## DISPERSION MODELING OF PARTICULATE EMISSIONS FROM LOW-LEVEL POINT SOURCES Bradley K. Fritz, Bryan W. Shaw and Calvin B. Parnell Texas A&M University College Station, TX

## <u>Abstract</u>

Dispersion modeling is increasingly being used (as opposed to downwind sampling) as the primary method for determining potential downwind particulate concentration levels resulting from a given source's release. Modeling is attractive as a regulatory tool because of its ease of use, low cost, and small time requirement. On-site sampling demands greater costs, more time and manpower, and more care, while yielding less concentration data. As a result, sampling is used only as a last resort, and even then, may be set aside in favor of modeling results. The majority of the dispersion models approved by the Environmental Protection Agency (EPA) are Gaussian (or normal distribution) based models. These models require source parameter inputs, such as location and dimensions of emitting points and on-site structures and types and emitting rate of pollutants, along with meteorological data (wind speed, wind direction, etc...). This paper deals with the meteorological data input, and its effect on the modeling results. Three variations of meteorological data input format are compared, sub-hourly (two-minute), hourly average, and "spot" recordings. In general, the sub-hourly data results in concentration predictions that are more representative of actual conditions and have a lesser degree of variation in the concentration predictions.

### **Introduction**

The Clean Air Act (CAA) is the predominate piece of legislation that provides guidance to the states in controlling sources of air pollution. These regulatory programs have traditionally fallen into three categories; prohibition of new and existing sources emitting pollution that exceeds the ambient air quality levels set to protect public health, more stringent controls and permitting requirements for new sources, and the addressing of specific pollution problems such and hazardous air pollutants and visibility impairment (Brownell, 1999). Related to all of these categories, are the national ambient air quality standards (NAAQS). These standards address pollution that endangers public health and welfare.

Six pollutants have been established as criteria pollutants: sulfur dioxide (SO<sub>2</sub>), nitrogen dioxide (NO<sub>2</sub>), particulate matter (PM), carbon monoxide (CO), ozone (O<sub>3</sub>), and lead (Pb). Specific concentration levels are set for each of these pollutants by both a primary and secondary standard. George T. Wolff, Chair of the Environmental Protection Agencies (EPA) Clean Air Scientific Advisory Committee (CASAC), in a written statement to the House Subcommittee on Energy and Environment, describes the purpose of the two standards. He states that the primary standards are set to protect human public health, and that the secondary standards are set to protect against adverse welfare effects which include protection of plants, animals, ecosystems, visibility, etc. He further states that the primary NAAQS are required to be set at a level sufficient to protect public health with an adequate margin of safety for the benefit of any sub-populations. The primary NAAQS are therefore health-based standards.

We will concern ourselves only with the PM standards, as only they come in to play when permitting most agricultural sources. The original NAAQS for PM was based on total suspended particulate (TSP) (particulate matter less than 40  $\mu$ g/m<sup>3</sup> aerodynamic equivalent diameter (AED)). The primary standard was 260  $\mu$ g/m<sup>3</sup> TSP, (dry standard cubic meter) 24 hour average, and the secondary standard was 150  $\mu$ g/m<sup>3</sup> TSP, 24 hour average (Perkins, 1974). The NAAQS were revised in 1987 by replacing TSP as an indicator that included particles with an aerodynamic diameter of less than or equal to 10 micrometers AED (PM10), with PM10. The new primary standard is 150  $\mu$ g/m<sup>3</sup> PM10, 24 hour average, and the new secondary standard is 150  $\mu$ g/m<sup>3</sup> PM10, 24 hour average. States, when establishing state air quality guidelines, must set state NAAQS at levels that are at least as stringent as those established by the EPA NAAQS, but may apply levels that are more stringent.

The ongoing trend when applying these standards is to require sources to demonstrate, either through sufficient sampling or dispersion modeling results that the emissions from the source do not result in off-property concentrations that exceed the levels set by the primary NAAQS. Given that a sources right to operate hinges on modeling output, it is essential that the model used is as accurate as possible and that the outputs are appropriately applied. The presently accepted model used by State Air Pollution Regulatory Agencies (SAPRAS) for sources like cotton gins, feed mills, and grain elevators, is Industrial Source Complex (ISC). This same model is also used to predict downwind concentrations from power plants and other industrial sources.

## **Gaussian Based Modeling**

Gaussian-based dispersion models are all based on the concept that at a given downwind distance from a source, the concentration of pollutant, in both the vertical and horizontal directions, can be represented by a normal, or Gaussian, distribution. The degree of spread of the normal distribution is a function of both the downwind distance and the variation in wind direction, and is represented by the stability parameters  $\sigma_v$  and  $\sigma_z$ .

The Gaussian dispersion equation is given by Equation 1.

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

where:

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

Q = emission rate,  $\mu g/s$ 

 $\sigma_{y_3}\sigma_z$  = 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
- H = effective stack height (H = h+ $\Delta$ h, where h = physical stack height and  $\Delta$ h = plume rise), m (Cooper, 1986)

Several input parameters are required to predict downwind concentrations. These can include, source emitting point locations and dimension, source structure locations and dimensions, source emission rates, and meteorological data. This paper will focus on the types of meteorological data input and the effects of each on modeling outcomes.

## Meteorological Data

Meteorological data tends to be collected in one-hour intervals. This is in accordance with EPA guidelines put in a publication entitled *Meteorological Monitoring Guidance for Regulatory Modeling Applications* (EPA, 2000) that describes protocol for collecting and processing various meteorological data. The primary meteorological variables addressed are wind speed and direction, temperature and temperature difference, humidity, precipitation, pressure, and radiation. For each variable, suggested equipment, equipment performance standards, suggested setup location guidelines, and data processing is addressed.

Section 6 of this document addresses meteorological data processing, which includes data averaging and stability class assignment. Section 6.1 address data averaging and sampling strategies (EPA, 2000). Hourly averages are assumed throughout the text unless otherwise noted. The hourly averages are obtained from data collected throughout a given hour with a recommended sampling rate of 1-5 seconds. Hourly averages may be the overall average for a given hour or and average based on smaller time interval averages (EPA, 2000). When using smaller time intervals, the use of 15-minute periods is suggested. It is further noted "... the use of shorter period averages in calculating on hourly value has advantages in that it minimizes the effects of meander under light wind conditions in the calculation of the standard deviation of the wind direction..." (EPA, 2000). This seems to imply a desire to smooth out short-term variations in wind directions. On the other extreme, at most weather observation sites the "hourly" wind direction is the result of a "spot" recording, or at best the average of only several minutes observation that is not representative of the average wind direction (Trinity Consultants, 2000).

Zwicke (1998) looked at a new method of incorporating meteorological data into the modeling algorithm. Meteorological data, in the form of two-minute average wind speeds and wind directions, was used. The concept behind the use of these short-term data points was to meet the assumption of steady-state conditions over each transport interval. Zwicke (1998) conducted controlled pollutant release and measurement tests, recording all appropriate input parameters. Each test was then modeled using ISC Short Term (ISCST) and the new model, and modeled concentrations where compared to measured values. Zwicke (1998) reports that ISCST over-predicted the measured concentrations anywhere from 2.5 to 10 times, while the new model predictions were around 2.5 times the measured concentrations.

# **Meteorological Data Simulation**

In order to compare the concentration predictions that result from the use of each of the meteorological data types, comparative modeling was performed. This required that meteorological data for a given time period, in the form of all three types, was needed. This proved very difficult to obtain. The short-time period data was limited to at most one to 2 days and had missing data points. There was also the difficulty that the meteorological patterns from one day to the next were extremely varied, which makes comparison of multiple days difficult. It was decided to develop a simulation program that would generate all three data types simultaneously. This allowed user control as to the daily meteorological patterns and allowed for replication by day and year.

Several assumptions were made when developing the meteorological data simulation program. These will be discussed, when appropriate, within the general program description. The first step in the development of the meteorological model was to establish the required data. These included wind speed, wind direction, and stability class. The base interval for the generation of the meteorological data was set at two minutes, with the hourly averaged and the hourly "spot" data being based on the 30 two minute data points within each hour period. When examining generation methods for these data, it was realized that they are all dependent upon each other, as well as other non-required meteorological conditions. For example stability classes E and F occur only at night, and are then distinguished from each other based on cloud cover and wind speed. This type of dependence is true of all the stability classes. Table 1 shows these dependences.

This led to several initial parameters being required in the data generation process. Daytime and nighttime conditions were distinguished by daytime being assigned from hours 0600 through 1900, and nighttime the remaining hours. A discrete probability distribution (of equal probabilities) was used to establish the insolation (strong, moderate, or slight) during daytime, and similarly the cloud cover for nighttime. It was assumed that the insolation and the cloud cover (These will be referred to as stability class (SC) conditions) were constant over each one-hour interval, but varied from hour to hour. A wind speed grouping was assigned to each hour (<2, 2-3, 3-5, 5-6, >6 m/s) based on a discrete probability distribution of equal probability, independent of time of day. Based on the combination of SC condition and wind speed group, the stability class for a given hour was assigned based on Table 1.

At this point, a given hour has an assigned stability class and wind speed group. The next step was to generate wind speed and direction data in two-minute increments for each hour. It was assumed that both the wind speed and wind direction were normally distributed within each hour. This allowed for speed and direction data to be generated based on a mean and standard deviation. The wind speed mean was assigned as the average value of the upper and lower boundary values of the wind speed group. For example if the wind speed group were 2-3 m/s, the mean wind speed would be 2.5 m/s. The wind speed standard deviation was assigned based on time of day. In general there is more variation in met conditions during daytime hours than nighttime. So, for daytime conditions the wind speed standard deviation was set at 0.75 m/s (based on rough estimates from existing measured 2-minute met data) and the nighttime wind speed standard deviation was set at 0.5 m/s.

A mean wind direction and standard deviation for each hourly period was required to generate the sub-hourly data based on a normal distribution. The wind direction hourly mean was set based on two typical meteorological data patterns. The first was a diurnal type behavior, or where daytime wind directions are offset from nighttime directions. The second type assumed both daytime and nighttime directions were similar (non-diurnal). It was desired to compare the concentration predictions based on the maximum 24-hour concentrations. Wind flowing directly from source to receptor will result in the highest concentration predictions. For this analysis, this direction (vector direction directly from source to sampler) was 180°. Therefore, the daytime hourly wind direction means were uniformly distributed from 135° to 225°. This range was arbitrarily chosen for this analysis. Narrowing or widening will vary the magnitude of the concentrations (increase or decrease respectively), but will yield results that have similar relationships to those presented later in this paper. The nighttime hourly wind direction means were also uniformly distributed, 135° to 225° for a non-diurnal pattern and 315° to 405° for a diurnal pattern. The standard deviation of the wind direction within each hourly period was set based on data presented in Table 2 along with comparison to available two-minute measured data. The values in Table 2 do not have a specified associated time period, but do provide a guide on the relationship of wind direction variance from one stability class to the next. Based on analysis of available meteorological data (in two-minute increments), the average standard deviation in wind direction for type A stability conditions was approximately 60°. Based on this, all values in Table 2 were modified accordingly. The wind direction standard deviation for each hour was then assigned based on the stability class and a uniform distribution between the upper and lower values as established by modified Table 2 values.

Using the conditions above, each hour was assigned a wind speed mean and standard deviation, and wind direction mean and standard deviation. The assigned parameters were consistent with the time of day and the atmospheric conditions. Based on the means and standard deviations, two-minute wind speed and direction data were generated based on normal distributions.

This data was recorded as the two-minute met data. The hourly averaged met data was calculated based on the generated two-minute data. Each hourly wind speed and direction was determined using vector analysis as outlined by USEPA (2000). The one-hour "spot" wind direction and speed values were taken as the direction and speed that occurred as the last two-minute data point within each hour. This process resulted in three distinct, but dependent, meteorological data files: a two-minute data file, a one-hour average data file, and a "spot" data file. For each 24-hour period, there were 720 data points (one data point is a wind speed/direction combination) in the two-minute file, and 24 data points in both the one-hour averaged and one-hour "spot" data files. This meteorological data generation process was repeated to generate 3 years worth of data for both diurnal and non-diurnal conditions.

Figures 1,2 and 3 are the wind direction frequency plots for one-year's worth of data for each of the meteorological data types for diurnal conditions. Similarly, Figures 3,4 and 5 are the wind direction frequency plots for one-year's worth of data for each of the meteorological data types for non-diurnal conditions.

# **Concentration Prediction Analysis of the Three Data Types**

An arbitrary source and receptor combination was used to compare the concentration predictions that resulted from the use of the three data types. The source was assigned an effective stack height of 10 meters and an emission rate of 4 g/s ( $PM_{10}$ ). The distance from source to receptor was set at 100 meters. Daily 24-hour concentrations were calculated using the generated met data. For each year, the average daily 24-hour concentration along with the standard deviation, 95% confidence interval, maximum and minimum values, and number of excedences (>150 µg/m<sup>3</sup> PM<sub>10</sub> as set by the NAAQS) was recorded.

Table 3 contains the summary statistics for the diurnal met conditions, and Table 4 contains the summary statistics for the non-diurnal met conditions.

The first observation to make from this data is that the mean 24-hour predicted concentrations for the two-minute and the "spot" data are not significantly different from each other, but are significantly different from the 24-hour concentrations predicted using the one-hour averaged data. The two-minute and "spot" data based concentrations are approximately 3 times lower than the one-hour averaged based concentrations. This agrees with the work done by Zwicke (1998). The next observation to make is that the variation of the concentrations in the "spot" data is greater than that of the two-minute data. The "spot" data also has higher maximum concentration values and lower minimum concentrations values.

In order to understand why this occurs it is necessary to examine the wind direction data. The maximum predicted concentration will occur when the wind direction is in the same direction as the directional vector that connects the source to the sampler (prime direction). The predicted concentration will decrease as the angle between the wind direction and prime direction increases. It is important to understand that the "spot" data is only a small picture of the total hour's data. The only difference between the "spot" data and the two-minute data is that the "spot" data has one point sampled from the total hours distribution while the two-minute data has 30 points. We can extend this to the daily data. In this simulation, each day's meteorological data is generated based on the same sets of distributions and relationships. Again, the only difference between the two-minute data and the "spot" data is the number of data points, 720 for the two-minute data and 24 for the "spot" data. Collecting enough samples using the meteorological simulation model should result in similar frequency plots for the two-minute and for the "spot" data should be the same, while the variance should differ (as a result of being based on a smaller number of data points), as the generated data demonstrates.

Looking at the concept of "spot" and average data collection from a purely statistical standpoint, we can look at a day's or year's overall meteorological distribution, regardless of shape or degree of variation, as a total population of data spots. If a number of data points were taken using the "spot" method, and a similar number of data points were obtained by taking each data point as the average of another sample, the "spot" data will return a distribution that is more representative of the population. The method of averaging to obtain each data point actually reduces the variation of the total population distribution. Very simply, the averaged data distribution will always be narrower than a distribution resulting from "spot" data collection. In terms of dispersion modeling and estimated concentrations based on meteorological data, the averaged data will always result in the highest expected concentration value.

The one-hour averaged data is distinctly different from both the two-minute and the one-hour "spot" data. It is similar to the "spot" data, in that it contains one data point per hour, but unlike the "spot" data, the one-hour averaged data is representative of the hourly meteorological conditions. It is, by definition, the average value. The average is based on the recorded two-minute data, and is therefore statistically representative. The difficulty with the hour averaged meteorological data is that fact that it is an average and because of that summarizes multiple data points with one value thereby smoothing any variation in

the wind direction within the hour. Basing a one-hour concentration estimate one this single data point results in overpredicting the maximum concentration and underestimating concentrations at other locations. Basically, all the pollutant is concentrated into a small area. In contrast, using each two-minute data point to estimate a concentration and then averaging the 30 two-minute concentrations to obtain the one-hour averaged concentration spreads the pollutant over a larger area. The result is that the maximum concentration is lower the that from the single data point estimate, but with higher concentration estimates at locations where the single point estimate predicted little or no concentration. Figure 7 illustrates this difference. This means that for any given day, all of the maximum one-hour concentrations predicted using the one-hour averaged met data are higher than the one-hour averages using the two-minute data. This also means that on any given day the maximum 24-hour concentration based on one-hour averaged data will be higher than that based on the two-minute data and the "spot" data. Another way to look at this is to examine the wind direction frequency plot. By averaging each hour of the directional data recorded in the two-minute format, the daily directional distribution is confined to a smaller range. Whereas, taking one "spot" sample per hour returns the same distribution with less data point. This is evident in Figures 1 through 6.

#### **Conclusions**

Based on the results of this analysis, we can see that the use of the "spot" meteorological data, as opposed to one-hour averaged data, is actually a better representation of the actual conditions. The "spot" data, although only a snapshot in time, actually accounts for more variation in meteorological data than using averaged data. Again, this can be seen in Figures 1 through 6. "Spot" data will, therefore, result in lower maximum 24-hour concentrations than one-hour averaged data. Based on the results presented in Tables 3 and 4, we can see the use of averaged data results in a higher overall 24-hour mean concentration and in more predicted concentrations of that exceed the levels set by the NAAQS. We can also see that the "spot" data actually returns the same expected value as does the two-minute data, although with a greater degree of variation.

Ongoing research is looking to return similar concentration predictions as those obtained by using the two-minute data. The concept is to use the one-hour data, which return a concentration profile as shown in Figure 7, and to adjust the shape of the normal curve through use of the standard deviation of the hourly wind direction. This approach will allow the hourly averaged distribution, as shown in Figures 2 and 5, and transform them into the two-minute distribution (Figure 1 and 4). This will allow the use of the hourly averaged data to predicted more representative downwind concentrations.

#### **References**

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	Insolation		Night		
Strong Moderate S		Slight	Thinly overcast or ≥ 4/8 low cloud	≤ 3/8 cloud	
А	A-B	В			
A-B	В	С	Е	F	
В	B-C	С	D	Е	
С	C-D	D	D	D	
С	D	D	D	D	
	A A-B	StrongModerateAA-BA-BBBB-C	StrongModerateSlightAA-BBA-BBCBB-CC	Thinly overcast orStrongModerateSlight≥ 4/8 low cloudAA-BBA-BBCEBB-CCD	

Table 1. Stability Parameters (Pasquill, 1983).

Notes:

1. Strong insolation corresponds to sunny midday in midsummer in England; slight insolation to similar conditions in winter.

2. Night refers to the period from 1 hr before sunset to 1 hr after sunrise.

3. The neutral category D should also be used, regardless of wind speed, for overcast conditions during day or night and for sky conditions during the hour preceding or following night as defined above.

Table 2. Atmospheric Stability Classification by Wind Direction Fluctuation (Zannetti (1990)).

Pasquill Stability Categories	Standard Deviation of the Horizontal Wind Direction Fluctuations (degrees)	Standard Deviation of the Vertical Wind Direction Fluctuations (degrees)			
А	Greater than 22.5°	Greater than 11.5°			
В	17.5° to 22.5°	10.0° to 11.5°			
С	12.5° to 17.5°	7.8° to 10.0°			
D	7.5° to 12.5°	5.0° to 7.8°			
E	3.8° to 7.5°	2.4° to 5.0°			
F	Less than 3.8°	Less than 2.4°			

## Table 3. Summary Statistics - Diurnal Meteorological Condition.

	Meteorological Data Type									
		2 Minute	•	One	Hour Av	erage	One	One-Hour "Spot"		
	Year			Year			Year			
	1	2	3	1	2	3	1	2	3	
Mean ( $\mu g/m^3$ )	44.4	44.8	44.1	133.3	127.5	130.4	42.7	44.3	44.8	
Standard Deviation	14.2	14.2	14.2	77.5	72.1	74.6	36.6	39.9	38.8	
95% C. I. (+/-)	1.24	1.23	1.24	6.73	6.26	6.48	3.18	3.47	3.37	
Maximum Value	85.3	97.8	113.7	690.3	414.1	442.6	178.8	226.9	212.8	
Minimum Value	13.9	9.4	15.1	5.8	6.4	10.2	0.01	0.06	0.17	
No. of Excedences	0	0	0	127	124	125	5	10	5	

Table 4. Summary Statistics - Non-Diurnal Meteorological Conditions.

	Meteorological Data Type									
	2 Minute Year			One-	One-Hour Average			One-Hour "Spot"		
				Year			Year			
	1	2	3	1	2	3	1	2	3	
Mean ( $\mu g/m^3$ )	45.0	45.4	44.6	134.0	128.2	131.1	43.2	44.8	45.3	
Standard Deviation	14.2	14.2	14.2	77.5	72.0	74.5	36.6	40.0	38.8	
95% C. I. (+/-)	1.24	1.23	1.24	6.73	6.26	6.48	3.18	3.48	3.37	
Maximum Value	86.0	98.4	114.2	691.8	414.1	443.8	179.7	227.6	214.7	
Minimum Value	14.8	10	15.5	6.8	6.7	11.0	0.24	0.06	0.38	
No. of Excedences	0	0	0	129	125	126	5	10	5	

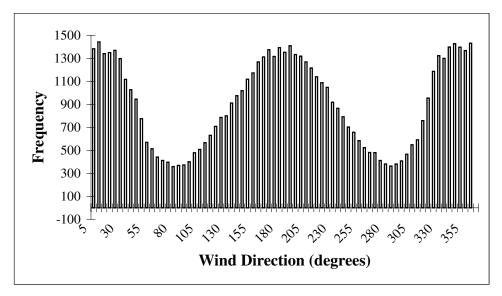


Figure 1. Frequency Plot: 2 Minute Wind Direction Data (Diurnal).

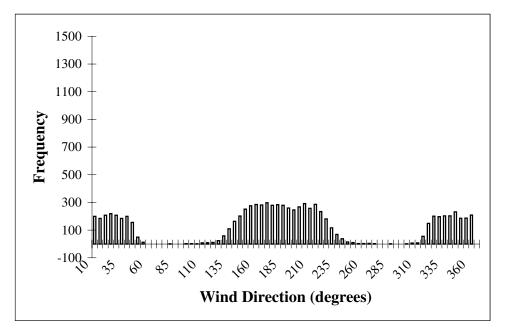


Figure 2. Frequency Plot: One-Hour Averaged Wind Direction Data (Diurnal).

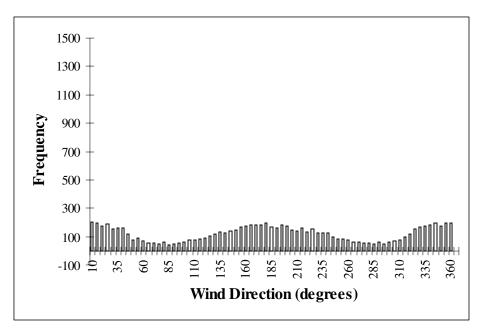


Figure 3. Frequency Plot: One-Hour "Spot" Wind Direction Data (Diurnal).

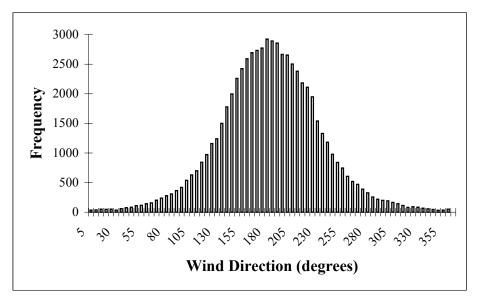


Figure 4. Frequency Plot: 2 Minute Wind Direction Data (Non-Diurnal).

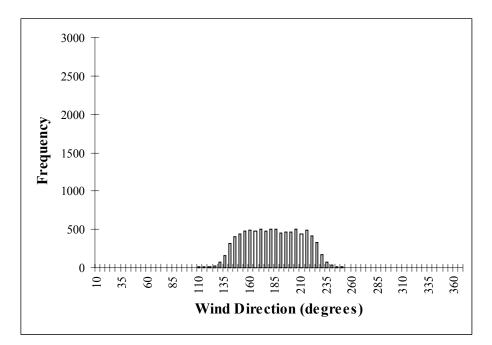


Figure 5. Frequency Plot: One-Hour Averaged Wind Direction Data (Diurnal).

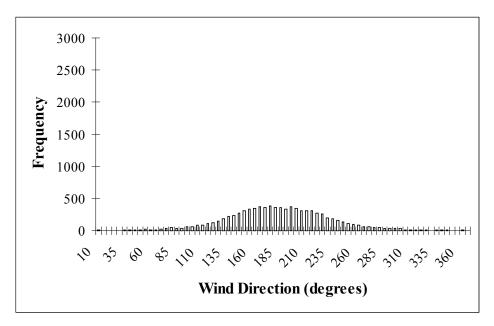


Figure 6. Frequency Plot: One-Hour "Spot" Wind Direction Data (Diurnal).

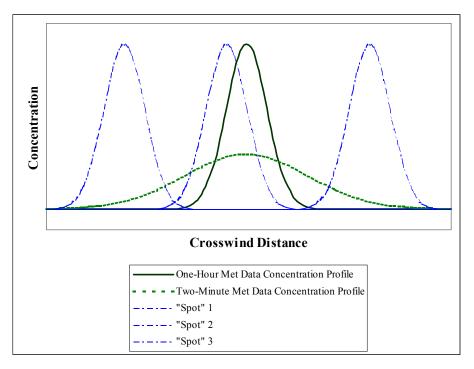


Figure 7. One-Hour Concentration Profile for One-Hour Averaged and Two-Minute Based Met Data.