DISPERSION MODELING OF PARTICULATE MATTER FROM GROUND-LEVEL AREA SOURCES

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Abstract

The new National Ambient Air Quality Standards (NAAQS) for particulate matter less than 2.5 µm in diameter ($PM_{2.5}$) and ozone will increase the number of nonattainment areas in the United States. Since a facility is responsible for *all* PM emissions originating from that property, an increased emphasis will be placed on the regulation of fugitive PM sources, as well. Dispersion modeling is often used by State Air Pollution Regulatory Agencies (SAPRA's) in determining whether the contribution of particulate matter from a facility meets the NAAQS. As such, a facility may be granted or denied an operating permit based on the results obtained from a dispersion model. However, the model currently approved by EPA over-predicts downwind concentrations of PM by as much as ten fold. This results in the possibility that a facility is denied a permit when, in fact, its emissions are well within the NAAQS. Dispersion models that provide accurate estimations of downwind concentrations of pollutant from these fugitive sources are needed to ensure reliable and fair regulation of pollutant sources. The presently accepted Gaussian-based models use dispersion profiles that do not accurately describe dispersion of pollutants from ground-level sources and inaccurately apply time averages to calculated concentrations. A new model, the Fritz-Meister Model, is being developed that contains a dispersion profile in the vertical plane that more accurately reflects dispersion from ground-level releases. The new model also applies a new area integration algorithm and uses a shorter time increment to allow for variation in wind direction and velocity. The result is a model that more accurately predicts concentrations downwind of ground-level sources and gives the modeler a greater degree of flexibility when modeling different pollutant types.

Introduction

The purpose of State Air Pollution Regulatory Agencies (SAPRAs) is to ensure the safety of the public. This is accomplished through the regulation of sources that emit airborne pollutants. Regulated pollutants are those established as criteria pollutants by the United States Environmental Protection Agency (US EPA). These criteria pollutants include particulate matter less than 10 µm in diameter (PM_{10}), particulate matter less than 2.5 µm in diameter ($PM_{2.5}$), sulfur dioxide (SO_2), nitrogen dioxide (NO_2), carbon monoxide (CO), and particulate lead. Criteria pollutants are regulated based on set acceptable ambient concentration levels as defined by the National Ambient Air Quality Standards (NAAQS). They are termed as criteria pollutants as a result of being set based on health-based criteria. The acceptable ambient concentration levels set by the NAAQS are used to determine if an area is in attainment or non-attainment. If an area is classified as non-attainment, all permitted sources within that area must reduce their allowable emissions in an effort to reduce the ambient levels. One of the tools used by SAPRA engineers to determine the impact of pollutant emissions from an individual source on the ambient level is dispersion modeling.

The SAPRAs must determine whether or not the release of a pollutant from a source, regardless of the area's attainment status, results in public exposure to pollutant concentrations in excess of the NAAQS. Dispersion modeling is a mathematical tool that allows for estimates of downwind concentrations of pollutants to be made based on the source emission rate and the meteorological conditions. Based on estimates from dispersion modeling, a source may be required to provide additional controls to further reduce pollutant emission rates, thus reducing public exposure levels.

The use of dispersion modeling in the regulatory process is increasing. SAPRAs utilizing these modeling tools are required to use models that are approved by the US EPA. One of the dispersion models approved by the EPA for regulatory use is Industrial Source Complex (ISC) which is based upon the concept of Gaussian dispersion. The current ISC models being used by SAPRAs are: ISC-ST3 (short term 3rd update) and ISC-SCREEN3 which is a simple version of ISC-ST3 with imbedded meteorological data.

These models apply the Gaussian equation and related dispersion parameters incorrectly. A one hour concentration prediction is determined using one hour averaged meteorological data. This process incorporates the assumption of a constant wind speed and wind direction throughout the entire one-hour time period. This implies that during a one hour time frame, there is no variation in the wind direction or speed. This in turn implies that pollutant released from a source is carried directly from that source to the receptor, and in no other direction. The result is an estimated concentration at the receptor that is significantly higher than if the wind direction and speed variation over the hour had been accounted for. This procedure for estimating downwind concentrations is inappropriate. The use of smaller time average meteorological data into the modeling algorithm will account for changes in downwind concentration due to wind speed and direction variation.

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For ground-level sources of pollutant, the vertical dispersion profile used by the Gaussian equation to model pollutant dispersion, may not be the most accurate representation of natural pollutant behavior. The vertical distribution, as described by Gaussian models, disperses half of the pollutant into the ground and "reflects" it back into the plume. This reflection of pollutant results in a distribution with a "spike" at or near ground-level (Figure 1). As a result, concentration estimates, at or near ground-level, have the potential of being excessively high. The incorporation of new distribution whose vertical profile is entirely above ground level will be a step towards improving the model's representation of natural dispersion. One such distribution is the triangular distribution. The triangular distribution has the advantage of having three separate independent indices which can be used to vary the distribution's profile characteristics.

Sources regulated based on models that may potentially over-estimate the downwind concentration are subject to unfair and unnecessary financial pressure. A source can potentially be required to install additional, expensive control devices as a result of inappropriately estimated downwind concentrations. The goal of this research is to provide a model for use by the regulatory agencies that accurately estimates downwind concentrations and provides a fair basis for regulation of pollutant sources.

Discussion

The Gaussian Dispersion Model

Equation 1 is used to calculate the ambient downwind concentration associated with Gaussian dispersion from a pollutant source (Cooper and Alley, 1994):

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

where

C = steady state concentration (µg/m³),
Q = emission rate (µg/s),
π = 3.141593,
u = wind speed at stack height(m/s),
σ_y = lateral dispersion parameter (m),
σ_z = vertical dispersion parameter (m),
z = receptor height above ground (m),
H = plume centerline height (m).

Figure 2 illustrates the horizontal and vertical dispersion of pollutants from a source (Turner, 1994). The basis for the Gaussian model are two density functions (equations 2 and 3) that approximate dispersion of pollutants in these two planes.

$$f(y) = \frac{1}{\sigma_y \sqrt{2\pi}} \exp\left(-\frac{y^2}{2\sigma_y^2}\right) \quad \text{(Eq. 2)}$$

$$f(z) = \frac{1}{\sigma_z \sqrt{2\pi}} \left\{\exp\left(-\frac{(z-H)^2}{2\sigma_z^2}\right) + \exp\left(-\frac{(z+H)^2}{2\sigma_z^2}\right)\right\} \quad \text{(Eq. 3)}$$

The second term in equation 3, $(z+H)^2$, takes into account eddy reflection. The division of the emission rate by the wind speed results in units of [MASS/LENGTH] . This value is multiplied by the two normal density functions, one for the horizontal direction, and one for the vertical direction. The product of the two density terms has units of [1/AREA]. The overall product is a concentration with units of [MASS/VOLUME].

Associated with the Gaussian model and all dispersion models based upon the Gaussian model are the following assumptions (Turner, 1994):

- Continuous Emissions - The emission rate of pollutant does not vary over time.
- Conservation of Mass - During transport, no pollutant is lost due to chemical reaction, settling, or turbulent impaction.
- Steady-State Conditions - Meteorological conditions remain constant over the time of transport.
- Crosswind and Vertical Concentration Distributions - Both concentration distributions are assumed to be well represented by a Gaussian, or normal, distribution at any distance downwind or any distance in the crosswind directions.

It is obvious that there are cases where some or all of these assumptions do not hold. "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." (Veigele and Head, 1978) 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.

Purpose of New Model

The overall purpose of developing a new air dispersion model is to provide a method that can be used to accurately predict concentrations of pollutants downwind from ground-level area sources.

More specifically:

- To develop a more appropriate dispersion model for ground-level area sources.
- To develop a dispersion model that has the potential to accurately predict downwind concentrations of different pollutants with

varying physical characteristics, e.g. odors and heavy PM.
- To develop a dispersion model that models only the portion of the area source that contributes to a downwind receptor.
- To provide a regulatory tool that can be used to accurately determine emission factors from measurements of downwind concentrations.

New Ground-Level Model Methodology

The major difference of the proposed new model relative to ISC is an alteration of the distribution used in the vertical plane. To improve performance for use with ground-level area sources the normal distribution in the vertical plane was replaced with a triangular distribution with indices that can be adjusted based on pollutant characteristics. Figure 3 shows the difference between the two distributions. The proposed new model also differs from ISC in the manner in which an area source contributes to a stationary receptor downwind. By breaking up an area source into a grid of equal sized point sources, the model determines the contribution of each unit to the total concentration measured by a receptor downwind of the source and calculates an emission rate based only on the amount each unit contributes. This algorithm is a function of wind speed and direction. The Gaussian calculation approach is used, but the concentration calculated by the equation uses the wind speed and wind direction for a 2 minute period, and is thus a 2 minute concentration. Zwicke, et al. (1999) published validation study results for modeling elevated point sources using concentrations that were measured at known downwind distances from a source with controlled emission rates.

Distribution in the Vertical Plane

The Gaussian model utilizes a normal distribution in the vertical plane. The new model will replace this normal distribution with a distribution whose vertical concentration profile is completely above ground. The proposed distribution to be used to replace the normal is the triangular distribution. Figure 3 illustrates how the triangular distribution is completely above ground, compared to the normal distribution. Note that the heavy dashed line is the vertical distribution after reflection and addition of the bottom half of the normal curve into the upper half of the curve.

Like the normal distribution, the triangular distribution can be mathematically represented by probability density functions. Figure 4 (Pritsker, 1979) is a graphical representation of the triangular distribution and the indices associated with it. Unlike the normal distribution, the triangular distribution allows for modification of the height of maximum concentration within the plume, and the height of the plume. The triangular distribution has three different indices that must be assigned values. By setting each of these indices, the size and shape of the plume is defined.

Equations 4 and 5 give the probability density function for vertical dispersion represented by a triangular distribution (Pritsker, 1979):

$$f(z) = \frac{2(z-A)}{(M-A)(B-A)} \rightarrow A \le z \le M \qquad \text{(Eq. 4)}$$

$$f(z) = \frac{2(B-z)}{(B-M)(B-A)} \rightarrow M \le z \le B \qquad \text{(Eq. 5)}$$

Index A is set at ground-level, or 0 meters, in the proposed new model. We have chosen the other two indices, B and M, to be linear functions of σ_z. This approach allows the use of existing science associated with the currently used Gaussian model can be used. The use of sigma z in the triangular distribution will allow for an accounting of changes in the vertical concentration profile as a function of stability class and distance downwind. Another benefit to using these parameters, is that they are accepted and being used by present dispersion models. Indices B and M have the ability to be varied independently of one another, this results in numerous possible vertical concentration profiles. This approach provides an added flexibility in adjusting the vertical dispersion rate to more accurately estimate downwind concentrations that will vary with physical characteristics of different pollutants.

The new model is derived by replacing the probability density function in the vertical plane with a new distribution. Mathematically, when the normal distribution in the vertical plane (Equation 3) is replaced by the a triangular distribution (Equations 4 and 5), the new model takes on the form of Equation 6.

$$C = \frac{Q}{U} * fy * fz \qquad \text{(Eq. 6)}$$

where:

fy is Equation 2; and
fz is Equations 4 and 5.

Figure 5 is the proposed method of setting the indices of the triangular distribution. B and M are both linear functions of sigma z, where K and L are scalar multipliers of sigma z. A is set at a constant 0 meters (ground level). Since the model assumes that no settling occurs, the total mass of particulate in the plume at the point of release equals the total mass in the plume at any point downwind. If a low value for K is used (a short plume), the mass of the particulate will be confined to a small area, resulting in the prediction of a high concentration. Conversely, if K is increased (resulting in a greater plume height), there exists a greater area in which the same amount of mass can be distributed. Thus, increasing K results in the prediction of a lower concentration.

The triangular distribution also has a unique advantage over the normal distribution, a variable height of maximum concentration. This is index M in Figure 5. The reflected normal probability density function in the vertical plane for a ground-level release results in a maximum concentration at, or near, ground-level regardless of downwind distance. In contrast, with index M being a linear function of sigma z, the height within the plume at which the maximum concentration occurs increases as the downwind distance increases.

A major component of this research is to determine the scalar multipliers, K and L, for the indices, B and M. The key to setting these indices is the ability to correlate the plume height and the maximum concentration height to the stability class and the downwind distance from the source. One of the initial methods proposed to accomplish this was to obtain plume profiling sampling data as related to source emission rate, downwind distance, and recorded meteorological data. The difficulty was in locating this information. No small scale plume profiling data was to be found. There were several sources containing information on single point sampling downwind from sources. The problem common to all of these was the lack of credible area source emission rates. The emission factors or emission rates available in literature were determined by a process of measuring downwind concentrations from a source and using dispersion modeling to back-calculate the emission rate. If the dispersion model inaccurately calculates downwind concentrations as we have determined, the use of these models to determine emission factors would also be in error.

There are three key components needed for dispersion model validation and testing. These are: accurate, controlled emission rates; appropriate meteorological data in 2 minute intervals; and measured downwind concentration at known sampler locations. The Department of Agricultural Engineering, Texas A&M University is in the process of obtaining validation data for this new model. Obtaining validation data for a new model is not a simple process. To illustrate the utility of a new model for predicting downwind concentrations from ground level area sources using a combination normal (horizontal plane) and triangular (vertical plane), several values for B and M were assumed. Equations 7 and 8 were used to determine the B and M values.

$$B = F\sigma_z \qquad \text{(Eq. 7)}$$

where, F is a scalar.

$$M = L\,B \qquad \text{(Eq. 8)}$$

where, L is a scalar.

The flexibility of the triangular distribution is illustrated in Figures 6 and 7. It was assumed that the value of B would never exceed $6\sigma_z$ since this should encompass 98% of the plume. Given a situation of a relatively heavy particulate, the height of the point of maximum concentration may be determined to be M = 0.1B (see Figure 6). Notice that, as B was increased from $2\sigma_z$ to $6\sigma_z$, the predicted downwind concentrations decreased. This result corroborates our assertions that as plume height increases, dispersion increases. Note, also, the performance of ISC's reflected "double normal" model. Figure 7 illustrates how we expected relatively lighter PM to behave. Setting our point of maximum concentration at M = 0.25B, we find that the predicted downwind concentrations were lower than those obtained with M = 0.1B (Figure 6). This illustrates that if the pollutant is lighter the slope of M will be greater and thus, the pollutant will disperse faster. Note that ISC predicted the same downwind concentrations no matter what the physical properties of the pollutant were.

The triangular distribution in the vertical, in the form declared above may not be the best representation of actual plume dispersion. However, we are convinced that it is an improvement over the use of ISC for ground level sources. This model is a first estimate of the vertical profile of a dispersion model that can be used to more accurately estimate downwind concentrations from ground level area sources. We are in the process of obtaining data that can be used to validate this model or to provide insight as to a more appropriate vertical distribution profile.

Effective Area

In order to accurately predict downwind concentrations from ground level fugitive sources, a modeler must have accurate data on the emission rate (emission factors). This requirement has presented problems in this research. From past experience, we have learned that the emission factors published by EPA in AP-42 are usually not accurate. It is likely that this is a consequence of using inaccurate dispersion models (such as ISC) along with accurate measurements of downwind concentrations to calculate Q in Equation 1. An alternative approach to determining emission factors from ground level area sources is to use the box model. With the box model, one may assume that the measured concentration at one point on the downwind edge of the field is constant throughout the box, the velocity through the box is constant during the sampling period and calculate the emission rate. The difficulty with this approach is that these assumptions do not hold. Additionally, the emission rate if the entire field is assumed to contribute to the measured concentration of the stationary sampler, which is intuitively incorrect.

Another, more accurate way of dealing with emissions from an area source is to model that area as a collection of equally-sized point sources and integrate, or sum, those individual point sources. So, for an area source, the edge closest to the receptor will have the least sensitivity (Figure 8). As you back deeper into the area towards the edge most distant from the receptor, the sensitivity of the concentration estimate to the variation in wind direction increases and the distance to the receptor increases, giving the pollutant more opportunity to disperse before it reaches the receptor. Another aspect is the impact of downwind distance, whether it be directly from source to sampler, or an X offset distance resulting from off prime wind direction. As the distance, X, increases, the predicted concentration decreases. This distance, X, increases from front of area to back of area, and from left to right of point in the perpendicular direction of the receptor. In either of these instances, there will be some distance downwind, depending on wind speed, emission rate, and wind direction variation, where the contribution to predicted concentration at the receptor will be extremely small if not zero. Therefore, some portion of the area source both upwind and crosswind, exists such that emissions outside of that area will not contribute to the concentration at the receptor. This was termed the "effective area" (Figure 9).

The size of this effective area depends on several parameters. The two most important of these parameters are the downwind distance and stability class. As the downwind distance increases, the effective area increases. Note, that even though the effective area increases, the predicted concentration decreases. As the distance between the source and receptor increases, the Y offset distance for the most distant points in the crosswind direction decreases.

These concepts are best illustrated in Figures 10 and 11. Given a receptor located 50 meters directly downwind of an area source and atmospheric stability class F (Class F is the most stable atmospheric conditions, usually found with very low wind speed and nighttime or overcast conditions), we see that the portion of the area source contributing most to the receptor is that portion located at the center edge of the area closest to the receptor (Figure 10). The most important illustration here is that as we travel away from the field's edge, the contribution relative to the rest of the area source decreases, because the pollutant has a greater distance to travel to reach the receptor and, thus, has dispersed more. Figure 11 illustrates the same conditions, but now the receptor is located 1000 meters downwind. Note that because of variations in wind direction, more of the area source is now contributing to the receptor. However, even at 1000 meters, the receptor is still not measuring contributions from the entire area. This demonstrates how modeling an area by integrating the contribution of PM from a collection of point sources may yield a more accurate emission rate than assuming the entire area contributes equally to the concentration at a stationary receptor.

Time Averaging

Knowing that the Gaussian dispersion model was derived specifically for steady state meteorological conditions, the conclusion can be drawn that this model is time independent. The only parameter that determines what time-average the modeled concentrations represent is the time period for which steady-state meteorological conditions exist.

The values of the σ_y and σ_z dispersion parameters are functions of meteorological stability class and downwind distance. Their function in the model is to define the horizontal and vertical boundaries of the plume at any point downwind. When these values are reported in literature, they are grouped according to stability class, which is based on the wind speed and incoming solar radiation. It is believed that when Pasquill (1961) originally formulated these values, he correlated the plume size to the wind speed. In other words, the use of the sigmas does not take into account significant variation in the wind direction, but are based on a time period of constant wind speed and wind direction. The size of the plume is, therefore, based on the atmospheric stability, as determined by the wind speed and incoming solar radiation. The application of the sigmas (σ_y and σ_z) in the new model should consist of utilizing these values in the dispersion model equation for small meteorological time increments (one to two minutes). This application is intended to ensure that the model predictions of downwind concentrations are for time periods when the meteorological conditions are constant.

Even within a small time period, such as ten minutes, the wind speed and more importantly, the wind direction does not remain constant. The stability classes and thus, the dispersion parameters, are grouped according to wind speed ranges and not according to wind direction variations. The result is that, in the present applications of the model, there is no method to account for changes in predicted downwind concentrations due to wind direction variations for periods of less than one hour. Another difficulty is that most weather data available to SAPRA modelers is reported as one-hour averages. Thus, even with a dispersion model that utilizes two-minute data, modelers have no choice but to model a source using one-hour averages. SAPRAs are in the process of revising their recording of meteorological data. In the state of Texas, for example, weather data is now being reported as one-hour averages of wind speed and direction, but includes their standard deviations. This is a significant step forward in that SAPRAs may now account for meteorological variation while maintaining the one-hour format.

Conclusions

The Fritz-Meister Model is a new approach to dispersion modeling. The use of small increment time averaging (2 minute time periods instead of 1 hour) results in concentration estimates that are based on dispersion parameters consistent with Pasquill's original work. This results in concentrations that are more representative and accurate. Another major step toward developing a dispersion model that more accurately represents actual conditions, is changing the distribution associated with the vertical plane. The normal distribution, with reflection, in the vertical plane, which produced a profile with a spike at ground level, was removed. This was replaced with a triangular distribution whose indices represent the plume height and the height of maximum concentration. Both indices increase as a function of sigma z, which signifies that the maximum concentration of the plume does not remain in height at ground-level, but increases as the distance downwind increases. The present values associated with this triangular distribution were set based on the only available sampling data that had known emission rates, measured downwind concentrations, and meteorological data recorded in two minute increments. Unfortunately, this source was a 10 meter stack source. Even so, the use of this sample data allowed development of a logical method to take a first cut at setting the indices of the triangular distribution.

This model is a step toward a more improved model. It provides the framework for a more robust model that can be adapted to predict dispersion of various pollutants ranging from particulate matter to gases and odors. It should also be realized that the ISC-ST3 area algorithm has not been validated. The comparison of the two models is only for the purpose of relating how one model performs compared to the other. Generally, The FM-GL model predicts higher concentrations closer to the source than does ISC-ST3, and predicts about the same, or lower, concentrations that ISC-ST3 at locations farther away from the source. This is because the triangular distribution allows for an increase in the height of maximum concentration, with increased downward distance whereas, the normal distribution always has its highest concentration at ground-level.

The science of dispersion modeling has remained relatively unchanged over the past several decades. The Gaussian dispersion equation and the stability classes and dispersion parameters developed by Pasquill have continued to be used from their inception to the present time. The application of a one hour time period to the Gaussian dispersion equation is still being used instead of the more commonly accepted 10 minute period for which the parameters were developed, because the original introduction of dispersion modeling into the regulatory process used the one hour period. Tradition is a hard barrier to overcome. The Fritz-Meister Ground-Level dispersion model in its present form is an attempt to take a step toward developing and validating a more accurate dispersion model for regulatory use.

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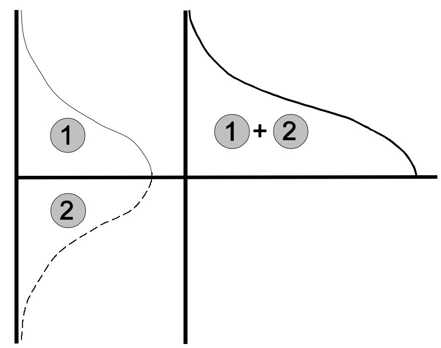

Figure 1. Mathematical reflection of normal distribution from a ground level source.

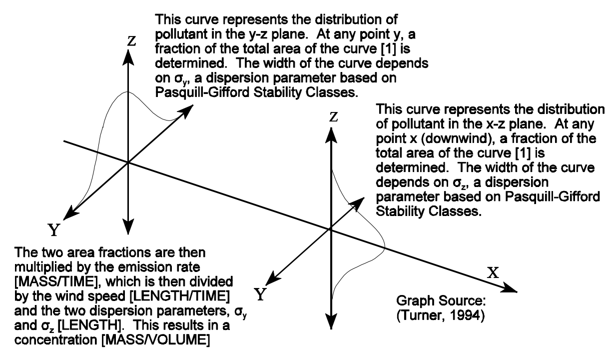

Figure 2. The Gaussian Model.

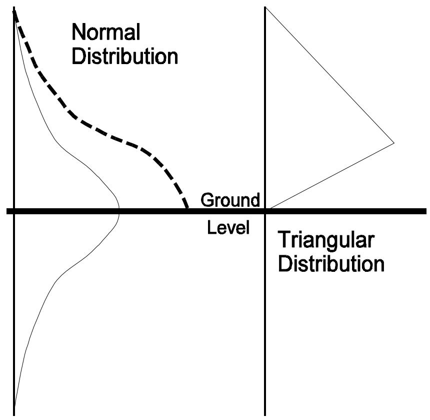

Figure 3. Distributions in the vertical plane: Reflected Normal vs. Triangular.

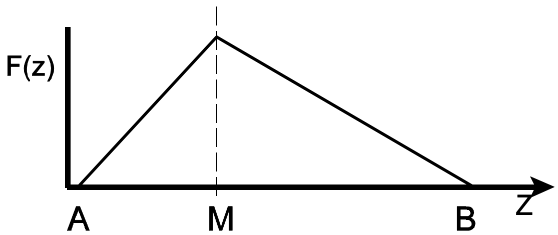

Figure 4. The triangular distribution (Pritsker 1979).

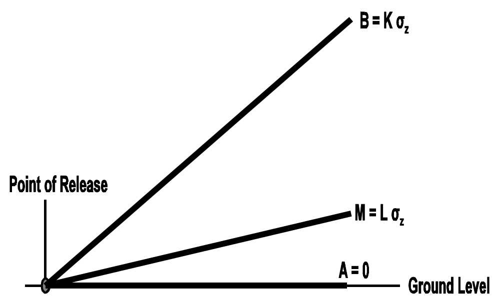

Figure 5. Indices of the triangular distribution.

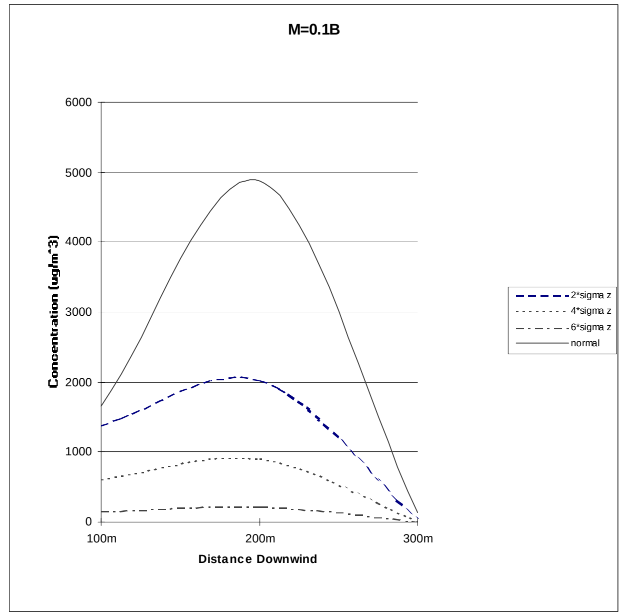

Figure 6. Model performance results illustrating versatility, compared with ISC.

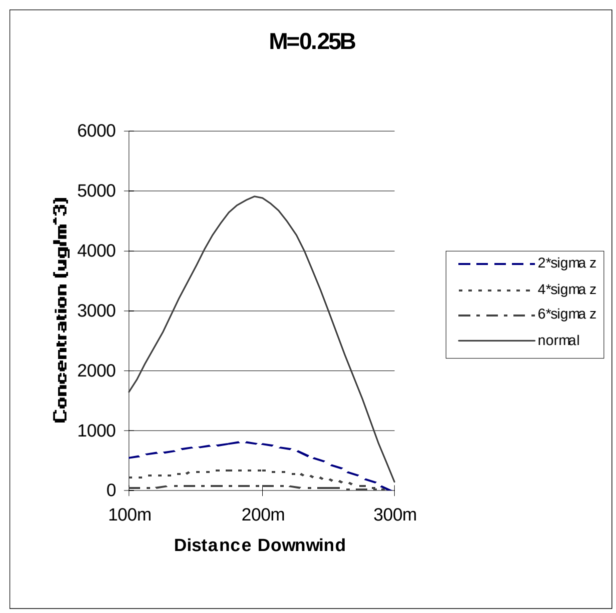

Figure 7. Model performance results illustrating versatility, compared with ISC.

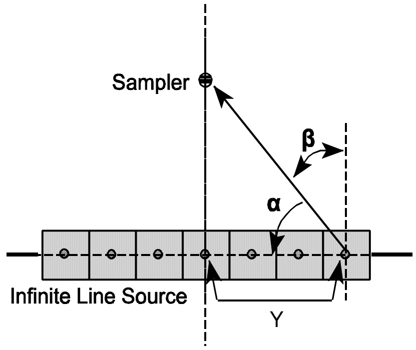

Figure 8. Contribution of individual point source to receptor.

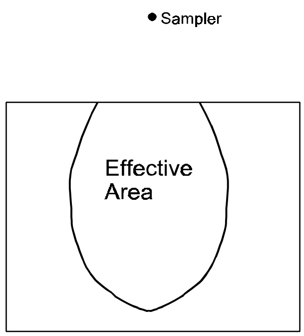

Figure 9. Illustration of effective area

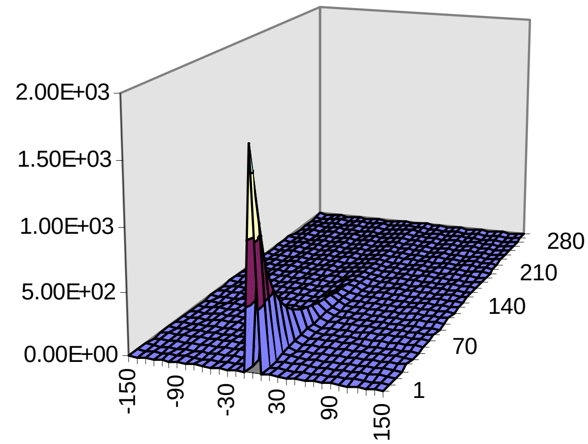

Figure 10. Relative contribution of area source to receptor located 50 m downwind (Stability Class F).

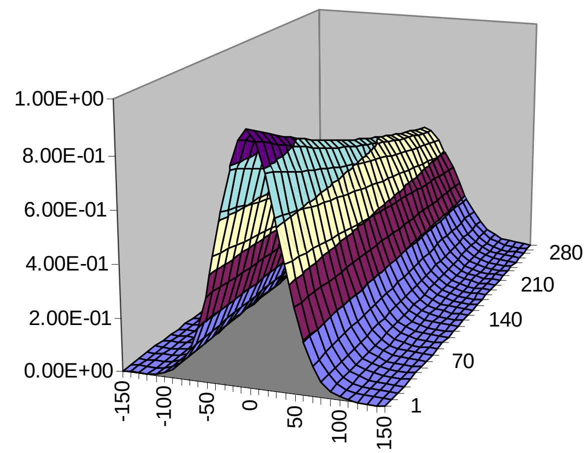

Figure 11. Relative contribution of area source to receptor located 1000 m downwind (Stability Class F).