

## **Regulatory Modeling-Current and Future Issues**

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### **ABSTRACT:**

A regulatory model has to meet special criteria for acceptance because it is governed by a legal framework. One of the most important is that concentration estimates from the model have empirical support through evaluation with observations under a variety of situations relevant to regulatory applications. This paper examines two situations in which current models have difficulty meeting this criterion. They are related to 1) surface releases under low wind speed conditions, and 2) prediction of short averaging time concentrations required for odour assessment. This paper analyzes the reasons for poor model performance under low wind speeds and provides suggestions on improving current models. The second part of the paper proposes a framework to estimate short concentrations averaged over time scales relevant to odour by using information on statistics comparing observed concentrations to one hour averaged model estimates. Finally, the paper examines some regulatory issues for which we have not yet developed adequate modeling tools.

### **INTRODUCTION:**

Air pollution models play an important role in the implementation of air pollution regulations. For example, before an industrial plant can be constructed, its impact on air

quality is determined through an air pollution model to show that emissions from the plant do not lead to ambient concentrations that are above a regulated level. Air pollution models that include chemistry are used to make decisions to control emissions that are precursors of ozone and acidifying pollutants.

This paper examines regulatory models applicable to scales of the order of tens of kilometers, when chemistry is not important. Examples of such models are AUSPLUME (Lorimer 1986), AERMOD (Cimorelli *et al.* 2005), the UK ADMS (Carruthers *et al.* 1994) and the Danish OML (Berkowicz *et al.* 1986) model. Because the results of applying a regulatory model have major financial and legal implications, the model has to meet some special criteria for acceptance: the model has to 1) be as simple as possible without sacrificing the essential physics of the problem, 2) provide realistic concentration estimates under a variety of conditions, 3) has extensive empirical support through evaluation with observations, 4) be robust in the sense that it is not very sensitive to certain model inputs, 5) should ensure consistency in application.

This paper examines two situations in which current models have difficulty meeting criterion (2), which ranks high among the criteria. These situations are related to 1) surface releases under low wind speed conditions, and 2) prediction of short averaging time concentrations required for odour assessment. This paper provides an analysis of the reasons for poor model performance in these situations and offers suggestions to improve the relevant modeling tools. The paper draws heavily from the authors' experience gained in developing and applying AERMOD (Cimorelli *et al.* 2005), USEPA's regulatory model for short range dispersion.

We first examine the treatment of dispersion under low wind speed conditions.

## **LOW WIND SPEEDS AND MEANDERING**

Estimating concentrations during low wind speeds, which occur frequently in urban areas, is one of the more important problems in regulatory modeling. We can make realistic estimates of concentrations under low wind speed conditions if measurements of turbulence levels, which govern dispersion, are available (Venkatram *et al.* 2004). But

such measurements are not available routinely, and we have estimate turbulence levels from measured mean wind speeds. In this situation, uncritical application of the Gaussian plume model can yield very high concentrations as seen by examining the expression for the ground-level concentration (Venkatram 1992 for example),

$$C \sim \frac{Q}{u_* x \sigma_y}, \quad (1)$$

where  $Q$  is the emission rate,  $u_*$  is the surface friction velocity,  $x$  is the downwind distance, and the horizontal plume spread,  $\sigma_y$ , is given by

$$\sigma_y = \frac{\sigma_v x}{U}, \quad (2)$$

where  $\sigma_v$  is the standard deviation of the horizontal velocity fluctuations. Because  $u_*$  and  $\sigma_v$  are generally taken to be proportional to the mean wind,  $U$ , we see from Equation (1) that the concentration becomes high when wind speed approaches zero. In the past, the “solution” to this problem was to set the wind speed equal to 1 m/s when it was smaller than this value.

AERMOD, and other currently used regulatory models, attempt to treat this situation more realistically by using the observation that when the wind speed is low, the plume meanders in the horizontal direction. When the mean wind speed is close to zero, the horizontal plume spread covers 360°. To model this situation, AERMOD and ADMS assume that the concentration is a weighted average of concentrations of two possible states: a random spread state, and plume state. In the random spread state, the release is allowed to spread radially in all horizontal directions. Then, the weighted horizontal distribution is written as:

$$H(x, y) = f_r \frac{1}{2\pi r} + (1 - f_r) \frac{1}{\sqrt{2\pi}\sigma_y} \exp\left(-\frac{y^2}{2\sigma_y^2}\right), \quad (3)$$

where the first term represents the random state in which the plume spread covers  $360^\circ$  or  $2\pi$  radians, and  $r$  the distance between the source and receptor. The second term is the plume state corresponding to the Gaussian distribution.

The plume is transported at an effective velocity given by

$$U_e = \left(2\sigma_v^2 + U^2\right)^{1/2}, \quad (4)$$

where  $U$  is the mean velocity. Note that the effective velocity is non-zero even when the mean velocity is zero, as long we can estimate the turbulent velocities. The minimum value of the transport wind,  $U_e$ , is  $\sqrt{2}\sigma_v$ .

The weight for the random component in Equation (3) is taken to be

$$f_r = \frac{2\sigma_v^2}{U_e^2}, \quad (5)$$

This ensures that the weight for the random component goes to unity when the mean wind approaches zero.

This approach works if measurements of  $\sigma_v$  are available; presumably, the measurements will reflect the large meandering when the wind speed is close to zero. If measurements are not available, we have to estimate  $\sigma_v$  from other meteorological variables. During the night, the wind speed is the primary routinely measured variable, and we end up with underestimating  $\sigma_v$ , which is assumed to be proportional to the wind speed. One tentative solution is to assume a minimum value of  $\sigma_v$ , say 0.25 m/s as suggested by Hanna *et al.* (2003). It might be preferable to use an empirical model for the behavior of  $\sigma_v$  near  $U=0$ . Let us examine some data to see whether such a model can be developed.

The data used in the analysis was measured on a tower operated by the UK meteorological office at Cardington, Bedfordshire. The tower, located on a large grassy field, has sonic anemometers measuring wind and temperature measurements at 10 m, 25 m, and 50 m above ground level. That data is sampled at 50 Hz, and the vector mean winds, temperatures, turbulent fluxes and variances are averaged over 1, 10, and 30 min.

We used the 30 minute averages from the 10 m in our analysis. The data set corresponds to all the stable periods (Monin-Obukhov length greater than zero) for 2005. These are the conditions under which the predicted concentrations can be high because the surface friction velocities are low. The estimated concentrations are high because both the horizontal as well as vertical turbulent velocities are taken to be proportional to the friction velocity.

Figure 1 (upper of P18) compares the estimated surface friction velocity with the observed values. The friction velocity is estimated using the one-level approach described in Venkatram and Princevac (2008).

We see that although there is scatter at low values of friction velocity, there is little bias in the estimated values, most of which are within a factor of two of the observations. This lack of bias does not transfer to the estimates of the standard deviations of horizontal and vertical turbulent velocities,  $\sigma_w$  and  $\sigma_v$ , as seen in Figure 2 (bottom of P18). The red lines in the figures correspond to the predictions:

$$\sigma_v = 2.5u_* \text{ and } \sigma_w = 1.3u_* . \quad (6)$$

The left top panel of Figure 2 indicates that even using a measured value of surface friction velocity does not allow us to obtain an adequate estimate of the horizontal velocity,  $\sigma_v$ . The observations are generally higher than the model estimates especially for low friction velocities. The situation is much better for  $\sigma_w$ : the right panel shows that the model estimates are mostly within a factor of two of the observations. The bottom panels show that, as expected, using the estimated value of the friction velocity increases the scatter in the estimates of  $\sigma_w$  and  $\sigma_v$ , and the negative bias in estimating  $\sigma_v$  is even larger.

To examine the effects of the uncertainty in estimating turbulent velocities on concentrations, let us define the dilution velocity,  $U_{dil}$ , using the expression for the ground-level concentration for surface releases in AERMOD (Cimorelli *et al.* 2005):

$$C(x,0) = \frac{Q}{u_*x} H(x,0) \equiv \frac{Q}{\pi U_{dil}x^2} , \quad (7)$$

where the horizontal distribution is given by Equation (3). We see that  $U_{dil}$  determines the effects of micrometeorology on ground-level concentrations. Substituting Equation (3) in (7) yields:

$$U_{dil} = \frac{u_*}{\left( \frac{f_r}{2} + \frac{(1-f_r)U}{\sigma_v} \sqrt{\frac{\pi}{2}} \right)}, \quad (8)$$

where  $f_r$ , the factor that determines the role of the random component in the horizontal concentration distribution, is computed from Equation (5).

We see in Figure 3 (upper of P19) that values of  $f_r$  based on estimates of  $\sigma_v$  from Equation (6) are much smaller than  $f_r$  based on observed values of  $\sigma_v$  and  $u_*$  when the mean wind speeds are less than 2 m/s. The right panel shows that computed dilution velocities are smaller than those based on observed variables. Furthermore, the estimated dilution velocity continues to decrease as the mean wind goes to zero while the observed values actually increase below a wind speed of 1.5 m/s; near  $U=0$ , the dilution velocity is of the order of 0.1 m/s.

It is clear that to avoid predicting unrealistically high concentrations at low wind speeds, we need to account for the increase in dilution velocity with the decrease in wind speed near zero wind speeds. At this stage, we are not aware of any regulatory models that incorporate any sort of formulation to account for this behavior. Once this behavior is modeled, we still need to evaluate the results from the dispersion model with observations from a field study that focuses on low wind speed conditions.

Another aspect of regulatory modeling that is uncertain is estimating concentrations for averaging times that are much shorter than the nominal 1 hour averaging time used in modeling. These short averaging time concentrations are used in applications related to odour and hazard assessment. We examine the modeling of these concentrations next.

## ODOUR MODELING

The sensation of odour at a location is related to the frequency with which a threshold concentration of the offending contaminant is exceeded. The threshold concentration is associated with an averaging time of a few seconds or minutes, which means that it is necessary to estimate the frequency distribution of concentrations at short time scales to quantify odour impact. Gifford (1959) showed that this frequency distribution can be estimated by modeling the time averaged plume in terms of an instantaneous plume fluctuating about the mean position of the time averaged plume. In a classic paper, Hogstrom (1972) showed how Gifford's (1959) fluctuating plume model could be adapted to estimate odour impact frequencies. However, as acknowledged in the paper (Hogstrom, 1972), there is great deal of uncertainty in modeling the spread of the instantaneous plume, which determines the relevant concentrations. There are other models such as SCIPUFF (Sykes *et al.* 2004) that purport to estimate concentration fluctuations using second-order closure methods. They have undergone limited evaluation, and could be useful if their computational requirements were manageable.

In view of the difficulty with applying models that estimate short averaging time concentrations, most regulatory methods estimate odour impact (Engel *et al.* 1997; Scire *et al.* 2000) by multiplying the time averaged model estimate,  $C_m$ , by a factor,  $f$ :

$$f = \left( \frac{T}{T_s} \right)^p, \quad (9)$$

where  $T_s$  is the time scale for odour impact, taken to be the order of seconds or minutes.  $T$  corresponds to averaging time of the model estimate, usually taken to be 1 hour. The values of the exponent,  $p$ , used in the literature, range from 0.2 to 0.5. Multiplication of the modeled concentration,  $C_m$ , by the factor  $f$  results in a "peak" concentration,  $C_s$ , corresponding to  $T_s$ , which is then compared to the threshold concentration.

Equation (9) is based on results obtained by Hino (1968) using an expression by Ogura (1959) for the plume spread of particles released in a turbulent flow over a time corresponding to the averaging time. Thus, it is based on a model that is conceptually

different from Gifford's fluctuating plume model, and cannot be justified for application to odour problems. However, the idea of multiplying the 1 hour modeled concentration with a factor to obtain a short averaging time concentration is attractive for regulatory applications. We next examine the possibility of retaining this simple idea within a more realistic model for concentration statistics.

## **BASIC CONCEPTS**

Imagine an experiment in which model inputs are kept constant, and instantaneous concentrations are observed at a receptor over an indefinitely long period. Figure 4 (bottom of P19) depicts a plausible time series. This time series can be used to construct sets of concentrations corresponding to different averaging times. Each one of these sets can be used to construct a frequency distribution. The distribution for an averaging time of a few seconds or minutes is relevant to odour impact, and that for an averaging time of 1 hour is relevant for the regulatory model estimate. Because all the concentration sets are derived from the same time series, the arithmetic means are exactly the same.

The basic motivation behind using Equation (9) is to incorporate the fact that the likelihood of observing a "high" concentration increases as the averaging time decreases. But the concept of a peak concentration,  $C_s$ , is not consistent with the observations made in this thought experiment, because the definition of a peak is not clear. Furthermore, comparing this ill defined peak to a threshold concentration is not equivalent to estimating the frequency with which the threshold concentration is exceeded.

We will explore the possibility of relating the ratio of the modeled 1 hour concentration to the threshold concentration as an indicator of this probability. The key to such a relationship is a model for the evolution of the pdf of concentrations as a function of averaging time.



## SIMULATING THE CONCENTRATION TIME SERIES

In a previous paper (Venkatram 2002), we modeled the pdf using a Binomial distribution. We showed that the distribution realistically mimics an exponential distribution at short averaging times, and a normal distribution at long averaging times. However, the distribution depends on intermittency, a parameter that cannot be readily estimated in practical modeling applications. In the analysis here, we will use an empirical approach based on assuming that time averaged concentrations follow a Weibull distribution. This distribution is useful because it can mimic distributions ranging from exponential to Rayleigh depending on the choice of its parameters,  $\alpha$  and  $\beta$ ,

$$f(C) = \alpha\beta(\beta C)^{\alpha-1} e^{-(\beta C)^\alpha}, \quad (10)$$

where  $C$  is the concentration.

To use this distribution we need to relate the mean and variance of the distribution at averaging time,  $T_1$ , to those at another averaging time,  $T_2$ . In view of the previous discussion, we assume that the arithmetic mean of the distribution does not change with averaging time. The arithmetic variances at the two averaging times are related

$$\frac{\sigma_{T_1}^2}{\sigma_{T_2}^2} = \left(\frac{T_2}{T_1}\right)^n. \quad (11)$$

Venkatram (2002) shows that  $n=1$  using a simple model for the concentration time series. This is consistent with the wind tunnel data presented by Aubrun and Leitl (2004).

Equations (10) and (11) can be combined to calculate the parameters of the Weibull distribution at any averaging,  $T$ , given the parameters at a nominal averaging time,  $T_0$ . The next section shows how these equations can be used to provide information relevant to concentrations at short averaging times.

## APPLICATION OF MODEL

Air pollution models are designed to estimate a value that lies in the middle of the distribution of observed concentrations, which suggests that the model estimate,  $C_p$ , corresponds to the median of the possible observations corresponding to the model inputs. If we assume that hourly averaged observations are log-normally distributed about this median (See Venkatram *et al.* 2005), it is reasonable to use the geometric standard deviation,  $s_g$ , of the ratio of observed to model estimated concentrations as a measure of the deviation of the 1 hour averaged concentrations about the geometric mean (also the median). Table 1 (bottom of P21) shows the variation of model performance measures found in some studies. We see that  $s_g$  varies from about 1.5 to 3. In the analysis that follows, we will present results corresponding to this range.

Figure 5 (upper of P20) shows the effects of averaging time on two statistics of the concentration distribution-the median and the standard deviation- for  $s_g = 1.5$ . As expected, the median approaches a small fraction of the model estimate as the averaging time becomes the order of seconds. The median approaches the model estimate when the averaging time is close to a nominal 60 minutes. The standard deviation of the distribution is 20 times the model estimate when the averaging time is 1 s, and is slightly less than 1 when the averaging time is 30 minutes. These results are consistent with our intuitive understanding of the effects of averaging on concentrations: when the averaging is small, we see a lot of concentrations close to zero, but the excursions from the model estimated concentration can be large, as signified by the large value of the standard deviation.

We can interpret these statistics by calculating the probability that the time average concentration,  $\bar{C}^T$ , exceeds a multiple,  $m$ , of the model estimate. Figure 6 (bottom of P20) plots for different values of averaging time and  $s_g = 1.5$ . We see that when the averaging time is 30 minutes, the probability that the observed concentration is more than the 3 times the model estimate is very small. On other hand, at the short averaging times of 1 second and 1 minute, the probability of exceeding a concentration that is 10 times the model estimate is about 1 %. The right panel shows that the shape of the distribution

changes with averaging time. At short averaging times, the distribution is close to exponential, while it becomes more symmetrical for an averaging time of 30 minutes.

To translate these results into a form that is familiar to the modeler who uses the power law of Equation (9), define a threshold concentration as the concentration that is exceeded once during an hour of sampling time. For example, if the averaging time is 1 minute, the threshold is the concentration that is exceeded once during the sixty consecutive 1 minute averages that can be derived from the sampled one hour period.

Figure 7 (upper of P21) indicates that when the averaging time is 1 minute, we expect a concentration that is about 15 times the model estimate to be exceeded once during a 1 hour interval. For an averaging time of 1 second, this peak concentration (defined in a special way) is about 500 times the model estimate. These peak concentrations are a function of 1 hour geometric standard deviation,  $s_g$ , which is a measure of the variation of the 1 hour averaged concentrations. The values of  $s_g$  can be assigned on the basis of experience with evaluating models with observations under varying source and meteorological conditions.

The preceding results allow us to construct rules of thumb, such as the probability that the one minute averaged concentration exceeds five times the modeled one hour concentration is about 5 %. This calculation suggests that one hour averaged concentrations from models such as ISC (EPA, 1995) and AERMOD can be used to examine the odour impact of sources. If odour is considered a problem if a threshold value is exceeded during three minutes of a 60 minute period, the impact of a source can be quantified by simply multiplying the one hour averaged model estimate by a factor of five, and comparing the resulting value with the threshold concentration.

## **DISCUSSION AND CONCLUSIONS**

AERMOD is one of a new generation of regulatory models that are being used in the US, Europe, and Australia. While the model is undoubtedly more scientifically acceptable than the older models, such as ISC, that it has replaced, its application to regulatory issues is not as straightforward as it used to be.

The meteorological inputs required by AERMOD are considerably more complex than those of ISC, and thus cannot be readily interpreted by modelers who are not versed in micrometeorology. More importantly, the inputs are relatively sensitive to the characteristics of the surface over which the model is applied. Thus, one can question the application of meteorological inputs derived from a measurement site with surface characteristics different from the application site. Furthermore, characterizing the surface characteristics of a non-homogeneous site is an ambiguous exercise that does not fit well within a legal regulatory framework. There is a need for a method that can adjust the input files for differences in surface characteristics between the official site and the application site. Luhar *et al.* (2006) have proposed one approach that models the modification of the boundary layer as it flows from one site to another. This approach has been evaluated with data from a field study conducted in Switzerland, but it has not yet gained the empirical support required for regulatory acceptance.

There are several other aspects of regulatory modeling that have not been discussed in this paper, but need attention. One is the effect of building downwash on plume rise and dispersion. A recent paper by Olesen *et al.* (2009) indicates that current regulatory models perform poorly in estimating building effects. As far as we know, none of the models deal with the effects of multiple buildings on plume rise and dispersion. There is need for adequate models for such situations because of the regulatory concern with risks posed by emissions of toxics in urban areas. There are also proposals to locate small power plants (Allison and Lents 2002; Carreras-Sospedra *et al.* 2008) in urban areas to gain efficiency through distributed energy generation. Emissions from these plants are buoyant but occur from stacks that are of the order of 10 m. Current models have not been evaluated for their ability to model such emissions, which are affected by downwash from multiple buildings. Future modeling improvements will also need to address concentrations at scales ranging from scales of few meters to hundreds of kilometers by combining large scale grid models with short range dispersion models, such as AERMOD. Although progress has been made in this area (Stein *et al.* 2007; Isakov *et al.* 2007), there are still unresolved issues related to combining concentrations and the associated chemistry at vastly different scales.

With the introduction of short term NO<sub>2</sub> standards in the US, the issue of conversion of emitted NO to more toxic NO<sub>2</sub> has become important. Current models do have elementary treatment (Hanrahan 1999 a, b) of the conversion, but there is room for improvement. Because most urban emissions of NO<sub>x</sub> originate from automobiles, there is a need for adequate treatment of dispersion of emissions from roads and highways at source-receptor distances of a few meters (Venkatram *et al.* 2008).

After being introduced in 2005, AERMOD has been applied to large number of regulatory problems. The feedback received to date suggests that scientific improvements by themselves are not enough for regulatory application. These improvements have to be embedded in a framework that satisfies the criteria for regulatory acceptance. A standing committee, set up the USEPA, is currently working on ensuring that AERMOD meets these criteria.

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## FIGURES AND TABLES

Figure 1: Comparison of estimated surface velocities with observations from the 10 m level at the Cardington site during 2005. Data correspond only to stable conditions.

Figure 2: Comparison of estimated values of  $\sigma_w$  and  $\sigma_v$  with observed values from Cardington site. Red lines in figures correspond to estimates from Equation (6).

Figure 3: Variation of  $f_r$  and dilution velocity with mean wind speed. The red lines are based on estimates of  $\sigma_v$  from Equation (6).

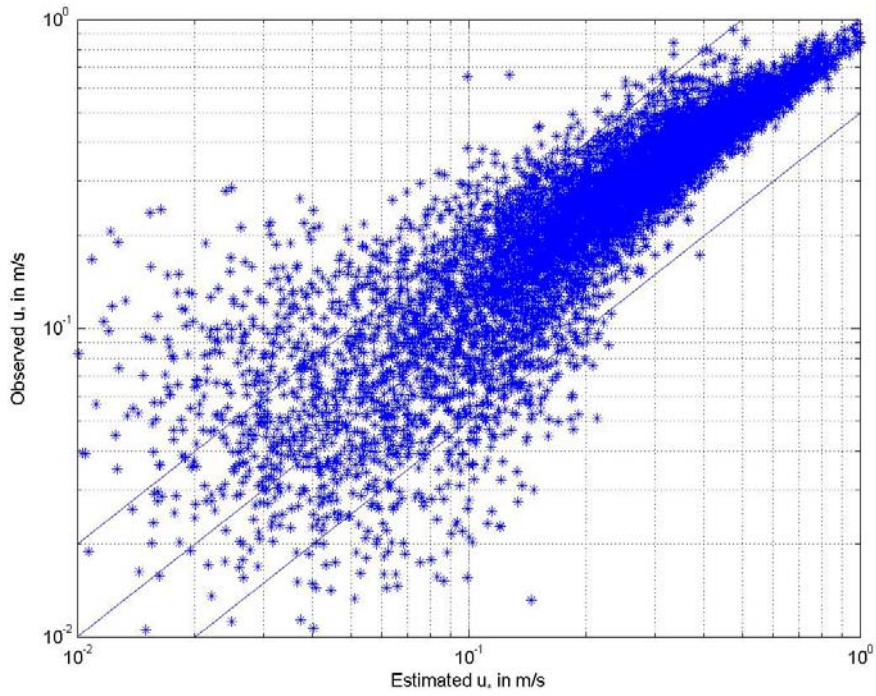
Figure 4: Time series of instantaneous concentrations.

Figure 5: The left panel shows the median as a function of averaging time. The right panel shows the standard deviation as a function of averaging time.

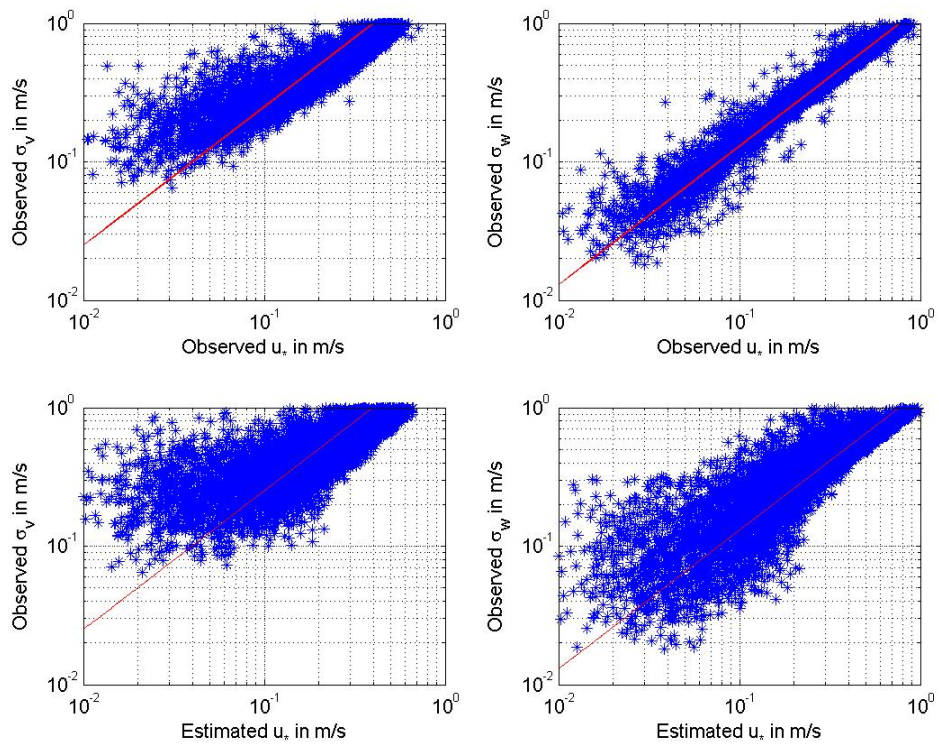
Figure 6: The left panel shows Equation (4) as a function of averaging time. The right panel shows the corresponding histograms.

Figure 7: Peak/model estimate as a function of averaging time.

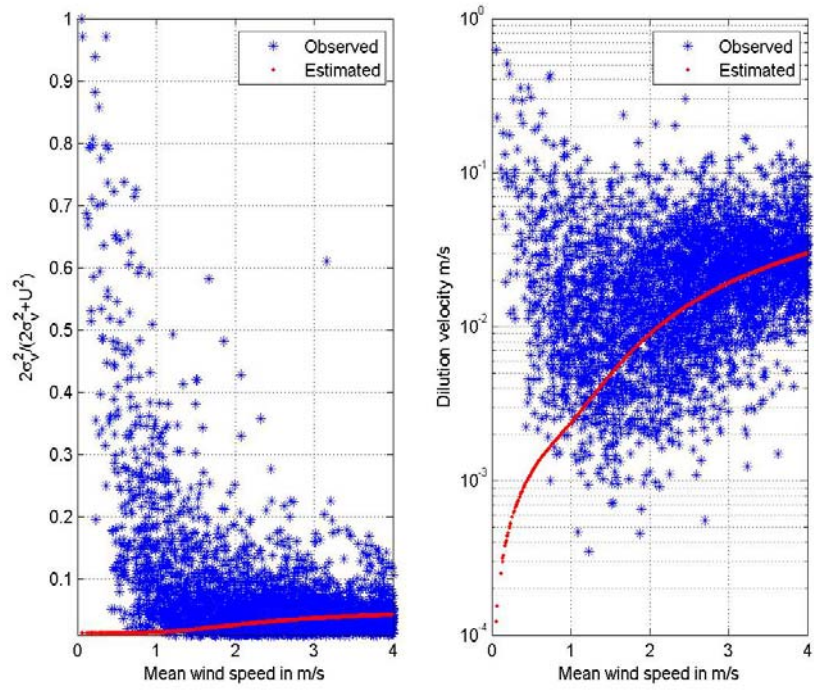
Table 1: Performance statistics from selected studies.



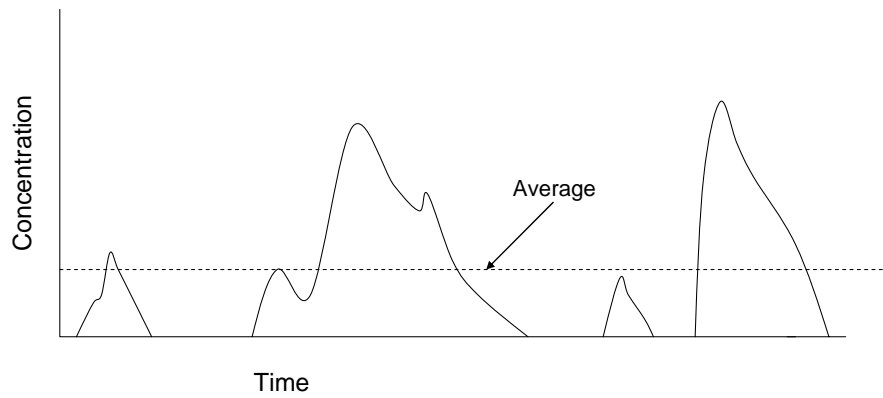
**Figure 1 (Venkatram)**



**Figure 2 (Venkatram)**



**Figure 3 (Venkatram)**



**Figure 4 (Venkatram)**

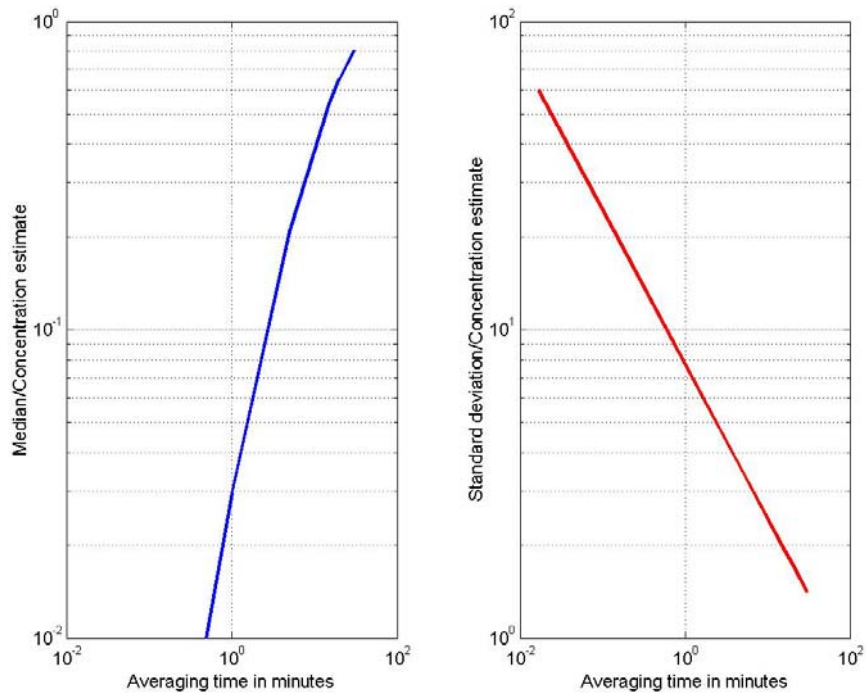


Figure 5 (Venkatram)

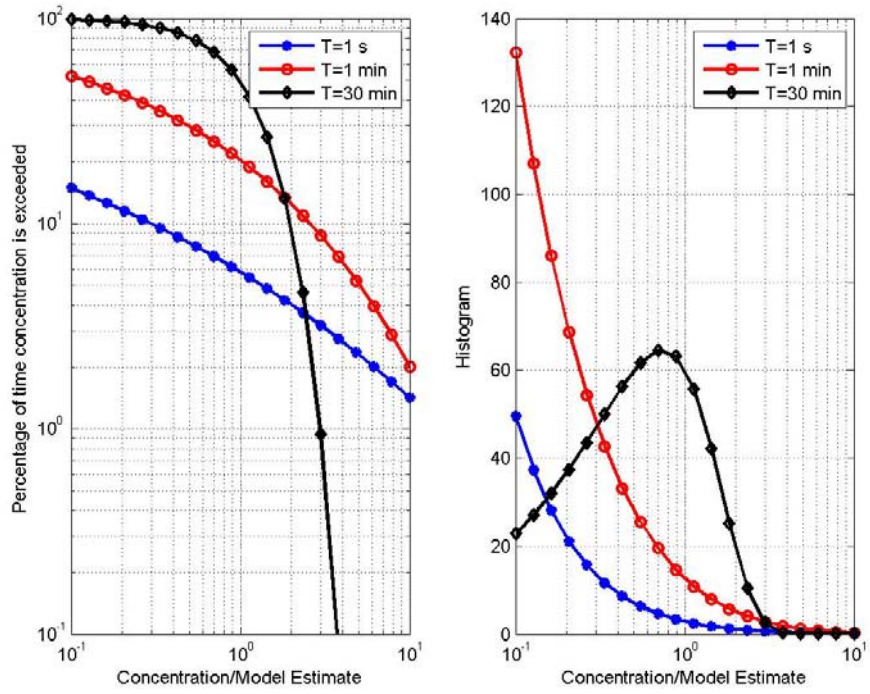


Figure 6 (Venkatram)

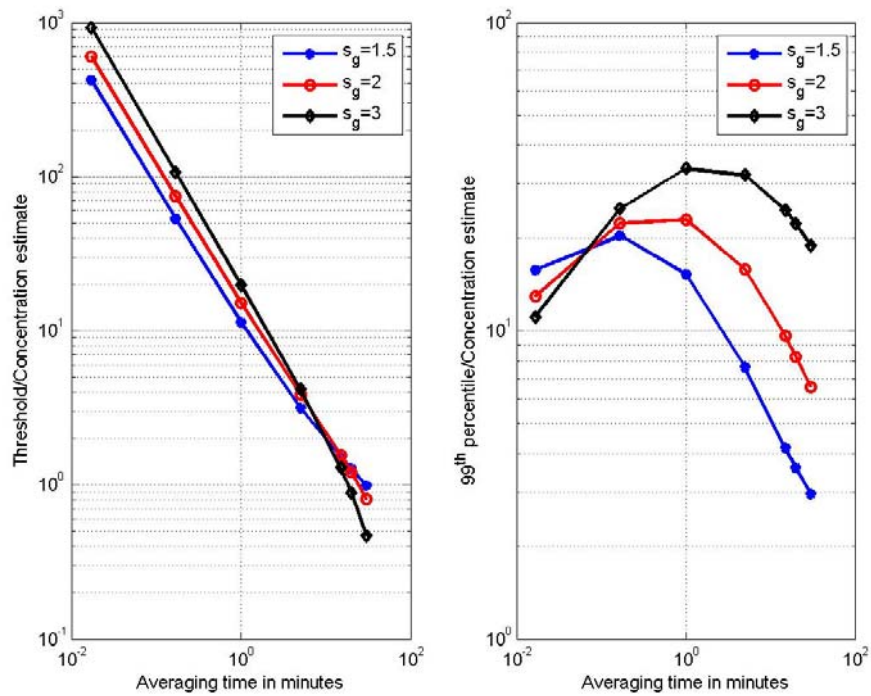


Figure 7 (Venkatram)

Field Study	Type of Source		Receptor Locations	$m_g$		$s_g$	References
Wilmington, CA 2004	surface release	release behind power plant	100, 400, 1000, 3000, 5000m arcs	0.92		1.71	Yuan <i>et al.</i> 2006
		release in open area		0.86		2.68	
Barrio Logan, CA 2001	surface release		200, 500, 1000, 2000m arcs	1.12		2.27	Venkatram <i>et al.</i> 2005
St. Louis, Missouri 1963-1965	near ground level	800m – 16km arcs	Briggs formulae	day	1.17	2.85	Venkatram 2005
				evening	0.92	2.02	
			Barrio Logan model	day	1.06	2.22	
				evening	0.97	1.87	

Table 1 (Venkatram)