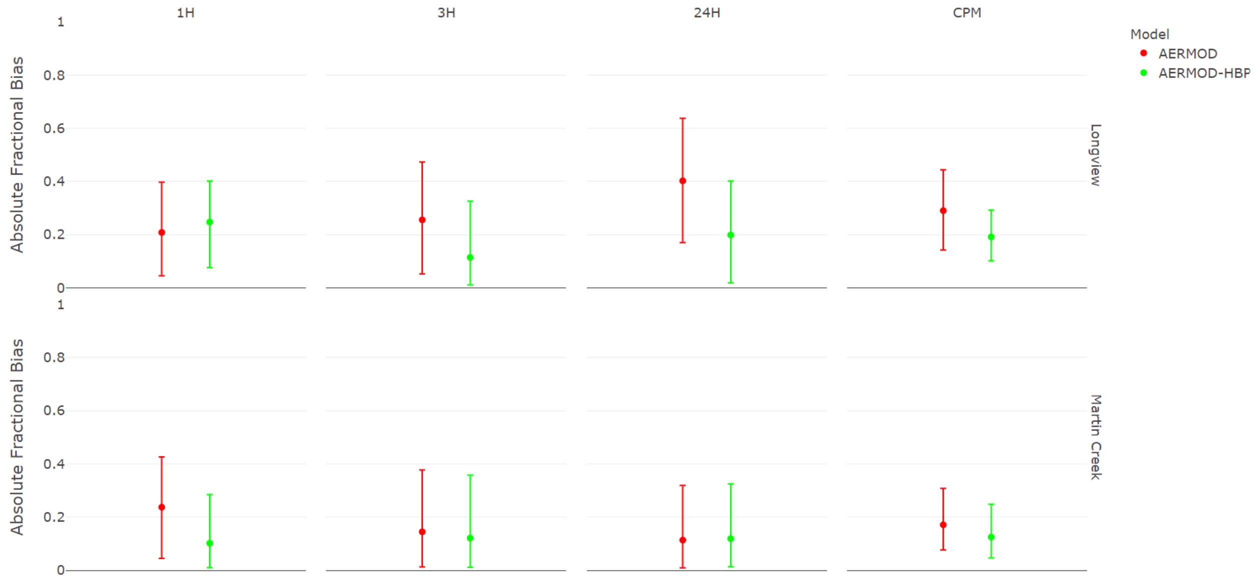
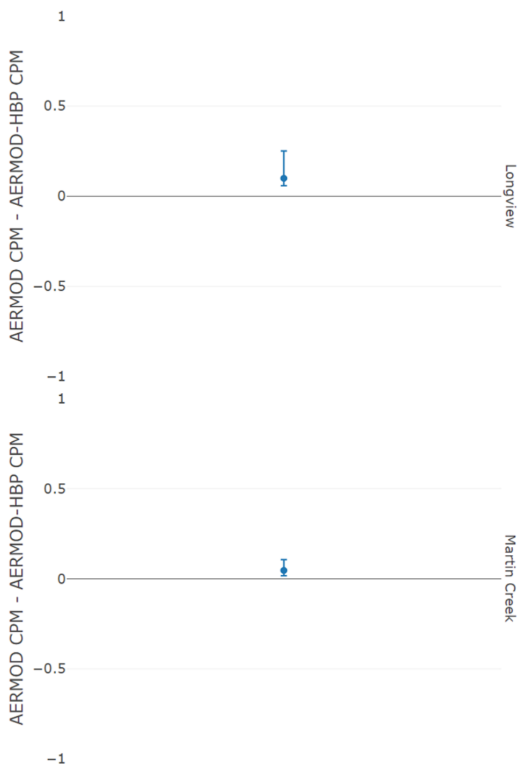


Figure 5.2-6 Model Comparison Measure Monitor Specific – Single Receptor



SITE	MCM (AERMOD - AERMOD-HBP)	BEST PERFORMING MODEL
Longview	0.10	AERMOD-HBP
Martin Creek	0.12	AERMOD-HBP

TCEQ's results are summarized in Figures 5.2-7 and 5.2-8. We note that for the CPM ratio it is 1.13 for Longview and 1.48 for Martin Creek, and Martin Creek is closer to the ratio cutpoint of what is typically considered statistically significant (± 1.7). We also note that the 1-hour ratio for Martin Creek is 4.71, much greater than the 1.7 cutpoint.

Figure 5.2-7 TCEQ Composite Performance Summary Monitor Specific – Single Receptor

SITE	AVERAGING PERIOD	ABSOLUTE FRACTIONAL BIAS		DIFFERENCE (D)	STD ERROR (S)	RATIO (D/S)
		AERMOD	AERMOD-HBP			
LONGVIEW	1hr	0.21	0.26	-0.04	0.10	-0.41
	3hr	0.26	0.12	0.13	0.16	0.83
	24hr	0.41	0.19	0.22	0.18	1.22
	CPM	0.30	0.19	0.10	0.09	1.13
MARTIN CREEK	1hr	0.43	0.15	0.28	0.06	4.71
	3hr	0.18	0.08	0.10	0.15	0.64
	24hr	0.26	0.25	0.01	0.17	0.08
	CPM	0.29	0.17	0.12	0.08	1.48

Figure 5.2-8 TCEQ's Cox-Tikvart Analysis (MCM values)

Scenario	Site	MCM (AERMOD - AERMOD-HBP)	Best Performing Model
Standard Methodology	All	0.04	AERMOD-HBP
Single Receptor	Longview	0.1	AERMOD-HBP
Single Receptor	Martin Creek	0.12	AERMOD-HBP

Using EPA Region 6's modeling with corrected stack locations, we conducted Cox-Tikvart analysis to confirm that the differences were minor and did not impact the final analysis of the Alternative AERMOD-HBP Model, especially since some of the TCEQ's metrics were close. AERMOD-HBP did improve 1-hour modeled to observed values, especially for Martin Creek in TCEQ's analysis. TCEQ's results were more mixed for the Longview monitor. However, the Longview monitor is 19 km away and has much lower modeled and monitored values as compared to the Martin Creek monitor, and because of the distance and travel time there may be some hours where the modeled plume does not reach the Longview monitor receptor. For these reasons, we weighed the Cox-Tikvart analysis results for modeled concentrations at the Longview monitor slightly less compared to the results at the Martin Creek monitor location in our evaluation of the two models.

EPA Region 6's Cox-Tikvart analysis results are included in Tables 5.2-1 through 5.2-6. EPA Region 6 looked at the data three ways: Longview and Martin Creek pooled together for 2018-2020 (Tables 5.2-1 and 5.2-2); Martin Creek monitor by itself for 2018-2020 (Tables 5.2-3 and 5.2-4); and Longview monitor with five years combined 2016-2020 by itself (Tables 5.2-5 and 5.2-6).

Martin Creek & Longveiw monitors pooled together (2018-2020)(Tables 5.2-1 and 5.2-2)
In looking at the 1-Hour RHC by meteorological bins in Table 5.2.1 for the Longview (monitor 1) and Martin Creek (monitor 2), a couple things are apparent. At the Longview monitor, for meteorological speed class 1 and stability class 3 as well as speed class 2 and stability class 3 both AERMOD and AERMOD-HBP have lower 1-hour RHC than observerved. At the Martin Creek monitor, for meteorological speed class 1 and stability class 2 both AERMOD and AERMOD-HBP have lower RHC than observerved. For the other meteorological bins, the 1-hour RHC indicated AERMOD-HBP performed better than AERMOD with the exception of speed class 1and stability class 1 at both monitors where the 1-hour RHC indicated some underestimation occuring compared to observations. We note that the Longview data set we included 2 extremely high value observations (greater than the 4th high value) that TCEQ felt should be dropped from the analysis and TCEQ did not include those two hourly data points in their analysis. TCEQ indicated via email that they thought these values were outliers and/or not impacted by Martin Lake.[14] Based on the information provided by TCEQ we were uncertain that they should be dropped and conservatively included those observations in our analysis to make sure exclusion did not significantly impact the model performance analysis results. Ultimately inclusion of these 2 monitored values did not change the conclusions of our analysis that AERMOD-HBP performs better than AERMOD.

In looking at the 3-Hour RHC values in Table 5.2-2, AERMOD-HBP resulted in lower 3-Hour RHC values that are closer to observed values for both monitors indicating better model performance. There was a very slight underestimation at the Longview monitor of less than 0.4 $\mu g/m^3$ (116.104 $\mu g/m^3$observed vs. 115.786 $\mu g/m^3$ modeled) but we note these values are significantly less than the NAAQS and a insignificant difference, so this is not thought to be of any consequence. In looking at the 24-Hour RHC values in Table 5.2-2, AERMOD-HBP resulted in lower 24-Hour RHC values that are closer to observed values at the Longview monitor and very similar to AERMOD values for the Martin Creek monitor. Overall AERMOD-

[14] Email From Shantha Daniel of TCEQ to Erik Snyder of EPA Region 6 dated August 6, 2021

HBP exhibited improved model performance for the 3-Hour RHC at both monitors and improved model performance for the 24-Hour RHC at the Longview monitor.

In looking at the AFB and CPM values in Table 5.2-2, AERMOD-HBP exhibited better model performance for the 1-Hour AFB, 3-Hour AFB and CPM values, and slightly better performance for the 24-Hour AFB. The MCM value indicates HBP improved model performance and the ratio of -1.53 is near the typically used threshold of ±1.7 of being statistically signficant.

Martin Creek monitor by itself (2018-2020)(Tables 5.2-3 and 5.2-4)
In addition to the traditional Cox-Tikvart method we also performed Cox-Tikvart analysis for each monitor individually.We did Cox-Tikvart for the Martin Creek monitor by itself using three years of data (2018-2020). As was indicated in Table 5.2-3, both AERMOD and AERMOD-HBP had some 1-Hour RHCs lower than observed for the same combinations of certain speed and stability classes (red text in Table 5.2-3) at the Martin Creek monitor. For the other combinations of speed and stability classes, AERMOD-HBP and AERMOD were similar except for speed Class 1 and stability Class 1 where AERMOD was much higher than observed and AERMOD-HBP was lower than observed for the Martin Creek monitor. In Table 5.2-4 AERMOD-HBP performed better for the 3-Hour RHC and was similar, but slightly better for the 24-RHC at Martin Creek monitor. AERMOD-HBP had lower to slightly lower AFB for the 1-Hour, 3-Hour, and 24-Hour AFB and better CPM value compared to AERMOD at Martin Creek monitor. The MCM indicated better performance and the ratio was -0.62459 which also indicated AERMOD-HBP performed better than AERMOD.

Longview monitor by itself (2016-2020)(Tables 5.2-5 and 5.2-6))
We also did Cox-Tikvart for the Longview monitor by itself using five years of data (2016-2020). As was indicated in Table 5.2-5, both AERMOD and AERMOD-HBP had some 1-Hour RHCs lower than observed for the same combinations of certain speed and stability classes (red text in Table 5.2-5) at the Longview monitor. For the other combinations of speed and stability classes AERMOD-HBP had lower 1-Hour RHCs than AERMOD (indicating AERMOD-HBP was performing better) except for speed Class 1 and stability Class 1 where AERMOD was higher than observed and AERMOD-HBP was lower than observed 1-Hour RHC for the Longview monitor. In Table 5.2-6, AERMOD-HBP performed much better than AERMOD (but slightly lower than observed) for the 3-Hour RHC and was similar but slightly better for the 24-RHC at Longview monitor. AERMOD-HBP had much lower AFB for the 1-Hour, 3-Hour, and 24-Hour AFB and better CPM value compared to AERMOD at Longview monitor. The MCM indicated better performance and the ratio was -4.97858 which also indicates AERMOD-HBP performed better than AERMOD and well above what is often considered the statistically significant threshold of ±1.7.

Overall EPA Region 6's modeling with corrected stack locations and downwash indicates that AERMOD-HBP performs better than AERMOD in this particular situation in looking at the Cox-Tikvart statistics in the traditional way of both monitors together and in the alternate way of looking at the Cox-Tikvart statistics at the monitors individually. From this perspective it appears that while not all the ratio statistic values are above/below the typical ±1.7 value used to represent significant statistical difference, the traditional approach yielded a value within 10% (-1.53445) and, in the individual monitor approach, the ratio indicated statistical significance at Longview monitor and was slightly less than statistically significant at Martin Creek but other statistics (RCH, AFB, and CPM) indicated that AERMOD-HBP still performed better than regulatory AERMOD. Statistical significance is not a pass/fail situation in an alternative model approval and in this case the Martin Creek value was close to the typical value used to represent significant statiscal difference. Overall, the different Cox-Tikvart analyses indicates that AERMOD-HBP performs better than AERMOD in this particular case-specific analysis for the modeling of the Martin Lake facility in East Texas.

Table 5.2-1 Martin Creek & Longview (2018-2020) combined 1-Hr RHC by meteorology bins.

1-HOUR RHC Values				MC & LV (2018-2020)
SCENARIO	RECEPTOR	SPEED Class	Stability Class	1-Hour RHC
OBS	1	1	1	225.516097
OBS	1	1	2	55.424227
OBS	1	1	3	135.965444
OBS	1	2	1	163.388297
OBS	1	2	2	101.320058
OBS	1	2	3	54.665554
OBS	2	1	1	427.871032
OBS	2	1	2	50.811419
OBS	2	1	3	181.634572
OBS	2	2	1	160.050508
OBS	2	2	2	397.017797
OBS	2	2	3	149.097297
DEFAULT	1	1	1	269.366211
DEFAULT	1	1	2	136.539036
DEFAULT	1	1	3	17.213028
DEFAULT	1	2	1	196.758883
DEFAULT	1	2	2	237.096966
DEFAULT	1	2	3	17.23659
DEFAULT	2	1	1	643.234896
DEFAULT	2	1	2	44.964058
DEFAULT	2	1	3	62.55248
DEFAULT	2	2	1	344.422436
DEFAULT	2	2	2	447.921916
DEFAULT	2	2	3	38.319427
HBP	1	1	1	179.311285
HBP	1	1	2	67.64557
HBP	1	1	3	17.213028
HBP	1	2	1	166.090986
HBP	1	2	2	162.703023
HBP	1	2	3	17.23659
HBP	2	1	1	346.542556
HBP	2	1	2	43.066775
HBP	2	1	3	62.55248
HBP	2	2	1	344.36141
HBP	2	2	2	447.921916
HBP	2	2	3	38.319427

SPEED-STABILITY HOUR COUNTS			
	SPEED	STABILITY	
SCENARIO	CLASS	CLASS	HOURS
OBS	1	1	2912
OBS	1	2	483
OBS	1	3	7956
OBS	2	1	3862
OBS	2	2	7908
OBS	2	3	2891
DEFAULT	1	1	2912
DEFAULT	1	2	483
DEFAULT	1	3	7956
DEFAULT	2	1	3862
DEFAULT	2	2	7908
DEFAULT	2	3	2891
HBP	1	1	2912
HBP	1	2	483
HBP	1	3	7956
HBP	2	1	3862
HBP	2	2	7908
HBP	2	3	2891

Table 5.2-2 Martin Creek & Longview (2018-2020) combined 3-Hr & 24-Hr RHC by meteorology bins and 1, 3 and 24-Hr AFB CPM values and MCM values.

3-HOUR RHC		MC & LV (2018-2020)
SCENARIO	RECEPTOR	3-HOUR RHC
OBS	1	116.104043
OBS	2	276.296567
DEFAULT	1	171.460538
DEFAULT	2	330.558016
HBP	1	115.7857
HBP	2	319.838038
24-HOUR RHC		MC & LV (2018-2020)
SCENARIO	RECEPTOR	24-HOUR RHC
OBS	1	31.829726
OBS	2	77.118223
DEFAULT	1	47.056906
DEFAULT	2	102.999489
HBP	1	39.495739
HBP	2	102.185124

CPM Values				
Scenario	1-HR AFB	3-Hr AFB	24-Hr AFB	CPM
DEFAULT	0.6779	0.17883	0.28738	0.38137
HBP	0.57364	0.14608	0.2796	0.33311

MCM Values			
Scenario	MCM	Std. Dev.	Ratio
HBP - Default	-0.04826	0.03145	-1.53445

Table 5.2-3 Martin Creek (2018-2020) combined 1-Hr RHC by meteorology bins.

1-HOUR RHC Values				MC (2018-2020)
SCENARIO	RECEPTOR	SPEED Class	Stability Class	1-Hour RHC
OBS	2	1	1	427.871032
OBS	2	1	2	50.811419
OBS	2	1	3	181.634572
OBS	2	2	1	160.050508
OBS	2	2	2	397.017797
OBS	2	2	3	149.097297
DEFAULT	2	1	1	643.234896
DEFAULT	2	1	2	44.964058
DEFAULT	2	1	3	62.55248
DEFAULT	2	2	1	344.422436
DEFAULT	2	2	2	447.921916
DEFAULT	2	2	3	38.319427
HBP	2	1	1	346.542556
HBP	2	1	2	43.066775
HBP	2	1	3	62.55248
HBP	2	2	1	344.36141
HBP	2	2	2	447.921916
HBP	2	2	3	38.319427

SPEED-STABILITY HOUR COUNTS			
SCENARIO	SPEED CLASS	STABILITY CLASS	HOURS
OBS	1	1	2912
OBS	1	2	483
OBS	1	3	7956
OBS	2	1	3862
OBS	2	2	7908
OBS	2	3	2891
DEFAULT	1	1	2912
DEFAULT	1	2	483
DEFAULT	1	3	7956
DEFAULT	2	1	3862
DEFAULT	2	2	7908
DEFAULT	2	3	2891
HBP	1	1	2912
HBP	1	2	483
HBP	1	3	7956
HBP	2	1	3862
HBP	2	2	7908
HBP	2	3	2891

Table 5.2-4 Martin Creek (2018-2020) combined 3-Hr & 24-Hr RHC by meteorology bins and 1, 3 and 24-Hr AFB CPM values and MCM values.

3-HOUR RHC Values		MC (2018-2020)
SCENARIO	RECEPTOR	3-HOUR RHC
OBS	2	276.296567
DEFAULT	2	330.558016
HBP	2	319.838038
24-HOUR RHC		MC (2018-2020)
SCENARIO	RECEPTOR	24-HOUR RHC
OBS	2	77.118223
DEFAULT	2	102.999489
HBP	2	102.185124

Martin Creek CPM Values				
Scenario	1-HR AFB	3-Hr AFB	24-Hr AFB	CPM
DEFAULT	0.58886	0.17883	0.28738	0.35169
HBP	0.56397	0.14608	0.2796	0.32988
MCM Values				
Scenario	MCM	Std. Dev.	Ratio	
HBP - Default	-0.02181	0.03491	-0.62459	

Table 5.2-5 Longview (2016-2020) combined 1-Hr RHC by meteorology bins.

Longview (2016-2020)				
1-HOUR RHC Values		SPEED	STABILITY	Longview (2016-2020)
SCENARIO	RECEPTOR	SPEED Class	Stability Class	1-Hour RHC
OBS	1	1	1	219.796496
OBS	1	1	2	67.593023
OBS	1	1	3	145.0537
OBS	1	2	1	157.246092
OBS	1	2	2	125.470549
OBS	1	2	3	61.580398
DEFAULT	1	1	1	272.925469
DEFAULT	1	1	2	175.434172
DEFAULT	1	1	3	17.260176
DEFAULT	1	2	1	197.612958
DEFAULT	1	2	2	253.295912
DEFAULT	1	2	3	17.271416
HBP	1	1	1	181.72801
HBP	1	1	2	88.532713
HBP	1	1	3	17.260176
HBP	1	2	1	168.349708
HBP	1	2	2	163.606162
HBP	1	2	3	17.271416

SPEED-STABILITY HOUR COUNTS			
	SPEED	STABILITY	
SCENARIO	CLASS	CLASS	HOURS
OBS	1	1	5036
OBS	1	2	748
OBS	1	3	13331
OBS	2	1	6685
OBS	2	2	12658
OBS	2	3	4564
DEFAULT	1	1	5036
DEFAULT	1	2	748
DEFAULT	1	3	13331
DEFAULT	2	1	6685
DEFAULT	2	2	12658
DEFAULT	2	3	4564
HBP	1	1	5036
HBP	1	2	748
HBP	1	3	13331
HBP	2	1	6685
HBP	2	2	12658
HBP	2	3	4564

Table 5.2-6 Longview (2016-2020) combined 3-Hr & 24-Hr RHC by meteorology bins and 1, 3 and 24-Hr AFB CPM values and MCM values.

3-HOUR RHC Values		LV (2016-2020)
SCENARIO	RECEPTOR	3-HOUR RHC
OBS	1	115.882421
DEFAULT	1	176.57567
HBP	1	113.608039

24-HOUR RHC		LV (2016-2020)
SCENARIO	RECEPTOR	24-HOUR RHC
OBS	1	77.118223
DEFAULT	1	102.999489
HBP	1	102.185124

Longview CPM Values				
Scenario	1-HR AFB	3-Hr AFB	24-Hr AFB	CPM
DEFAULT	0.78402	0.41506	0.42877	0.54261
HBP	0.5814	0.01982	0.24547	0.28223

Longview MCM Values				
Scenario	MCM	Std. Dev.	Ratio	
HPB - Default	-0.26038	0.0523	-4.97858	

5.3 Q-Q Plots

In the following figures EPA Region 6 provides modified Q-Q Plots from EPA Region 6's modeling and from TCEQ's alternate model package provided to EPA Region 6 in July and August 2021. Since EPA Region 6 is particulary interested in how the higher end distribution performs and since the standard is the 99th percentile of maximum 1-hour daily SO_2 concentrations, we added a number of additional percentiles to EPA Region 6's Q-Q plots that are based on 8760 hours per year. In addition to the typical 5% increments between 0.05 percentile and 0.95 percentile we added a number of additional percentile points between 0.95 and 1.0. EPA Region 6 added 0.97, 0.9725, 0.975, 0.9775, 0.98, 0.9825, 0.0985, 0.98775, 0.99, 0.9925, 0.995, 0.975, and 0.999 percentile points. To help read the Q-Q plots, we modified the markers for the 99th percentile (square shape), 98 percentile (triangle shape), and 95th percentile (diamond shape). We note that TCEQ plots are also modified and have many more percentiles in the upper end between 95th and 100th percentile.

LONGVIEW MONITOR

Figure 5.3-1 is a composite of the five years (2016-2020) of modeled and observed data. Excluding the one outlier observation of greater than 160 ppb at Longview, the composite shows that AERMOD-HBP had one other percentile below the one-to-one line (indicating a slight underestimation at that percentile) while the rest of the percentiles were above the one-to-one line for AERMOD and AERMOD-HBP (indicating the modeling was overestimating for those percentiles). Figure 5.3-2 is a plot of each year's percentiles for 2016-2020 combined onto one plot that indicates AERMOD-HBP and AERMOD result in a few of these highest percentiles being underestimated. For further understanding we also generated yearly Q-Q plots. In evaluating EPA Region 6's Q-Q plots for 2016-2020 (Figures 5.3-3 through 5.3-7) we do see AERMOD-HBP results in some slight underprediction between 99th percentile and 100th percentile in all years but not for all the datapoints. AERMOD results are all overpredictions for the 99th percentile to 100th percentile, with the exception of 2018 which AERMOD also has some datapoints underpredicting. TCEQ's modeling resulted mostly in similar results to EPA Region 6's Q-Q plots. We note that TCEQ removed two of the highest monitored exceedances in 2018 from Longview's observations datasets as they didn't think they were attributable to Martin Lake emissions. EPA Region 6 reviewed the information provided and conservatively decided to keep those monitored values in the observations datasets to determine if they would impacting the results for this evaluation. Ultimately, inclusion of these 2 monitored values did not change the conclusions of our analysis that AERMOD-HBP performs better than AERMOD.

MARTIN CREEK MONITOR

Figure 5.3-8 is a composite of the three years (2018-2020) of modeled and observed data that indicates that AERMOD-HBP had two percentiles below the one-to-one line (indicating a slight underestimation at those percentiles), and the rest of the percentiles were above the one-to-one line for AERMOD and AERMOD-HBP (indicating the modeling was overestimating for those percentiles). Figure 5.3-9 is a plot of each years percentiles for 2018-2020 combined onto one plot that indicates AERMOD-HBP and AERMOD result in a few of these highest percentiles being underestimated in the above 99th percentile range. For further understanding we also generated yearly Q-Q plots. In evaluating EPA Region 6's Q-Q plots for 2018-2020 (Figures 5.3-10 through 5.3-13) we do see AERMOD-HBP results in some slight underprediction between 99th percentile and 100th percentile in 2018 and 2020 but not for all the datapoints and no underprediction for these percentiles in 2019. AERMOD results are all overpredictions for the 99th percentile to 100th percentile for each year. TCEQ's modeling resulted mostly in similar results to EPA Region 6's Q-Q plots.

Overall, the slight underestimations that are indicated in the Q-Q plots are mostly relatively small and close to the one-to-one line. Even though there are cases where AERMOD-HBP underpredicts by some small amount and largely at values on the extreme high end and not relative to the NAAQS, the overall information does not indicate that there is a bias to underpredict. EPA Region 6 considers this to be relatively close in a few caases but still can be considered acceptable in this case-specific alternative model evaluation for the Rusk-Panola 1-Hour SO_2 Attainment Demonstration SIP modeling.

Figure 5.3-1 EPA Region 6 Longview 2016-2020 Composite Q-Q Plot

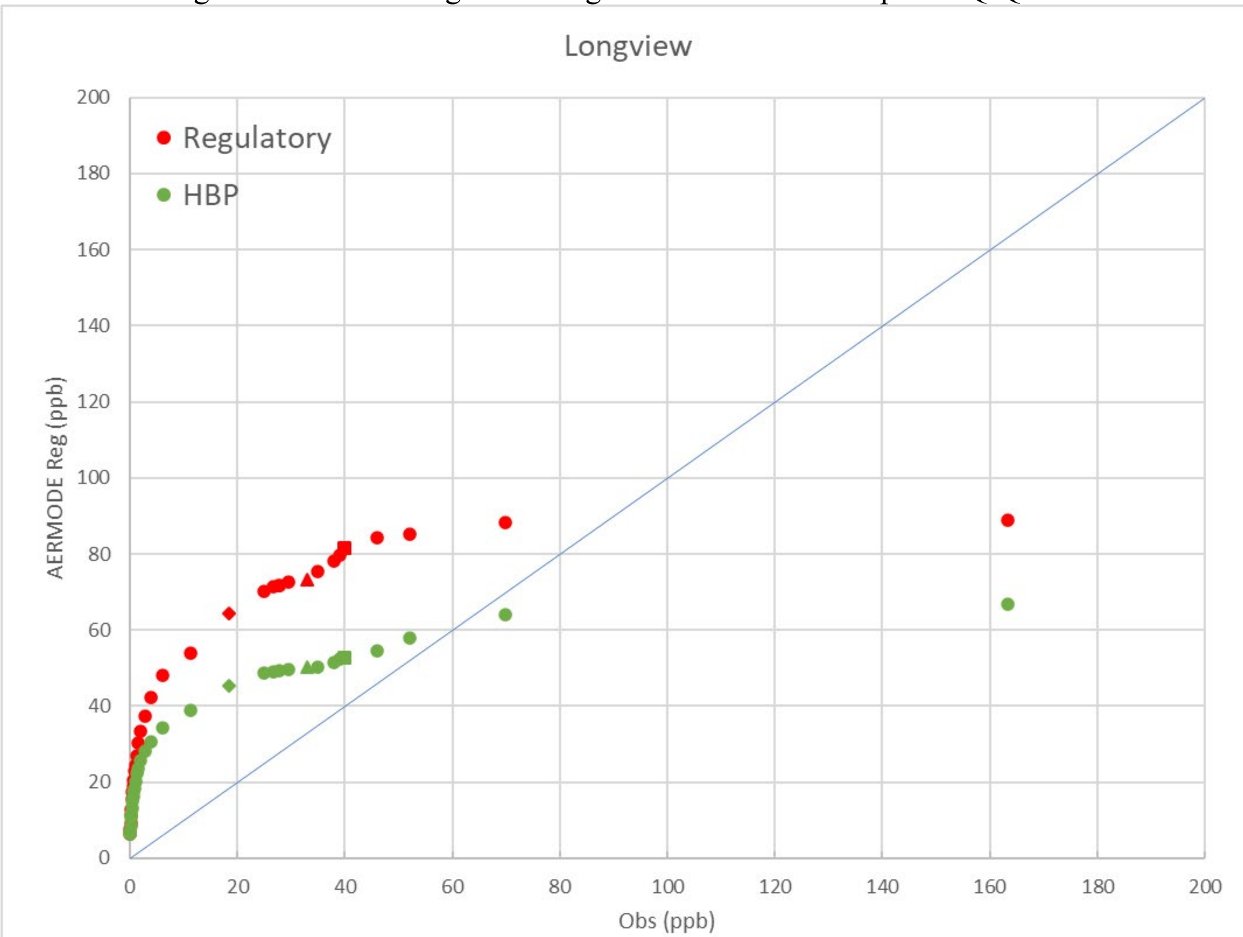


Figure 5.3-2 EPA Region 6 Longview 2016-2020 Q-Q Plot Each Year Plotted Separately.

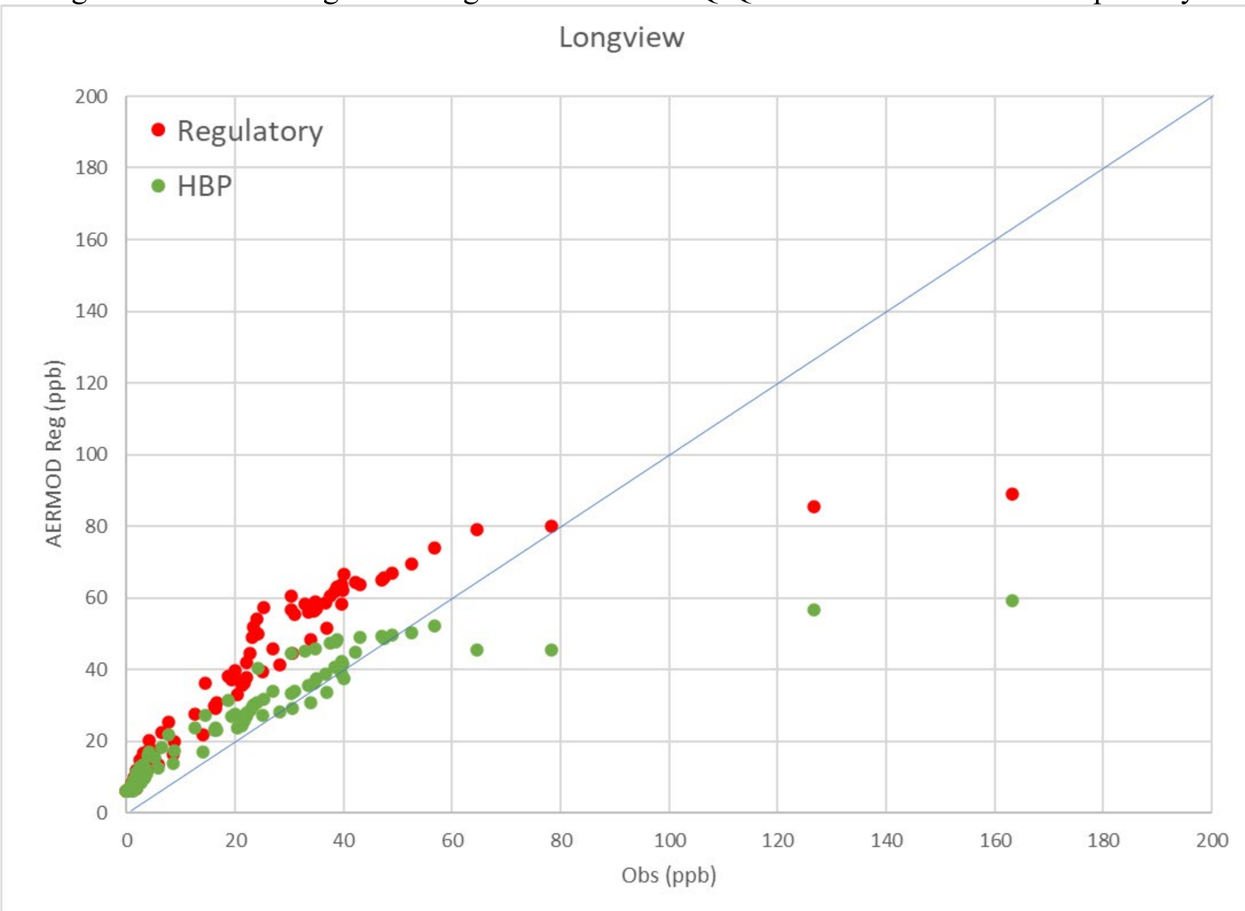
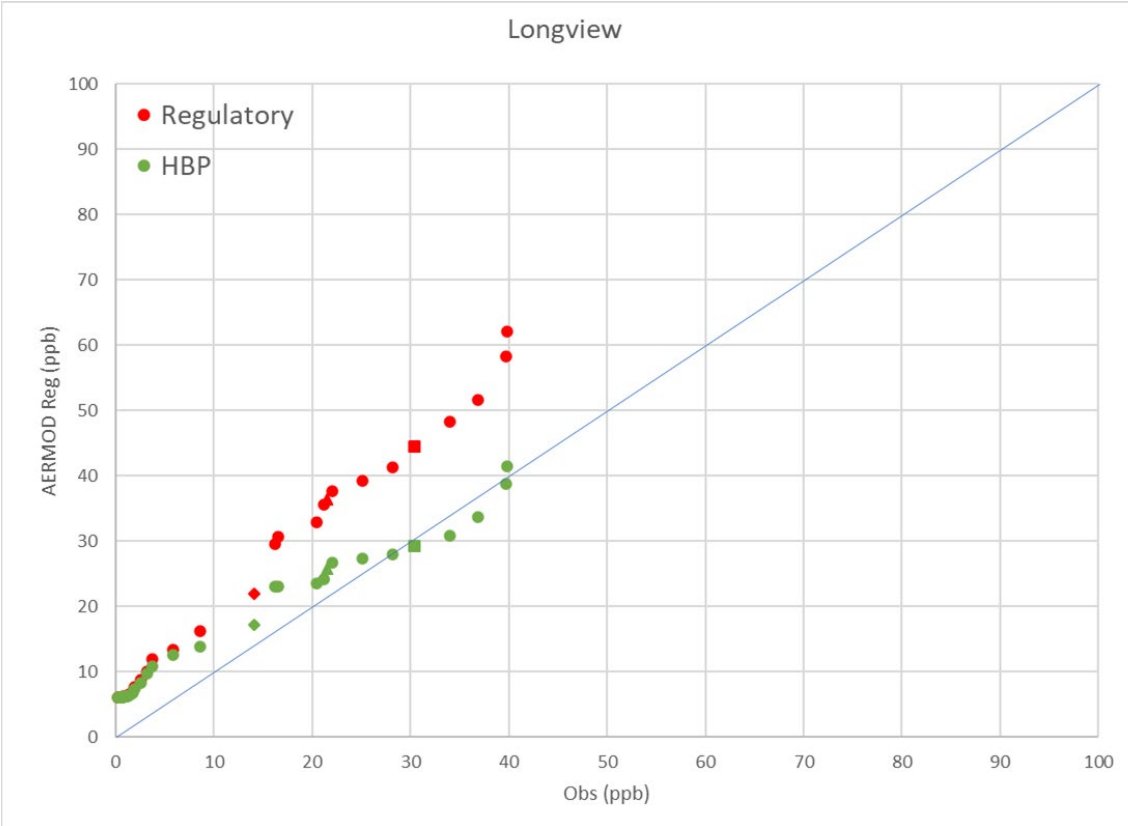


Figure 5.3-3 Longview Q-Q Plot 2016 EPA Region 6 on Top and TCEQ on Bottom (different scales).



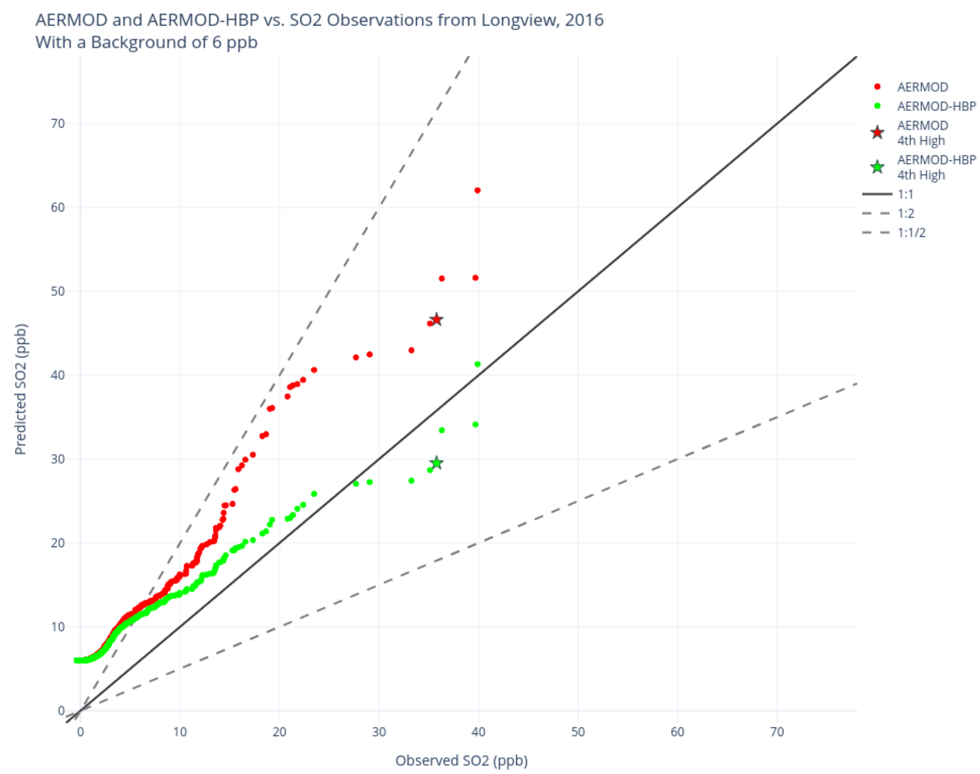

AERMOD and AERMOD-HBP vs. SO2 Observations from Longview, 2016
With a Background of 6 ppb
Predicted SO2 (ppb)
Observed SO2 (ppb)
0
10
20
30
40
50
60
70
AERMOD
AERMOD-HBP
AERMOD 4th High
AERMOD-HBP 4th High
1:1
1:2
1:1/2

Figure 5.3-4 Longview Q-Q Plot 2017 EPA Region 6 on Top and TCEQ on Bottom (different scales)

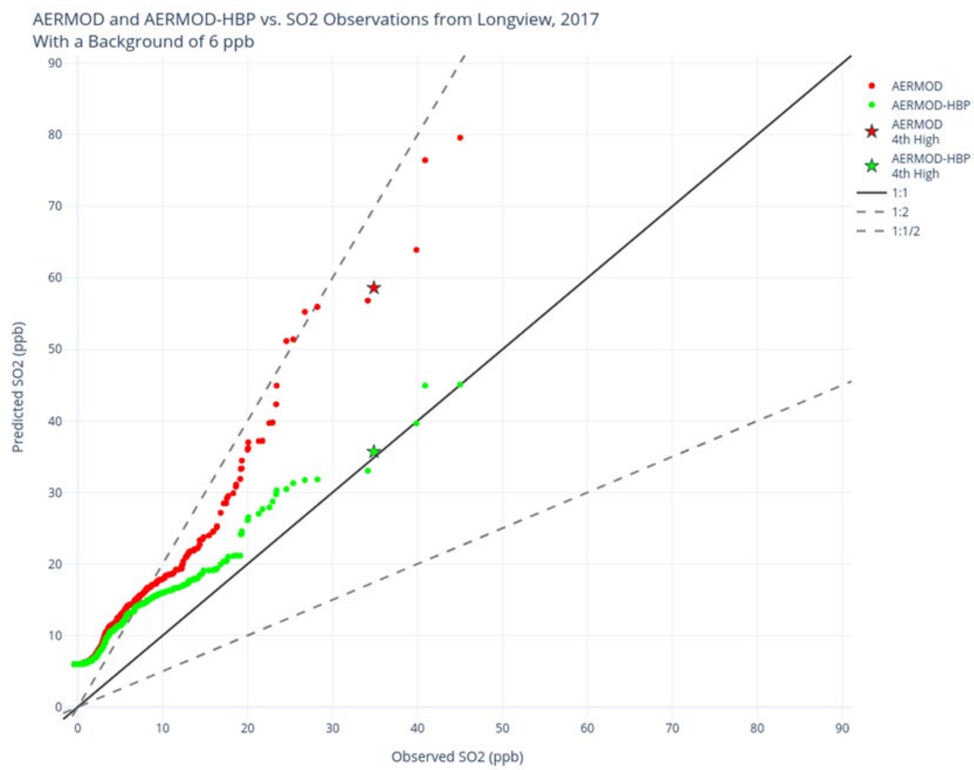
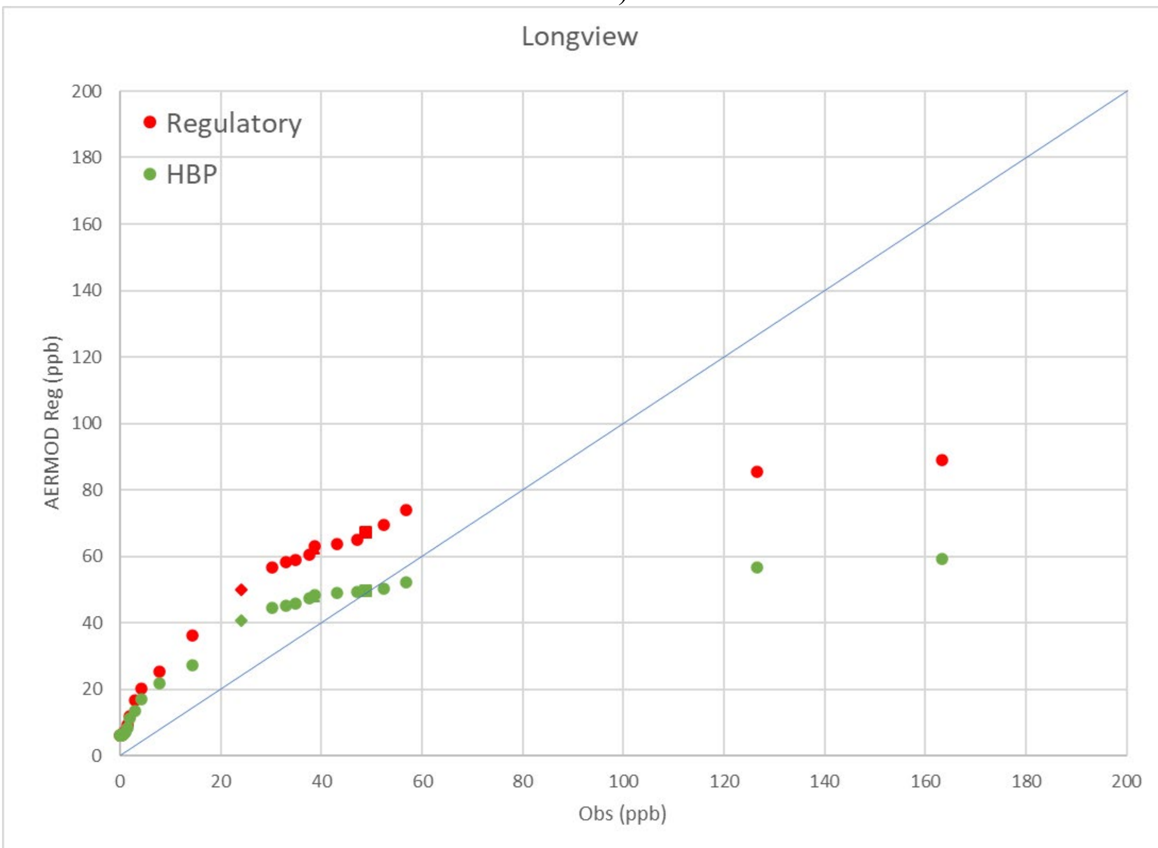

AERMOD and AERMOD-HBP vs. SO2 Observations from Longview, 2017
With a Background of 6 ppb
Predicted SO2 (ppb)
Observed SO2 (ppb)
0
10
20
30
40
50
60
70
80
90
AERMOD
AERMOD-HBP
AERMOD 4th High
AERMOD-HBP 4th High
1:1
1:2
1:1/2

Figure 5.3-5 Longview Q-Q Plot 2018 EPA Region 6 on Top and TCEQ on Bottom (different scales)



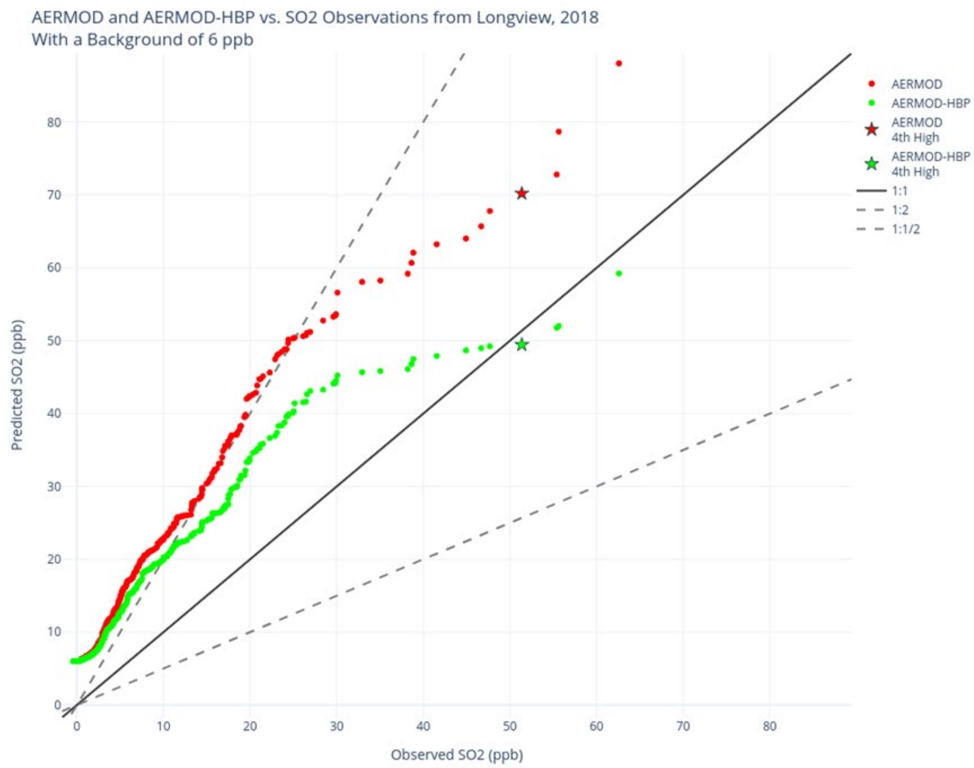
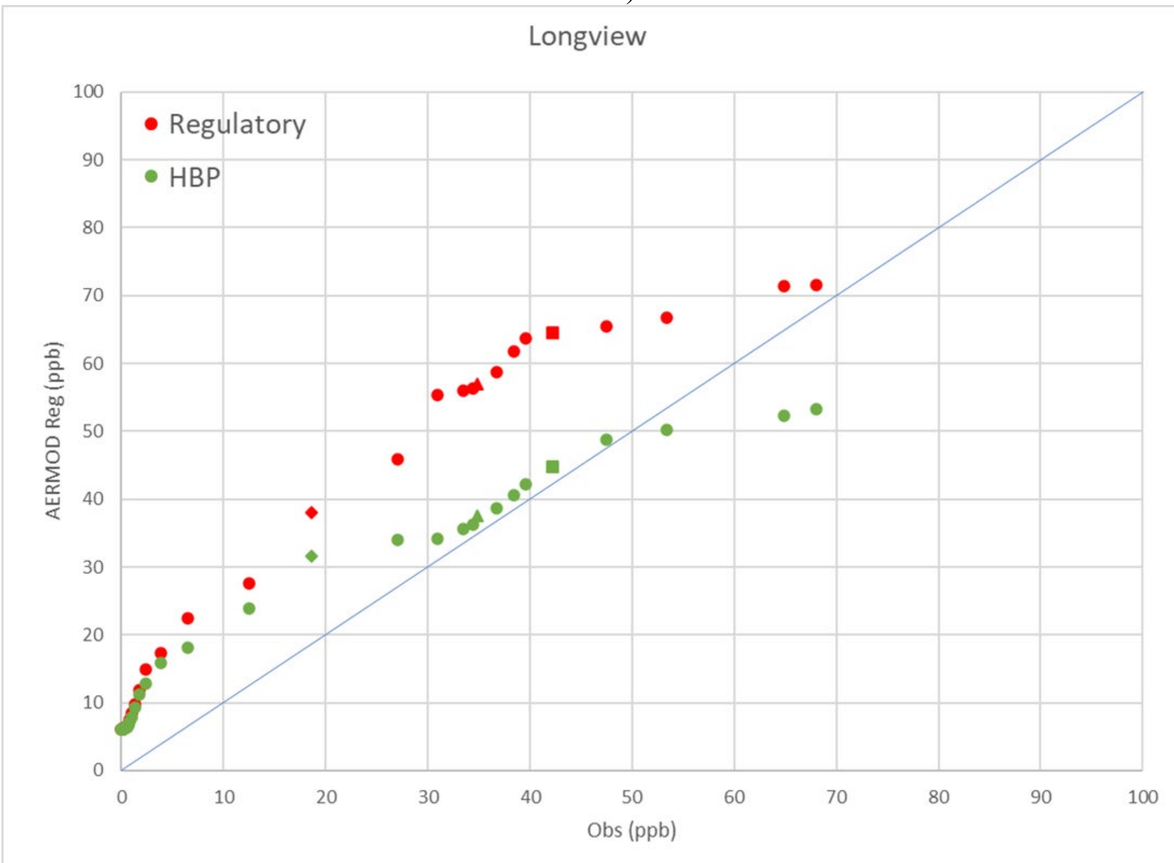

AERMOD and AERMOD-HBP vs. SO2 Observations from Longview, 2018
With a Background of 6 ppb
Predicted SO2 (ppb)
Observed SO2 (ppb)
0
10
20
30
40
50
60
70
80
AERMOD
AERMOD-HBP
AERMOD 4th High
AERMOD-HBP 4th High
1:1
1:2
1:1/2

Figure 5.3-6 Longview Q-Q Plot 2019 EPA Region 6 on Top and TCEQ on Bottom (different scales)



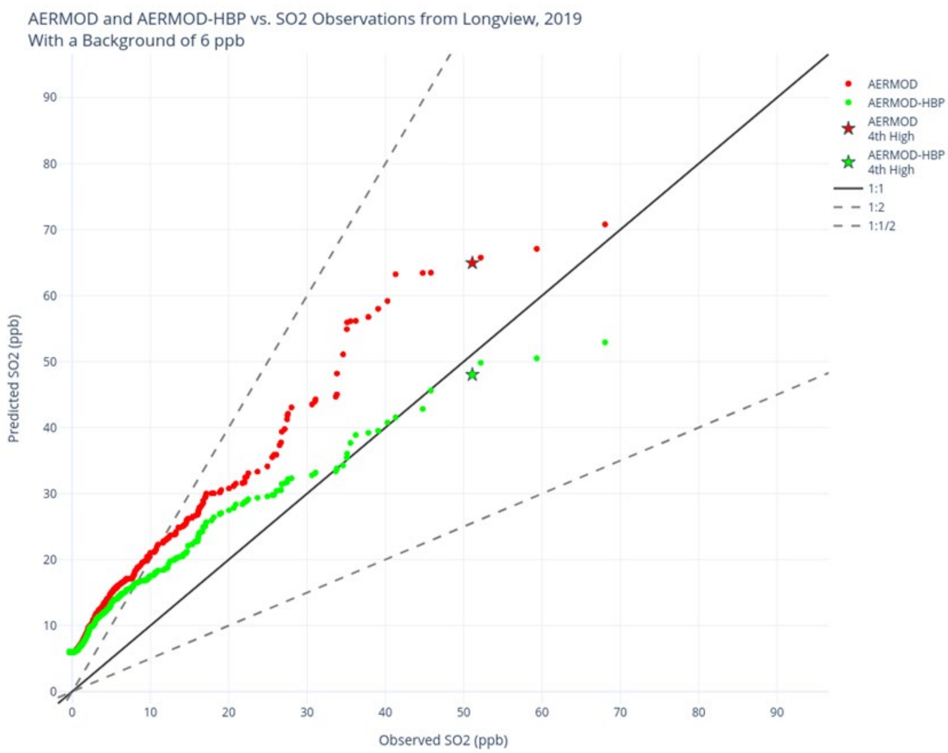
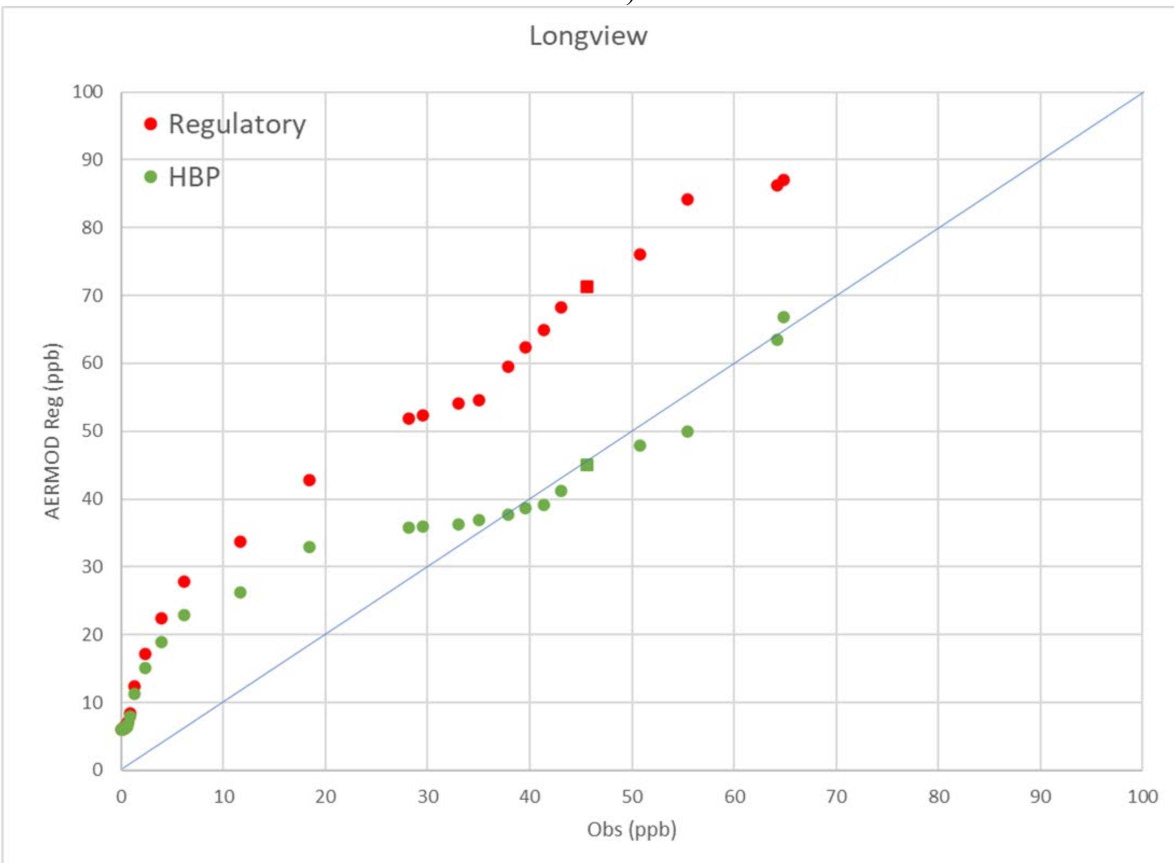

AERMOD and AERMOD-HBP vs. SO2 Observations from Longview, 2019
With a Background of 6 ppb
Predicted SO2 (ppb)
Observed SO2 (ppb)
AERMOD
AERMOD-HBP
AERMOD 4th High
AERMOD-HBP 4th High
1:1
1:2
1:1/2
0
10
20
30
40
50
60
70
80
90

Figure 5.3-7 Longview Q-Q Plot 2020 EPA Region 6 on Top and TCEQ on Bottom (different scales)



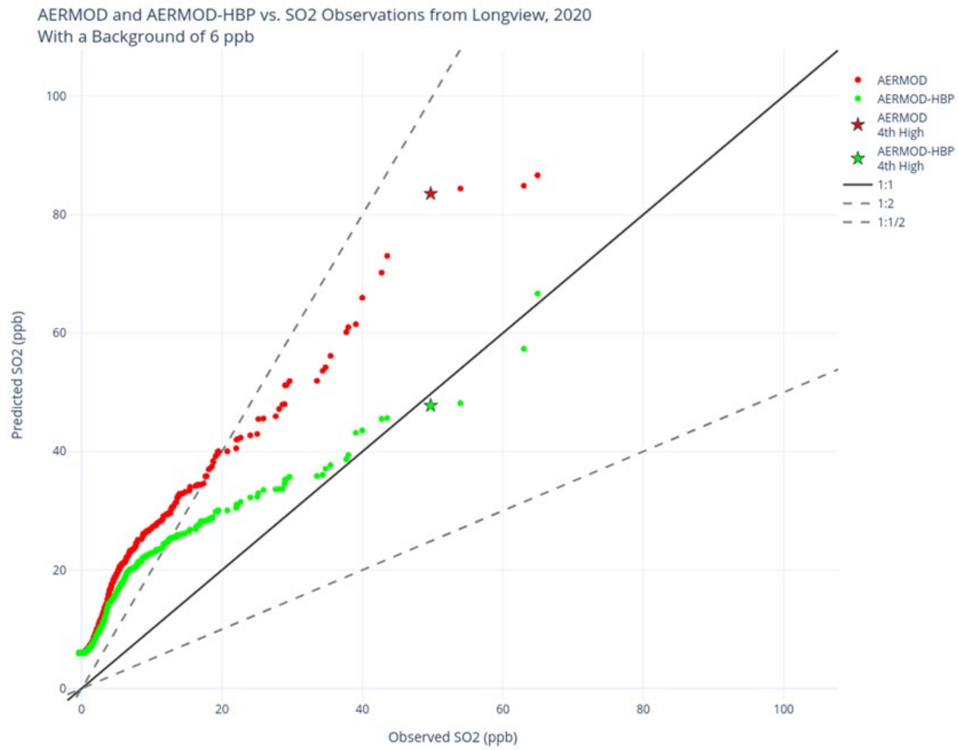

AERMOD and AERMOD-HBP vs. SO2 Observations from Longview, 2020
With a Background of 6 ppb
Predicted SO2 (ppb)
Observed SO2 (ppb)
0
20
40
60
80
100
AERMOD
AERMOD-HBP
AERMOD 4th High
AERMOD-HBP 4th High
1:1
1:2
1:1/2

Figure 5.3-8 EPA Region 6 Martin Creek 2018-2020 Composite Q-Q Plot

Figure 5.3-9 EPA Region 6 Martin Creek 2018-2020 Q-Q Plot Each Year Plotted Separately

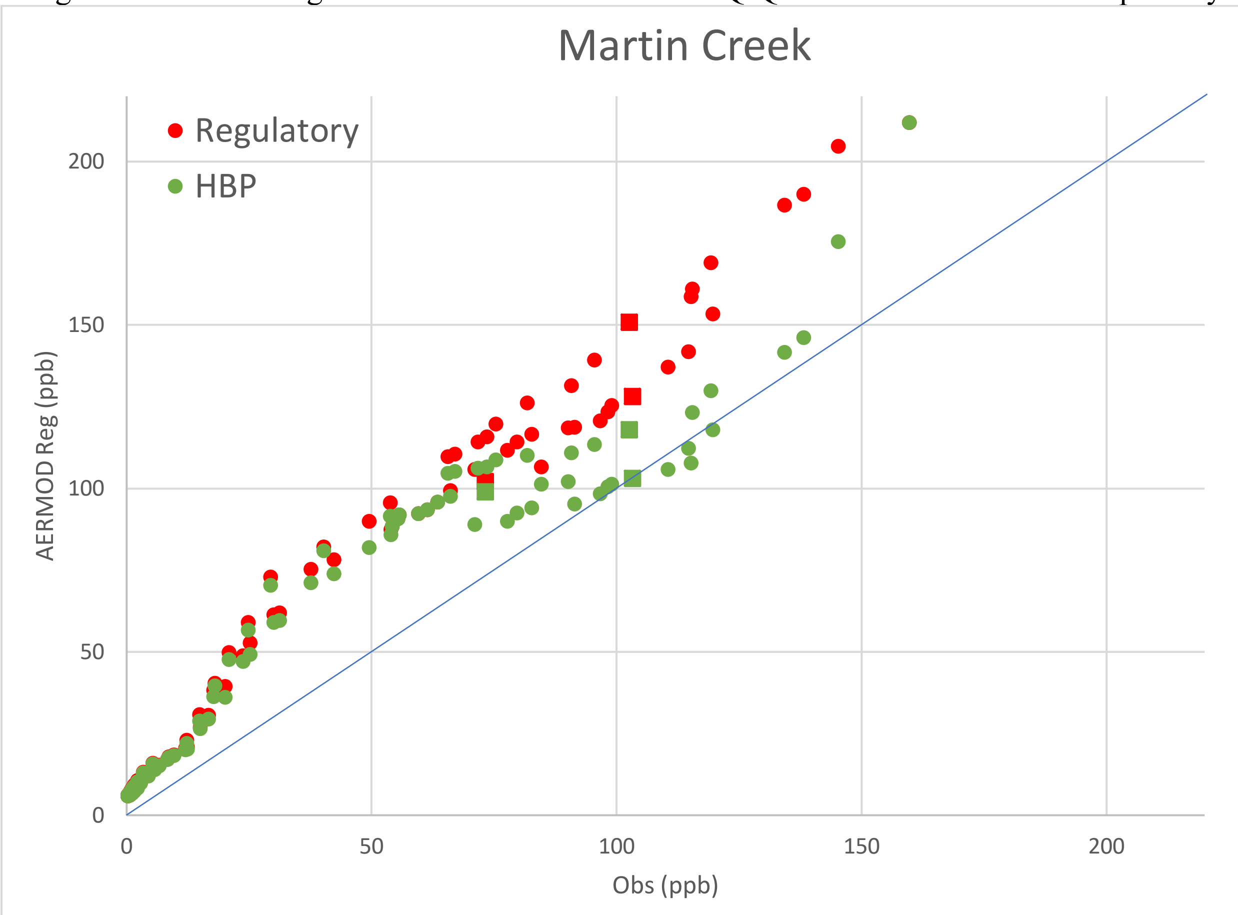
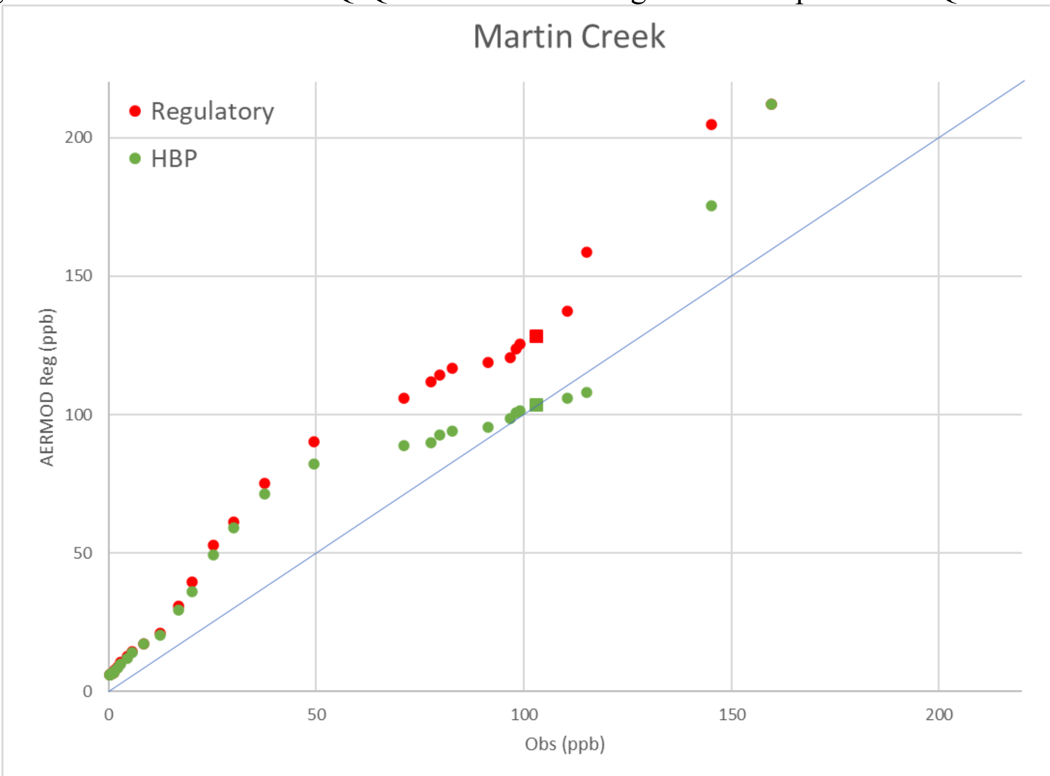


Figure 5.3-10 Martin Creek Q-Q Plot 2018 EPA Region 6 on Top and TCEQ on Bottom



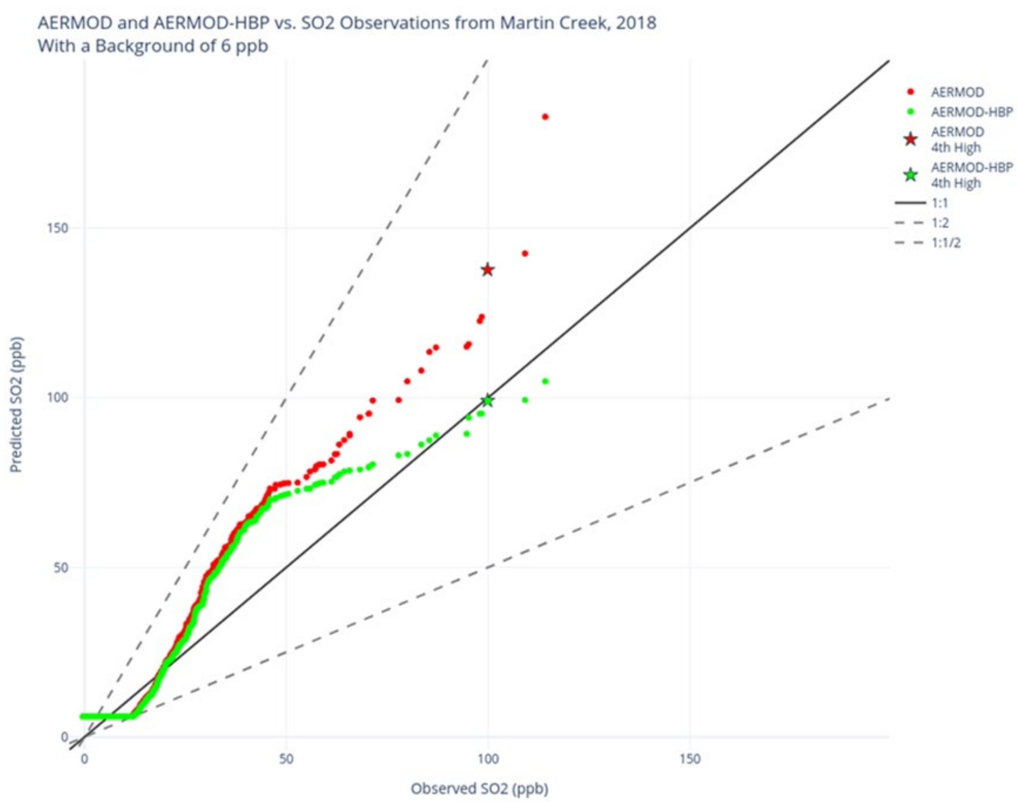
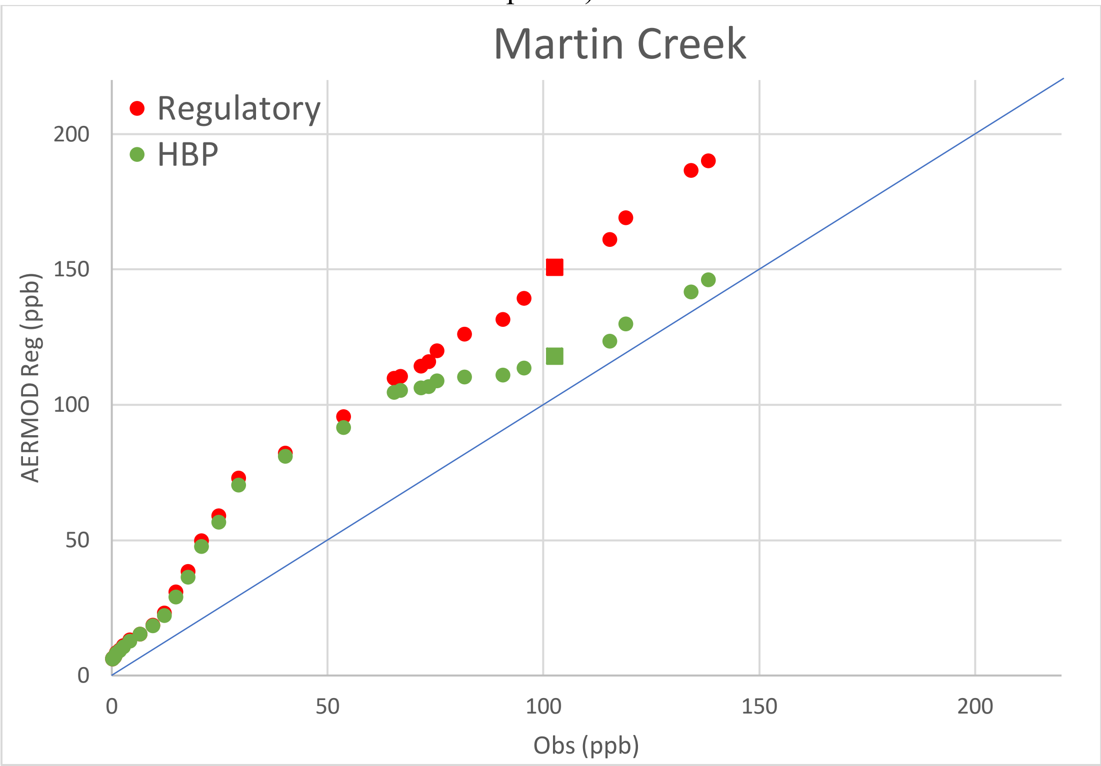


Figure 5.3-10 Martin Creek Q-Q Plot 2019 EPA Region 6 on Left and TCEQ on Right (extra points)



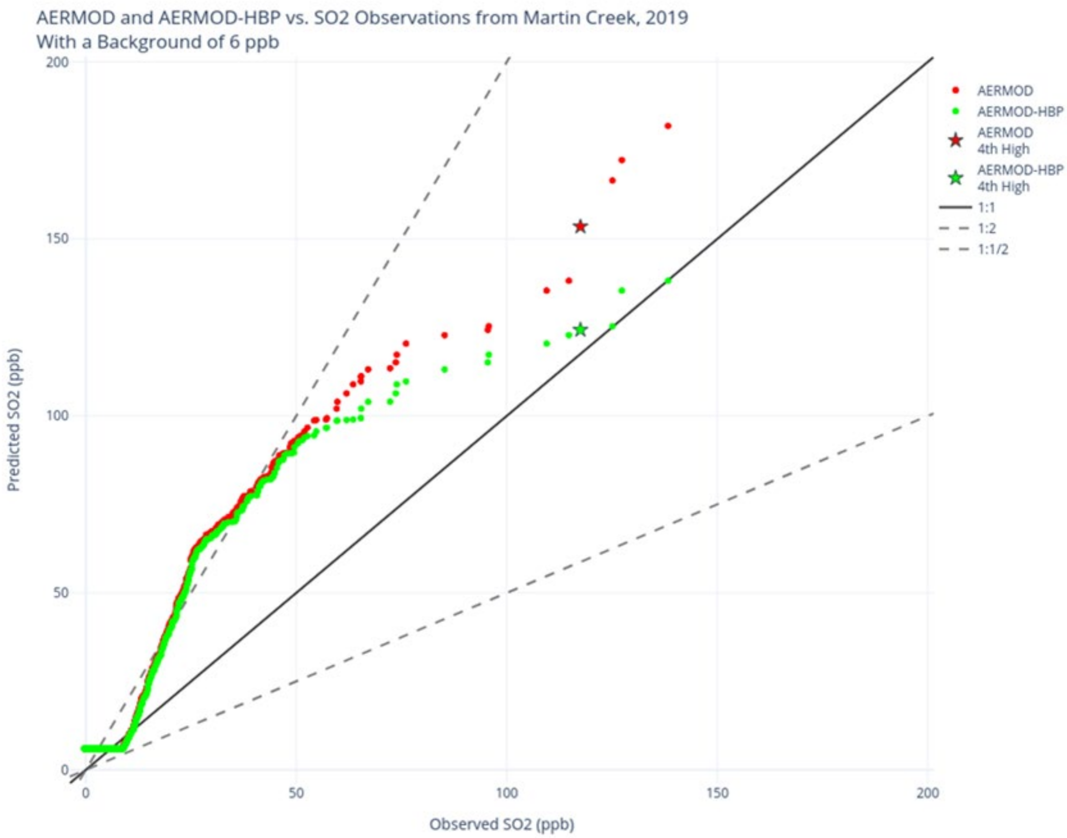
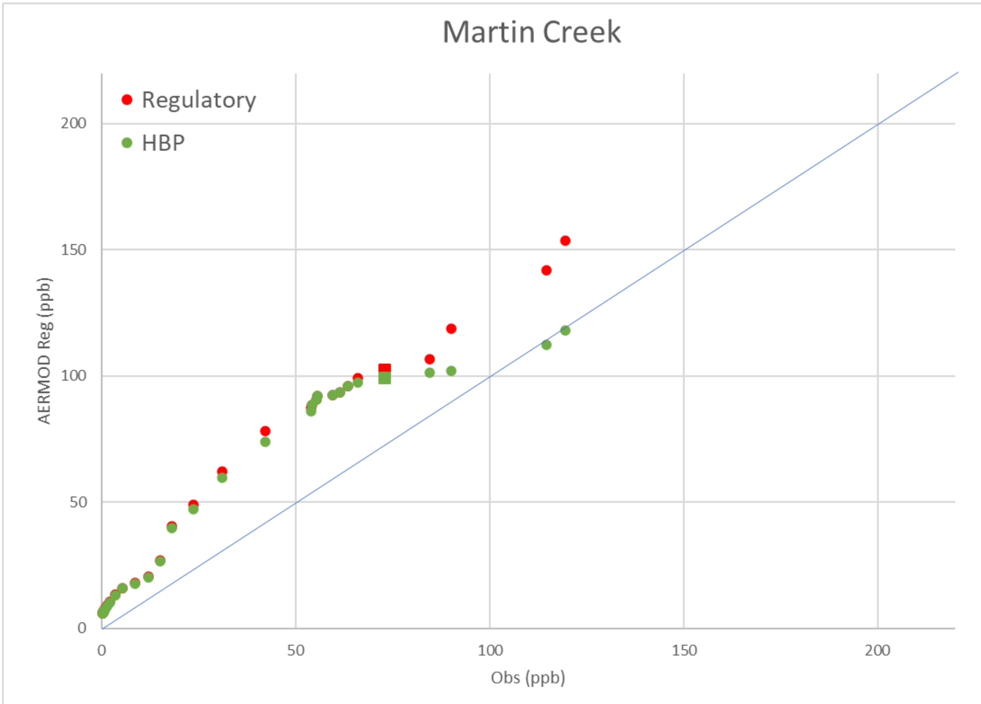
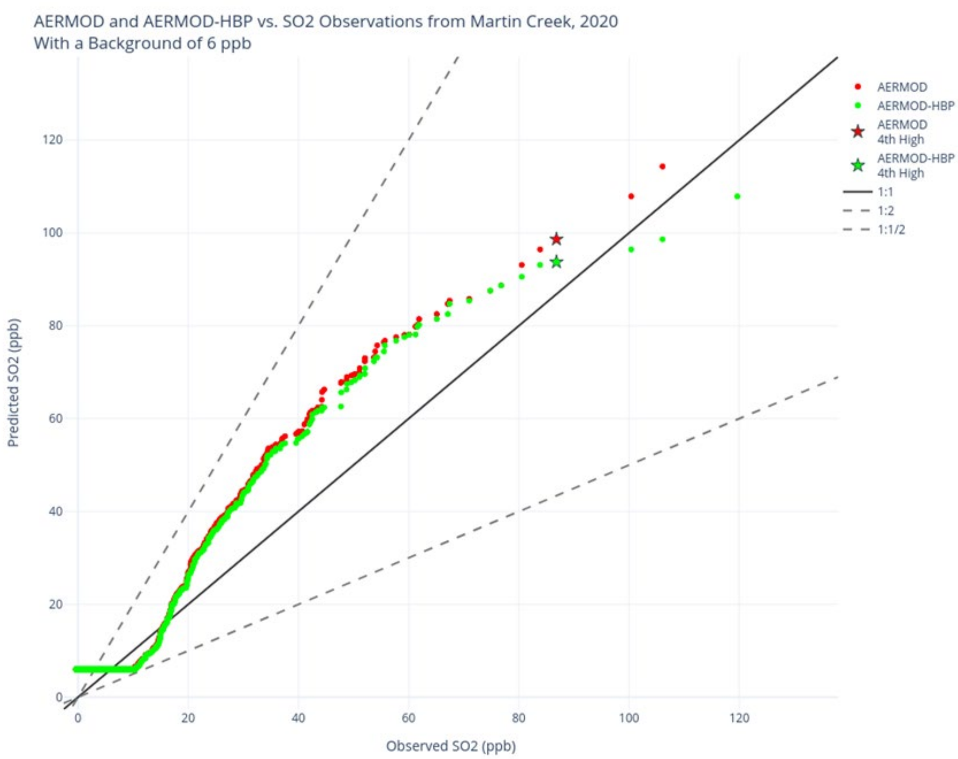

AERMOD and AERMOD-HBP vs. SO2 Observations from Martin Creek, 2019
With a Background of 6 ppb
Predicted SO2 (ppb)
Observed SO2 (ppb)
0
50
100
150
200
AERMOD
AERMOD-HBP
AERMOD 4th High
AERMOD-HBP 4th High
1:1
1:2
1:1/2

Figure 5.3-10 Martin Creek Q-Q Plot 2020 EPA Region 6 on Top and TCEQ on Bottom (extra points)





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5.4 Time Series Plots

TCEQ provided time series plots of observed, AERMOD v21112, and AERMOD-HBP results for each monitor (Martin Creek and Longview). For the Longivew monitor they provided yearly time series (replicated in Figure 5.3-1) of the Daily Maximum 1-Hour SO_2 Concentrations for modeled values at the monitor location. For the Longview monitor they also provided yearly time series (replicated in Figure 5.3-2) of the 1-Hour SO_2 value for all hours. TCEQ provided similar time series for the Martin Creek monitor in Figures 5.3-3 and 5.3-4, respectively.

For the modeling that EPA Region 6 conducted with the corrected stack locations, we also generated 1-Hour SO_2 time series for each year and monitor; they are included as Figures 5.3-5 through 5.3-9 for the Longview monitor and Figures 5.3-10 through 5.3-12 for the Martin Creek monitor. EPA Region 6's time series and the data are included in an EXCEL spreadsheet named "AltModel_timeseries.xlsx" that is available upon request.

For these time series, in general AERMOD-HBP does result in lower values than AERMOD on many of the highest hours, although there are some of the higher concentration hours where AERMOD-HBP does result in higher concentrations than AERMOD. For the higher concentration hours, both models tend to be higher than the observations for the lion's share of the time with some hours one or both models are not resulting in as high values as were observed. While results are mixed when concentrations are compared hour-by-hour, modeled concentrations are generally biased to overpredict at the upper end of the distribution and there is clearly not a bias to underpredict across the entire distribution. Overall the time series over the course of the period modeled does not indicate that AERMOD-HBP is underestimating the highest observed concentrations relevant to the NAAQS relevant data points (most of such data points are higher than the NAAQS and not relevant for determining attainment) when evaluated from a standpoint of not pairing in time.

Figure 5.3-1 TCEQ Daily Maximum 1-Hour SO_2 Concentrations Time Series (Longview- Single Receptor)

Figure 5.3-2 TCEQ Hourly 1-Hour SO_2 Concentrations Time Series (Longview - Single Receptor)

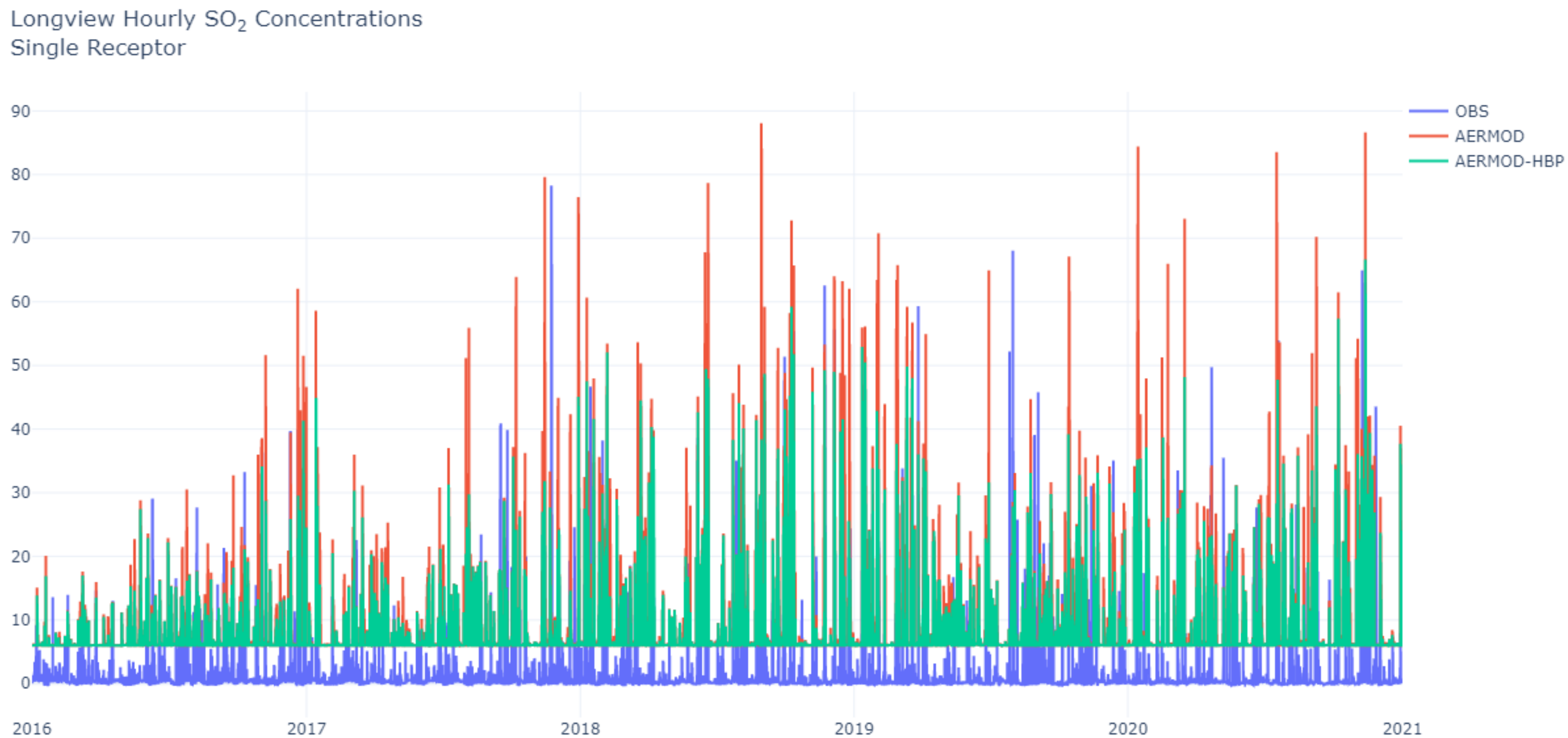


Figure 5.3-3 TCEQ Daily Maximum 1-Hour SO_2 Concentrations Time Series (Martin Creek - Single Receptor)

Figure 5.3-4 TCEQ Hourly 1-Hour SO_2 Concentrations Time Series (Martin Creek - Single Receptor)

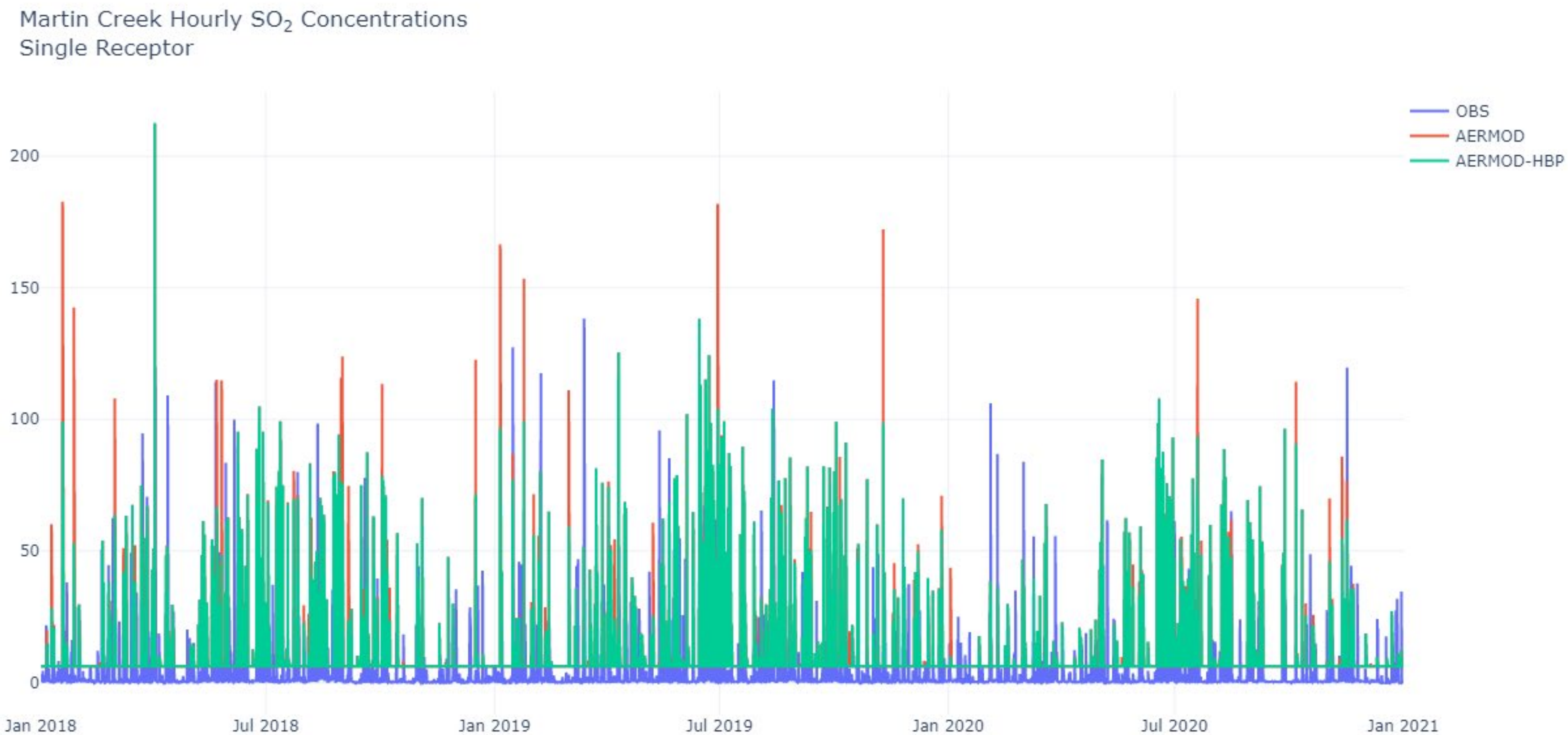


Figure 5.3-5 EPA Region 6 2016 Hourly 1-Hour SO_2 Concentrations Time Series (Longview - Single Receptor)

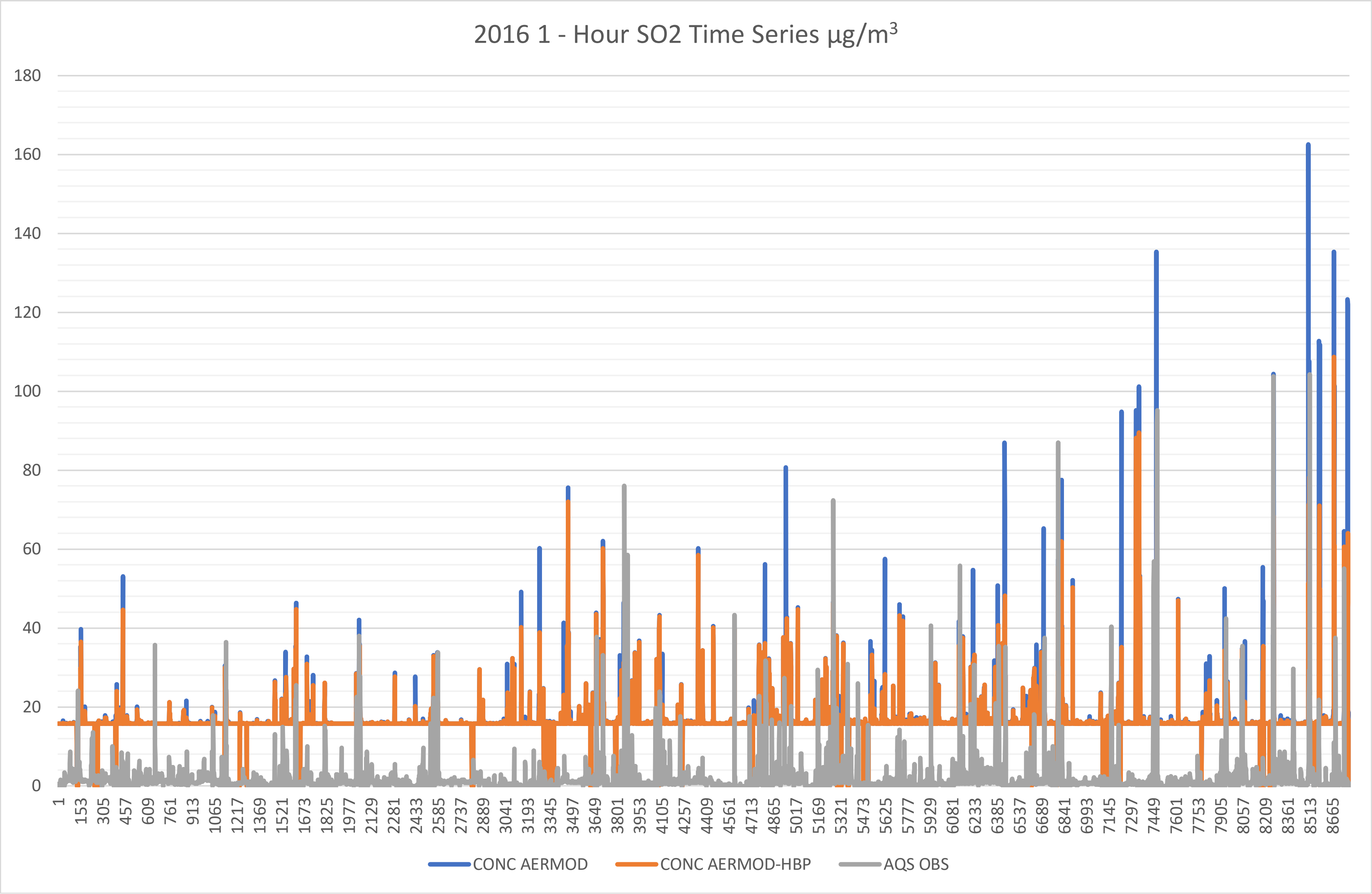


Figure 5.3-6 EPA Region 6 2017 Hourly 1-Hour SO_2 Concentrations Time Series (Longview - Single Receptor)

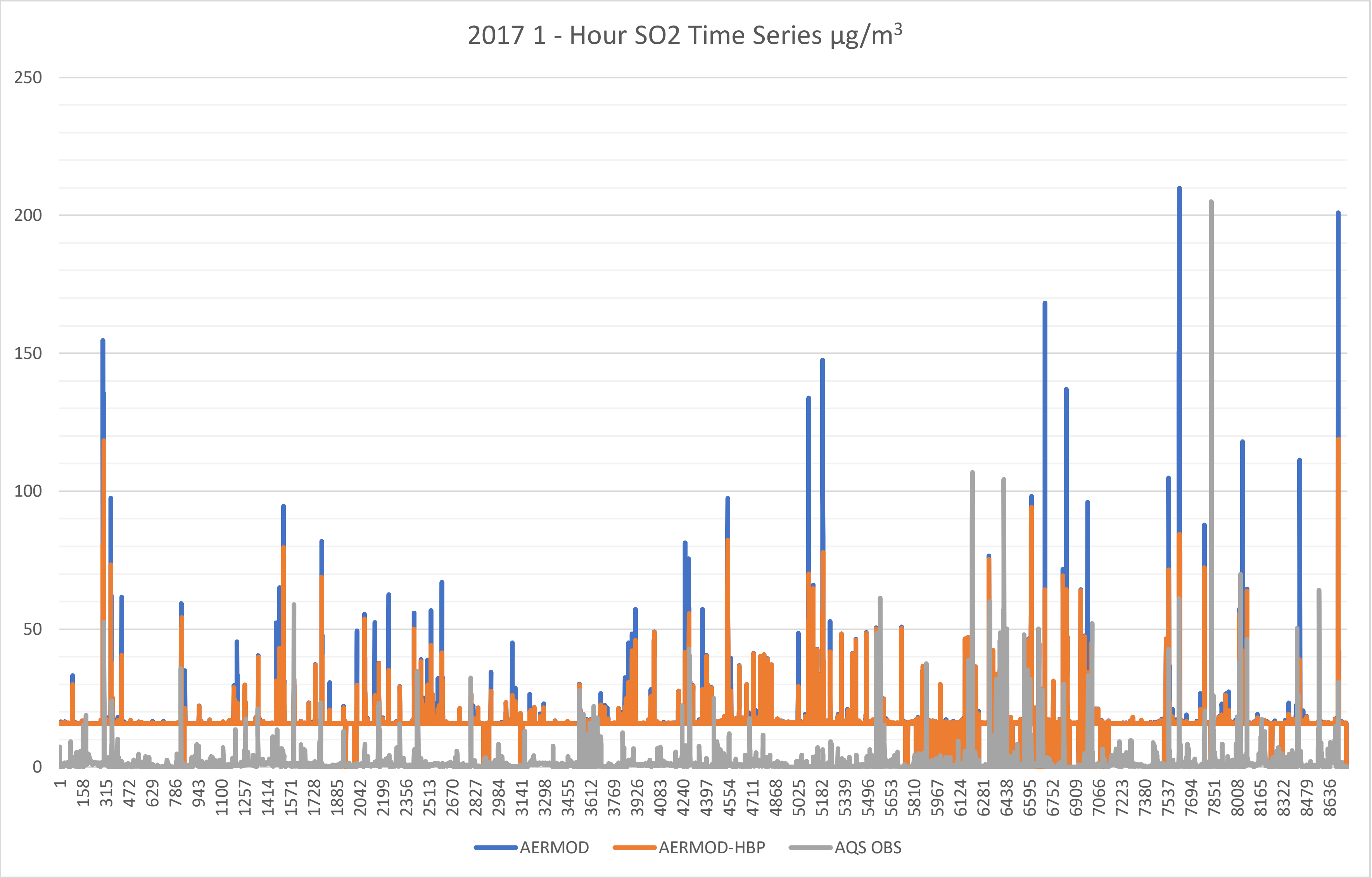


Figure 5.3-7 EPA Region 6 2018 Hourly 1-Hour SO_2 Concentrations Time Series (Longview - Single Receptor)

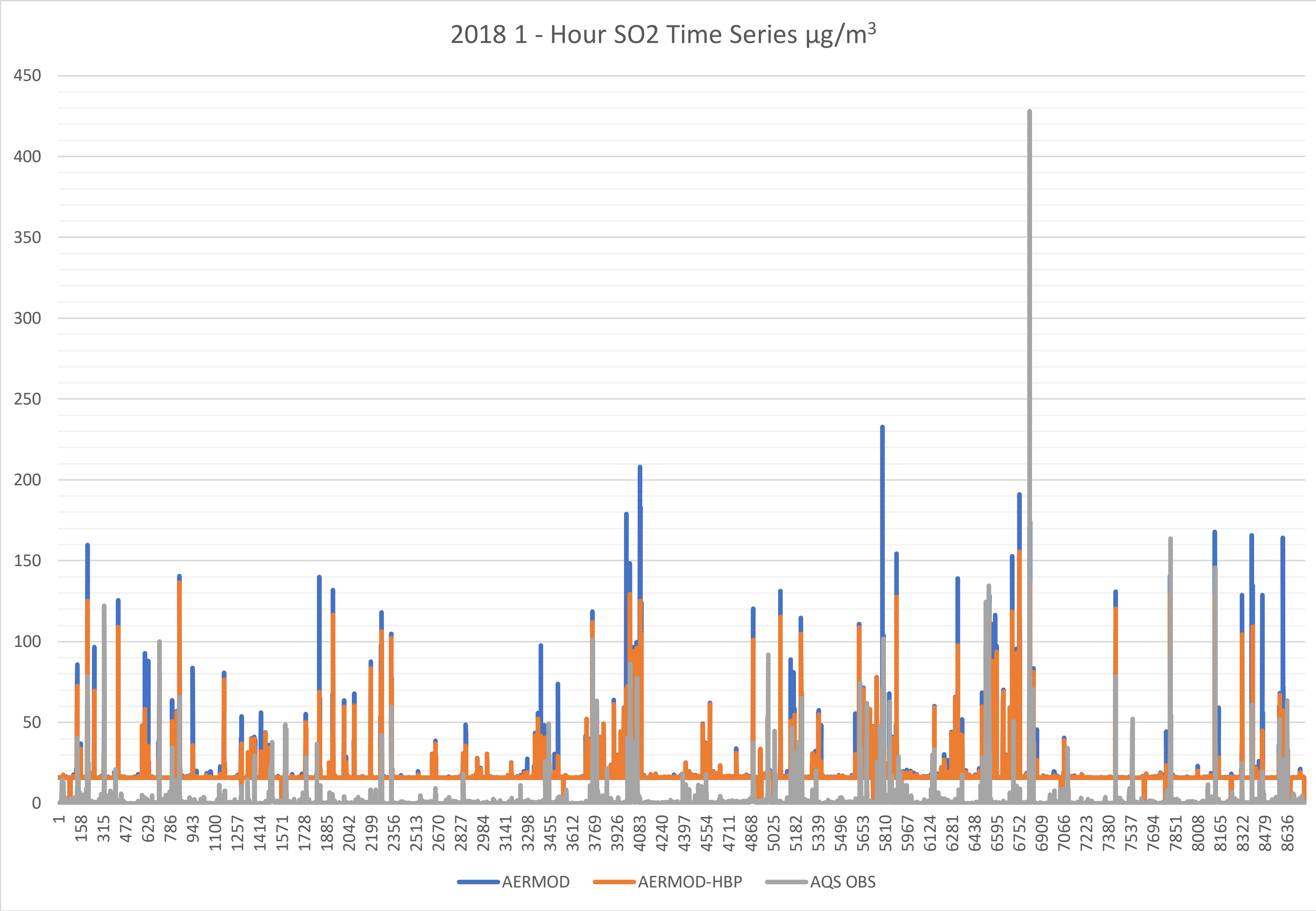


Figure 5.3-8 EPA Region 6 2019 Hourly 1-Hour SO_2 Concentrations Time Series (Longview - Single Receptor)

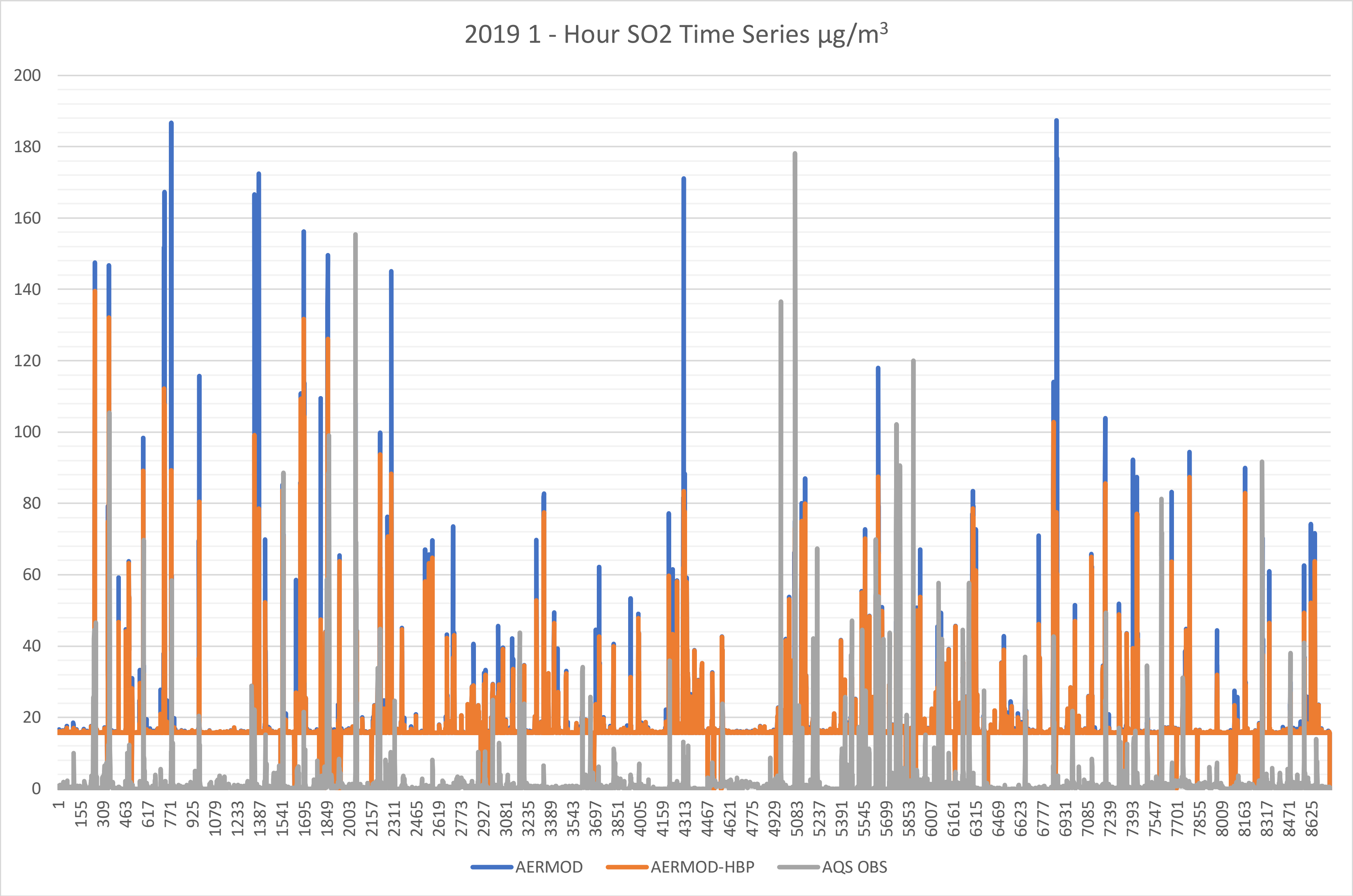


Figure 5.3-9 EPA Region 6 2020 Hourly 1-Hour SO_2 Concentrations Time Series (Longview - Single Receptor)

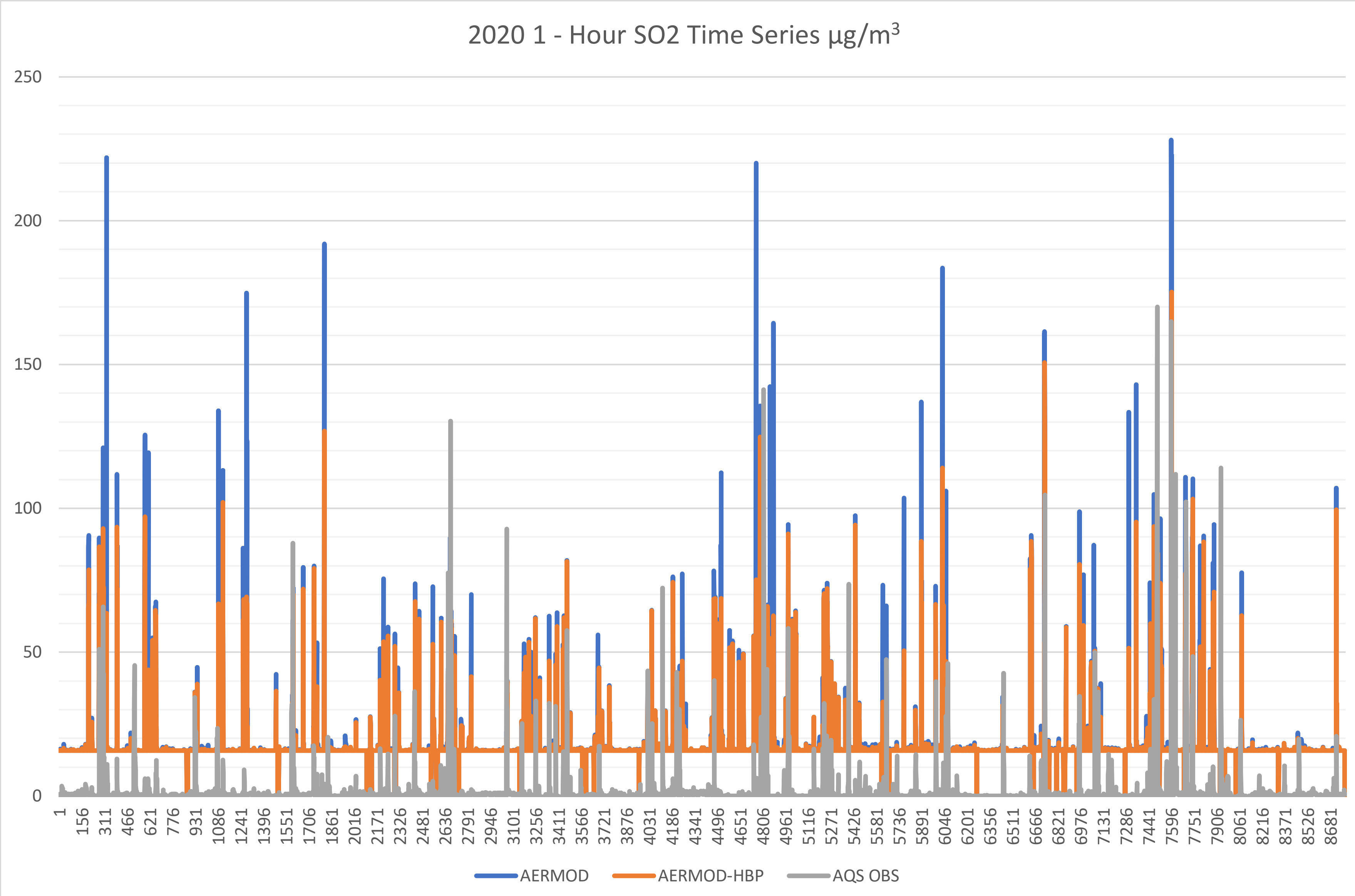


Figure 5.3-10 EPA Region 6 2018 Hourly 1-Hour SO_2 Concentrations Time Series (Martin Creek - Single Receptor)

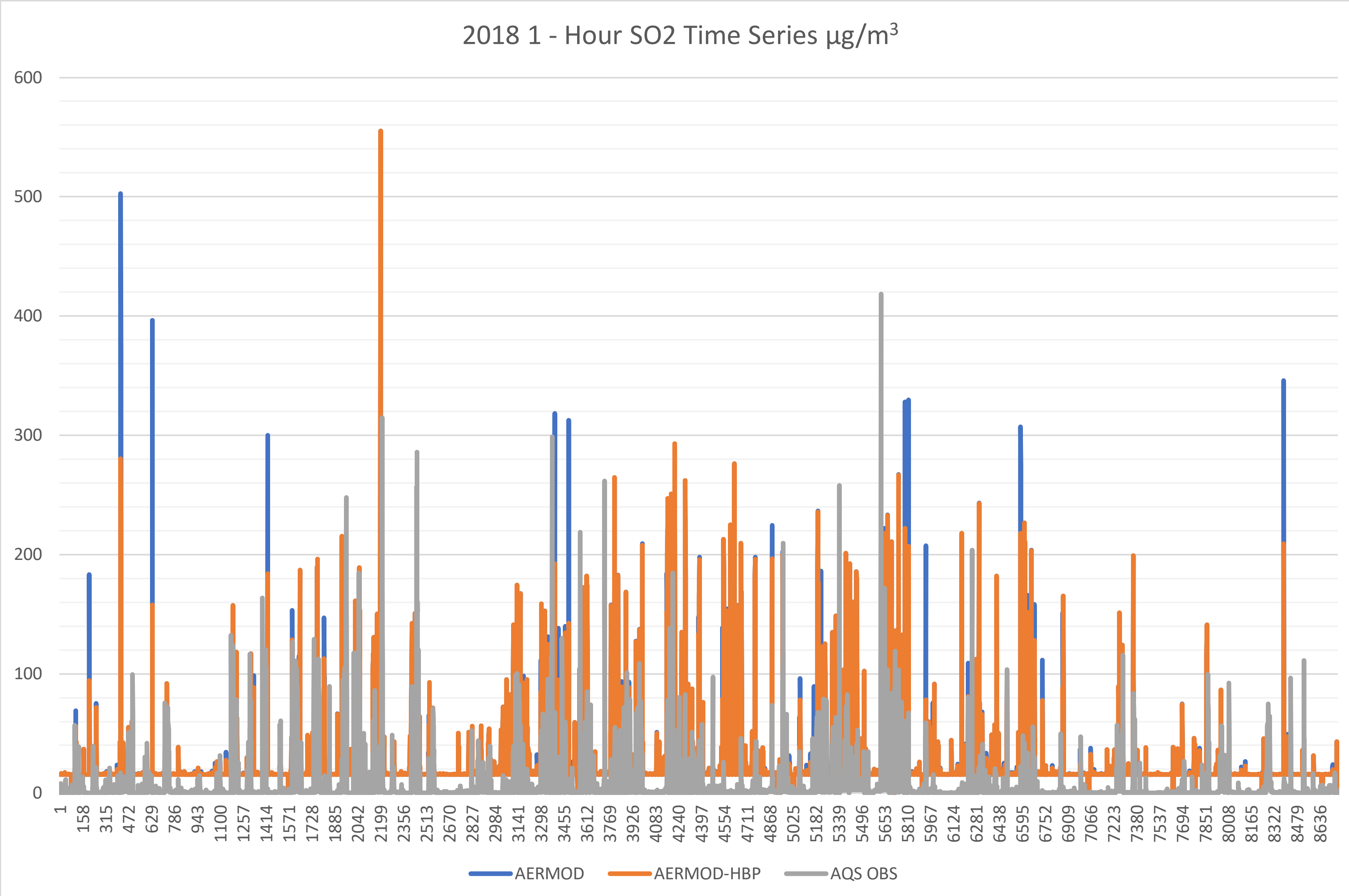


Figure 5.3-11 EPA Region 6 2019 Hourly 1-Hour SO_2 Concentrations Time Series (Martin Creek - Single Receptor)

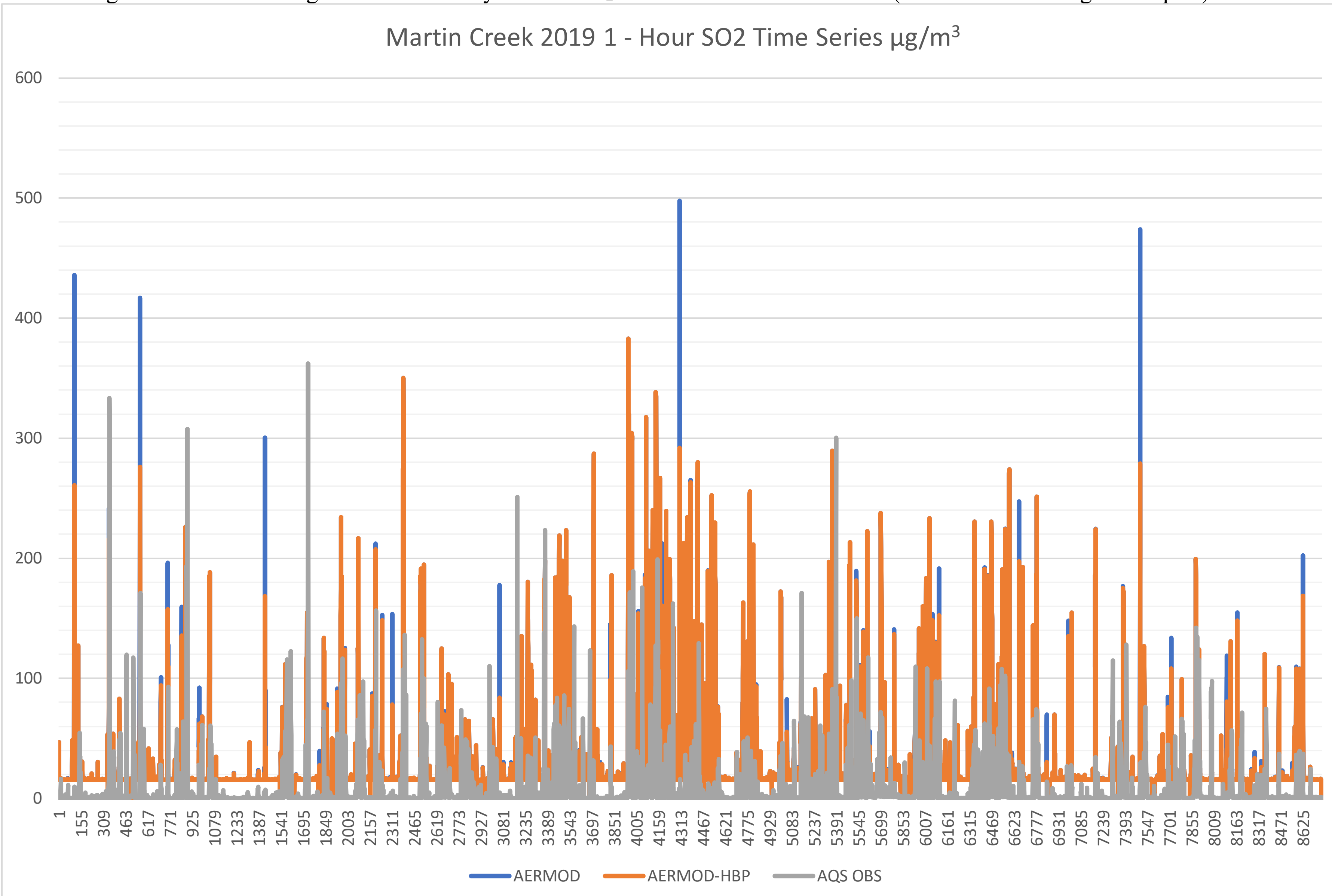
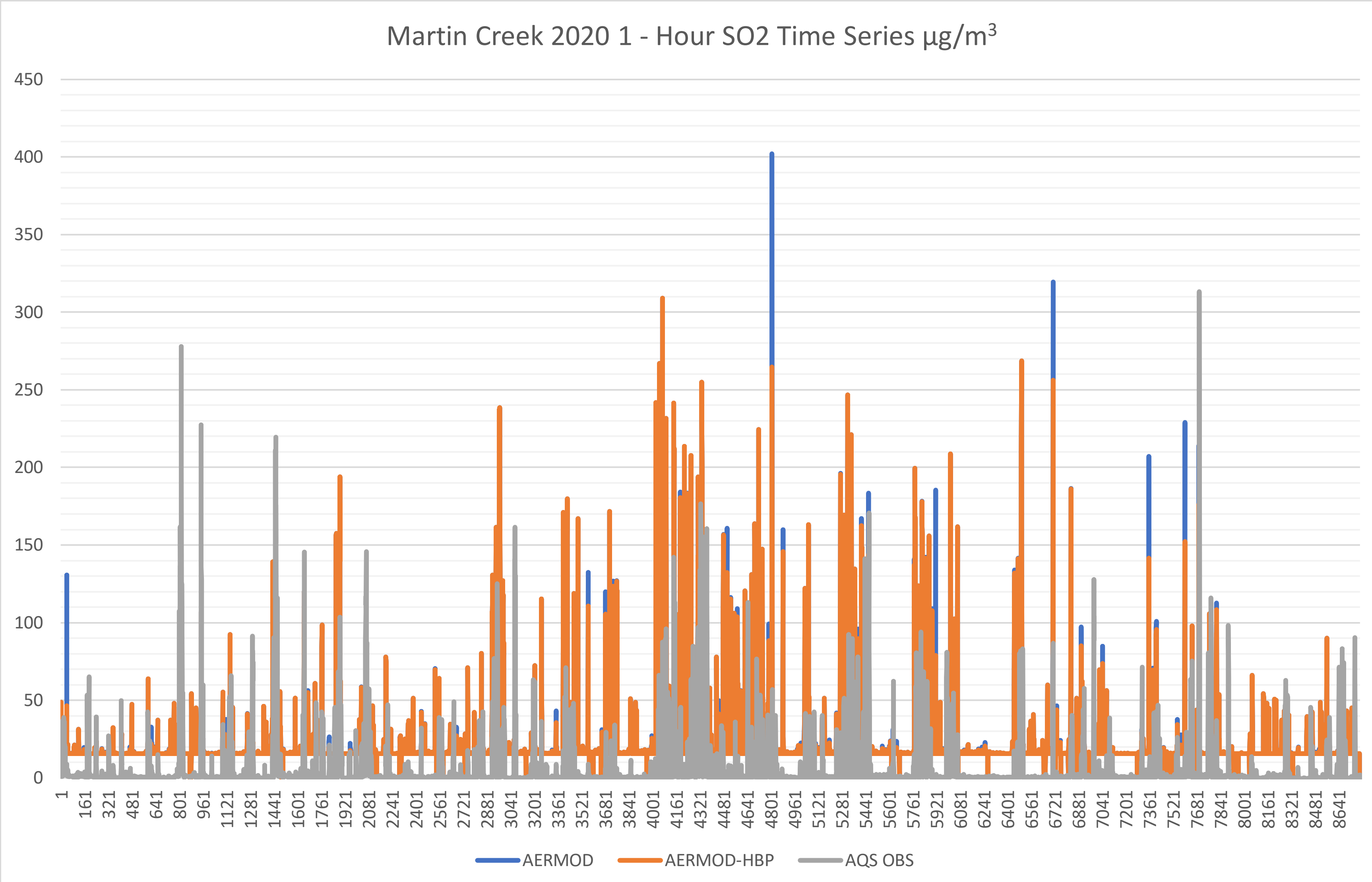


Figure 5.3-12 EPA Region 6 2020 Hourly 1-Hour SO_2 Concentrations Time Series (Martin Creek - Single Receptor)



5.5 Percentile Plots

TCEQ included many percentile plots. All of the the plots that TCEQ provided are included in Appendices E, F, and G.

Appendix E includes 10 figures for each of the three years that there are observations (2018-2020)(30 figures in total) for the 1st through 10th highest observed values. Appendix E also includes figures for AERMOD-HBP 1-hour daily maximum days (includes all 24 hours of values for each day) and also indicates the regulatory AERMOD results on those days. For example, the First Figure on Page E-2 for the Martin Creek monitor had a 1st high observed value on August 23rd (159.8 µg/m^3) and the AERMOD-HBP 1st high modeled value was on April 2nd (218.6 µg/m^3). That figure includes the modeled values for AERMOD and AERMOD-HBP values for both days to evaluate how the model values differ between the regulatory version of AERMOD and the alternative model AERMOD-HBP on both days and how they differ with the observed value. In evaluating these top 10 modeled and top 10 observed maximum 1-hour days for each year we can assess model results and observations to understand what differences may exist between the data sets and if there are any potential concerns overall for these days around the values that drive whether the area models attainment or nonattainment values.

As previously noted, AERMOD and AERMOD-HBP modeled concentrations are not expected to always match nearly or exactly with monitored concentrations when paired in both space and time but are expected to perform well in a statistical assessment replicating the statiscial distribution of monitored concentraions of datasets, especially for concentration values around the NAAQS. AERMOD is expected to result in similar maximum design values (within a factor of two) over the course of multiple years of meteorological data in an upaired time and space assessment. We do this particular type of assessment to be informative and detect if there are any potential major concerns. In general, while the days will often differ between maximum observed and maximum modeled values, the informative part is if overall the top 10 maximum daily values are similar in magnitude between modeled and monitored values not paired in time, especially since these are still paired in space because of the limited number of monitors in the area. Normally we do not constrain assessment of AERMOD's performance to pairing in time and space but in an alternative model review we do a combination of ansalyes to fully assess the changes and compare with relevant monitoring data available.[15]

Appendix F includes six years of the same type of plots as Appendix A but for the years 2015-2020 (six years) for the Longview monitor. There are 60 figures on pages Appendix F-2 through Appendix F-61 based on the observed value and AERMOD-HBP values and another 60 figures on pages Appendix F-62 through F-121.

[15] 40 CFR Part 51 Appendix W

Appendix G includes the 90th percentile and 95th percentile plots (for each year 2018-2020) of observed & AERMOD-HBP 1-hour daily maximum days (includes all 24 hours of values for that day) and also indicates the regulatory AERMOD results on those days on the first 6 figures on pages F-2 through F-7. The 90th percentile and 95th percentile plots (for each year 2018-2020) of observed & AERMOD 1-hour daily maximum days (includes all 24 hours of values for that day) and also indicates the regulatory AERMOD-HBP results on those days on the 6 figures on pages G-8 through G-13.

Overall these plots indicate that AERMOD and/or AERMOD-HBP are generally matching up with the diurnal pattern on some days and not on other days. In looking at all the plots in these three appendices, AERMOD and AERMOD-HBP results in maximum observed values near observed values on some days but not other days. It does appear that overall the maximum values (top 10, 90th percentile, and 95th percentile), while not occuring on the same days, have similar values when evaluated unpaired in time.

5.6 Day Specific Analysis

EPA Region 6 analyzed the hours of the day that AERMOD-HBP was resulting in a change at both the Longview and Martin Creek monitors and also the magnitude of the changes that HBP adjustment was resulting in and compared that to AERMOD regulatory version (both version are AERMOD v21112 as base code) using the 5 years of meteorology (2016-2020). See Tables 5.6-1 and 5.6-2. For Martin Creek monitor, out of the 43,800 hours modeled for the 5-year period, the HBP code resulted in 541 hours that the modeled concentration changed by more than 1 $\mu g/m^3$ (approximately 1.2% of the hours modeled). Of those hours, only 118 hours had a change in the modeled impact of greater than 10 $\mu g/m^3$. As expected the changes were mostly from 10 a.m. to 1 p.m. For the Longview monitor that is 19 km away, out of the 43,800 hours modeled for the 5-year period, the HBP code resulted in 1288 hours that the modeled concentration changed more than 1 $\mu g/m^3$ (approximately 2.9% of the hours modeled). Of those hours, only 370 hours had a change in the modeled impact of equal to or greater than 10 $\mu g/m^3$. Given the distance to the Longview monitor of 19 km, the changes and larger changes tended to be in the earlier hours of the day with changes primarily from 8 a.m. through 4 p.m. and starting to decrease in number after 1p.m.

This analysis helps to confirm that the HBP changes are only impacting modeled concentrations during hours of the day when the convective mix layer is typically increasing and could entrain a penetrated plume that was above the mix lay in previous hours.

Table 5.6-1 HBP Hour of Day when values changed and magnitude of change for Martin Creek Monitor.

HR of Day	Number of Hours of HBP adjustment > 1 ug/m3	Number of Hours of HBP adjustment > 10 ug/m3	Number of Hours of HBP adjustment > 50 ug/m3
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	0	0	0
6	0	0	0
7	1	1	0
8	11	3	2
9	55	16	7
10	98	22	7
11	106	29	9
12	89	20	5
13	68	10	4
14	46	7	1
15	33	5	1
16	18	3	1
17	14	2	1
18	2	0	0
19	0	0	0
20	0	0	0
21	0	0	0
22	0	0	0
23	0	0	0
24	0	0	0
Total	541	118	38

Table 5.6-2 HBP Hour of Day when values changed and magnitude of change for Longview Monitor.

HR of Day	Number of Hours of HBP adjustment > 1 ug/m3	Number of Hours of HBP adjustment > 10 ug/m3	Number of Hours of HBP adjustment > 50 ug/m3
1	0	0	0
2	0	0	0
3	0	0	0
4	0	0	0
5	0	0	0
6	0	0	0
7	55	22	2
8	150	59	14
9	218	69	14
10	200	52	12
11	163	41	5
12	123	36	6
13	109	20	4
14	77	19	3
15	66	19	0
16	64	20	2
17	46	9	2
18	13	2	0
19	4	2	0
20	0	0	0
21	0	0	0
22	0	0	0
23	0	0	0
24	0	0	0
Total	1288	370	64

5.7 Diagnostic Modeling

EPA Region 6 also requested TCEQ to do some diagnostic modeling to evaluate the overall change in modeling results using receptor grid of approximately 25 km by 25 km around Martin Lake (same receptor grid that TCEQ used for attainment demonstration modeling for the area). TCEQ has provided the model runs and some output data for the highest DV run using 2015-2019 actual emissions and meteorology. TCEQ provided Maximum 1-hour SO_2 concentration time series for AERMOD v2112 regulatory version and AERMOD-HBP in Figure 5.7-1.[16]

[16] For interactive time series see file "25km_Hourlyts.html" and "25km_maxDailyts.html" available upon request.

TCEQ also provided daily maximum 1-hour SO_2 concentration time series for the two model versions in Figure 5.7-2. Figure 5.7-3 is the 1st through 10th rank highest averaged 5-year modeled SO_2. Figures 5.7-4 and Figure 5.7-5 are 5-year design value isopleths. We note that TCEQ's model run did not include any emissions from the auxillary boilers,only the three main boilers. As expected there is a sizeable difference between model results using the regulatory version of AERMOD and AERMOD-HBP.

Figure 5.7-1 TCEQ Maximum Hourly SO_2 Concentrations over 25km receptor grid (actual emissions and meteorology 2015-2019).

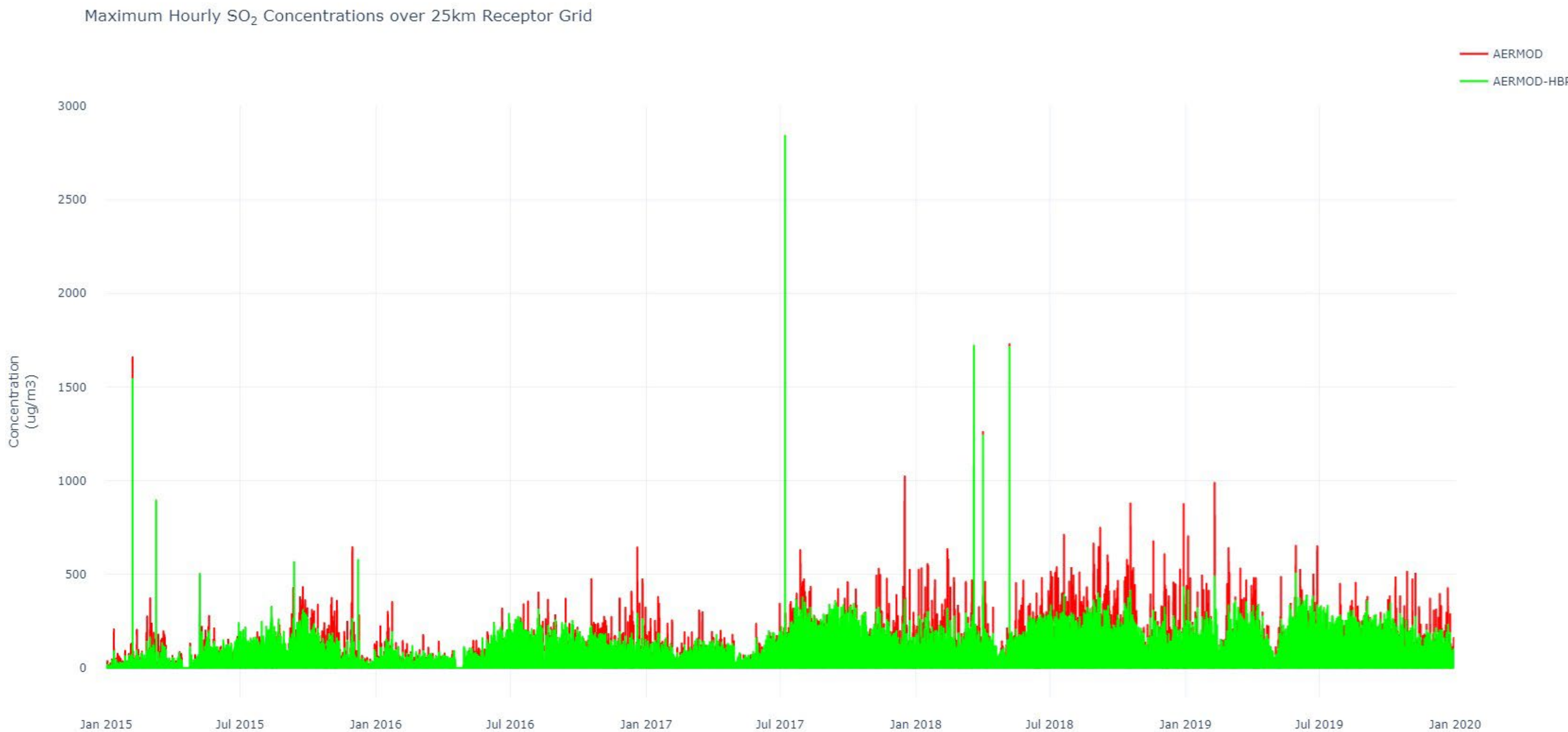


Figure 5.7-2 TCEQ Maximum daily 1-Hour SO_2 Concentrations over 25km receptor grid (actual emissions and meteorology 2015-2019).

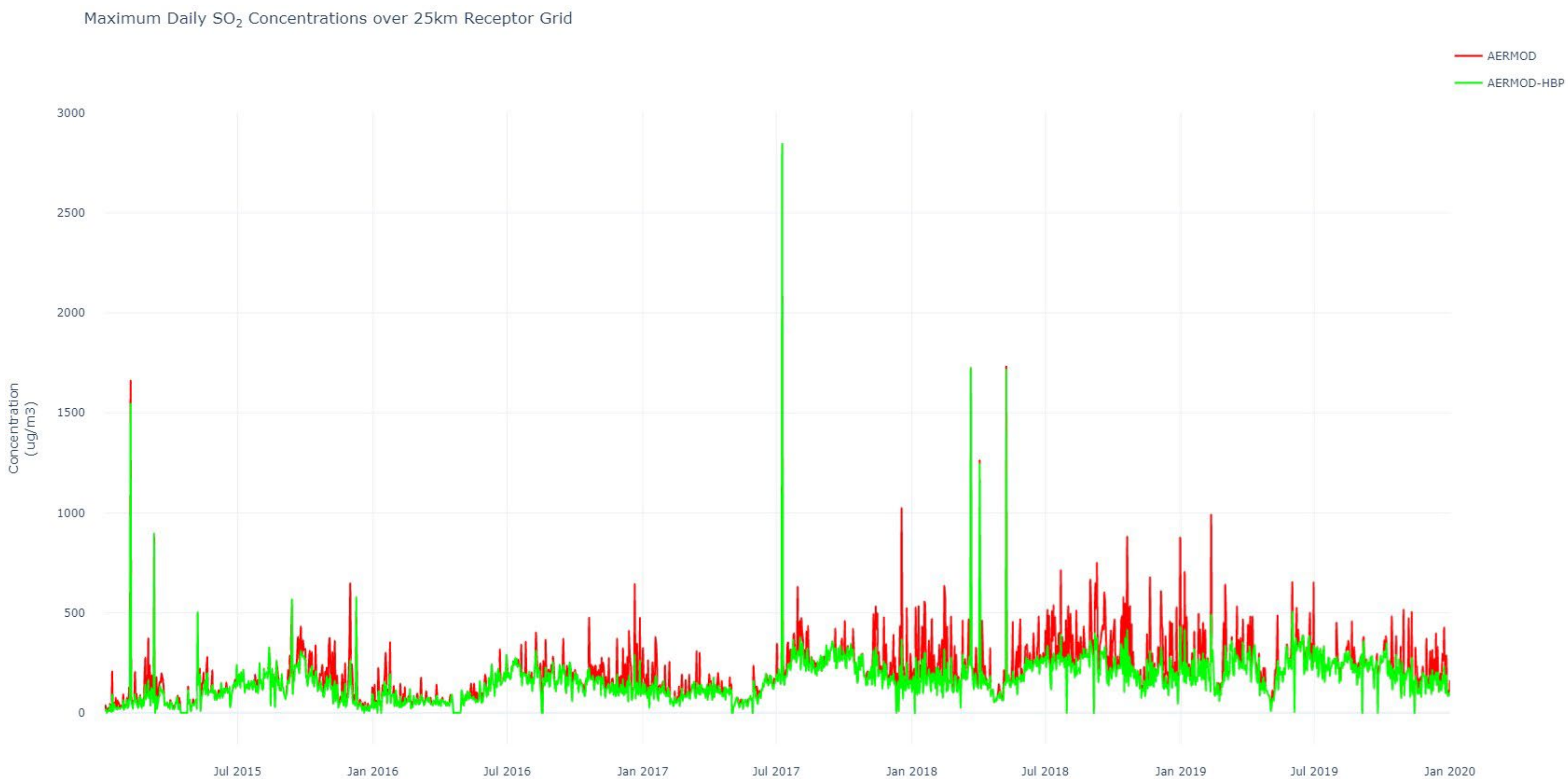


Figure 5.7-3 TCEQ 1st through 10th Rank Highest Average 5-year modeled SO_2 (includes 6 ppb background, meteorology and actual emissions for 2015-2019).

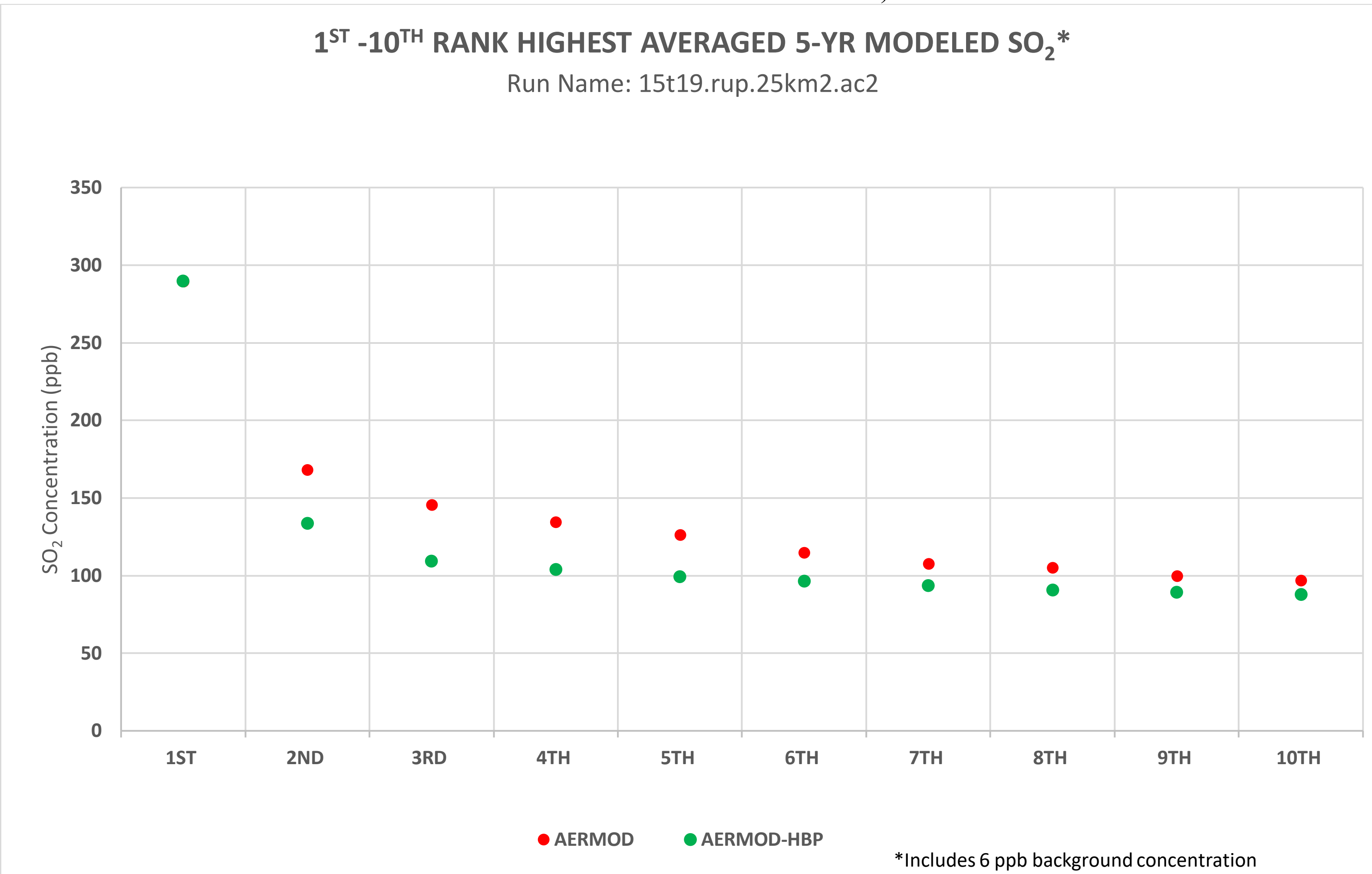


Figure 5.7-4 TCEQ isopleth AERMOD-v21112 regulatory with actual emissions 2015-2019.

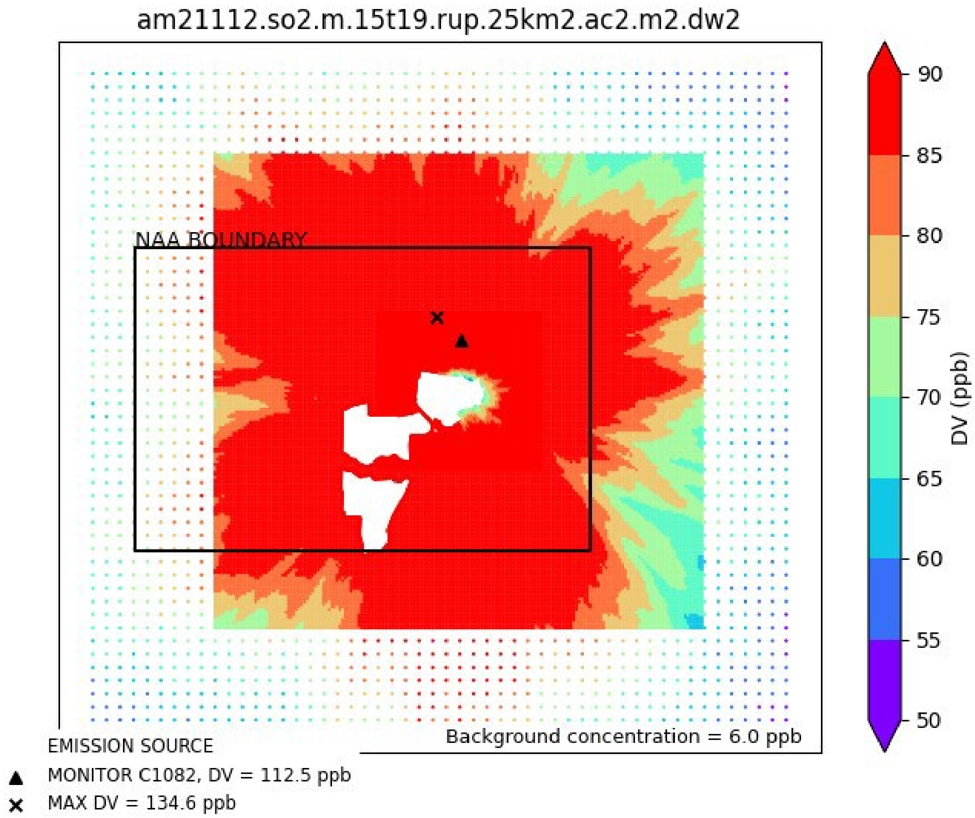
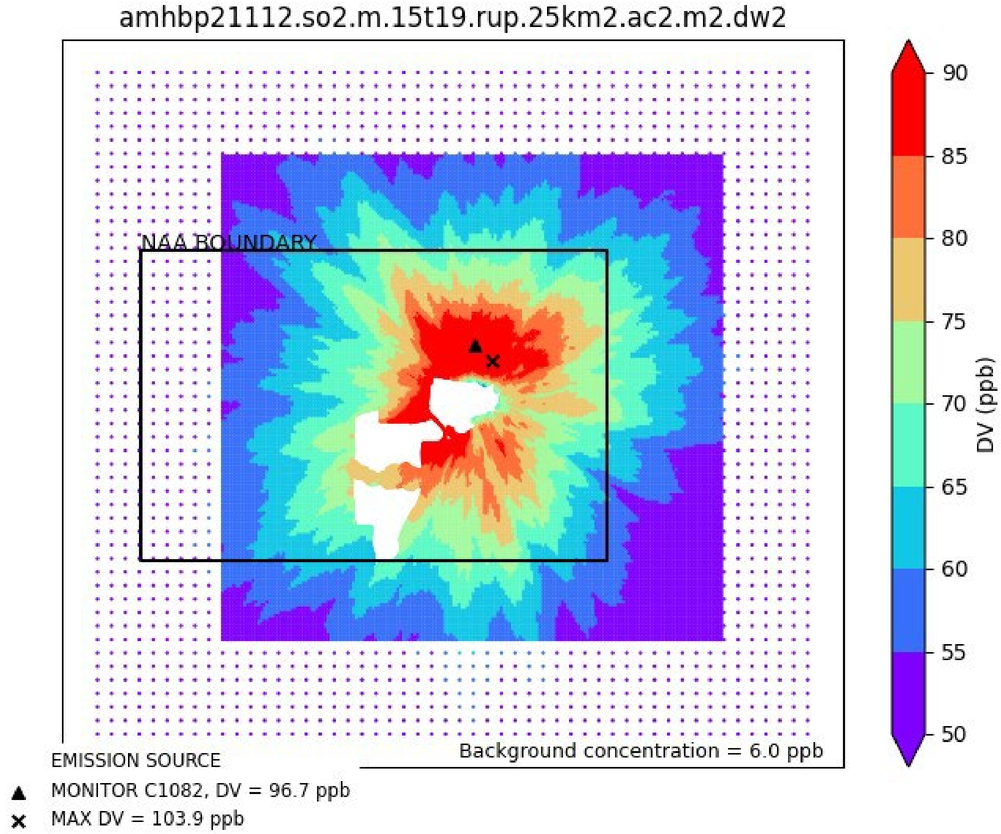


Figure 5.7-5 TCEQ AERMOD-HBP Diagnostic model run with 2015-2019 actual emissions.



EPA Region 6 also did some diagnostic runs as part of our review. EPA Region 6 used the 2016-2020 actual emissions, stack parameters provided by Vistra, and meteorological files provided by TCEQ for this alternative model review. EPA Region 6 did include the auxillary boiler source in this modeling. Figures 5.7-6 and 5.7-7 are isopleths of the concentration in micrograms/meter cubed using the attainment demonstration SIP receptor grid and the regulatory version of AERMOD v 21112 in the first figure and a zoom in on the second figure. Figures 5.7-8 and 5.7-9 are isopleths of the concentration in micrograms/meter cubed using the attainment demonstration SIP receptor grid and the alternate model AERMOD-HBP (version of AERMOD v 21112 with HBP code) in the first figure and a zoom in on the second figure. The regulatory version of AERMOD results in an area that is indicated having a design value exceeding the 1-hour SO_2 NAAQS of 196.4 μg/m^3 while the AERMOD-HBP model results a maximum DV of 191.5 μg/m^3 with no area exceeding the 1 -hour SO_2 NAAQS. This is similar to TCEQ's modeling for a different period, even though it is not directly comparable,both indicate that HBP results in significant reductions in design value concentrations in the Rusk-Panola area.

Figure 5.7-6 EPA Region 6 isopleth AERMOD-v21112 regulatory with actual emissions 2016-2020.

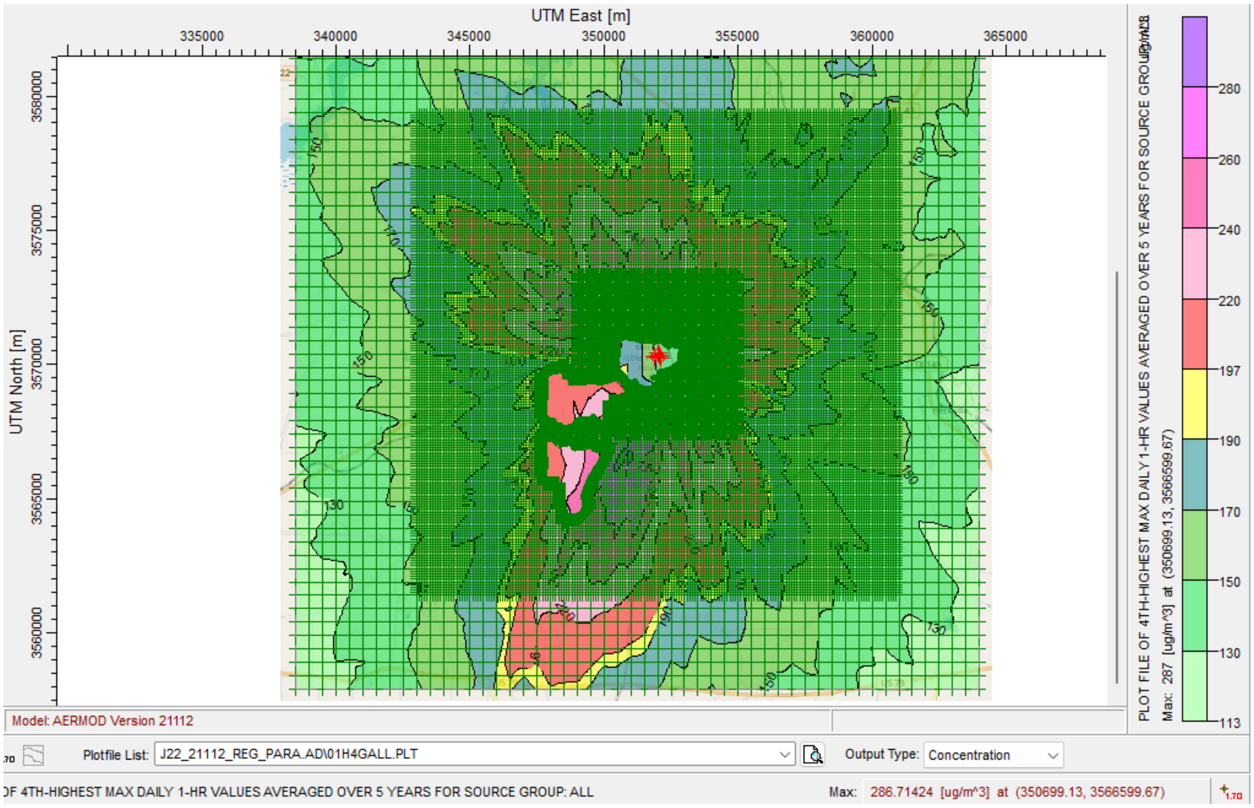


Figure 5.7-4 EPA Region 6 isopleth AERMOD-v21112 regulatory with actual emissions 2016-2020 (Zoom-in).

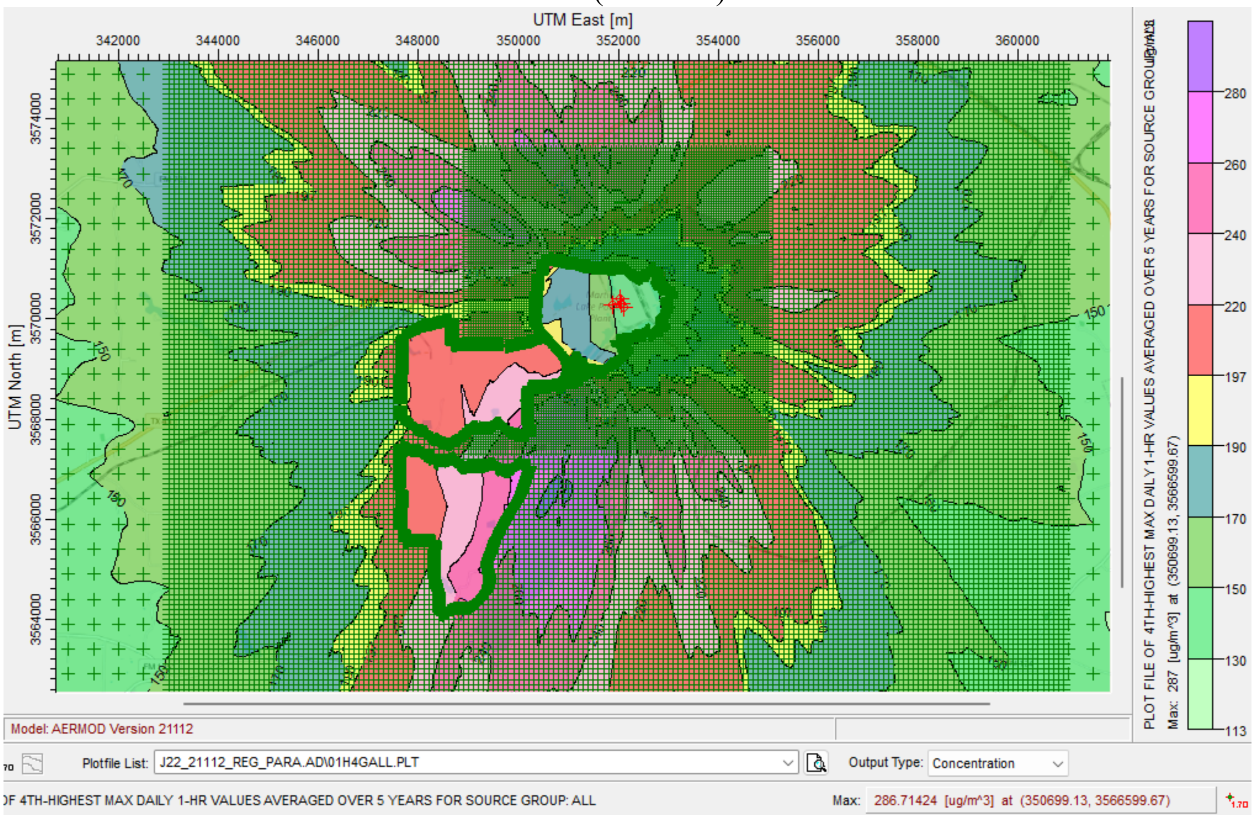


Figure 5.7-4 EPA Region 6 isopleth AERMOD-v21112 -HBP with actual emissions 2016-2020.

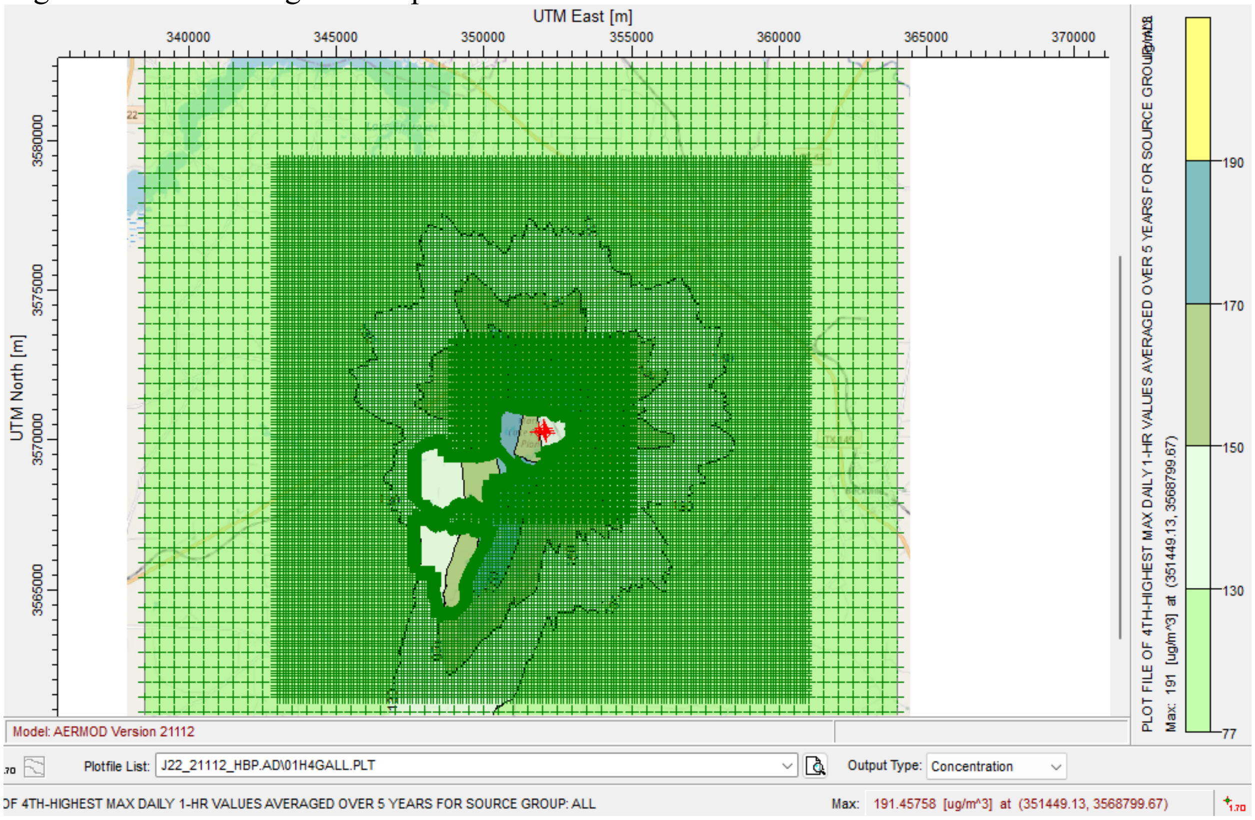
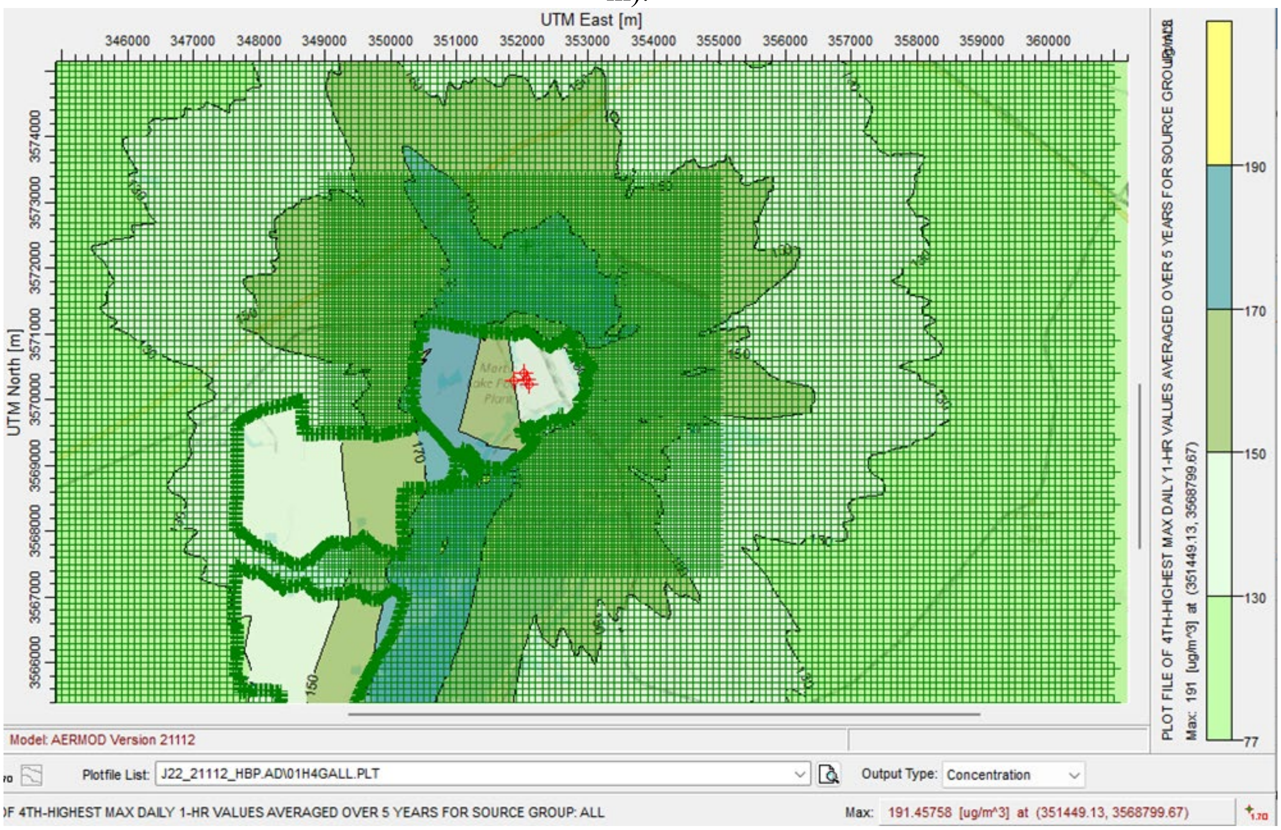


Figure 5.7-4 TCEQ isopleth AERMOD-v21112 HBP with actual emissions 2016-2020 (Zoom-in).



5.8 Comparison to EPA Model Evaluations

TCEQ provided a summary of different EPA AERMOD model evaluation studies with a summary of the 1-hour and 3-hour Modeled/Observed RHC ratio that AECOM had prepared. TCEQ proposed that comparing the Modeled/Observed RHC ratio of AERMOD-HBP with these other studies that had similar sources and distances would provide context to the Cox-Tikvart results of the comparison of AERMOD regulatory and AERMOD-HBP. TCEQ examined EPA's Model Evaluation Databases[17] and their discussion in EPA's 2003 paper "AERMOD: Latest Features and Evaluation Results".[18] The EPA studies' RHC values used the top 25 values for all monitors in the dataset, irrespective of space and time, so for comparison the AECOM used the RHC for the top 25 values from the combination of Martin Creek and Longview monitors.

We note that EPA Region 6 did not have all the information or time to review these other studies for how they might compare or be different from the Rusk-Panola Attainment Demonstration

[17] https://www.epa.gov/scram/air-quality-dispersion-modeling-preferred-and-recommended-models

[18] https://gaftp.epa.gov/Air/aqmg/SCRAM/models/preferred/aermod/aermod_mep.pdf (454-R-03-003)

alternative model request situation in source specific information and location and number of monitors and prevailing winds. EPA Region 6 did not review the results of this AERMOD-HBP modeling analysis for Martin Lake area against the results from these other studies but evaluated this alternative model request solely on the information and analysis available for the use of AERMOD-HBP vs. AERMOD regulatory v21112 in this case and site specific determination.

6. Alternative Model AERMOD-HBP EPA Region 6 Review Conclusions

As EPA Region 6 performed this review and created this TSD the elements included are formulated to address the specific requirements of an alternative model review. In this section we go over each relevant part of the Guideline on Air Quality Models, how those are being addressed, and EPA Region 6's conclusions.

40 CFR Part51 App. W 3.2.2(b) states:

- App. W 3.2.2(b) "An alternative model shall be evaluated from both a theoretical and a performance perspective before it is selected for use. There are three separate conditions under which such a model may be approved for use:[19]"

Sections 2, 3, and 5.6 of this TSD address EPA Region 6's review and conclusions of the theoretical analysis and determine the proposed Alternate approach is reasonable in this one-time case-specific evaluation for the modeling for the Rusk-Panola 1-Hour SO_2 Attainment Demonstration (Martin Lake area).

App. W 3.2.2 provides three separate conditions under which such a model may be approved for use and TCEQ's alternative model request is being evaluated pursuant to Condition 2. Condition 2 states:

- App. W 3.2.2(b)(2) {also referred to as 'Condition 2'} "If a statistical performance evaluation has been conducted using measured air quality data and the results of that evaluation indicate the alternative model performs better for the given application than a comparable model in appendix A"

Also directly relevant to meeting the conditions of App. W 3.2.2(b)(2) is the App. W 3.2.2(d), which states:

- App. W 3.2.2(d) "For condition (2) in paragraph (b) of this subsection [above], established statistical performance evaluation procedures and techniques[20] for determining the acceptability of a model for an individual case based on superior performance should be followed, as appropriate. Preparation and implementation of an evaluation protocol that is acceptable to both control agencies and regulated industry is an important element in such an evaluation."

In respect to App. W 3.2.2(d), EPA Region 6, OAQPS, TCEQ and their contractor Ramboll, and Vistra and their contractor AECOM had several calls to discuss and work out different elements

[19] The other 2 conditions discussed in App. W 3.2.2.(b)(1) and b(3) do not apply in this situation as the applicant has asked for approval in accordance with App. W 3.2.2(b)(2).

[20] Endnotes 28 and 29 "28. ASTM D6589: Standard Guide for Statistical Evaluation of Atmospheric Dispersion Model Performance. (2010). 29. U.S. Environmental Protection Agency, 1992. Protocol for Determining the Best Performing Model. Publication No. EPA–454/R–92–025. Office of Air Quality Planning and Standards, Research Triangle Park, NC. (NTIS No. PB 93– 226082)."

of a protocol in late 2020 and through July 2021. In addition to these meetings a draft model evaluation protocol was shared with EPA and EPA reviewed and provided comments back on several occasions including in early July 2021. TCEQ finalized the protocol and shared it with EPA Region 6 at the end of July. This final protocol (Appendix B of this TSD) dated July 29, 2021 meets this requirement.

In respect to App. W 3.2.2(b)(2) {Condition 2}, EPA Region 6's evaluation of the Cox-Tikvart results indicates that AERMOD-HBP performs better than AERMOD in this case/site specific evaluation of AERMOD-HBP. The Cox-Tikvart results are statistically significant (for one of the two monitors in alternative CT approach) or close to statistically signicant (standard method). Statistical significance is not a requirement but a goal point to give context to the magnitude of benefit. The test under App. W 3.2.2(b)(2) is that the model has to perform better for a given application than a comparable model in appendix A (AERMOD in this case). In looking at the Cox-Tikvart results and other plots and analysis in Section 5 of this TSD, EPA Region 6 concludes that AERMOD-HBP performs better than the regulatory model AERMOD in this site specific analysis for the area around Martin Lake Power Plant. This best performing model analysis of AERMOD-HBP is limited to this one site specific situation and should not be construed as validitating AERMOD-HBP for use in regulatory related actions other than this specific Rusk-Panola 1-Hour SO_2 Attainment Demonstration SIP for the area around the Martin Lake Power Plant.

As previously discussed, while not specifically cross-referenced, App. W 3.2.2(e) sets forth five conditions that must be satisfied for alternative model approval under Condition 2 of 3.2.2(b)(2) by providing a framework on how to address the requirements of App. W 3.2.2 and on how to perform an analysis from both a theoretical and performance perspective.

Other relevant App. W.:

- App. W 3.2.2(e) "Finally, for condition (3) in paragraph (b) of this subsection, an alternative model or technique may be approved for use provided that:
    i. The model or technique has received a scientific peer review;
    ii. The model or technique can be demonstrated to be applicable to the problem on a theoretical basis;
    iii. The databases which are necessary to perform the analysis are available and adequate;
    iv. Appropriate performance evaluations of the model or technique have shown that the model or technique is not inappropriately biased for regulatory application [21]; and
    v. A protocol on methods and procedures to be followed has been established."

[21] Footnote a "For PSD and other applications that use the model results in an absolute sense, the model should not be biased toward underestimates. Alternatively, for ozone and PM2.5 SIP attainment demonstrations and other applications that use the model results in a relative sense, the model should not be biased toward overestimates."

In respect to App. W 3.2.2.(e)(i) and (ii), Sections 2 and 3 includes EPA Region 6 evaluation of the materials provided which included a peer reviewed scientific article (Weil, 1997), several reports and presentations (see materials included in Appendices A, C, and D to this TSD) on the theoretical problem and proposed theoretical solution, and proposed code changes to AERMOD to address the problem. EPA Region 6 has reviewed these materials as discussed in the sections and consider the alternate treatment of penetrated plume is applicable in the specific situation of modeling for Rusk-Panola 1-Hour SO_2 Attainment Demonstration modeling. Materials provided included evaluations of a couple of alternate treatments of penetrated plumes (AECOM's HBP and Weil's HIPMOD) at several other locations in the U.S and Australia but EPA Region 6 did not do a full review of these materials as this is a site and case specific evaluation just for the nonattainment area around the Martin Lake Power Plant facility. EPA Region 6 does conclude that all the information provided indicates that the proposed alternate treatment of penetrated plume is a problem on a theoretical basis for this specific situation of modeling emissions from the Martin Lake Power facility, so EPA Region 6 concludes that App. W 3.2.2(e)(i) and (ii) have been met in this case specific situation.

In respect to App. W 3.2.2.(e)(iii), Sections 2 and 5 are pertinent. Initially, only 3 years of monitoring data at the nearby Martin Creek monitor was proposed to be used. EPA Region 6 did not consider one monitor to necessarily be enough observation data for conducting an alternative model evaluation, so we also requested the Longview monitor that is further away but whose modeled concentrations would also be expected to be impacted by the proposed alternate penetrated plume treatment. The Longview monitor also has the benefit of being a long-term 1-Hour SO_2 monitor so five years of data was available for use that included the years the Martin Creek monitor also had collected data. While it was a limited dataset, EPA determined that this dataset provided enough monitoring data for this case specific alternative model evaluation. Vistra also provided hourly emissions and stack parameters (temperature and velocity) based on CEMs collected data, so there was good emission and stack parameters for the evaluation. With the inclusion of the Longview monitor EPA Region 6 is determining that App. W 3.2.2(e)(iii) is met.

In respect to App. W 3.2.2.(e)(iv), Sections 5 includes EPA Region 6 evaluation of AERMOD-HBP. There were a few metrics that indicated AERMOD-HBP might have a slight underprediction under certain situations but overall this was not deemed to be be a significant concern. EPA Region 6 concludes that looking at all the information that AERMOD-HBP was not inappropriately biased for this case specific determination for the Rusk-Panola 1-Hour SO_2 attainment demonstration modeling.

In respect to App. W 3.2.2.(e)(v), as discussed above there were a number of meetings and emails between EPA Region 6, OAQPS, TCEQ and their representatives, and Vistra and their representatives to develop what analyses needed to be included for EPA Region 6 to evaluate an alternative model request. Draft protocol was shared and EPA provided comments and feedback on several issues up through July 2021. TCEQ finalized the protocol and shared it with EPA Region 6 at the end of July. This final protocol (Appendix B of this TSD) dated July 29, 2021 meets this requirement.

In looking at the different parts of App. W Section 3.22, EPA Region 6 concludes that TCEQ's Alternate Model evaluation and EPA Region 6's additional modeling and evaluation provide adequate information for review and decision on this request in accordance with the pertinent requirements of App. W Section 3.

Each site-specific alternative model request is unique, so this analysis and proposed approval of the use of AERMOD-HBP for Texas' 1-Hour SO_2 Attainment Demonstration SIP is a site-specific analysis based on the datasets available at this time. Overall AERMOD-HBP has improved model performance compared to the regulatory version of AERMOD (both versions use AERMOD v21112 model system) with some indication of slight underestimation bias at the extreme high end of the distribution for some years. Given this is an alternative model assessment and is based on three years of data for one monitor two kilometers from Martin Lake and five years at another monitor 19 km away, it is a relatively small data set for this evaluation, but EPA Region 6 agrees that this is all the pertinent data available when the state submitted and the data set is adequate for EPA Region 6 to perform this alternative model review.

EPA Region 6 finds that AERMOD-HBP is a better performing model than AERMOD for this specific situation in modeling the area around the Martin Lake Facility in East Texas. EPA Region 6's finding is a site-specific and time-specific analysis determination and does not imply that AERMOD-HBP can or should be considered as available to use at another facility elsewhere in the country in a regulatory review without a site specific evaluation based on information in the area that AERMOD-HBP is requested to be used as an Alternate Model to AERMOD. EPA Region 6 also notes that our approval is narrowly drawn and that use of AERMOD-HBP in future modeling of the Martin Lake facility would likely require another alternative model request, review, and approval by EPA Region 6 using all additional data that may be available at that time.