Use of Probabilistic Statistical Techniques in AERMOD Modeling Evaluations

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ABSTRACT

The advent of the short term National Ambient Air Quality Standards (NAAQS) prompted modelers to reassess the common practices in dispersion modeling analyses. The probabilistic nature of the new short term standards also opens the door to alternative modeling techniques that are based on probability. One of these is the Monte Carlo technique that can be used to account for emission variability in permit modeling.

Currently, it is assumed that a given emission unit is in operation at its maximum capacity every hour of the year. This assumption may be appropriate for facilities that operate at full capacity most of the time. However, in most cases, emission units operate at variable loads that produce variable emissions. Thus, assuming constant maximum emissions is overly conservative for facilities such as power plants that are not in operation all the time and which exhibit high concentrations during very short periods of time.

Another element of conservatism in NAAQS demonstrations relates to combining predicted concentrations from the AMS/EPA Regulatory Model (AERMOD) with observed (monitored) background concentrations. Normally, some of the highest monitored observations are added to the AERMOD results yielding a very conservative combined concentration.

A case study is presented to evaluate the use of alternative probabilistic methods to complement the shortcomings of current dispersion modeling practices. This case study includes the use of the Monte Carlo technique and the use of a reasonable background concentration to combine with the AERMOD predicted concentrations. The use of these methods is in harmony with the

probabilistic nature of the NAAQS and can help demonstrate compliance through dispersion modeling analyses, while still being protective of the NAAQS.

INTRODUCTION

Annual ambient standards have historically been addressed with deterministic methods. Under these standards, the highest predicted concentration is compared to a set threshold. However, this paradigm has changed with short term probabilistic NAAQS. Instead of comparing the maximum value to a given threshold, with probabilistic standards we compare a percentile value from the predicted concentrations to a specific threshold. For example, for the 1-hour SO_2 NAAQS, the high-fourth-high (H4H) predicted concentration is compared to the 1-hour NAAQS of 196 $\mu g/m^3$. That is the case because the distribution of maximum hourly values each day is equal to 365 values (one per day) and the 99^{th} percentile value from such a distribution is the 3.6^{th} highest value which rounds to 4^{th} highest value also referred to as the high-fourth-high (H4H). The aim of probabilistic standards is to reduce the likelihood of concentrations exceeding a threshold. This means that for a modeling evaluation with a H4H concentration at the level of the 1-hour SO_2 NAAQS, the likelihood of exceeding 196 $\mu g/m^3$ is less than 1% (1.0-0.99). Thus, probabilistic standards provide a stringent level of protection based on the likelihood of complying with the NAAQS. The switch from deterministic to probabilistic standards allows for alternative modeling techniques that are based on probability.

Whereas the use of probability in modeling demonstrations may seem foreign in dispersion modeling, probability has been used for a long time to evaluate AERMOD's performance. Additionally, EPA allows the use of probabilistic methods such as the Monte Carlo approach in other fields including health risk assessments. More recently EPA used this method in the modeling guidance for 1-hour SO_2 non-attainment designations. With this in mind, the use of the Monte Carlo statistical technique for permitting dispersion modeling evaluations should also be allowed. Justification for the use of a reasonable background concentration to combine with the AERMOD predicted concentrations is included in this analysis. The use of these two methods is in line with the probabilistic nature of the short term NAAQS and can help demonstrate compliance through dispersion modeling analyses while still being protective of the NAAQS.

AERMOD's Probabilistic Performance Evaluations

The American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD) was rigorously evaluated before it was incorporated by EPA as the preferred near-field dispersion model for regulatory applications in the Guideline on Air Quality Models (Appendix W to 40 CFR Part 51). These evaluations involved comparisons between predicted (modeled) and observed (monitored) concentrations from 17 studies. The databases from these studies are available in EPA's Support Center for Regulatory Atmospheric Modeling.[1]

EPA employed Quantile-Quantile (Q-Q) plots to evaluate AERMOD's performance for predicting compliance with air quality regulations.[2] These plots compare predicted and observed concentrations from the databases available. While these values are originally paired in time and space, the spatial and temporal alignment is lost in the ranking process. That is the case because Q-Q plots compare the sorted list of predicted concentrations with the sorted list of observed concentrations.

A more rigorous test would involve comparing predicted and observed concentrations on a scatterplot with data paired in time and space. However, AERMOD has been shown to have poor correlation on a spatial and temporal basis. [3-7] Nonetheless, EPA uses Q-Q plots to evaluate model performance because the distribution of maximum and minimum values tends to follow a similar pattern between predicted and observed concentrations. This means that, whereas the model is not able to predict the exact location and the exact time of a maximum concentration, the model is able to provide with good accuracy the likelihood of experiencing a maximum occurrence within a given time period (5 years or 1 year if using on-site meteorological data). Section 9.1.2 Studies of Model Accuracy from Appendix W summarizes this as follows:

> *Models are reasonably reliable in estimating the magnitude of highest concentrations occurring sometime, somewhere within an area.*

This means that we cannot assume that the highest concentration obtained with AERMOD will be located at the exact receptor and at the exact time identified by AERMOD. On the other hand, measured concentration distribution is similar to the one predicted in AERMOD. Thus, it should be recognized that the results from AERMOD are probabilistic in nature. With this in

mind, the EPA has established probabilistic standards (e.g., 98th percentile) for the new NAAQS (e.g., 1-hour NO_2, 24-hour $PM_{2.5}$).

Regardless of the lack of temporal and spatial correlation between predicted and observed concentrations, AERMOD is able to predict the likelihood of exceedances happening in a given receptor grid over a given period of time (e.g., 5 years).

Monte Carlo Statistical Technique

The Monte Carlo technique is the probabilistic technique proposed to address some of AERMOD's conservative assumptions is. Numerous fields of science and industry widely use and accept this statistical procedure. The Manhattan Project scientists developed this statistical approach in the 1940's to estimate neutron multiplication rates to predict the explosive behavior of neutron chain reactions in fission weapons.[8] The EPA already has a long standing policy in place to allow Monte Carlo analyses in risk assessments.[9,10,11] More recently, EPA pioneered the use of the Monte Carlo technique in its evaluation included in the *Guidance for 1-hr SO2 Nonattainment Area SIP Submissions*.[12] In Appendix B of this guidance EPA introduces the concept of using of a longer term average emission limit to be comparable in stringency with the 1-hour average limit. EPA performed a Monte Carlo analysis to justify this approach by using 100 randomly reassigned emission data and single years of emissions data to characterize emission variability over a 5-year period of meteorology. This evaluation concluded that if periods of hourly emissions above the critical emission value were rare occurrences at a source, these periods would be unlikely to have a significant impact on air quality, insofar as they would be very unlikely to occur repeatedly at the times when the meteorology is conducive for high ambient concentrations. In other words, the method outlined by EPA allows for sporadic emission spikes that would not be allowed with a 1-hr limit, but compensates by adopting a lower average emission rate over a longer averaging time such that the likelihood (probability) of having high emissions and poor dispersion characteristics is minimized.

Emission Variability Processor (EMVAP)

The Electric Power Research Institute (EPRI) commissioned the EMVAP technique a tool to incorporate the transient and variable operations of emission units in a modeling analysis.

EMVAP employs the Monte Carlo statistical technique, which as discussed earlier, has been allowed by EPA for risk assessments and 1-hr SO_2 non-attainment modeling. EMVAP creates a frequency distribution from given emission sources by assigning emission rates from a pool of emissions (usually from CEMS data) at random over numerous iterations. The resulting distribution yields a more realistic approximation of actual modeled impacts. EMVAP has been evaluated extensively[13-15] for dispersion modeling applications.

The assumption of constant emissions is not appropriate for emission units that operate infrequently, at variable loads, or that have infrequent high emissions. For these cases the EMVAP probabilistic approach is more suitable to accurately characterize the effect from these emission profiles.

Combining Background Concentrations in NAAQS Modeling Evaluations

Background concentrations are commonly obtained from representative ambient monitors. However, most of these monitors are sited to capture maximum impacts in a given area[16]. Thus, finding ambient monitors that are truly representative of background levels of ambient air is challenging. Additionally, it is a common practice to pair predicted concentration from AERMOD with maximum recorded observation from the ambient monitor. EPA made some concessions on this practice[17,18] and now allows a Tier 2 approach where a reduced subset of monitored observations are grouped by seasons and combined with predicted AERMOD concentrations on a seasonal basis. This approach assumes that AERMOD concentrations are sufficiently correlated with monitored concentrations on a temporal basis (hour by hour). However, as discussed previously, AERMOD results are evaluated irrespective of time and space (i.e., with Q-Q plots) since model performance significantly decreases when analyzed on a temporal basis[3-7]. Thus, temporal pairing of modeled and monitored concentrations is unjustified.

Screening of Background Concentrations

When meteorological data is available, it may be possible to exclude the monitored observations that occur when the monitor is being impacted from these sources.

Nicholson[19] described a screening technique to obtain a representative background concentration by analyzing hourly $PM_{2.5}$ monitored data from the Santa Fe, New Mexico airport monitoring site. Nicholson screened out monitoring observations from unusual events and occurrences when the monitor was downwind of a major emission source. After screening out exceptional events, the resulting 98th percentile concentration was 6 $\mu g/m^3$ compared to 18 $\mu g/m^3$ obtained from the unscreened data set. Nicholson cautioned against the use of background concentrations based upon extreme values since these are not representative of the background in a dispersion modeling domain.

The EPA defines exceptional events as unusual or naturally occurring events that can affect air quality but are not reasonably controllable.[20] However, the flagging of exceptional events is only performed by State agencies when there are attainment issues. Therefore, the data collected from these monitors contains observations that overpredict background concentrations.

The challenge in determining a representative background value is how to screen out the observations from times when the monitor is downwind from a given emission source to avoid double counting emissions. However, it is possible to filter out the effects from explicitly modeled sources and exceptional events (e.g., forest fires, sand storms, etc.) by analyzing the distribution of monitored observations as proposed below.

Combining Modeled Results and Background Concentrations

The 1-hour SO_2 NAAQS was promulgated as the 99th percentile of maximum daily concentrations. Thus, the probability of this standard is 1.00 - 0.99 = 0.01. This is equivalent to 1 exceedance every 100 days (1/100 = 0.01). When we extrapolate this ratio to the number of days in a year (365) we get 3.6 exceedances in a year which is rounded up to the 4th highest value in a year. Thus, the form of the standard is the high-fourth-high (H4H) value from the daily maximum 1-hour values across a year. However, by assuming that the 99th percentile modeled concentration is combined with the 99th percentile background concentration, the probability equals 0.0001 or (0.01) * (0.01). This is equivalent to the 99.99th percentile or one exceedance every 10,000 days (1/10,000 = .0001), representing one exceedance every 27 years. The probabilistic inappropriateness of such an approach has been described previously.[6]

Furthermore, this degree of conservatism is well beyond the level necessary to protect the NAAQS.

A more realistic approach in NAAQS dispersion modeling analyses is to combine AERMOD's concentrations with the 50th percentile background concentration.[21] This approach conserves the use of the modeled 99th percentile value from AERMOD and allows for a more representative background level by selecting the median instead of the tail of the distribution. Additionally, this approach will still be protective of the NAAQS because it results in a marginal probability of 0.005 or (0.01) * (0 .50). This is equivalent to the 99.5th percentile combined concentration which is more conservative than the 99th percentile standard. Therefore, this method is statistically sound and provides a reasonable level of conservatism that ensures the protection of the NAAQS.

EXPERIMENTAL METHODS

The current study evaluates the predicted concentrations based on three cases:

1. Using AERMOD by assuming a constant maximum emission rate (current modeling practice)
2. Using AERMOD by assuming a variable emission rate
3. Using EMVAP to account for emission variability

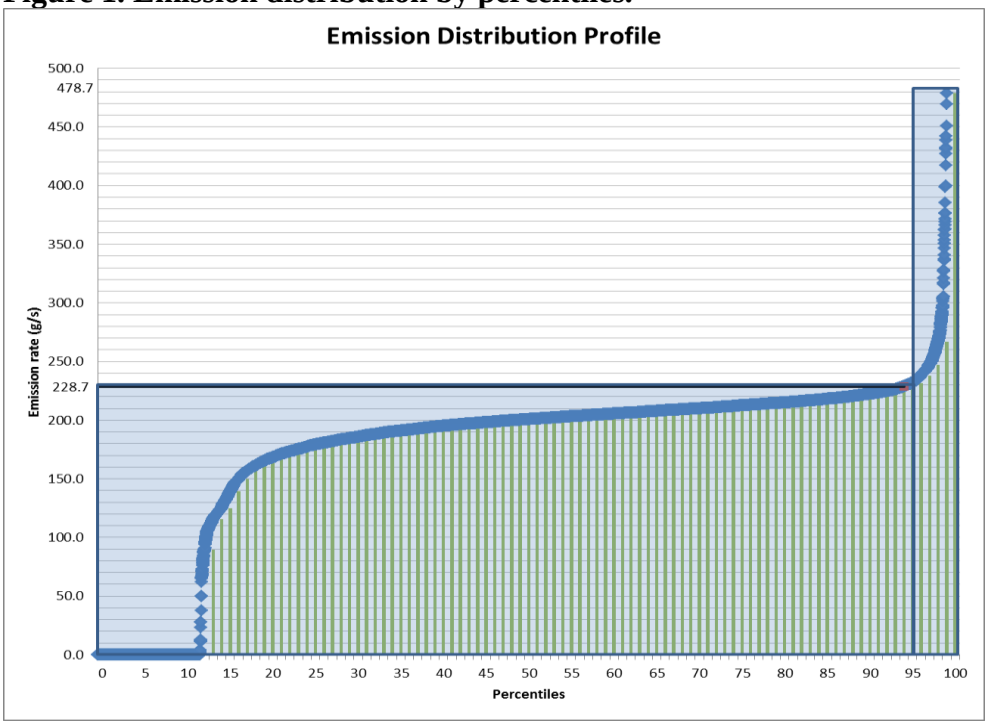
The modeling evaluation is based on one year of emission data from a power plant. These data were scaled up for the following example. In other words, its emission profile is the same but the magnitude has been adjusted. A graphical representation of the emission profile for this hypothetical power plant is shown in Figure 1.

The assumptions and the modeling parameters for these cases are summarized in Table 1. AERMOD version 14134 was used with meteorological data processed for one year with AERMET version 12345. The receptor grid is comprised of 1,080 polar receptors extending 7,500 meters from the source.

Table 1. Three cases used to model the power plant.

Input parameter	Case 1	Case 2	Case 3
Description of Dispersion Modeling	Current Modeling Practices	AERMOD with hourly emission	EMVAP (500 iterations)
SO_2 Emission rate (g/s)	478.7	Actual emission rates from CEMS data	Bin1: 478.7 (5.0% time) Bin 2: 228.7 (95% time)
Stack height (m)	122		
Exit temperature (degrees K)	416		
Diameter (m)	5.2		
Exit velocity (m/s)	23		

Figure 1. Emission distribution by percentiles.



RESULTS AND DISCUSSION

The results for the three cases described are summarized below (Table 2). Case 1 produced the highest concentrations and exceeded the NAAQS. This is not surprising given that Case 1 assumes continuous emissions at the highest emission rate. Case 2 resulted in the lowest concentration; about 40% of the NAAQS. However, this is presented for comparison purposes only and should be viewed with caution because AERMOD has negligible correlation with

monitored concentrations on a temporal basis. Case 3 was calculated from 500 iterations in EMVAP and resulted in a 99th percentile concentration that is 92% of the NAAQS. These results do not include impacts from neighboring sources and background concentrations.

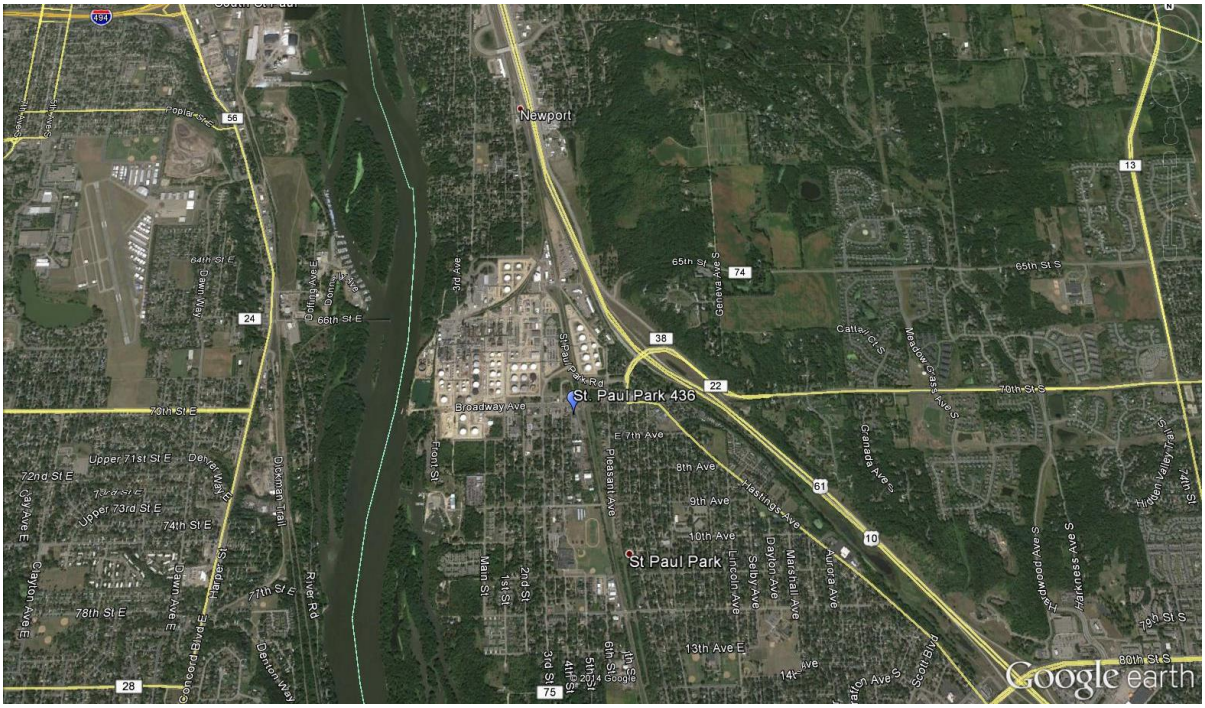
Table 2. Results of 1-hour SO_2 concentrations for the three cases.

	Case 1 (µg/m^3)	**Case 2 (µg/m^3)**	**Case 3 (µg/m^3)**
Description of Dispersion Modeling	Current Modeling Practices	AERMOD with hourly emission	EMVAP (500 iterations)
H4H	229.9	78.6	179.3
Percent of NAAQS	117%	40%	92%

Background Concentrations

According to the Annual Air Monitoring Network Plan for Minnesota,[22] the MPCA monitors SO_2 at six sites. The 2011-2013 average 99th percentile 1-hr SO_2 concentrations range from 5.2 µg/m^3 to 89.0 µg/m^3. Out of these, the Saint Paul Park 436 monitor was selected since it records the second highest three year average concentration (26.2 µg/m^3). The Saint Paul Park 436 monitor is located about 9 miles southeast of downtown St. Paul, Minnesota. The location is east of the Mississippi River and is surrounded by industrial land including an oil refinery (Figure 2).

Figure 2. St. Paul Park 436 ambient monitor location.



Hourly ambient air monitoring data was obtained from EPA's Airdata web site[23] for the Saint Paul Park 436 monitor for the years 2011 through 2013. The monitoring data is recorded in parts per billion (ppb) and contained only the maximum hourly observations by day. Therefore, there were 365 maximum hourly values for 2011 and 2013, and 366 maximum values for 2012 (leap year). These values were analyzed to find a representative 1-hour background concentration. The observations were analyzed in the histogram below (Figure 3). The histogram exhibits a long right tail due to few very high observations. However, the most frequent observation recorded was 2.6 $\mu g/m^3$ (1 ppb) which occurred 40 percent of the time. Table 3 presents the distribution of concentrations at different percentiles. The Annual Air Monitoring Network Plan for Minnesota shows the three-year average of the annual 99th percentile daily maximum 1-hour SO_2 concentrations to be 10 ppb (about 26.2 $\mu g/m^3$), which is one order of magnitude higher than the most frequent observation (1 ppb). Thus, from the histogram below, it is overly conservative to assume that a 10 ppb concentration is present every hour of the year.

Figure 3. Histogram of 1-hour SO_2 monitoring observations for the Saint Paul Park 436 monitor for years 2011-2013.

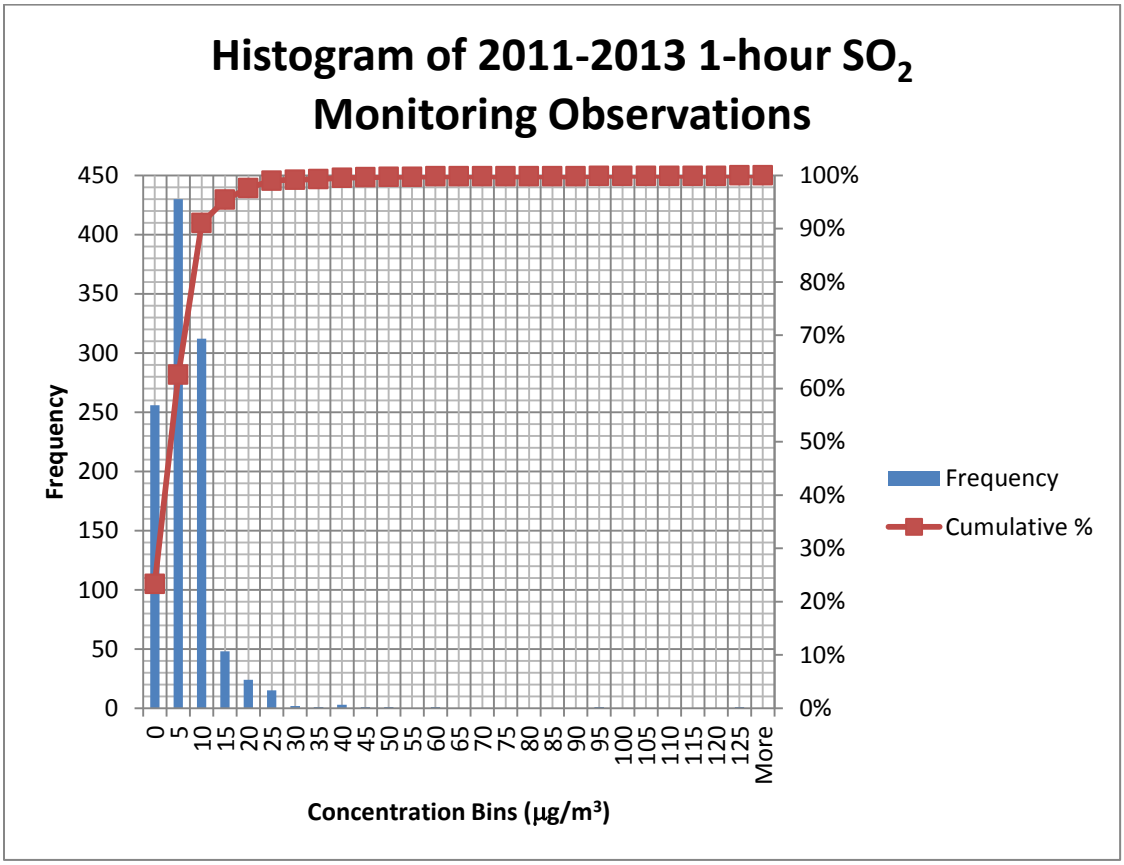


Table 3. Concentrations at different percentiles for the St. Paul Park 436 monitor.

Percentile	µg/m^3
50th	2.6
60th	3.5
70th	5.2
80th	6.1
90th	9.6
95th	12.9
98th	20.1
99th	25.6
99.9th	69.5
99.99th	84.7

Case 3 was further analyzed by combining it with three background values that include the following:

1. Bkg 1: Three year average of maximum daily 1-hour SO_2 observations.
2. Bkg 2: Three year average of the 99th percentile daily maximum 1-hour SO_2 observations.
3. Bkg 3: Three year average of the 50th percentile daily maximum 1-hour SO_2 observations.

Bkg 1 is representative of the value initially recommended by EPA (Tier 1). In more recent guidance[14] EPA allowed the use of the three year average 99th percentile daily maximum observations for the 1-hour SO_2 concentrations. However, as discussed previously, assuming that two exceptional events occur at the same time is excessively conservative. Thus, the use of the 50th percentile is a more reasonable assumption that was evaluated as Bkg 3. The results in Table 4 show that Bkg 1 and Bkg 2 exceed the 1-hour SO_2 NAAQS. However, by assuming a more reasonable background concentration (i.e., Bkg 3), the 1-hour SO_2 NAAQS are met in this hypothetical analysis.

Table 4. Case 3 with three different background values.

	Case 3 with Bkg 1 (µg/m^3)	**Case 3 with Bkg 2 (µg/m^3)**	**Case 3 with Bkg 3 (µg/m^3)**
H4H	179.3	179.3	179.3
Background	86.4	25.6	2.6
Total	265.7	204.9	181.9
Percent of NAAQS	135.6%	104.5%	92.8%

SUMMARY

The newly promulgated NAAQS herald a new era of dispersion modeling with its probabilistic nature. The use of probabilistic techniques is consistent with the evaluations performed to validate the use of AERMOD. Combining the use of AERMOD with the Monte Carlo technique is appropriate when used to account for emission variability inherent in many emission sources. Furthermore, this technique is already allowed by EPA for risk assessments and more recently for modeling of non-attainment modeling of 1-hour SO_2. Consequently, the use of EMVAP to account for the emission variability of emission units allows for more reasonable results in dispersion modeling analyses. EMVAP is especially useful in cases where the emission units evaluated have an infrequent use or variable load. The use of this modeling technique can result

in more reasonable predicted concentrations that are still protective of the NAAQS. Furthermore, as shown in this study, combining the 50th percentile monitored concentration with the 99th percentile predicted concentration (1-hr SO_2) should be considered in regulatory applications. In summary, more realistic results can be obtained from AERMOD by addressing emission variability with a Monte Carlo approach and by pairing predicted concentrations with the median observed values.

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KEYWORDS

Monte Carlo, AERMOD, background concentrations, EMVAP