

ERRORS ASSOCIATED WITH TIME AVERAGE CONCENTRATIONS IN GAUSSIAN MODELING

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Abstract

Cotton gins are required to have an air quality permit in order to operate. Some states permit gins are based upon predicted PM_{10} concentration levels from dispersion modeling. The use of dispersion modeling allows regulators to estimate downwind concentrations that potentially could impact the public off-property. Industrial Source Complex – Short Term version 3 (ISCST3) is the EPA approved dispersion modeling program used by most states to regulate industrial sources. The product of ISCST3 is a 24-hour average downwind concentration of particulate matter given an emission rate. Concentrations predicted by ISCST3 are based upon the Gaussian dispersion model, using Pasquill-Gifford dispersion parameters (σ_y, σ_z)

It is generally known that ISCST3 over-predicts downwind concentration from low-level point sources (LLPS) such as cotton gins, grain elevators and feed mills. ISCST3 does not account for horizontal wind direction variations within an hour. Accounting for these variations results in a significantly lower predicted PM_{10} concentration at the receptor. This paper describes a unique approach for estimating 24-hour concentrations using USEPA (2000) data on horizontal wind direction variations, Monte-Carlo simulations, and the Gaussian model. The results include power law coefficients by stability class for estimating 60-minute concentrations from 10-minute concentrations (Gaussian equation) and the ratios of C_{60}/C_{10} for 10 days of meteorological data. It is concluded that the current downwind concentrations estimated by regulatory agencies using ISCST3 over-predicts PM_{10} by a factor of 2.5.

Introduction

An important feature of the regulation of PM_{10} emissions of low-level point sources (LLPS), such as cotton gins, is the use of dispersion modeling programs. The purpose of dispersion modeling is to obtain an estimate of downwind concentrations without resorting to field sampling. The most common EPA approved dispersion model used by State Air Pollution Regulatory Agencies (SAPRAS) is the Industrial Source Complex – Short Term, version 3 (ISCST3). Unfortunately, ISCST3 results in over-estimates of downwind concentrations. The SAPRA goal is to limit the concentrations crossing the property boundaries to a concentration less than the National Ambient Air Quality Standards (NAAQS). The NAAQS for PM_{10} is a 24-hour average concentration of 150 micrograms per cubic meter ($\mu\text{g}/\text{m}^3$).

The intent of this paper is to explore the basis for ISCST3 dispersion modeling and create a simple approach to correct the over-estimate of downwind concentrations through which more accurate estimates can be made. ISCST is based upon Gaussian modeling. The classical Gaussian modeling approach using the Pasquill-Gifford stability classification system is used to estimate downwind concentrations from emission rates, wind velocities, dispersion parameters (based upon atmospheric stability), and effective height of emission. These concentrations are 10-minute concentrations (Cooper and Alley, 1994) in that the Pasquill-Gifford dispersion parameters were based upon 10-minute (or less) field data. However, ISCST3 does not account for this fact. The 10-minute concentrations of the Gaussian model (the basis for ISCST3) are assumed to be 60-minute concentrations in ISCST3. It is hypothesized and demonstrated in this paper that this error in ISCST3 results in a significant over-estimate of downwind concentrations of PM_{10} from LLPS. The consequences of these over-estimates are that many agricultural operations including cotton gins are inappropriately regulated. When modeling results are used for permitting purposes for agricultural LLPS, the dispersion modeling estimates of downwind concentrations are incorrect.

The simple reason why a 10-minute concentration is always higher than a 60-minute concentration is the variation in wind direction. In 60 minutes, the wind direction may vary ± 45 degrees or more. In 10 minutes, it is assumed that the wind direction is from the source to the sampler. When the wind direction is other than directly toward the sampler, the stationary sampler captures less PM. By incorporating changes in wind direction (within an hour), this approach will demonstrate that the sixty-minute average concentration is significantly less than a ten-minute average concentration. The current available data assumed for this paper are the Pasquill-Gifford stability classification system (Cooper and Alley, 1994), estimates of standard deviation of horizontal wind direction published by the EPA (2000), and meteorology data collected and published by Fritz (2002b). This method incorporates the Gaussian Model as the basis for determining downwind concentration levels and the Power-Law Model (Cooper and Alley, 1986). The power law is a standard method for estimating longer-term time average concentrations using a known power (p-value). P-values for different stability classes were determined using simulation (Crystal Ball, 2000). With a constant emission rate, the Gaussian equation was used to estimate 10- and 60-minute concentrations. The 10-minute concentrations were assumed to be the numerical values that would have resulted utilizing ISCST3. The

60-minute concentrations were, in the view of the authors, more accurate estimates of downwind concentrations for agricultural LLPS based upon science.

Methods

The Gaussian Model

Equation 1 is used to calculate downwind concentrations with the classical Gaussian model (Cooper and Alley, 1994).

The Pasquill–Gifford dispersion parameters (σ_y , and σ_z) are integral to the calculations.

$$C = \frac{Q}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{1}{2} \frac{y^2}{\sigma_y^2}\right) \left\{ \exp\left(-\frac{1}{2} \frac{(z-H)^2}{\sigma_z^2}\right) + \exp\left(-\frac{1}{2} \frac{(z+H)^2}{\sigma_z^2}\right) \right\} \quad (\text{Equation 1})$$

where:

C = steady state concentration at a point (x,y,z), $\mu\text{g}/\text{m}^3$

Q = emission rate, $\mu\text{g}/\text{s}$;

σ_y, σ_z = horizontal and vertical spread parameters, m;

u = average wind speed at stack height, m/s;

y = horizontal distance from plume centerline, m;

z = height of receptor with respect to ground, m; and

H = effective stack height ($H=h+\Delta h$, where h = physical stack height and Δh = plume rise), m.

Atmospheric Stability Classification

The most commonly used method for estimating the dispersion parameters associated with the Gaussian dispersion model is the Pasquill-Gifford atmospheric stability classification system and stability parameter methodology. Atmospheric stability as a function of wind speed, cloud cover, and angle of the sun are used. The stability classification system was introduced by Pasquill (1961) and customized by Gifford (1960) and Turner (1967). Stability class A corresponds to very unstable conditions, B represents moderately unstable conditions, C represents slightly unstable conditions, D represents neutral conditions, E represents slightly stable conditions, and F represents stable conditions. Stability classes A through D are only utilized for daytime conditions while D through F are associated with night-time conditions. Class D should always be used when cloud cover is present. The stability classes are essential criteria utilized in calculating the horizontal and vertical spread parameters (σ_y , and σ_z) used in the Gaussian Model. The horizontal spread parameter, σ_y , is calculated using Equation 3. The vertical spread parameter, σ_z , is calculated using Equation 4.

$$\sigma_y = ax^b \quad (\text{Equation 3})$$

$$\sigma_z = cx^d + f \quad (\text{Equation 4})$$

where:

a,b,c,d,f = curve-fit constants for calculating spread parameters (See Table 1); and

x = distance downwind to point of concentration measurement, km.

Power-Law Model

Equation 1 will yield concentration estimates (C) based upon Pasquill-Gifford dispersion parameters, wind velocity, height of emitting point, and emission rate. Because the Pasquill-Gifford dispersion parameters were based upon 10-minute (or less) field measurements, it is commonly assumed that the 'C' in equation 1 is an average 10-minute concentration (Cooper and Alley, 2002; Warke et al., 1998). Dispersion modeling is used to estimate concentrations that are compared to the NAAQS. The NAAQS for PM_{10} is a 24-hour average concentration of $150 \mu\text{g}/\text{m}^3$. It is essential for the air pollution regulatory process that a 24-hour concentration be the results of dispersion modeling in order to insure that the public is not exposed to concentrations exceeded the 24-hour NAAQS. The difficulty faced by the developers of ISC was how to get from a predicted 10-minute concentration using dispersion modeling to a predicted 24-hour concentration. They chose to assume that the wind direction was constant each hour. Hence, the average of 24 10-minute concentrations would equate to the average of 24 1-hour concentrations.

It is common to use the power-law model to obtain concentrations associated with time periods longer than 10 minutes (Cooper and Alley, 2002; Warke et al., 1998). The Power-Law Model is given in Equation 2.

$$C_t = C_{10} \left(\frac{10}{t} \right)^p \quad \text{(Equation 2)}$$

where:

- t = the desired averaging time, min;
- C_t = concentration for averaging time t, $\mu\text{g}/\text{m}^3$; and
- p = p-value.

The power law p-value will vary with the magnitude of horizontal wind direction variations and the source of the pollutant. For example, the p-value for a ground-level area source will be much smaller than if the source were a LLPS. Smaller p-values will result in less difference between C_t and C_{10} .

The Problem

In order to determine whether modeled concentrations would be in compliance with the NAAQS, modeled 24-hour concentrations (C_{1440}) were needed. The NAAQS are 24-hour average concentrations. The problem faced by the ISC developers was how to get from C_{10} (equation 1) to C_{1440} ? The simple method was to assume that the wind direction was constant within each hour. If the wind directions were constant within each hour, $C_{10} = C_{60}$. However, wind directions are not constant within each hour. EPA (2000) published wind direction changes by stability class. (See table 2.) As a consequence, the calculation of C_{10} using equation 1 is an over-estimate of C_{60} and the average of 24 over-estimates of C_{60} will likely be an over-estimate of C_{1440} .

Figure 1 illustrates the impact of wind direction changes on the resulting time-averaged concentrations. 1-hour concentrations are always less than C_{10} if there are any within-hour variations of wind direction.

ISC results utilize an average of 24 C_{10} estimates of downwind concentration as the 24-hour modeled concentration to be compared to the NAAQS. In effect, the ISC 24-hour modeled **concentration is an average of 24 10-minute concentrations not 24 1-hour concentrations!** It was hypothesized in this research that 24 10-minute concentrations would be significantly different than 24 1-hour concentrations! In order to test this hypothesis, the authors developed a process of estimating 60-minute concentrations (C_{60}) from 10-minute concentrations (C_{10}). The approach was to use the power-law and Monte Carlo simulation (Crystal Ball, 2000). Simulation was used to determine to correct 'p' value for each stability class for equation 2. The following procedure was used:

- Six random wind directions were used for each stability class to estimate C_{60} with multiple replications. {Crystal Ball (2000) was used to generate wind directions using a normal distribution and standard deviations reported by EPA (2000).}
- The average of each of the six C_{10} concentrations (equation 1) was assumed to be a more accurate estimate of C_{60} .
- Equation 5 was used to calculate 'p' with the C_{10} and C_{60} calculations.

$$p = \frac{\ln\left(\frac{C_{60}}{C_{10}}\right)}{\ln\left(\frac{10}{60}\right)} \quad \text{Equation 5}$$

- This procedure was replicated for each stability class twenty four times. The average of the 24 p-values was designated as the p-value for that specific stability class. This procedure was repeated for stability classes A through F. With p-values for each stability class, it was possible to compute sixty-minute concentrations from C_{10} .

Example Application and Results

With an assumed emission factor of 3.05 lb TSP/bale emitted from a twenty bale per hour cotton gin, the resulting emission rate was 7.69 (10^6) $\mu\text{g}/\text{s}$. Ten-minute concentrations (C_{10}) were calculated using this emission rate, distance from source to receptor (D) of 500 meters, an average wind velocity of 3 m/s, a height of receptor, z, equal to zero meters, and an effective stack height, H equal to 10 meters. Using simulation (Crystal Ball, 2000), six different ten-minute concentrations were de-

terminated, taking into consideration varying wind direction. The average of these six C_{10} concentrations was the estimate of the sixty-minute or hourly concentration. Table 3 shows a set of data for one hour of stability class A where the P-value was determined. Notice that C_{60} is always less than C_{10} . Table 4 depicts the ten-minute concentrations calculated for these variables along with the average P-values for each stability class.

Using meteorological data (Fritz, 2002), calculations are made to generate a C_{10} from the Gaussian model, with the actual wind direction and speed, for each hourly measurement. The C_{10} concentrations were used with equation 2 to determine C_{60} concentrations using the p-values listed in table 4. Table 5 illustrates several hours of met data including wind direction, wind speed, stability class, and the calculated concentrations. (These calculations have been made assuming the receptor was located in the average wind direction for the twenty four hour period. For Table 5, the receptor is located at 240 degrees.) Again, notice that C_{60} is less than C_{10} .

Further analysis of the average C_{10} and C_{60} values shows that the ratio of C_{10} to C_{60} was 2.45:1. This is illustrated in Table 6.

Summary and Conclusions

The goal of this research was to demonstrate the error associated with a lack of consideration of within hour variations of horizontal wind direction which was the method used by the developers of ISC to approximate 24-hour concentrations for comparison to the NAAQS for regulatory purposes. The EPA published standard deviations of horizontal wind directions were used to simulate within hour wind directions and calculate C_{10} . One-hour concentrations were determined by averaging six C_{10} . This process was replicated numerous times to obtain p-values for each stability class. An example was used to compare average 24-hour concentrations typical of ISCST3 (the average of 24 10-minute concentrations) and the average of 24 1-hour concentrations calculated with p-values previously determined. The results demonstrate that **not** correcting for sub-hourly wind direction changes causes the prediction of downwind PM concentrations to be overestimated by 250%. ISCST3 does not correct for the sub-hourly wind direction shifts. This over-prediction causes cotton gins to be inappropriately regulated. Reducing the predicted concentration from ISCST3 by a factor of 2 would yield conservative yet more accurate estimates of downwind PM concentration from LLPS.

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Table 1. Constants used for calculating dispersion coefficients as a function of downwind distance and atmospheric stability classes (Cooper and Alley, 2002). Stability classes A through D are used for daytime conditions where E and F are for nighttime conditions. Table values are used to calculate σ_y and σ_z (Equations 3 and 4) used in the Gaussian equation (Equation 1) to predict a steady state concentration at the receptor (point x,y,z).

Stability	a	b	c	d	f
A	213	0.894	440.8	1.941	9.27
B	156	0.894	106.6	1.149	3.3
C	104	0.894	61	0.911	0
D	68	0.894	33.2	0.752	-1.7
E	50.5	0.894	22.8	0.678	-1.3
F	34	0.894	14.35	0.74	-0.35

*This table is utilized for $x < 1\text{km}$. (Cooper and Alley, 2002)

Table 2. Standard deviations of horizontal wind direction variations by stability class reported by EPA (2000). It was assumed that wind direction variations were normally distributed.

Stability Class	Range of Standard Deviation of Horizontal Wind Direction Fluctuations (degrees)
1 (A)	> 22.5
2 (B)	17.5 – 22.5
3 (C)	12.5 – 17.5
4 (D)	7.5 – 12.5
5 (E)	3.8 – 7.5
6 (F)	< 3.8

Table 3. One-hour of simulated ten-minute concentrations for stability class A. These values are the predicted concentrations at the receptor for stability class A taking into account changes in wind direction as specified by the standard deviations in horizontal wind direction published by the EPA (2000). C_{10} is the highest concentration of the six – ten minute concentrations during the hour. C_{60} is the average of the six – ten minute concentrations during the hour. The p – value was found using equation 5.

Wind Direction	C ($\mu\text{g}/\text{m}^3$)
159	48.710
213	5.349
225	0.050
156	36.695
180	171.624
184	166.409

C_{10} =171.631

C_{60} =71.473

P-value=0.49

Table 4. Simulated ten-minute concentrations and p-values for stability classes A-F. These values were calculated based upon six – ten minute concentrations simulated using Crystal Ball. C_{10} is the highest concentration of the six – ten minute concentrations during the hour. C_{60} is the average of the six – ten minute concentrations during the hour. The P – value is found using equation 5.

Stability Class	C_{10} ($\mu\text{g}/\text{m}^3$)	P-value
A	171.63	0.498
B	557.17	0.460
C	1286.16	0.547
D	3139.23	0.607
E	5164.16	0.436
F	7778.21	0.172

Table 5 Example of hourly meteorological data (Fritz, 2002) with respective calculated C_{10} and C_{60} values. These calculations were made assuming the receptor was at a location equal to the average wind direction for the twenty-four hour period. The receptor was located at 240 degrees.

Hour	Direction (degrees)	X (m)	Speed (m/s)	Class	p	C_{10} ($\mu\text{g}/\text{m}^3$)	C_{60} ($\mu\text{g}/\text{m}^3$)
10	254.050	145.356	0.820	B	0.460	2368.902	1039.473
11	284.150	107.182	1.820	B	0.460	0.018	0.008
12	295.990	83.371	1.590	A	0.498	0.002	0.001
13	243.430	149.692	1.740	A	0.498	1526.501	624.940
14	244.410	149.505	2.530	B	0.460	1634.769	717.336
15	318.190	30.075	5.590	D	0.607	0.000	0.000
23	324.560	13.585	2.650	D	0.607	0.000	0.000
24	303.740	65.794	1.950	E	0.436	0.000	0.000
AVERAGE						230.425	99.240

*Concentration values for all hours not listed are zero.

Table 6. 24-hour average concentrations predicted for ten days using simulation (Crystal Ball, 2000) to determine an average wind direction. Note that the C_{10} values are higher than the C_{60} values. The ratio of the average C_{10} to average C_{60} values indicated that ISCST3 over predicted concentrations by 245%.

Day	C_{10}	C_{60}
1	21.769	9.435
2	3.421	1.283
3	441.054	164.663
4	100.678	37.734
5	192.176	97.832
6	168.801	74.435
7	268.158	99.858
8	270.474	115.811
9	345.623	140.943
10	397.735	160.929

Ratio of C_{10} to C_{60} = 2.45

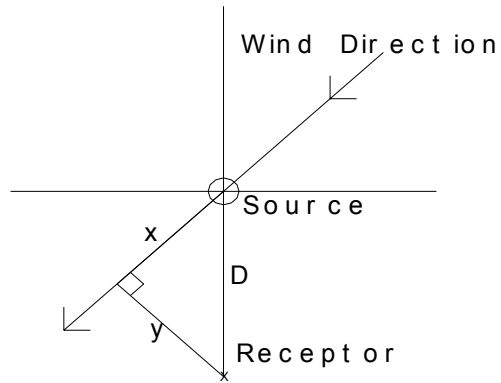


Figure 1. Schematic diagram illustrating a wind direction other than directly from source to receptor. The calculated concentration that would result from using the Gaussian equation would be less for any wind direction that is not directly from the source to the receptor. The magnitude of the reduced concentration would equal $[\exp(-y^2/2\sigma_z^2)]$. (See equation 1.)