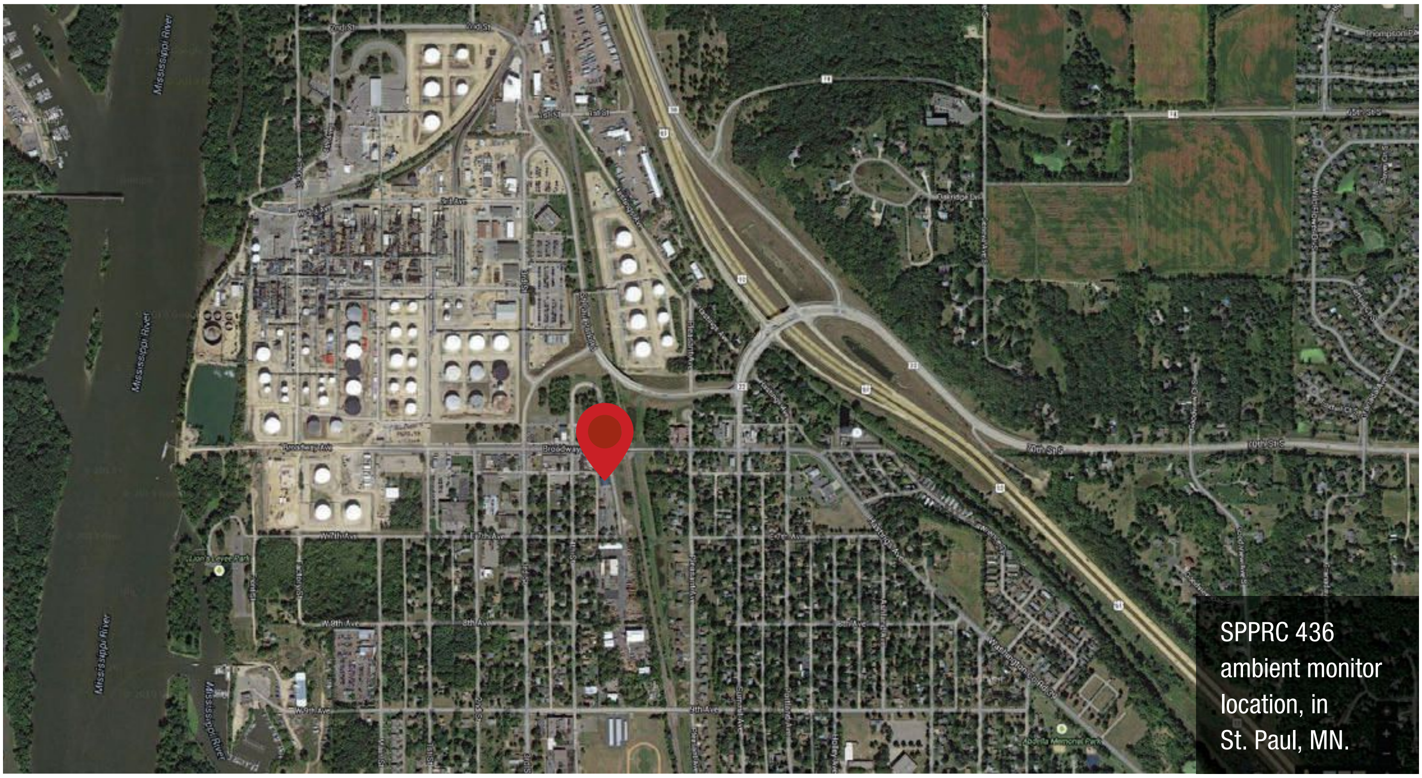
Innovative Dispersion Modeling

Practices to Achieve a Reasonable Level of Conservatism in AERMOD Modeling Demonstrations


SPPRC 436 ambient monitor location, in St. Paul, MN.

An overview of a case study that presents two modeling techniques to address areas of excessive conservatism in dispersion modeling analyses.

by Sergio A. Guerra

Sergio A. Guerra, Ph.D., is an environmental engineer at Wenck Associates Inc., Bloomington, MN, who specializes in air quality and air dispersion modeling. E-mail: info@SergioAGuerra.com.

Annual ambient standards have historically been met with a high level of conservatism in dispersion modeling evaluations, in large part, because it is easier for regulatory agencies to approve modeling practices that are conservative in nature, since it ensures the protection of the National Ambient Air Quality Standards (NAAQS). However, the advent of the short-term NAAQS has prompted a reassessment of the assumptions commonly used in air dispersion modeling analyses.

One area of conservatism relates to the assumption that a given emission unit is in operation at its maximum capacity every hour of the year. This assumption may be appropriate for some facilities that operate at full capacity most of the time. However, in most cases, emission units are used at variable loads that produce variable emissions. Thus, assuming a constant maximum emission value 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 (e.g., startup, shutdown, and malfunction [SSM] events) due to technical limitations of pollution control equipment.

Another element of conservatism in NAAQS demonstrations relates to combining predicted concentrations from the U.S. Environmental Protection Agency (EPA)'s AERMOD model with observed (monitored) background concentrations. Normally, some of the highest monitored observations are added to the AERMOD results yielding a very conservative combined concentration. The case study below evaluates modeled concentrations obtained by using the current modeling methods and by applying a Monte Carlo technique. Justification for the use of a reasonable background concentration to combine with the AERMOD predicted concentrations is also presented. The use of these methods can help demonstrate compliance through dispersion modeling analyses while still being protective of the NAAQS.

Case Study Overview

This study presents two modeling techniques to address areas of excessive conservatism:

1. The Emission Variability Processor (EMVAP) Modeling System
2. The use of the 50th percentile monitored concentration as background

Emission Variability Processor (EMVAP)

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, a probabilistic approach is more suitable to accurately characterize the effect from these emission profiles.

The EMVAP technique was commissioned by the Electric Power Research Institute (EPRI) to provide a tool that could incorporate the transient and variable operations of emission units in a modeling analysis. EMVAP is based on the Monte Carlo statistical technique that is widely used and accepted in numerous fields of science and industry. The use of this method was pioneered by the Manhattan Project scientists who developed the first atomic weapon in the 1940s. In particular, this statistical approach was used to estimate neutron multiplication rates to predict the explosive behavior of neutron chain reactions in fission weapons.[1]

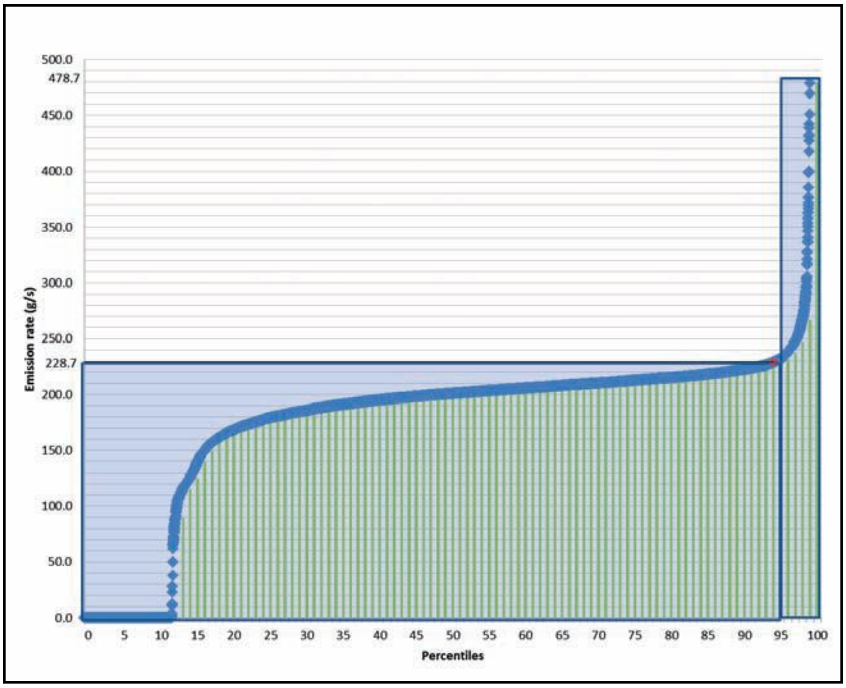
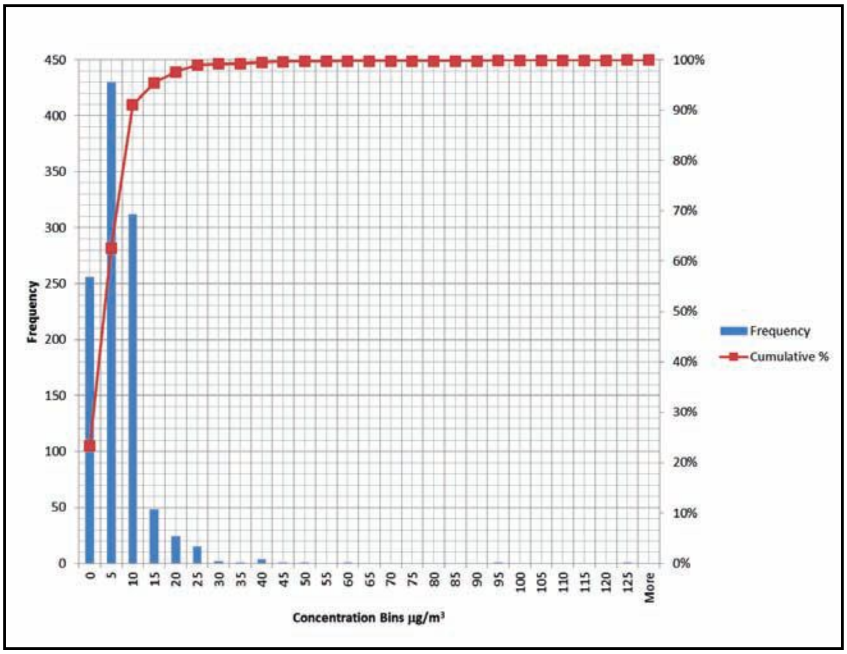


Figure 1. Emission distribution by percentiles.

The Monte Carlo technique is used in EMVAP to create a frequency distribution from a given emission source or sources by assigning emission rates from a given pool of emissions (usually from Continuous Emissions Monitoring System [CEMS] data) at random over numerous iterations. The resulting distribution yields a more realistic

Figure 2. Histogram of 1-hr SO_2 monitoring observations for the SPPRC 436 monitor, 2011–2013.



approximation of actual modeled impacts. EMVAP has been evaluated extensively[2-4] for dispersion modeling applications.

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.[5] Thus, finding ambient monitors that are truly representative of background levels of ambient air is challenging. Additionally, it is a common practice to pair the predicted concentration from AERMOD with the maximum recorded observation from the ambient monitor. EPA has made some concessions on this practice[6,7] 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, AERMOD results are evaluated irrespective of time and space (i.e., with Q-Q plots) because model performance significantly decreases when analyzed on a temporal basis.[8-12] Thus, temporal pairing of modeled and monitored concentrations is unjustified.

Combining AERMOD's concentrations with the 50th percentile background concentration conserves the use of the modeled 99th percentile value from AERMOD and allows for a more representative background level.

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

Nicholson[13] described a screening technique to obtain a representative background concentration by analyzing hourly fine particulate matter ($PM_{2.5}$) monitored data from the Santa Fe, NM, 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.

EPA defines exceptional events as unusual or naturally occurring events that can affect air quality but are not reasonably controllable.[14] However, the flagging of exceptional events is only performed by state agencies when there are attainment issues. Therefore, the data collected from these monitors contain 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-hr sulfur dioxide (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-hr 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 = 0.0001), which is equal to one exceedance every 27 years. The probabilistic inappropriateness of such an approach has been described previously.[11] 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.[15] 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 form of the standard (99th percentile). 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; and
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 m from the source.

Results and Discussion

The results for the three cases described are summarized below (see Table 2). Case 1 was the highest of the cases 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; approximately 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.

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/sec)	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/sec)	23		

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

	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%

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

Background Concentrations

According to the Annual Air Monitoring Network Plan for Minnesota,[16] the Minnesota Pollution Control Agency (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 at monitoring site 443 to 89.0 µg/m^3 at monitoring site 420. Out of these, the St. Paul Park Refinery Company (SPPRC) 436 monitor was selected, since it records the second highest three year average concentration (26.2 µg/m^3). The SPPRC 436 monitor is located about 9 miles southeast of downtown St. Paul, MN. The location is east of the Mississippi River and is surrounded by industrial land including an oil refinery (see map on page 24).

Hourly ambient air monitoring data were obtained from EPA's Airdata Web site[17] for the SPPRC 436 monitor for the years 2011 through 2013. The monitoring data were 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

Table 3. Concentrations at different percentiles for the SPPRC 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

366 maximum values for 2012 (a leap year). These values were analyzed to find a representative 1-hr background concentration and are analyzed in a histogram (see Figure 2).

The histogram exhibits a long right tail due to few very high observations. However, the most frequent observation recorded was 2.6 µg/m^3 (1 ppb), which occurred 40% of the time. The distribution of concentrations at different percentiles is also shown (see Table 3). The Annual Air Monitoring Network Plan for Minnesota shows the three-year average of the annual 99th percentile daily maximum 1-hr SO_2 concentrations to be 10 ppb (approximately 26.2 µg/m^3), which is one order of magnitude higher than the most frequent observation (1 ppb). Thus, from looking at the histogram, it is overly conservative to assume that a 10-ppb concentration is present every hour of the year.

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

Bkg 1 is representative of the value initially recommended by EPA (Tier 1). In more recent guidance,[7] EPA allowed the use of the three year average 99th percentile daily maximum observations for the 1-hr 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-hr SO_2 NAAQS. However, by assuming a more reasonable background concentration (i.e., Bkg 3), the 1-hr SO_2 NAAQS are met in this hypothetical analysis.

	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%

Table 4. Case 3 with three different background values.

Summary

The newly promulgated 1-hr NAAQS pose a challenge to the dispersion modeling community. However, a reasonable level of conservatism that is protective of the NAAQS can be achieved by implementing the modeling techniques discussed herein. First, the use of EMVAP to account for the emission variability of emission units can allow for more reasonable results in dispersion modeling analyses. This tool is especially useful in cases when 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.

The second element of conservatism in current modeling techniques deals with the combining of predicted and monitored concentrations. As shown in this case study, if this element of conservatism is not addressed, modeling analyses will continue to overestimate predicted concentrations. As a consequence, new and expansion projects may be halted, or additional expense in mitigation techniques may be incurred with minimal benefits to the environment. Therefore, we cannot continue to assume that two exceptional events happen at the same time. That is why combining the 50th percentile monitored concentration with the 99th percentile predicted concentration (1-hr SO_2) should be considered in regulatory applications. In summary, the level of conservatism in current dispersion modeling practices needs to be addressed with modeling techniques like the ones presented herein. **em**

References

1. Eckhardt, R. Stan Ulam, John von Neumann, and the Monte Carlo Method; *Los Alamos Science*, Special Issue, 1987. See http://library.lanl.gov/cgi-bin/getfile?15-13.pdf.
2. Paine, R.; Hamel, R.; Heinold, D.; Knipping, E.; Kumar, N. Early Experiences with EMVAP Implementation and Testing In *Proceedings of the Air & Waste Management Association's Annual Conference and Exhibition in Chicago, IL, June 25-28, 2013; Paper # 12827.*
3. Kumar, N. Development, Testing and Evaluation of EMVAP and SCICHEM Presented at the *EPA Regional/State/Local Modelers Workshop in Dallas, TX. April 23, 2013.*
4. Paine, R.; Hamel, R.; Kaplan, M.; Heinold, D.; Knipping, E.; Kumar, N. Progress Report: Further EMVAP Development, Testing, and Evaluation. Presented at the *Air & Waste Management Association's Specialty Conference in Raleigh, NC. March 19-21, 2013.*
5. *Ambient Monitoring Guidelines for Prevention of Significant Deterioration (PSD);* EPA-450/4-87-007; U.S. Environmental Protection Agency, Research Triangle Park, NC, 1987.
6. *Additional Clarification Regarding Application of Appendix W Modeling Guidance for the 1-hour NO_2 NAAQS*; U.S. Environmental Protection Agency; Tyler Fox memorandum dated March 1, 2011.
7. *Guidance for $PM_{2.5}$ Permit Modeling*; EPA-454/B-14-001; U.S. Environmental Protection Agency, Research Triangle Park, NC, May 20, 2014.
8. Bowne, N.E.; Londergan, R.J. *Overview, Results, and Conclusions for the EPRI Plume Model Validation and Development Project: Plains Site*; EPRI EA–3074; Electric Power Research Institute, Palo Alto, CA, 1983.
9. Moore, G.E.; Stoeckenius, T.E.; Stewart, D.A. *A Survey of Statistical Measures of Model Performance and Accuracy for Several Air Quality Models*; EPA–450/4–83–001; U.S. Environmental Protection Agency, Office of Air Quality Planning & Standards, Research Triangle Park, NC, 1982 (NTIS No. PB 83–260810).
10. *Urban Power Plant Plume Studies*; EPRI EA-5468; Electric Power Research Institute, Palo Alto, CA, 1988.
11. Murray, D.R.; Newman, M.B. Probability Analyses of Combining Background Concentrations with Model-Predicted Concentrations; *J. Air Waste Manage. Assoc.* **2014**, *64* (3), 248-254.
12. Frost, K.D. AERMOD Performance Evaluation for three Coal-fired Electrical generating Units in Southwest Indiana; *J. Air Waste Manage. Assoc.* **2014**, *64* (3), 280-290.
13. Nicholson, B.R. Background Concentration and Methods to Establish Background Concentrations in Modeling. Presented at *the Guideline on Air Quality Models: The Path Forward. Raleigh, NC, 2013.*
14. Treatment of Data Influenced by Exceptional Events; Final Rule (pursuant to the 2005 amendment of U.S. Clean Air Act Section 319); *Federal Register* **2007**, *72*, 13560.
15. Guerra, S.A.; Olsen, S.; Anderson, J. Evaluation of the SO_2 and NO_x Offset Ratio Method to Account for Secondary $PM_{2.5}$ Formation; *J. Air Waste Manage. Assoc.* **2014**, *64* (3), 265-271.
16. Gavin, K.; McMahon, C. *Annual Air Monitoring Network Plan for Minnesota*; Minnesota Pollution Control Agency, Saint Paul, MN, 2014.
17. EPA Airdata Web site. See http://www.epa.gov/airquality/airdata/.