DISPERSION MODELING OF PARTICULATE FROM POINT AND MULTIPLE POINT SOURCES

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Abstract

The Industrial Source Complex (ISC) model is currently the most popular air pollutant dispersion model approved for use by the United States Environmental Protection Agency (EPA) for modeling the dispersion of particulate matter. Agricultural sources of particulate pollutant are among the sources affected by the use of this model. The authors feel that the application of the parameters of the Gaussian dispersion equation, upon which the ISC model is based, is incorrect and results in extreme inaccuracy in estimation of concentrations of particulate downwind from a source. A new dispersion model, the Fritz-Zwicke Model ©, has been developed by the authors to more accurately predict downwind concentrations of particulate.

Introduction

Dispersion modeling is quickly becoming an increasingly more important part of the air pollution regulatory process. The use of air dispersion modeling can allow a modeler to predict the contribution of pollutant to the ambient concentration downwind from an emission source, including an agricultural source, such as a cotton gin. The accuracy of this prediction depends upon the accuracy of the dispersion model being used, as well as the accuracy of the emissions information and meteorological conditions observed. Since air dispersion modeling has become such a significant part of the regulatory process, it is essential to use an accurate model.

In order to ascertain the contribution from agricultural operations of particulate matter to the ambient concentration, dispersion modeling is used. The Environmental Protection Agency (EPA) recommended computer dispersion model is Industrial Source Complex (ISC), which is based upon the Gaussian model. The ISC model has three main components:

- SCREEN--a simple screening algorithm used to determine a one-hour average concentration,
- ST--uses weather data recorded in one-hour intervals to determine shorter-term (up to one year) average concentrations, and
- LT--used to determine longer-term (greater than one year) average concentrations.

The National Ambient Air Quality Standards (NAAQS) for particulate matter are based on 24-hour and one year average concentrations. Therefore, only the use of SCREEN and ST will be relevant for the purposes of this research.

There are problems inherent in these models that result in errors in estimation. One problem is the misapplication of the dispersion parameters found in the Gaussian model. The Pasquill-Gifford dispersion parameters were not intended to be used to estimate 1 hour concentrations, as done by ISC-SCREEN3 and ISC-ST3. These dispersion parameters were developed based on concentrations that were taken over small time increments. The result of this misapplication is the calculation of an inaccurate one hour concentration, and, subsequently, the 24 hour concentration of particulate.

The EPA-approved ISC models are inaccurate. This inaccuracy could result in a cotton gin or other agricultural source to be deemed out of compliance with the NAAQS by a regulatory agency, causing possible economic hardship for the operators of the source as they struggle to correct a perceived problem, which, in reality, may not be a problem at all. A more accurate computer dispersion model is needed to better estimate downwind particulate concentrations. The key variable that will result in more accurate downwind estimates of particulate matter concentrations is the time frame used for concentration calculations. An attempt will be made to incorporate the time period used by Pasquill and Gifford in developing their dispersion parameters.

Literature Review

The Gaussian dispersion model is the most popular basis for determining the impact of nonreactive pollutants, such as particulate matter. (EPA, 1986) This model may be used to estimate the ground-level concentrations downwind in a plume from a source with a specific emission rate. (Gifford, 1975) A coordinate system is incorporated where the origin is placed at the base of the stack with the x-axis aligned in the downwind direction. “The contaminated air stream (normally called a plume) rises from the stack and then levels off to travel in the x-direction and spread in the y- and z-directions as it travels. For Gaussian plume calculations, the plume is assumed to be emitted from a point with coordinates (0,0,H), where H refers to the effective stack heigh, which is the sum of the physical stack height (h) and the plume rise (Δh).” (DeNevers, 1995) The Gaussian dispersion equation for determining ground-level concentrations is shown in equation (1):

$$C=\frac{Q}{2\pi u\sigma_y\sigma_z}\exp(-\frac{1}{2}\frac{y^2}{\sigma_z{}^2})[\exp(-\frac{1}{2}\frac{(z-H)^2}{\sigma_z{}^2})+\exp(-\frac{1}{2}\frac{(z+H)^2}{\sigma_z{}^2})] \qquad (1)$$

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where: C = steady-state concentration ($\mu g/m^3$),
Q = emission rate ($\mu g/s$),
π = 3.14159...,
u = wind speed at stack height (m/s),
σ_y = lateral dispersion parameter (m),
σ_z = vertical dispersion parameter (m),
z = receptor height (m), and
H = plume centerline height (m).

The following assumptions are associated with the use of the Gaussian model (Turner, 1994):

- The emission rate of pollutant does not vary over time.
- No pollutant is lost due to chemical reaction, settling, or turbulent impaction during transport.
- The crosswind and vertical concentration distributions are well-represented by a Gaussian, or normal, distribution at any distance downwind or any distance in the crosswind directions.
- Meteorological conditions remain constant over the time of transport.

Veigele and Head (1978) noted, “The assumptions used in the derivation, frequently, do not hold. Emissions may vary with time. Pollutants may be lost due to settling or chemical reactions. Wind fields may vary with height. Inversion layers may exist. The diffusion constants may vary. Because of these and other cases where the assumptions do not hold, care must be taken when using the Gaussian equation.” In order to produce concentration estimates that are as accurate as possible, the Gaussian dispersion model should be applied to a situation that satisfies as many of these assumptions as possible. (Fritz, et al., 1997)

While it may be simple for the purposes of modeling to assume that a source has a constant emission rate, the particulate pollutants observe the law of conservation of mass, and the distributions of the pollutant in the crosswind and vertical directions follow a normal distribution, meteorological conditions are ever-changing. For short time periods, wind speed and direction can be assumed to remain relatively constant. However, over longer time periods, there can be much variation in wind speed and direction, resulting in an invalid assumption of constant meteorological conditions. For this reason, the authors feel that any particulate dispersion model, in order to be accurate, must incorporate small time-averaging periods. This is important, since the time average concentration is greatly influenced by the variation in wind speed and direction over the time period. For example, given a particular sampling location in a downwind direction over a two-minute time period, there is a good chance that wind speed and direction will remain constant. This will result in a relatively high two-minute average concentration at that sampling location. For a 24-hour time period at the same sampling location, however, there may be a great variation in wind speed and direction. This will cause the 24-hour concentration to be lower than the two-minute concentration, since there will periods in the averaging time when no particulate is being sampled, due to the flow of wind in a direction away from the sampler. In general, “a longer time-averaged concentration would be expected to be less than a short time-average, owing to wind shifts and turbulent diffusion.” (Cooper and Alley, 1994) Regardless, a period of constant wind speed and direction modeled using the Gaussian equation will result in a concentration that is valid for that period, since the Gaussian equation “...refers to a stationary state (i.e., C is not a function of time...” and it “...uses meteorological conditions (wind and turbulence states) that must be considered homogeneous and stationary in the modeled area...” (Zanetti, 1990)

The dispersion parameters, σ_y and σ_z, used in the Gaussian equation were developed by Pasquill (1961), who observed plumes of sulfur dioxide (SO_2) and smoke (gases and particulate matter) over small (2-10 minute) time intervals. In theory, they represent the distance of horizontal and vertical spread of the plume of pollutant. Mathematically, they are the standard deviations associated with the normal distributions in the Gaussian equation. Figure 1 (Turner, 1994) illustrates the function of the dispersion parameters in the double normal distribution of concentration estimates.

Since the dispersion parameters were developed from observations over small time intervals, it should be reasonable to assume that the use of the Gaussian equation incorporating these parameters should yield a concentration representing a small time average. These shorter time average concentrations can then be used to calculate longer time average concentrations. There is still much controversy surrounding the valid time period of application of these dispersion parameters, however.

Zanneti (1990), referencing Gifford (1976), stated that σ_y and σ_z were derived based on concentration readings taken every three minutes. Pasquill (1961) also denotes that the measurements used in developing the sigmas were from a source with three minute duration periods. Venkatram (1996), alluding to the Prairie Grass Experiment that was the basis for Pasquill’s estimates of the sigmas, states that the experiment consisted of 70 runs, and that each run was about ten minutes in length. Cooper and Alley (1994) explicitly say that the “...concentration predicted by [the Gaussian Model], using the σ_y and σ_z values from [the Pasquill-Gifford-Turner curves], is a 10-minute-average concentration.” Given the variation of time periods among the literature, there is no universally agreed upon time frame of application. Beychok (1996), in the following paragraph, provides a good summation of this issue.

> “A major problem with the Gaussian dispersion equation is defining what the calculated concentration C represents when using Pasquill’s dispersion coefficients. D.B. Turner states that C

> represents a 3- to 15-minute average; and American Petroleum Institute dispersion modeling publication believes C represents a 10- to 30-minute average; S.R. Hanna and P.J. Drivas believes C is a 10-minute average; and others attribute averaging times from 5 minutes to 30 minutes. Most agree on a range of 10 minutes to 15 minutes. However, many Environmental Protection Agency computer models used to determine regulatory compliance assume that the Gaussian dispersion equation yields 60-minute average concentrations."

The 24-hour concentrations obtained from both SCREEN and ST are calculated directly from the one-hour concentrations predicted from the use of these models. Because both SCREEN and ST are used to predict a one-hour concentration from a direct application of the Gaussian model, the authors assert that the use of these models results in an inaccurate prediction of downwind concentrations. This application involves the assumption that wind speed and direction remain completely constant over a one-hour period. It is difficult, if not impossible to find any example of atmospheric conditions in which this assumption is true. Williams (1996), in her research, concluded: "The current method of using ISC SCREEN results in inaccurate (excessively high) predictions of downwind concentrations. Any method used to model air quality should be conservative in nature. However, an extremely conservative prediction of property line concentrations used as a permitting tool could result in unjustified, mandated controls on an industry. Therefore, it is essential that a new model be developed for the purpose of accurately predicting downwind concentrations when compared to ISC SCREEN."

When predicting downwind concentrations with SCREEN, many regulators use only the full-meteorology option. The use of this option allows the modeler to find the combination of atmospheric stability class and wind speed at which the highest downwind concentration is predicted. The modeler adds an excessive degree of conservatism to the predicted concentrations when using this option, as will be shown in the results section of this paper. The use of ST requires the input of weather data recorded at one-hour intervals. This data is the resultant wind direction and speed over a particular one-hour interval; however, it definitely does not accurately represent the variation in wind speed and direction that may take place during the one-hour period.

In order to more accurately predict the ambient concentration of pollutant downwind from an emission source, the authors of this paper have developed a new dispersion model--the Fritz-Zwicke Model ©. This model is based on the Gaussian dispersion equation and requires the input of weather data in small time (two-minute) intervals to predict downwind concentrations, which is the same time interval used to develop the dispersion parameters of the Gaussian equation. The Fritz-Zwicke Model © also contains a simple screening model, which incorporates an alternative method of calculating σ_y, the dispersion parameter in the horizontal plane, from the standard deviation of the horizontal wind direction over a particular time period, as described by Pasquill. (Turner, 1997)

Procedure

As a part of the model development, a validation study was preformed. As this data has been previously reported, only a brief description is included. A site was chosen at the Riverside campus of Texas A&M University on an unused airport runway. A stack which was ten meters high was constructed to supply a constant emission rate of particulate with a known particle size distribution. The particulate used was fly ash, of which approximately 65% consisted of particles less than or equal to ten microns in aerodynamic equivalent diameter (PM_{10}). EPA reference method PM_{10} samplers were also located in various positions downwind from the source to measure the concentration of PM_{10} at those locations. A weather station was placed at the site to record the wind speed and direction at two-minute intervals. Each test was conducted for approximately a one-hour period, which correlates to the time-averaged concentration predicted by the use of SCREEN and ST. A comparison of the sampled concentrations and to the concentrations predicted by the models using appropriate weather data, showed that the Fritz-Zwicke model did in fact result in concentration estimates closer the measured values than those predicted by the ISC models.

To point out the significance that the new model will make in real world applications, a comparison of the ISC model concentration predictions to the Fritz-Zwicke predictions for a real world source is desired. For this demonstration, a hypothetical cotton gin with a processing capacity of 40 bales per hour was modeled over a 24-hour period using each of the dispersion models. The gin was assumed to have an overall emission factor of 3.05 lb/bale of total suspended particulate, which is consistent with the 1996 AP-42 emission factors published by EPA. The overall emission factor was distributed to each of ten process exhausts, as described by Flannigan (1997) and shown in Table 1. Hypothetical samplers were assumed to be located at 100, 200, 300, 400, 500, 600, 700, 800, 900, and 1000 meters in each of the north, south, east, west, northeast, northwest, southeast, and southwest directions.

Results

Figures 2-10 represent the results of the 24-hour cotton gin simulation. Figure 11 displays the windrose of the weather data for the 24-hour period from the two-minute data file used in the Fritz-Zwicke Model ©. Figure 12 displays the windrose of the weather data for the same 24-hour period, but was determined from the one-hour resultant wind speed and direction vectors used in ST. The use of SCREEN with the full-meteorology option resulted in predicted concentrations of PM_{10} in exceedance of the NAAQS even as far as 1000 meters downwind from the gin, and the use of SCREEN with the average wind speed and atmospheric stability class resulted in predicted concentrations in exceedance of the NAAQS as far as 700 meters downwind. The use of ST and the regular and simple Fritz-Zwicke Models © did not result in an exceedance of the NAAQS for this source.

It can be observed from Figure 2 that the use of the simple Fritz-Zwicke Model © resulted in predicted concentrations that were much lower than the concentrations predicted by the use of SCREEN with either the full-meteorology option or with the average weather. Figures 3-10 represent a comparison of the concentrations predicted from the use of ST and the regular Fritz-Zwicke Model © in the north, south, east, west, northeast, northwest, southeast, and southwest directions, respectively. In the north, west, and northeast directions, the predicted concentrations from ST are greater than those predicted from the regular Fritz-Zwicke Model © for shorter distances, but less than the concentrations from the Fritz-Zwicke Model © at farther distances. The use of the regular Fritz-Zwicke Model © resulted in greater predicted concentrations than ST in the south, east, southeast, and southwest directions. The use of ST resulted in a greater predicted concentration than the regular Fritz-Zwicke Model © at each of the distances in the northwest direction. An examination of the windroses for each of the models helps to show how the use of a single wind speed and direction for a one-hour period can affect the estimation of predicted concentrations downwind from a source.

Further Validation of the Fritz-Zwicke Dispersion Model

Preliminary sampling tests using a constructed stack system (Zwicke, et al, 1998) have shown that the Fritz-Zwicke model is a more accurate method for predicting PM_{10} concentrations downwind from a source than SCREEN and ISCST. It was desired, however, to compare predicted concentrations from the ISC set of models and the Fritz-Zwicke dispersion model with measured concentrations from an agricultural point source. A cotton gin, permitted at 18 bales per hour, was chosen as the facility at which ambient sampling would be conducted for comparison to the model predicted concentrations.

Ambient sampling of the cotton gin was conducted on each of the four boundary lines. Stations 1, 2, 3, and 4 represent the sampling stations on the south, east, north, and west property lines, respectively. Station 1 consisted of a high-volume PM_{10} sampler, a high-volume TSP sampler, and a federal reference method (FRM) $PM_{2.5}$ sampler. The TSP sampler at station 1 was used solely to determine a particle size distribution of the collected particulate. Stations 2, 3, and 4 each consisted of a high-volume PM_{10} sampler and a high-volume TSP sampler. Each of the PM_{10} and TSP samplers was operated at a flow rate of approximately 40 cfm. A weather station located at the site collected meteorological data on a two minute interval. Meteorological data collected were temperature, relative humidity, barometric pressure, wind speed, and wind direction.

These data will be analyzed to determine background, maximum, and gin contribution to property line particulate matter concentrations during the sampling period. The concentration data, gin processing rate, and meteorological data will be utilized to further validate the Fritz-Zwicke model.

Conclusions

The EPA-approved ISC models, SCREEN and ST, are inaccurate. The assumption of constant wind speed and direction for a one-hour period, which is incorporated in these models, is not valid. The use of this assumption in SCREEN results in an excessively high estimation of the one-hour concentration, and, ultimately, the 24-hour concentration. The use of this assumption in ST results in a wide variation of the estimated one-hour and 24-hour concentrations in different locations. The use of ST will result in the predicted concentrations in a particular location to be over-estimated, while also under-estimating the predicted concentrations in another location.

The use of weather data in small (2-10 minute) time increments will allow for more accurate predictions of particulate concentrations downwind from an emission source, including agricultural sources. This increased accuracy is desperately needed, as dispersion modeling becomes an increasingly more important tool in the regulatory process.

Initial validation efforts indicate that the Fritz-Zwicke Model © more accurately predicts downwind particulate matter concentrations. Further validation and efforts to obtain approval for State Air Pollution Regulatory Agencies (SAPRA's) to use this model , if successful, will facilitate fair regulation of agricultural sources of particulate matter.

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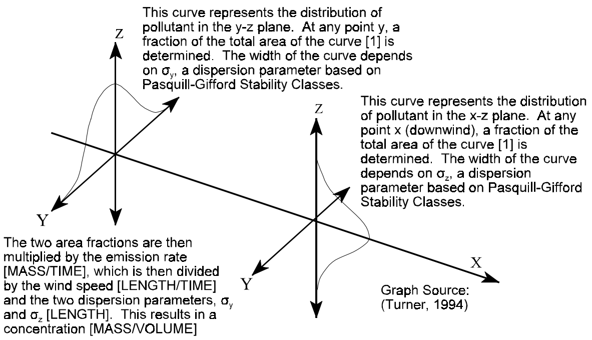

This curve represents the distribution of pollutant in the y-z plane. At any point y, a fraction of the total area of the curve [1] is determined. The width of the curve depends on σ_y, a dispersion parameter based on Pasquill-Gifford Stability Classes.

This curve represents the distribution of pollutant in the x-z plane. At any point x (downwind), a fraction of the total area of the curve [1] is determined. The width of the curve depends on σ_z, a dispersion parameter based on Pasquill-Gifford Stability Classes.

The two area fractions are then multiplied by the emission rate [MASS/TIME], which is then divided by the wind speed [LENGTH/TIME] and the two dispersion parameters, σ_y and σ_z [LENGTH]. This results in a concentration [MASS/VOLUME]

Graph Source: (Turner, 1994)

Figure 1. Graphical Representation of the Gaussian Dispersion Model

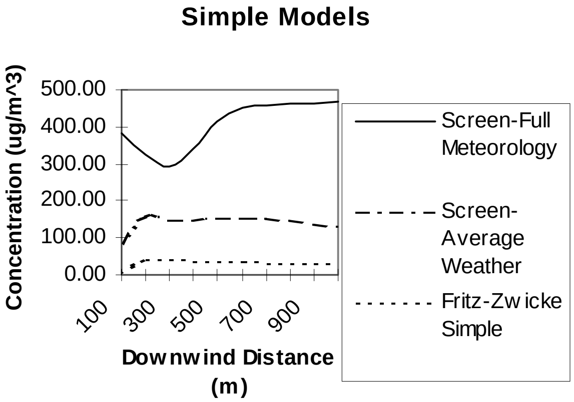

Figure 2. Simple Model Comparison

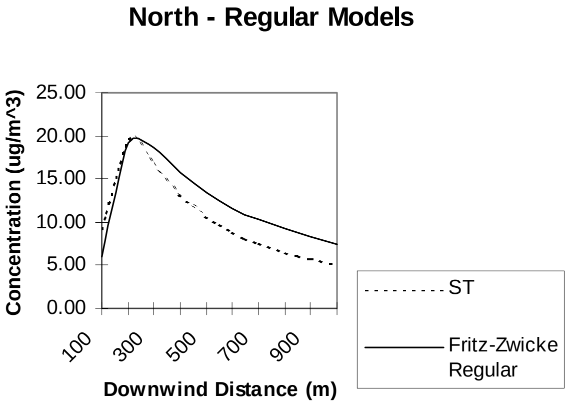

Figure 3. Regular Model Comparison-North Axis

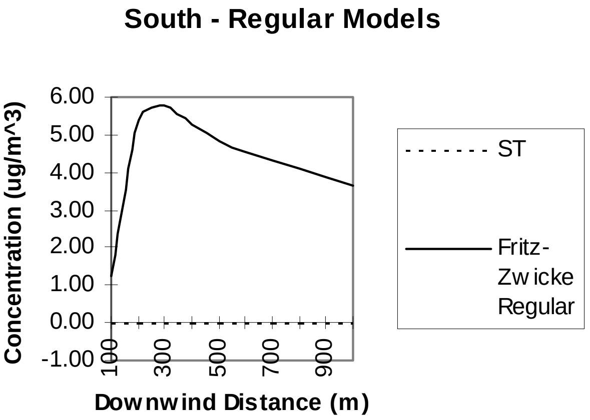

Figure 4. Regular Model Comparison-South Axis

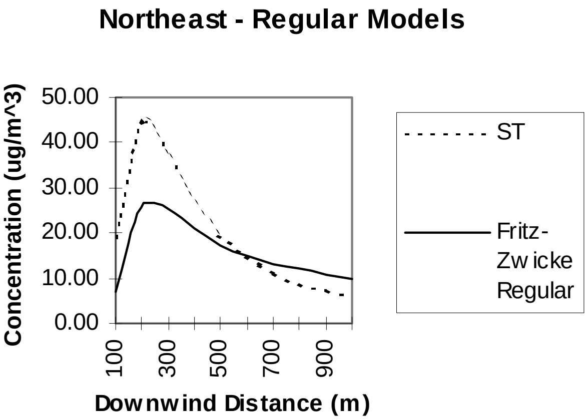

Figure 7. Regular Model Comparison-Northeast Axis

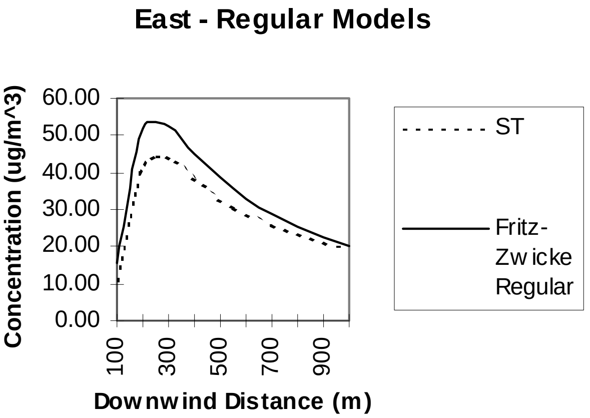

Figure 5. Regular Model Comparison-East Axis

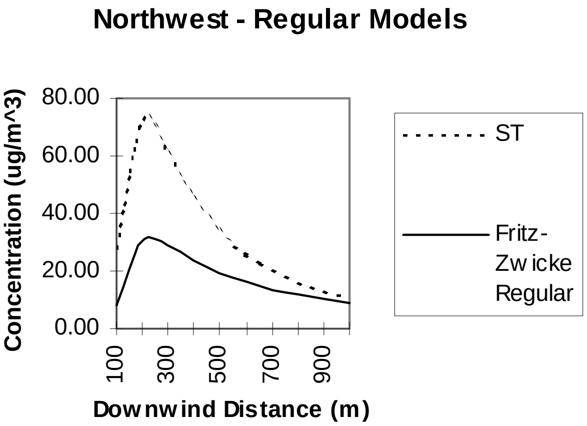

Figure 8. Regular Model Comparison-Northwest Axis

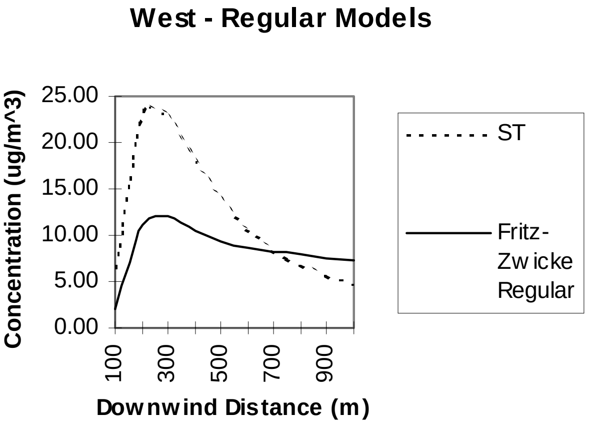

Figure 6. Regular Model Comparison-West Axis

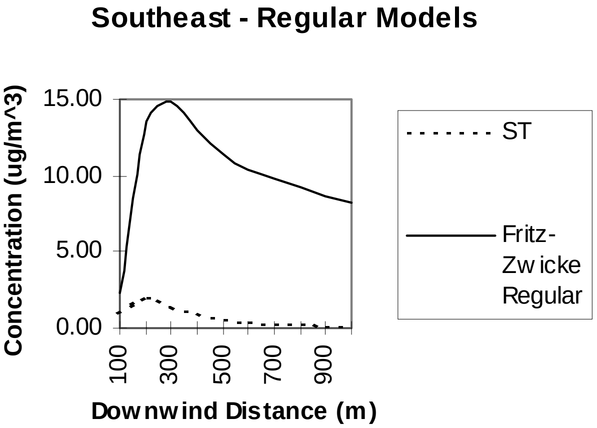

Figure 9. Regular Model Comparison-Southeast Axis

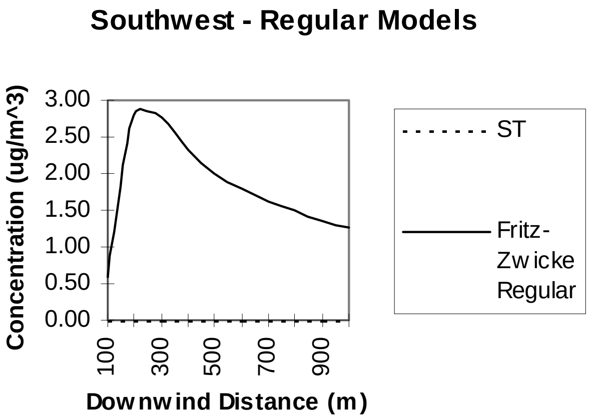

Figure 10. Regular Model Comparison-Southwest Axis

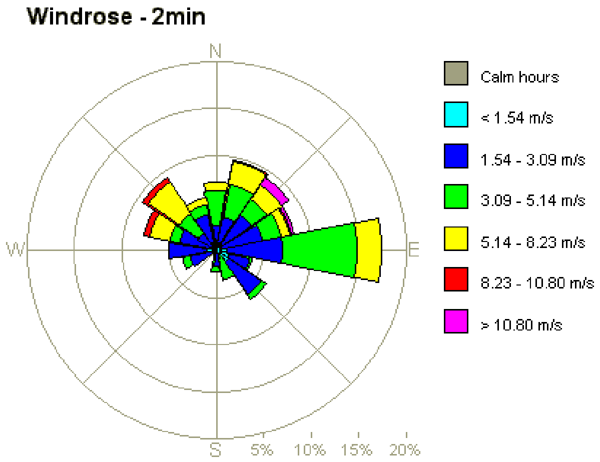

Figure 11. Cotton Gin Simulation Windrose-2 minute interval

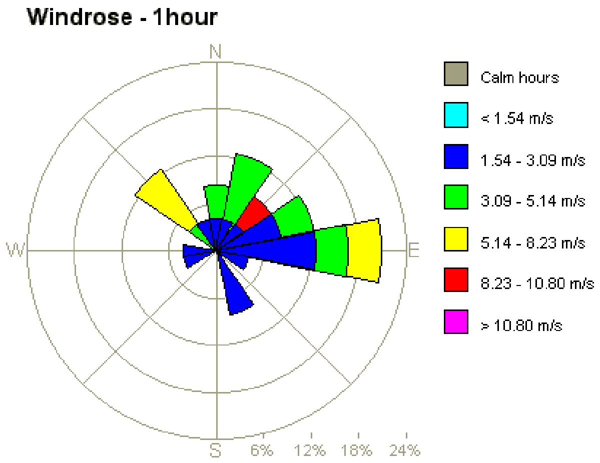

Figure 12. Cotton Gin Simulation Windrose-1 hour interval

Table 1: Hypothetical Cotton Gin Processes

Process	Process Name	Emission Factor (lb/bale TSP)
1	Unloading System	0.38
2	1st Push/Pull	0.33
3	2nd Push/Pull	0.21
4	Auger Distributor Separator	0.03
5	Master Trash	0.44
6	Overflow	0.09
7	Mote System	0.30
8	1st Stage Lint Cleaning	0.93
9	2nd Stage Lint Cleaning	0.17
10	Battery Condenser	0.17

Table 2: Test 1 Results

Model	Sampler					
	1	2	3	4	5	6
SCREEN-Full Met.	1560.00	1462.00	1341.00	1560.00	1462.00	1341.00
SCREEN-Avg. Weather	266.85	129.61	74.42	266.85	129.61	74.42
ST	312.88	156.53	93.02	0.00	0.00	0.00
Fritz-Zwicke Simple	64.15	55.33	50.57	64.15	55.33	50.57
Fritz-Zwicke Regular	75.58	33.81	18.29	59.76	25.99	13.62
Measured	35.35	30.12	19.22	56.31	33.55	24.82

Table 3: Test 2 Results

Model	Sampler		
	1	2	3
SCREEN-Full Met.	1540.00	1446.00	1301.00
SCREEN-Avg. Weather	212.50	146.30	101.50
ST	16.33	7.29	3.97
Fritz-Zwicke Simple	66.14	58.21	52.22
Fritz-Zwicke Regular	31.40	20.87	14.14
Measured	17.87	9.39	12.13

Table 4: Test 3 Results

Model	Sampler			
	1	2	3	4
SCREEN-Full Met.	1563.00	1468.00	1321.00	1340.00
SCREEN-Avg. Weather	190.32	130.86	90.74	66.06
ST	39.52	19.13	11.13	7.08
Fritz-Zwicke Simple	67.31	59.28	53.13	46.58
Fritz-Zwicke Regular	74.23	49.88	34.11	24.61
Measured	25.70	32.32	28.43	18.92