APPENDIX L

HOWARD COUNTY MONTE CARLO SIMULATIONS

Howard County Attainment Demonstration State Implementation Plan Revision for the 2010 One-Hour Sulfur Dioxide National Ambient Air Quality Standard

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APPENDIX L: A MONTE CARLO METHOD TO DEMONSTRATE ATTAINMENT OF THE 2010 SULFUR DIOXIDE (SO_2) NATIONAL AMBIENT AIR QUALITY STANDARD IN HOWARD COUNTY, TEXAS

Appendix L provides details of the dispersion modeling and Monte Carlo method, referred to as the MC approach, used to demonstrate compliance with the 2010 One-Hour SO_2 NAAQS in the Howard County nonattainment area. The TCEQ contracted with Ramboll US Consulting, Inc., (Ramboll) to aid with the modeling of emissions sources and application of a Monte Carlo approach in Howard County nonattainment area. Appendix L is the technical report from Ramboll detailing the MC approach.

Prepared for:

Texas Commission on Environmental Quality
12100 Park 35 Circle MC 164
Austin, TX 78753

Prepared by:

Ramboll US Corporation
19020 33rd Ave W, Suite 580
Lynnwood, WA, 98036

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A MONTE CARLO METHOD TO DEMONSTRATE ATTAINMENT OF THE THE 2010 SULFUR DIOXIDE (SO2) NATIONAL AMBIENT AIR QUALITY STANDARD IN HOWARD COUNTY, TEXAS

PREPARED UNDER A CONTRACT FROM THE
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CONTENTS

1.	**Introduction**	**4**
2.	**AERMOD Modeling Approach**	**4**
2.1	Source Characterization	4
2.1.1	Continuous Sources	5
2.1.2	Tokai Big Spring Carbon Plant	5
2.1.3	Delek Big Spring Refinery	5
2.2	Background	6
2.3	Receptor Grid	7
3.	**MC Approach**	**9**
3.1	Intermediate Processing	9
3.2	Monte Carlo Methodology	9
3.3	Monte Carlo Simulations Performed	10
3.4	Emission Scaling Verification	11
4.	**Results of MC Approach**	**11**
4.1	Maximum Concentrations from Each Tokai Scenario	11
4.2	Evaluation of Run Simulation Size	14
4.3	Additional Evaluation of Controlling Scenario	14
4.4	Maximum Concentration by Receptor	19
4.5	Monte Carlo Analysis Within the Big Spring Carbon Black Plant (Tokai) Property Boundary	20
5.	**References**	**21**

TABLES

Table 1. Emission Rate and Occurrences per Year of Delek Intermittent Sources 6

Table 2. Hourly SO_2 Background Concentrations in PPB by Season and Hour of Day 7

Table 3. Maximum Monte Carlo-Derived Concentrations for Top Ten Tokai MSS and Routine Scenarios 12

FIGURES

Figure 1. Receptors Included in Howard County Monte Carlo Analysis 8

Figure 2. Maximum Monte Carlo-Generated Design Values by Tokai Operational Scenario 13

Figure 3. Comparison of Monte Carlo Runs with 10,000 and 20,000 Simulations for top 10 MSS and Routine Scenarios 15

Figure 4. Distribution of Monte Carlo Design Values from Top 10 MSS Scenarios 16

Figure 5. Distribution of Monte Carlo Design Values from Top 10 Routine Scenarios 17

Figure 6. Monte Carlo-Generated Design Values After 220,000 Simulations of Scenario Routine 24D 18

Figure 7. Maximum 1-hr SO_2 Design Values over all Monte Carlo Simulations 19

Figure 8. Non-Tokai Maximum 1-hr SO_2 Design Values Within Tokai Site from Monte Carlo Analysis 21

1. Introduction

A Monte Carlo (MC) method is a statistical technique for investigating how model outputs respond to variation in model inputs by randomly sampling from the possible input data to create many different scenarios and thereby determine the likelihood of certain outcomes. MC methods are useful when the number of possible input scenarios is enormous and evaluating every scenario is impractical. This report describes the application of a MC method to evaluate modeled sulfur dioxide (SO_2) concentrations from sources with intermittent emissions in combination with continuous (deterministic) emission sources and background concentrations.

This study examines dispersion modeling using AERMOD of several sites in Howard County, Texas, an area designated as nonattainment for the 2010 1-hour SO_2 National Ambient Air Quality Standard (NAAQS). The Texas Commission in Environmental Quality (TCEQ) contracted with the Ramboll US Corporation (Ramboll) to aid with the modeling of the emissions sources in the nonattainment area and application of a MC approach to demonstrate compliance.

Howard County contains several significant sources of SO_2 emissions from three sites: the Delek US Holdings' Big Spring Refinery (Delek Big Spring Refinery), BHER Power Resources' Big Spring Cogeneration (BHER Big Spring Cogeneration) and Tokai Carbon CB LTP's Big Spring Carbon Black Plant (Tokai Big Spring Carbon Plant). Some sources at these sites intermittently and non-deterministically emit SO_2. The Delek Big Spring Refinery and the Tokai Big Spring Carbon Plant will be referred as the Delek and Tokai in the MC approach. Modeling these intermittent sources as if the emit continually results in unrealistic and overly conservative SO_2 concentrations. Therefore, a MC approach was applied to create intermittent emission scenarios that better simulate real-world operating conditions, and to demonstrate NAAQS compliance with statistical certainty.

2. AERMOD Modeling Approach

This section describes the application of AERMOD to generate concentrations and dispersion factors. Model input files are available electronically on the TCEQ's FTP site[1].

2.1 Source Characterization

This section describes the sources included in the AERMOD dispersion modeling and MC analysis. For a complete description of included sources, along with a derivation of their emission rates and source parameters, please refer to TCEQ's Howard County Attainment Demonstration State Implementation Plan for the 2010 One-Hour Sulfur Dioxide National Ambient Air Quality Standard (hereafter referred to as the Howard County AD SIP revision).

[1] ftp://amdaftp.tceq.texas.gov/so2/mc_approach

2.1.1 Continuous Sources

While several sources emit SO_2 within Howard County, most were modeled with the standard practices outlined in Appendix W[2], *Guideline on Air Quality Models*, which prescribes the use of AERMOD for regulatory purposes. These sources, along with continuously operating sources at the BHER Big Spring Cogeneration (BHER), the Delek Big Spring Refinery (Delek) and the Tokai Big Spring Carbon Plant (Tokai) sites, were assumed to operate on a continuous basis over the 5-year modeling period of 2016 through 2020.

All continuous sources were included in a single AERMOD run, along with background concentrations varying by season and hour of day, as described in **Section 2.2**. This run generates a single AERMOD "POST" file with SO_2 concentrations at each receptor for each hour of the modeling period.

2.1.2 Tokai Big Spring Carbon Plant

Two sources at Tokai operate in a continuous, deterministic fashion and were included in the continuous model run. However, emissions from four sources (EPN 7A, EPN 12A, EPN 13A, and EPN FLARE 4), are capped, i.e., instead of individual emission limits the four sources have a combined emissions cap limitation. In addition, only one of Tokai sources EPN 13A and EPN FLARE 4 are in operation at a time, depending on the mode of operation - either routine or planned maintenance, startup, and shutdown (MSS).

The standard method of modeling capped sources involves running AERMOD for each possible operational scenario that can distribute the emissions cap among the four capped sources. By examining each permutation of operating conditions at a site, compliance can be demonstrated if all scenarios fall below the standard. This approach was applied when modeling Tokai. The modeled emission rates, as well as stack exit gas velocities and temperatures for each scenario are provided in an Excel spreadsheet ("Tokai_cap_load_scenario_model_inputs.xlsx"), available on the TCEQ FTP site.

Each of these capped sources was modeled in AERMOD with a unit emission rate of 1 gram per second (g/s) to create one POST file per source. Since concentration scales linearly with emission rate (for a given dispersion factor), the resultant POST files can be scaled to examine multiple emission scenarios without the need to rerun AERMOD.

Since Tokai operational scenarios also vary in source parameters (exit gas velocity and temperature), separate POST files are generated for each scenario.

2.1.3 Delek Big Spring Refinery

Most sources at Delek were modeled on a continuous basis, with the MC approach applied to four intermittent sources. Each of these four sources were modeled in two operational modes: routine and planned maintenance, startup, and shutdown (MSS).

[2] https://www.epa.gov/sites/production/files/2020-09/documents/appw_17.pdf

For each operation mode for each of the four intermittent sources, the TCEQ provided a range of possible emissions. The maximum emission rate was selected for use in the MC approach. Each scenario was also assigned a maximum number of occurrences per year. While occurrences normally last a few hours, it was assumed that each occurrence would last a full calendar day to ensure that the daily maximum hourly concentration would be captured.

The model ID, operation mode, maximum emission rate, and number of occurrences per year for each source is provided in **Table 1**.

Table 1. Emission Rate and Occurrences per Year of Delek Intermittent Sources

Model ID	Operational Mode	Emission Rate (lb/hr)	Occurrences per Year
02CRUDEF	MSS	750	3
		250	14
	Routine	51.8	348/349[a]
05REFMRF	MSS	750	5
		250	4
	Routine	103.7	356/357[a]
14NEASTF	MSS	1500	2
		500	6
		250	4
	Routine	25	354/354[a]
16SOUTHF	MSS	1695	2
		500	12
		250	4
	Routine	118.7	347/348[a]

a - Remaining days in a calendar year taking into consideration leap years

2.2 Background

Background values were included in AERMOD by season and hour of day using the SEASHR keyword. These background values are provided in **Table 2**. The derivation of these background values is described in the Howard County AD SIP revision.

Table 2. Hourly SO_2 Background Concentrations in PPB by Season and Hour of Day

Hour of Day	Winter	Spring	Summer	Fall
1	1.50	1.18	1.71	1.59
2	2.37	0.79	0.98	1.84
3	2.06	1.00	0.89	1.44
4	1.69	1.40	0.73	1.45
5	1.33	1.28	0.72	1.38
6	1.60	0.96	0.73	1.27
7	1.43	1.15	0.77	1.56
8	1.59	1.22	0.66	1.30
9	2.31	1.09	0.98	1.33
10	4.02	1.78	1.55	1.88
11	3.29	2.13	2.16	2.08
12	2.82	1.78	0.94	2.20
13	2.48	1.83	0.89	2.85
14	1.93	1.49	0.85	2.25
15	2.30	2.45	1.12	2.02
16	1.99	2.07	0.84	1.85
17	2.30	2.13	0.87	1.41
18	1.50	1.46	0.77	1.43
19	1.45	1.16	0.60	1.07
20	1.45	1.07	0.48	1.02
21	1.42	0.92	0.85	1.13
22	2.09	1.04	0.76	1.32
23	1.44	1.30	0.81	1.38
24	1.41	1.33	1.07	1.67

2.3 Receptor Grid

To reduce simulation run time, a reduced receptor grid was used for the MC simulations. First, the modeling grid that covered the entire nonattainment area was screened to remove receptors with no possibility of a modeled NAAQS exceedance. This was done by running AERMOD for each Tokai operational scenario and all Delek (including the four intermittent sources and BHER) sources at maximum emission rates for each day of a five-year period. After combining with a background concentration, the design value at each receptor was determined. Maximum concentrations at each receptor in the original modeling domain were compared to a screening threshold. While the NAAQS for 1-hr SO_2 is 75 ppb, a screening value of 70 ppb was selected to ensure that sufficient receptors were included in the areas with highest concentrations. Receptors with a value exceeding this screening threshold of 70 ppb are shown in **Figure 1**. Receptors below 70 ppb were removed from further consideration.

To illustrate concentration gradients derived from the MC approach, and to demonstrate that the standard will not be exceeded in any area of the modeling domain, additional receptors were placed in the following locations:

- In a 100m grid within 500m of a receptor exceeding 70 ppb;
- Every 100m along property boundaries near receptors exceeding the NAAQS;
- Every 100m along the rail line;
- Every 100m along Interstate 20;
- Every 50, 100, or 200m along the fenceline, with closer spacing near high concentration areas; and
- Every 200m offset 100m from the fenceline.

The locations of the 648 receptors included in the analysis is provided in **Figure 1**.

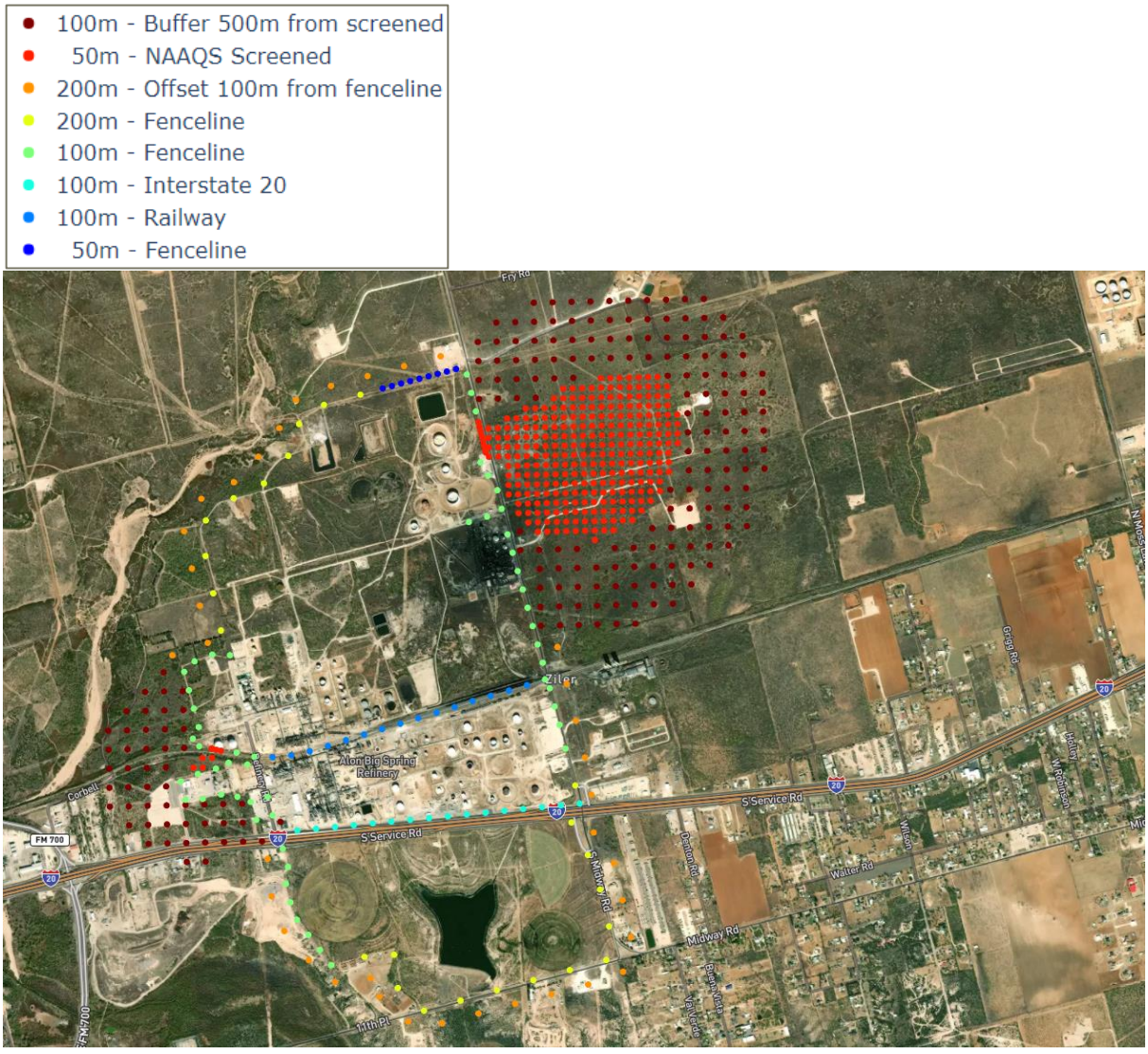

Figure 1. Receptors Included in Howard County Monte Carlo Analysis

3. MC Approach

This section describes the methodology used to conduct the MC analysis, and the various analyses performed to demonstrate compliance with the NAAQS.

Ramboll's Monte Carlo simulation program was developed in Python. It is available on the TCEQ's FTP site, and includes a README with instructions for installing and configuring a Python environment for running the program, and instructions on processing data and running the Monte Carlo analysis. It should be noted that this program was written for the Howard County Attainment Demonstration and is not intended to be broadly applicable to dispersion modeling projects. Ramboll's Python MC program was set up and run on the TCEQ computer system successfully for the Howard County Attainment Demonstration modeling.

3.1 Intermediate Processing

The program first converts an AERMOD POST file into a matrix of concentrations organized by receptor and time. The matrices are saved to disk in the "Parquet" format to streamline processing.

Next, dispersion factors from capped Tokai sources are scaled to generate a concentration matrix for each operational scenario and added to the continuous + background concentrations. This involves the following steps:

1. Read dispersion factors for capped Tokai sources from the appropriate Parquet cache file;
2. Read emission rates from the "Tokai_cap_load_scenario_model_inputs.xlsx" workbook;
3. Convert emission rates from lb/hr to g/s (453.59237 g/lb)/(3600 s/hr);
4. Multiply dispersion factors by the emission rate in g/s to produce a concentration matrix; and
5. Add the Tokai concentration matrix to continuous + background concentrations.

These Tokai scenario-specific concentration matrices, as well as the dispersion factor matrices for each Delek source, are then separated by year. These yearly matrices of concentration (including constant sources, Tokai sources, and background) are the final input to the MC simulation, and are saved as a formatted binary file on disk.

3.2 Monte Carlo Methodology

When running the Monte Carlo script, the user can specify the following: the Tokai operational mode (MSS/Routine), Cap Rate (A-D), Load scenario (1-24), and the number of simulations to run. The script then reads in 5 years of data including:

- Continuous source + background + Tokai concentration matrix; and
- Intermittent Delek source dispersion factor matrix (1 per source).

Each Delek source operates independently, meaning that multiple intermittent sources can operate at once. However, each source can only be in one operation mode per day. Each intermittent source's total possible MSS occurrences (days of operation) were assumed to occur each year.

Most runs were completed with 10,000 simulations of random sampling. However, several runs were performed with 20,000 simulations, to demonstrate that 10,000 is sufficient to achieve statistical convergence.

The Monte Carlo analysis processes each year independently, producing 10,000 simulated highest 4th high daily maximum values (H4H) at each receptor. From these 5 annual sets, values are averaged sequentially to generate concentrations comparable to the 1-hour SO_2 Design Value (DV). The program writes the maximum DV from each simulation across all receptors, as well as the maximum DV over all simulations at each receptor.

Each MC simulation involves the steps below.

1. Reset the "total" matrix to the continuous matrix (Tokai + Continuous + Background)
2. For each intermittent source:
    a. Create a list of all "remaining" days for the year
    b. For each of that source's operational modes:
        i. Randomly select days without replacement from the list of remaining days, and remove them from the list
        ii. Multiply each selected day's dispersion factors by the mode's emission rate in g/s to produce concentrations
    c. Multiply dispersion factors for all "remaining" days by the Routine operation emission rate
    d. Add the resultant concentration matrix to the "total" matrix
3. After all sources have been sampled and added, calculate the H4H value at each receptor

In this report, one "run" consists of either 10,000 or 20,000 simulations. Results are grouped by run for ease of comparison.

Compliance is demonstrated if every simulation in every Monte Carlo run falls below the 1-hr SO_2 standard.

3.3 Monte Carlo Simulations Performed

It was anticipated that 10,000 simulations of each Tokai operational scenario would suffice to capture the distribution of concentrations that could be produced by the MC approach. However, to ensure that no simulation would exceed the standard in any scenario, the following additional runs were conducted:

- 10,000 simulations of the top 10 scenarios under MSS conditions;
- 10,000 simulations of the top 10 scenarios under Routine Operation conditions; and
- 450,000 simulations of the controlling scenario (Routine 24D).

The top 10 Routine, top 10 MSS, and controlling scenarios were determined based on the maximum modeled design value across all 10,000 simulations for each of the 192 Tokai scenarios. Additionally, to demonstrate that convergence is achieved at 10,000 simulations, the top ten MSS and Routine scenarios were run with 20,000 simulations.

3.4 Emission Scaling Verification

MC inputs for each intermittent source were modeled in AERMOD using unit emissions of 1 g/s to generate dispersion factors. These dispersion factors are then scaled by selected emission rates in the MC simulation to generate concentrations. To verify that scaling of dispersion factors produced identical results to running AERMOD with final emission rates, two model runs were conducted for the continuous sources. In the first, all sources were modeled in AERMOD with specified emission rates in g/s to generate a single output post file. In the second run, AERMOD was run again to generate multiple post files – one for each source with unit emissions to generate dispersion factors. The dispersion factors in these post files were then scaled by each source's emission rate in g/s and summed.

From the resultant post files (one direct from AERMOD and one generated with sources scaled is post-processing), the 1-hr SO_2 design value was calculated. This resulted in concentrations of 110.74491 and 110.74488 µg/m^3, with the difference of 0.00003 µg/m^3 resulting from the fact that AERMOD writes concentrations to 5 decimal places.

Modeling inputs used to verify the emission scaling procedure are available at the TCEQ's FTP site.

4. Results of MC Approach

This section describes the results of the MC approach, including plots of maximum modeled concentration by receptor and a comparison of simulated design values to the standard. All concentrations presented are design values comparable to the 1-hr SO_2 NAAQS. Concentrations are presented in µg/m³ to avoid a rounding step since AERMOD outputs values in µg/m³.

4.1 Maximum Concentrations from Each Tokai Scenario

To identify the scenarios with the highest predicted DVs, the MC analysis was run for each Tokai scenario with 10,000 simulations. This was used to identify the top ten scenarios under MSS and Routine operation, as identified in **Table 3**. Additional simulations were performed for these scenarios.

The maximum design value over all simulations for each Tokai operational scenario is presented in **Figure 2.** The 1-hr SO_2 NAAQS of 196.4 µg/m^3 is shown as a black line for comparison. Ranked concentrations of the top 10 scenarios under MSS and Routine operational conditions over all MC runs are provided in **Table 3**.

Table 3. Maximum Monte Carlo-Derived Concentrations for Top Ten Tokai MSS and Routine Scenarios

Rank	Tokai Cap/Load Scenario (MSS)	Max Concentration ($\mu g/m^3$)	Tokai Cap/Load Scenario (Routine)	Max Concentration ($\mu g/m^3$)
1	24D	159.1	24D	193.8
2	24C	155.4	21D	188.9
3	21D	154.5	23D	187.7
4	23D	153.6	18D	183.4
5	21C	151.6	21C	182.5
6	18D	149.4	20D	182.0
7	23C	149.2	24A	181.8
8	20D	148.7	22D	181.1
9	18C	148.2	23C	180.8
10	22D	147.4	18C	178.9

Table 3 shows that routine operations at Tokai consistently result in higher concentrations than MSS. The highest concentration overall occurs in scenario Routine 24 D. Load scenario 24 assumes 100% capacity from all sources, resulting in the highest emission rates. Cap scenario D consistently shows the highest concentrations among the four Cap scenarios.

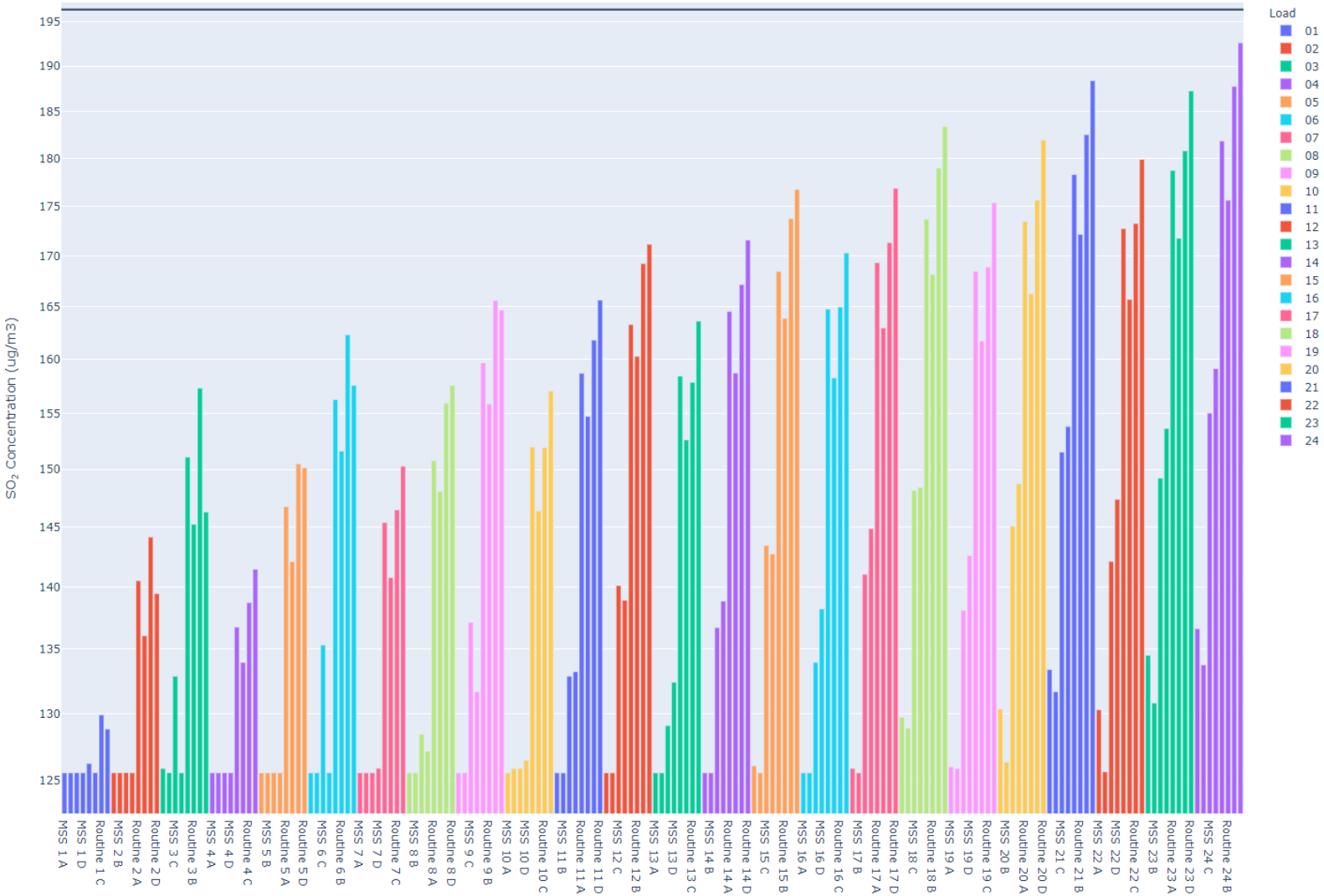

Figure 2. Maximum Monte Carlo-Generated Design Values by Tokai Operational Scenario

4.2 Evaluation of Run Simulation Size

To verify that statistical convergence is achieved at 10,000 simulations, the top ten scenarios for MSS and Routine were run with 20,000 simulations. The concentration distribution of each of these runs is compared in **Figure 3**. Note that a separate concentration scale was used for each scenario to provide higher detail, which means that results cannot be visually compared between scenarios.

For each scenario, the distributions are statistically identical, with similar medians, upper percentiles, and maximum values. These results indicate that the model converges after 10,000 simulations.

To show the distribution of output concentrations, and to compare this distribution between runs, 10,000 simulations were taken from the set of 20,000 simulations and compared to the original 10,000 simulations in a histogram. **Figures 4 and 5** show the distribution of design values for the top ten MSS and Routine scenarios, respectively. Concentration bins are placed along the X axis, and the total count in each bin is plotted along the Y axis. Box plots are also provided to focus on concentration ranges and highlight outliers. **Figure 5** includes a line showing the 1-hr SO_2 standard for reference.

Figures 4 and 5 show that the distribution of design values between runs is very consistent. Median, quartile, and extreme values never differ by more than 0.1 µg/m³. While this shows that 10,000 simulations is more than enough to capture the distribution of values, maximum values are the primary consideration for this analysis. MSS 24 D, for example, shows a maximum concentration of 157.7 µg/m³ in one run, and 159.1 µg/m³ in another. The high number of simulations performed for the controlling scenarios is necessary to ensure that significant outliers of maximum concentration are captured.

4.3 Additional Evaluation of Controlling Scenario

To ensure that extreme outliers were captured, the scenario with the highest measured concentration was run an additional 20 times with 10,000 simulations per run, for a total of 220,000 simulations. The results of this additional analysis are presented in **Figure 6** and are compared to the 1-hr SO_2 NAAQS.

Comparing the distribution of design values from both the histograms and box plots shows excellent agreement between runs. Maximum values between runs also agreed well, with a range between 192.4 and 193.7 µg/³.

Figure 3. Comparison of Monte Carlo Runs with 10,000 and 20,000 Simulations for top 10 MSS and Routine Scenarios

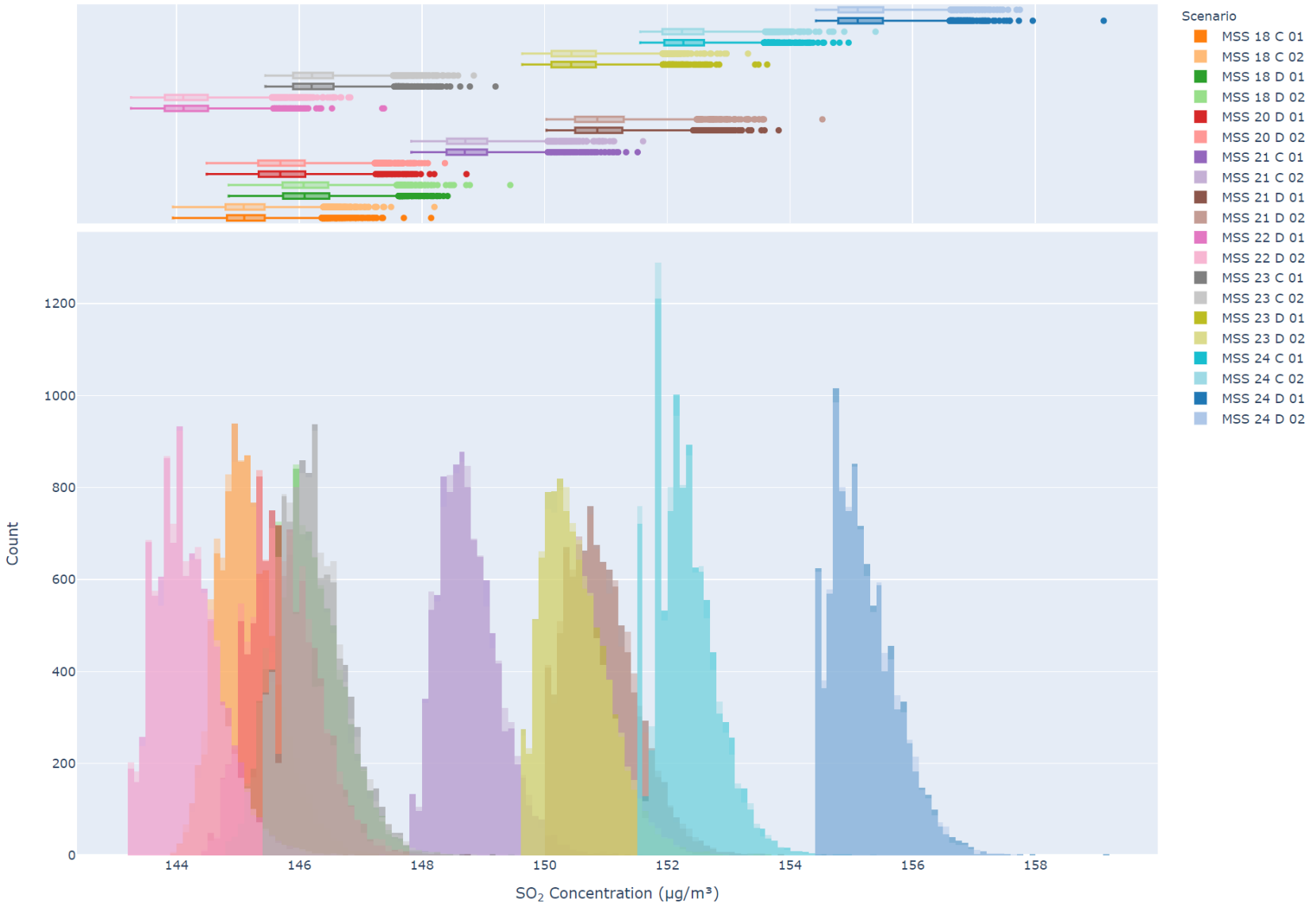

Figure 4. Distribution of Monte Carlo Design Values from Top 10 MSS Scenarios

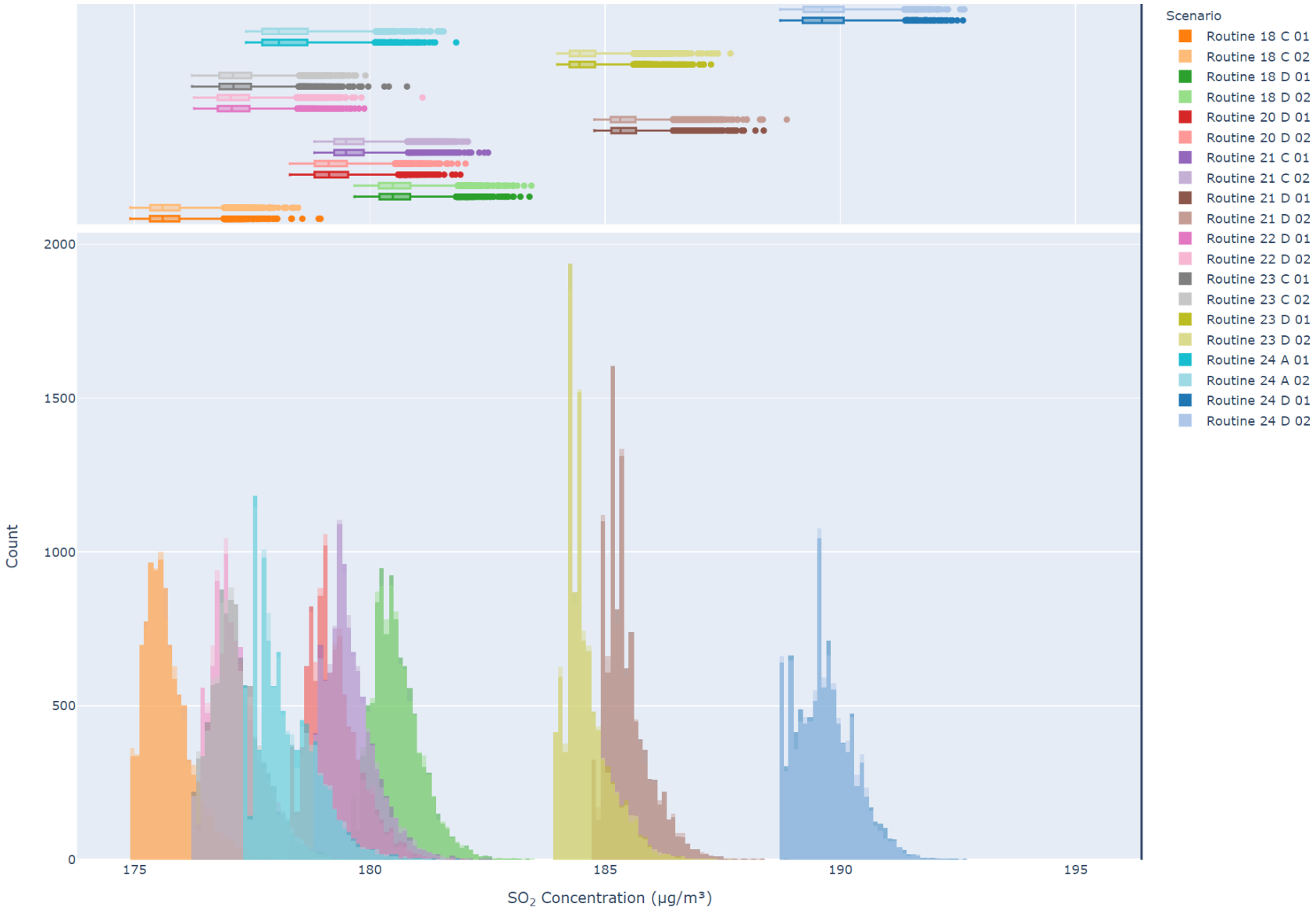

Figure 5. Distribution of Monte Carlo Design Values from Top 10 Routine Scenarios

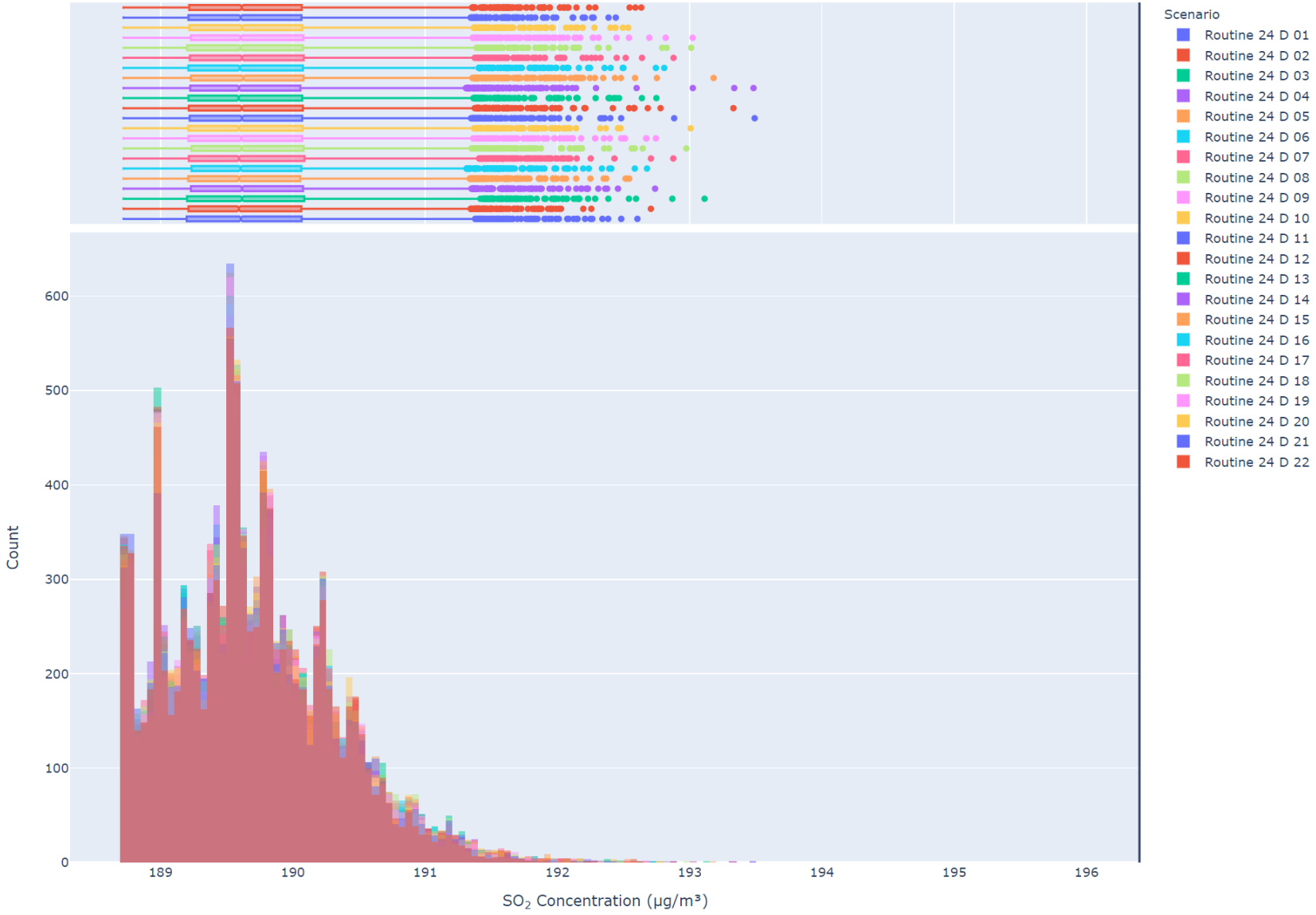

Figure 6. Monte Carlo-Generated Design Values After 220,000 Simulations of Scenario Routine 24D

4.4 Maximum Concentration by Receptor

To illustrate spatial variations in concentration, the maximum Monte Carlo-generated value at each receptor was determined, as shown in **Figure 7**. This value represents the maximum design value derived from over two million model simulations. With a maximum value of 193.8 µg/m³, the 1-hr SO_2 NAAQS of 196.4 µg/m³ was not exceeded in any scenario at any receptor.

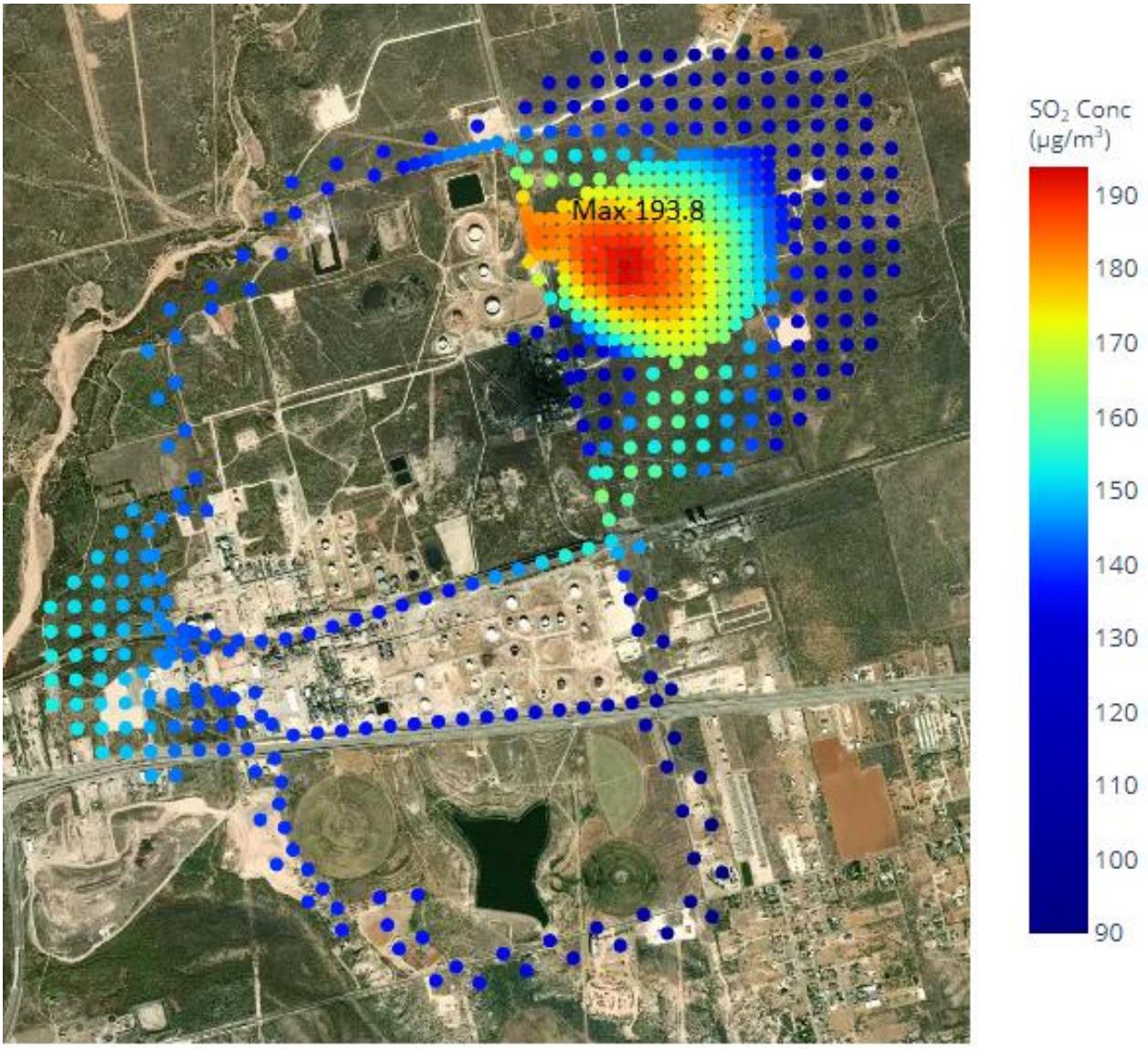

Figure 7. Maximum 1-hr SO_2 Design Values over all Monte Carlo Simulations

4.5 Monte Carlo Analysis Within the Big Spring Carbon Black Plant (Tokai) Property Boundary

Results thus far have been intended to demonstrate compliance with the NAAQS for ambient, publicly-accessible areas. Areas within the property boundary of emitting sites have been excluded from consideration. However, it is also required that no combination of sites will result in a NAAQS exceedance within the boundary of a neighboring site.

To demonstrate that no exceedances occur within BHER and Delek, TCEQ has completed traditional dispersion modeling, as described in the Howard AD SIP revision. Within the bounds of Tokai, however, emissions from Delek must be considered. For the sake of consistency, the MC approach was used to combine contributions from intermittent Delek sources with concentrations from constant sources at BHER and Delek, as well as a background.

A 50m receptor grid was generated for the area within the Tokai site. Additionally, receptors were placed every 25m along its boundary. AERMOD was run with this receptor grid using the methods described in **Section 2** of this report to generate a post file with constant + background concentrations, and post files of dispersion factors for each intermittent Delek source. No Tokai sources were included in the modeling.

Next, the methods described in **Section 3** were applied to process the post files, and 10,000 MC simulations were conducted to determine concentrations at each receptor within the site. After 10,000 simulations, a maximum design value of 54.3 µg/m³ was produced, demonstrating compliance with the 1-hr SO_2 NAAQS.

Figure 8 shows the receptor grid used for this analysis, as well as the maximum design value at each modeled receptor resulting from the Monte Carlo analysis.

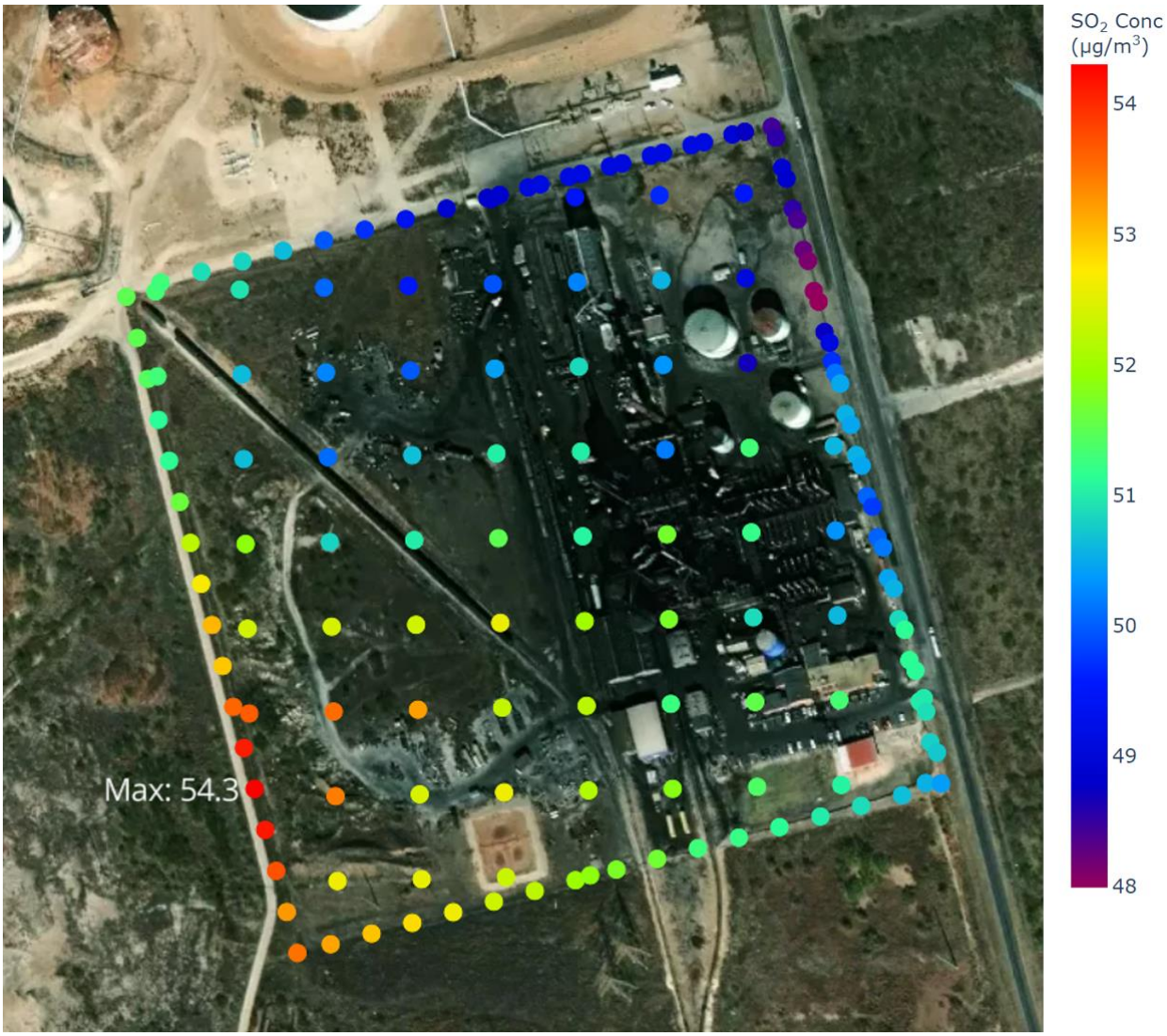

Figure 8. Non-Tokai Maximum 1-hr SO_2 Design Values Within Tokai Site from Monte Carlo Analysis

5. References

1. Revisions to the Guideline on Air Quality Models: Enhancements to the AERMOD Dispersion Modeling System and Incorporation of Approaches to Address Ozone and Fine Particulate Matter. 40 CFR Part 51. EPA–HQ–OAR–2015–0310; FRL–9956–23– OAR. January 2017. Available at https://www.epa.gov/sites/production/files/2020-09/documents/appw_17.pdf