

**A SIMULATED APPROACH TO ESTIMATING PM₁₀ AND PM_{2.5} CONCENTRATIONS
DOWNWIND FROM COTTON GINS**

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Abstract

Cotton gins are required to obtain operating permits from state air pollution regulatory agencies (SAPRA) which regulate the amount of particulate matter that can be emitted. Industrial Source Complex Short Term version 3 (ISCST3) is the Gaussian dispersion model currently used by some SAPRAs to predict downwind concentrations used in the regulatory process in the absence of field sampling data. The maximum ambient concentrations for PM₁₀ and PM_{2.5} are set by the National Ambient Air Quality Standard (NAAQS) at 150 µg/m³ and 65 µg/m³ respectively. Some SAPRAs use the NAAQS concentrations as property line concentrations for regulatory purposes. This paper reports the results of a unique approach to estimating downwind PM₁₀ and PM_{2.5} concentrations using Monte Carlo simulation, the Gaussian dispersion equation, the Hino Power Law, and a particle size distribution that characterizes the dust typically emitted from cotton gin exhausts. These results were then compared to a ten minute concentration (C₁₀) and the concentrations that would be theoretically measured by a FRM PM₁₀ and PM_{2.5} sampler. The total suspended particulate (TSP) emission rate, particle size distributions, and sampler performance characteristics were assigned to triangular distributions to simulate the real world operation of the gin and sampling systems. The TSP emission factor given in AP-42 for cotton gins was used to derive the PM mass emission rate from a 40 bale per hour plant. The Gaussian equation was used to model the ambient TSP concentration downwind from the gin. The performance characteristics for the PM₁₀ and PM_{2.5} samplers were then used to predict what the measured concentration would be for two PSD conditions. The first PSD assumption was that the mass median diameter (MMD) and geometric standard deviation (GSD) were constant at 12µm and 2 and the second scenario assigned a triangular distribution to the MMD and GSD of {15, 20, 25}µm and {1.8, 2.0, 2.2} respectively. The results show that the PM_{2.5} fraction of the dust emitted under either PSD condition was negligible when compared to the NAAQS for PM_{2.5} of 65µg/m³. The results also demonstrate that correcting for wind direction changes within the hour using the power law reduces the ambient concentration by a factor of 2.45. The measured downwind concentrations from the samplers reported higher 24-hour averages for each of the ten days modeled than the concentrations predicted by the new model.

Introduction

While the NAAQS for criteria pollutants were originally intended for use as ambient concentration standards, some air pollution regulations for cotton ginning facilities are based upon compliance with the NAAQS as a 24-hour average property line concentrations (PLC). PM₁₀ is the criteria pollutant emitted by cotton gins requiring the facility to obtain an operating permit from the SAPRA. True PM₁₀ is defined as the mass fraction of dust particles with aerodynamic equivalent diameter (AED) less than 10µm. True PM_{2.5} is defined as the mass fraction of dust particles with AED less than 2.5µm. It should be noted that PM_{2.5} is currently not regulated by the EPA, but is listed as a criteria pollutant in the NAAQS. The two methods regulators have to obtain the PLCs of PM₁₀ for regulatory purposes are dispersion modeling and field sampling. There are inherent errors in the protocol for both of these processes that result in the inappropriate regulation of cotton gins and other low level point sources (LLPS).

ISCST3 is the current dispersion model approved by the EPA for use in permitting a LLPS. ISCST3 uses the Pasquill-Gifford atmospheric stability classification system to calculate the horizontal and vertical plume dispersion coefficients (σ_y and σ_z respectively) used in the Gaussian dispersion equation. Pasquill

(1961) reports that the field data used to develop σ_y and σ_z were 3 to 5 minute averages. Turner (1994), assumes that the Pasquill-Gifford σ_y and σ_z produce concentrations that are **ten-minute averages** (C_{10}). As such, the concentrations obtained from the Gaussian equation are a function of the time dependence of σ_y and σ_z . ISCST3 uses this C_{10} as a one-hour average concentration (C_{60}) (Williams, 1996). This assumption that $C_{10} = C_{60}$ results in an **inappropriate overestimation of downwind concentration**. The assumption by the developers of ISCST3, in essence, states that the wind direction and wind velocity does not change within a one hour time period. **This is clearly not the case!** Hino (1968) suggests that using a power law model with a p-value of .5 is appropriate to use in converting short time average concentrations to longer time average concentrations ranging from ten minutes to five hours. Research by Stiggins et. Al. (2003) and Wanjura et. Al. (2003) shows that converting C_{10} s to C_{60} s using the power law approach results in concentration reductions of approximately 2.5 times.

The performance characteristics of a federal reference method (FRM) ambient PM_{10} sampler are characterized by a lognormal distribution with a cut point (d_{50}) of $10 \pm 0.5 \mu\text{m}$ and slope of 1.5 ± 0.1 (Hinds, 1982). EPA defines the performance characteristics of the FRM $PM_{2.5}$ sampler as having a $d_{50} = 2.5 \pm 0.2 \mu\text{m}$ with no slope specifically stated. Work by Peters and Vanderpool (1996) suggests a slope of the fractional efficiency curve for the WINS Impactor of 1.18. Further work by Buch (1999) indicates the performance characteristics of the WINS Impactor to have a slope of 1.3 ± 0.03 . The lognormal distributions defined for the PM_{10} and $PM_{2.5}$ samplers describe the fractional efficiency curve (FEC) in which the samplers are expected to operate. The FEC gives the expected collection efficiency of the sampler for any given particle diameter or stated differently, it gives the percentage of particles in the PSD that should be prevented from penetrating to the filter. Buser et. Al. (2001) report that inherent sampler errors exist for PM_{10} samplers when sampling in dusts with MMDs larger than $10 \mu\text{m}$ and also for $PM_{2.5}$ samplers when sampling in dusts with MMDs greater than $2.5 \mu\text{m}$. Buser goes further to report that the ratio of the measured concentration by the sampler to the true concentration for PM_{10} samplers sampling a dust with MMD = $20 \mu\text{m}$ and GSD = 1.5 ranges from 1.81 with the sampler operating with $d_{50} = 9.5$ and slope = 1.4 to 3.43 with the sampler operating with $d_{50} = 10.5 \mu\text{m}$ and slope = 1.6. The ratio of the measured concentration to the true concentration for a $PM_{2.5}$ sampler sampling the same PSD range from 14.8 with the sampler operating at $d_{50} = 2.3 \mu\text{m}$ and slope = 1.27 to 183 with the sampler operating with $d_{50} = 2.7 \mu\text{m}$ and slope = 1.33. The mass and PSD of the particulate matter penetrating the abatement systems of cotton gins varies depending upon the trash content of the cotton processed. The average PM_{10} percentage of TSP reported by AP-42 is 39% which corresponds to a PSD with a $12 \mu\text{m}$ MMD assuming a GSD of 2. Buser et. Al. (2002) reported MMDs in excess of $15 \mu\text{m}$ for gin exhausts. Agricultural dusts typically have PSDs characterized by an MMD ranging from 15 to $25 \mu\text{m}$ with GSD typically ranging from 1.5 to 2.0 (Redwine et. Al., 2001). Over-sampling errors caused by larger MMDs result in great inaccuracies in measuring downwind concentrations. This in turn causes the inappropriate regulation of cotton gins. It is the intent of this manuscript to demonstrate the use of a new model that predicts more accurate downwind concentrations than the current LLPS modeling method of using a C_{10} as a C_{60} through the use of the power law and assuming a PSD of the PM emitted from the source. It is also the intent of this manuscript to compare the concentrations predicted by the new model to those that would be theoretically measured by FRM PM_{10} and $PM_{2.5}$ samplers sampling in the same conditions downwind from a LLPS.

Methods

A spreadsheet model was developed to simulate the performance of a FRM ambient PM_{10} and $PM_{2.5}$ sampler operating downwind from a simulated cotton gin for two different scenarios. Scenario A was performed under the assumption that the PSD of the dust being sampled was constant and had an MMD = $12 \mu\text{m}$ and GSD = 2. Scenario B assigned a triangular distribution to the MMD and GSD of the PSD of the dust being sampled. The triangular distribution was also used to simulate the TSP emission rate from the gin exhausts, and the d_{50} and slope of the PM_{10} sampler in both scenarios. The range of a random variable defined by a triangular distribution will be denoted by {A, C, B} with the triangular distribution defined as follows:

$$\Theta = \frac{C - A}{B - A} \quad (1)$$

$$X = A + \sqrt{(B - A) * (C - A) * R} \quad \text{For } 0 \leq R \leq \theta \quad (2)$$

$$X = B - \sqrt{(B - A) * (B - C) * (1 - R)} \quad \text{For } \theta < R \leq 1 \quad (3)$$

where:

- Θ = constant ratio;
- A = minimum value of the simulated variable;
- B = maximum value of the simulated variable;
- C = most likely value of the simulated variable;
- X = simulated/random variable;
- R = random number.

The TSP emission factor for the 40 bale per hour gin was defined by a triangular distribution {0.91, 1.39, 1.82} kg/bale. It was assumed that the emission factor would change based upon the trash content of the incoming seed cotton and so an emission factor range was arbitrarily assigned as ± 1 lb from the total 1996 AP-42 TSP emission factor of 3.05 lbs/bale. Equation 4 was used to calculate the TSP emission rate for the gin.

$$ER_{TSP} = EF_{TSP} * GR * \frac{10^9}{3600} \quad (4)$$

where:

- ER_{TSP} = TSP Emission Rate, $\mu\text{g/s}$;
- EF_{TSP} = AP-42 TSP Emission Factor, kg/bale;
- GR = Ginning Rate, bales/hour;
- 10⁹/3600 = unit conversion constants.

The TSP emission rate was then used as the emission rate in the Gaussian equation as follows.

$$C_{10} = \frac{ER_{TSP}}{2\pi u \sigma_y \sigma_z} \exp\left(-\frac{1}{2} \frac{y^2}{\sigma_y^2}\right) \left\{ \exp\left(-\frac{1}{2} \frac{(z - H)^2}{\sigma_z^2}\right) + \exp\left(-\frac{1}{2} \frac{(z + H)^2}{\sigma_z^2}\right) \right\} \quad (5)$$

where:

- C₁₀ = ten minute average steady state concentration at a point (x, y, z) ($\mu\text{g/m}^3$);
- 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);
- H = effective stack height (H=h+Δh, where h = physical stack height and Δh = plume rise)(m);
- σ_y, σ_z = horizontal and vertical plume dispersion coefficients, m.

The values for σ_y and σ_z were calculated according to the procedure outlined in Cooper and Alley (2002). It should be noted that the value for σ_y calculated using the procedure described by Cooper and Alley is less than the value calculated by ISCST3 (Turner, 1994). This in turn will cause the 10 minute concentrations calculated using this method to be slightly higher than those calculated by ISCST3. Therefore, the C_{10s} reported in this manuscript are more conservative than those reported by ISCST3.

$$\sigma_y = a * x^b \quad (6)$$

$$\sigma_z = c * x^d + f \quad (7)$$

where:

- a, b, c, d, f = constants dependent upon stability class
(for stability class D: a=68, b=0.894, c=33.2, d=0.725, f=-1.7)
- x = downwind distance, km.

The downwind distances used for scenarios A and B were 550 and 300 meters respectively. These distances were chosen to demonstrate the effect of the particle size distribution on the required distance between the property-line and the emission point in order to be in compliance with the NAAQS at the property line. The following assumptions were made for the model:

- Constant wind speed of 6 m/s
- Stability class D
- Average wind direction is directly from source to receptor ($y=0$)
- Concentrations calculated at ground level ($z=0$)
- Effective stack height of 10 meters (typical cyclone height with rain cap preventing momentum plume rise).

The assumptions pertaining to the meteorological conditions were made to simplify the model setup for the demonstration of the proposed method. It is in no way the intent of the authors to suggest that these meteorological conditions would be typical of those encountered during a typical gin season. Again, it is the intent of this manuscript to demonstrate the methodology used by the proposed model.

The C_{10} values were then converted to C_{60} values using the power law model with p-value of 0.5 as shown below.

$$C_{60} = C_{10} * \left(\frac{10}{60} \right)^{0.5} \quad (8)$$

where:

C_{60} = one hour TSP concentration, $\mu\text{g}/\text{m}^3$;

10/60 = time ratio used to convert a 10 minute concentration to a 60 minute concentration.

The PM_{10} and $\text{PM}_{2.5}$ concentrations were calculated using the TSP C_{60} values calculated using equation 8 and the lognormal distribution defined by $\text{MMD} = 12\mu\text{m}$ and $\text{GSD} = 2$ for scenario A and by $\text{MMD} = \{15, 20, 25\}\mu\text{m}$ and $\text{GSD} = \{1.8, 2.0, 2.2\}$ for scenario B. The lognormal mass density function is defined as:

$$f(d_p, \text{MMD}, \text{GSD}) = \frac{1}{d_p \ln(\text{GSD}) \sqrt{2\pi}} \exp \left[\frac{-\left(\ln(d_p) - \ln(\text{MMD}) \right)^2}{2(\ln(\text{GSD}))^2} \right] \quad (10)$$

where:

d_p = particle diameter, μm .

$f(d_p, \text{MMD}, \text{GSD})$ = mass percentage of particles having diameter d_p .

The mass percentage of particles less than a given size is found by integrating equation 10 from 0 to the particle diameter of interest, this is known as the lognormal cumulative distribution function. To find the concentration of a particular size range of particles in a TSP concentration, equation 11 is used.

$$C(x) = C_{60} * \int_0^x f(d_p, \text{MMD}, \text{GSD}) dd_p \quad (11)$$

where:

x = Particle size of interest, μm (PM_{10} : $x = 10$, $\text{PM}_{2.5}$: $x = 2.5$)

$C(x)$ = One hour concentration of particles less than $x \mu\text{m}$, $\mu\text{g}/\text{m}^3$.

The d_{50} for the PM 10 ambient air sampler in scenarios A and B varied according to the triangular distribution $\{9.5, 10, 10.5\}$ and the slope varied according to $\{1.4, 1.5, 1.6\}$. The d_{50} for the $\text{PM}_{2.5}$ sampler in both scenarios was constant at $2.5\mu\text{m}$ with slope constant at 1.18. The lognormal density distribution function of the collection efficiency of a sampler is given by equation 12.

$$\eta(d_p, d_{50}, slope) = \frac{1}{d_p \ln(slope) \sqrt{2\pi}} \exp \left[\frac{-(\ln(d_p) - \ln(d_{50}))^2}{2(\ln(slope))^2} \right] \quad (12)$$

where:

$\eta(d_p, d_{50}, slope)$ = collection efficiency of the pre-separator for particles of diameter d_p .

The cumulative distribution function of the collection efficiency curve is given by equation 13.

$$N(x, d_{50}, slope) = \int_0^x \eta(d_p, d_{50}, slope) \quad (13)$$

where:

$N(x, d_{50}, slope)$ = the cumulative collection efficiency of particles less than x μm in diameter.

The collection efficiency $N(x, d_{50}, slope)$ is used in equation 14 to find the cumulative penetration efficiency.

$$P(x, d_{50}, slope) = 1 - N(x, d_{50}, slope) = 1 - \int_0^x \frac{1}{d_p \ln slope \sqrt{2\pi}} \exp \left[\frac{-(\ln d_p - \ln d_{50})^2}{2(\ln slope)^2} \right] \quad (14)$$

where:

$P(x, d_{50}, slope)$ = the cumulative penetration efficiency of particles less than x μm in diameter.

The concentration theoretically measured by the sampler is given by equation 15.

$$M(MMD, GSD, d_{50}, slope) = C_{60} * \int_0^{\infty} f(d_p, MMD, GSD) * P(d_p, d_{50}, slope) dd_p \quad (15)$$

where:

$M(MMD, GSD, d_{50}, slope)$ = the concentration measured by the sampler using a one hour TSP concentration PSD and sampler performance characteristics, $\mu\text{g}/\text{m}^3$.

The ratio of the theoretical measured concentration to the true concentration is found by dividing the theoretically measured concentration from equation 15 by the true concentration found from equation 11.

Results

24-hour average concentrations for all C_{10} s and C_{60} s for scenarios A and B are listed in tables 1 and 2 respectively. The C_{10} values for PM_{10} and $\text{PM}_{2.5}$ are the values that would be compared to the NAAQS for regulation purposes using the current modeling techniques. The C_{60} values for PM_{10} and $\text{PM}_{2.5}$ are the values that would be compared to the NAAQS for regulation purposes using the new model.

Using the power law to convert ten-minute concentrations to sixty-minute concentrations reduces the concentrations by a factor of 2.45 using a P-value of 0.5. Tables 3 and 4 list the 24-hour average ratios of the theoretically measured concentrations to the C_{60} values for PM_{10} and $\text{PM}_{2.5}$ for scenarios A and B respectively. This ratio of the theoretically measured concentration to the actual concentration (C_{60}) is known as the over-sampling rate. The average over-sampling rates for PM_{10} and $\text{PM}_{2.5}$ for scenario A are 1.04 and 1.17 respectively. The average over-sampling rates for PM_{10} and $\text{PM}_{2.5}$ for scenario B are 1.21 and 1.27 respectively. This indicates that larger MMDs cause the samplers to have higher over-sampling rates.

The mass fraction of particles less than 2.5 μm in the ambient TSP concentrations characterized by the given lognormal distribution in both scenarios results in a **negligible concentration** when compared to the

NAAQS of $65\mu\text{g}/\text{m}^3$. As the MMD of the ambient PSD increases, the mass fraction of PM_{10} and $\text{PM}_{2.5}$ decrease. However, the same increase causes a higher instance of over-sampling by the ambient samplers. Tables 5 and 6 show the affect on the over-sampling ratio from a change in MMD, GSD, d_{50} , or slope while the other three are held constant. Tables 5 and 6 denote the over-sampling ratio by the letter E. With the PSD and the d_{50} held constant, a decrease in slope causes a decrease in E, where an increase in slope causes an increase in E. Holding the PSD and slope constant, a decrease in D_{50} causes a decrease in E while an increase in d_{50} causes an increase in E. With the sampler performance characteristics (FEC) and MMD held constant, a decrease in GSD causes an increase in E, where an increase in GSD causes a decrease in E. Holding the FEC and the GSD constant, a decrease in MMD results in a decrease in E where an increase in MMD causes an increase in E.

Conclusions

The results from this study demonstrate a more appropriate method, based on science, by which to predict downwind concentrations. The downwind concentrations predicted by this model are dependent, to a high degree, on the particle size distribution used to define the ambient dust. It has been shown in previous research that the PSD for cotton gin dusts is in excess of that implied by AP-42 (MMD = 12, GSD = 2.0). The error encountered in AP-42 that the percentage of TSP that is PM_{10} is 39% was a result of dividing a flawed PM_{10} emission factor by the TSP emission factor ($0.54 \text{ kg } \text{PM}_{10} \text{ per bale} / 1.4 \text{ kg TSP per bale} = .39$ or 39%). If a more accurate PSD with a higher MMD is used to characterize the ambient dust at the gin property line, the PM_{10} PLCs will be reduced. This will allow gins in closer proximity to property lines to meet SAPRA regulations of PM_{10} concentrations more easily.

The assumption that the gin will operate at its designed throughput capacity (40 bales per hour) for 24 hours per day also causes the predicted concentrations to be conservative. Future analysis of this model should integrate the hourly change in stack tip wind speed and stability class. In addition, the ginning rate could be assigned to a statistical distribution as well as assigning different distributions to the simulated parameters to increase the accuracy of the real world simulation of the gin.

Disclaimer

Mention of a trade name, propriety product or specific equipment does not constitute a guarantee or warranty by the United States Department of Agriculture and does not imply approval of a product to the exclusion of others that may be suitable.

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Tables

Table 1. Scenario A PM₁₀ and PM_{2.5} concentrations based upon a lognormal particle size distribution with MMD = 12 μm and GSD = 2 at 550 meters downwind. The darkened columns list the 24 hour average concentrations predicted by the new model.

Day	Modeled Downwind Concentrations						Theoretically Measured Downwind Concentrations	
	TSP 24-Hour Avg.		PM ₁₀ 24-Hour Avg.		PM _{2.5} 24-Hour Avg.		PM ₁₀ 24-Hour Avg.	PM _{2.5} 24-Hour Avg.
	C ₁₀	C ₆₀	C ₁₀	C ₆₀	C ₁₀	C ₆₀	C ₆₀	C ₆₀
	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³
1	892	364	353	144	10.5	4.3	149	5.0
2	908	371	360	147	10.7	4.4	151	5.1
3	887	362	351	143	10.5	4.3	149	5.0
4	904	369	358	146	10.7	4.4	151	5.1
5	902	368	358	146	10.7	4.4	151	5.1
6	899	367	356	145	10.6	4.3	149	5.1
7	893	364	354	144	10.5	4.3	150	5.1
8	932	380	369	151	11.0	4.5	157	5.3
9	946	386	375	153	11.2	4.6	159	5.4
10	920	376	365	149	10.9	4.4	155	5.2

Table 2. Scenario B PM₁₀ and PM_{2.5} concentrations based upon lognormal particle size distributions with simulated MMD and GSD values from Triangular distributions {15, 20, 25} μm and {1.8, 2.0, 2.2} respectively at 300 meters downwind. The darkened columns list the 24 hour average concentrations predicted by the new model.

Day	Modeled Downwind Concentrations						Theoretically Measured Downwind Concentrations	
	TSP 24-Hour Avg.		PM ₁₀ 24-Hour Avg.		PM _{2.5} 24-Hour Avg.		PM ₁₀ 24-Hour Avg.	PM _{2.5} 24-Hour Avg.
	C ₁₀	C ₆₀	C ₁₀	C ₆₀	C ₁₀	C ₆₀	C ₆₀	C ₆₀
	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³	μg/m ³
1	2047	836	320	131	3.2	1.3	159	1.7
2	2059	841	318	130	3.6	1.5	159	1.8
3	1855	757	305	124	3.2	1.3	152	1.7
4	2070	845	349	142	3.7	1.5	170	1.9
5	2028	828	349	143	4.0	1.6	174	2.1
6	2050	837	324	132	3.4	1.4	160	1.7
7	2007	819	368	150	4.2	1.7	181	2.2
8	2008	820	322	131	2.9	1.2	161	1.5
9	1956	799	323	132	3.1	1.3	159	1.6
10	2114	863	384	157	4.2	1.7	190	2.2

Table 3. 24-hour average over sampling rates for scenario A.

Day	24-Hour Average of the Ratio of Theoretically Measured Concentration to C ₆₀	
	PM ₁₀	PM _{2.5}
1	1.03	1.17
2	1.03	1.17
3	1.04	1.17
4	1.03	1.17
5	1.04	1.17
6	1.03	1.17
7	1.04	1.17
8	1.04	1.17
9	1.04	1.17
10	1.04	1.17

Table 4. 24-hour average over sampling rates for scenario B.

Day	24-Hour Average Ratio of Theoretically Measured Concentration to C ₆₀	
	PM ₁₀	PM _{2.5}
1	1.21	1.27
2	1.22	1.25
3	1.22	1.27
4	1.20	1.26
5	1.22	1.25
6	1.21	1.27
7	1.21	1.26
8	1.22	1.28
9	1.21	1.28
10	1.21	1.26

Table 5. Comparison of varying d₅₀ and Slope while holding the PSD constant on the over sampling rate (E)

Constant PSD (MMD=20μm, GSD=2.0)				
Constant	D ₅₀	Slope	E	%Δ E
d ₅₀	10	1.5	122.29	0.00%
	10	1.275	108.83	-11.01%
	10	1.725	136.11	11.30%
Slope	10	1.5	122.29	0.00%
	8.5	1.5	90.33	-26.13%
	11.5	1.5	154.66	26.47%

Table 6. Comparison of varying MMD and GSD while holding the FEC constant on the over sampling rate (E).

Constant FEC (d ₅₀ =10μm, Slope=1.5)				
Constant	MMD	GSD	E	%Δ E
MMD	20	2	122.29	0.00%
	20	1.7	156.32	27.83%
	20	2.3	112.09	-8.34%
GSD	20	2	122.29	0.00%
	17	2	114.6	-6.29%
	23	2	130.56	6.76%