An Approach to Developing Air Quality Models for Regulatory Applications

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Introduction

Studies indicate that models that incorporate current understanding of micrometeorology and dispersion generally provide better estimates of observed concentrations than older models based on empirical Pasquill-Gifford dispersion curves. However, improvements in model performance are not always apparent because of large deviations between model estimates and observations. Hanna et al. (1999) show that the geometric standard deviations of the ratios of the model estimated to the observed concentrations, derived from several field studies, for two of the most recently developed models are close to 2.5. It is clear that such large deviations between model estimates and observations are unavoidable, and thus need to be accounted for in both judging model performance and in applying them. Under these circumstances, it is useful to make the assumption that errors in model inputs are unavoidable, and that these errors are the major contributors to the deviations between model estimates and observations. Then, if a model is adequate, it should reproduce the distribution of observations as long as the range of model inputs is similar to that of the observations. The distribution of concentrations provides enough information for regulatory questions such as: What is the probability that a certain concentration is exceeded?

In estimating the distribution of concentrations, we can assume that a chosen receptor is affected by the source and then estimate concentrations for a range of meteorological conditions. As a first approximation, we can take this range of meteorological conditions to correspond to that at the source. Since we are not trying to estimate the concentration at a precise time, this assumption is reasonable. The model used to estimate the concentration at the receptor can be simple because it can focus on estimating the magnitudes of possible concentrations rather than concentrations at specific locations and times. We can than construct the simplest possible model, and see whether it works by comparing the estimated distribution with the observed distribution of concentrations. It is clear that the validity of such a model is critically dependent on evaluation of model results with a range of data sets. The next section describes the application of this approach to the development of a model for dispersion in complex terrain.

Complex Terrain Model

The complex terrain model described here is a modified version of that incorporated into the AMS/EPA Regulatory Model (AERMOD; Cimorelli, et al., 1996; Paine et al., 1998). The model is essentially an interpolation of knowledge of flow and dispersion in complex terrain in two asymptotic states. Under very stable conditions, the flow and hence the plume embedded in it, tends to remain horizontal when it encounters an obstacle. Under unstable conditions, the plume is more likely to climb over the obstacle. Thus, the very stable and very unstable conditions represent the two asymptotic states.

Under unstable conditions, the plume is depressed towards the surface of the obstacle as it goes over it. The implied compression of streamlines is associated with speed-up of the flow and amplification of vertical turbulence. These and other effects are accounted for in models such as the

Complex Terrain Dispersion Model (CTDMPLUS, Perry 1992) that attempt to provide accurate concentration estimates for plumes dispersing in complex terrain.

AERMOD uses a much simpler approach because the objective is to estimate the frequency distribution of possible concentrations. It assumes that the concentration at a receptor, located at a position (x,y,z), is a weighted combination of two concentration estimates: one assumes that the plume is horizontal, and the other assumes that the plume climbs over the hill. The concentrations associated with the horizontal plume dominate during stable conditions, while that caused by the terrain-following plume are more important during unstable conditions. These assumptions allow us to write the concentration, $C(x,y,z)$, as

$$C(x,y,z) = fC_f(x,y,z) + (1-f)C_f(x,y,z_e) \tag{1}$$

The first term on the right-hand side of Equation (1) represents the contribution of the horizontal plume, while the second term is the contribution of the terrain-following plume. The weighting factor, f, is discussed in the next section.

The concentration, $C_f(x,y,z)$, is that associated with a plume unaffected by the terrain: the plume axis remains horizontal. Thus, $C_f(x,y,z)$ is evaluated at the receptor height, z, to simulate a horizontal plume. In the second term, the concentration is evaluated at an effective height, z_e, given by

$$z_e = (z - z_h), \tag{2}$$

which assumes that the plume climbs over the hill. Here, z_h represents the height of the terrain at (x,y), so that $(z-z_h)$ represents the height of the receptor above local terrain.

The Weighting Factor f

The formulation of the weighting factor, f, uses the concept of the dividing streamline height, H_c. Consider a receptor at height z embedded in stably stratified flow. Then, if we neglect drag forces on a parcel moving upwards, we can use simple energy arguments to show that there is a height, H_c, below which the fluid does not have enough kinetic energy to overcome the potential energy difference between the initial height of the parcel and the receptor height z (Snyder et al., 1985). Although the concept of dividing streamline height is based on an idealized scenario, towing tank experiments by Snyder et al.(1985) indicate that it can usefully characterize flow of a stably stratified fluid around a three-dimensional obstacle. This leads to the tentative assumption that f is a function of the fraction, ϕ, of the plume that is below H_c,

$$\phi = \frac{\int_0^{H_c} C_f(x,y,z)\,\mathrm{d}z}{\int_0^{\infty} C_f(x,y,z)\,\mathrm{d}z} \tag{3}$$

This fraction goes to zero under unstable conditions because H_c is zero. The weight, f, is taken to be

$$f = \tfrac{1}{2}(1+\phi). \tag{4}$$

When ϕ goes to unity, the entire plume lies below H_c, and f goes to unity. Under these conditions, the hill concentrations are entirely determined by the horizontal plume. When ϕ goes to zero under unstable conditions, f becomes $1/2$. Thus, under unstable conditions, the concentration at an elevated receptor is the average of the contributions from the horizontal plume and the terrain-following plume.

In a region with a number of irregular hills, the dividing streamline height, H_c, is not likely to describe the two-layer flow seen around a simple isolated hill in a laboratory (Snyder et al., 1985). However, we can apply the underlying concepts to real terrain by assuming that the plume can potentially affect the receptor if the flow can carry the plume over a vertical distance, H, equal to the local terrain height, z_h, plus the effective plume height, h_e,

$$H = z_h + h_e . \tag{5}$$

Then, H_c, is calculated relative to $z=H$.

Because the focus of this paper is a model for dispersion in complex terrain, we do not describe the model used to estimate concentrations in the absence of the hill. Details of this model and its performance against observations are provided elsewhere (Cimorelli et al., 1996, Paine et al., 1998). The next section describes the evaluation of the simple complex terrain model with concentration observations made around sources in four different complex terrain sites.

Model Evaluation

As indicated in the last section, we will evaluate the performance of the complex terrain model by comparing the estimated distribution of concentrations with the observed distribution. These distributions can be most readily compared through scatter-plots between observations ranked from high to low and similarly ranked model estimates. Such plots are referred to as Quantile-Quantile (Q-Q) plots because each point corresponds to a specific quantile of the data set.

The performance of the complex terrain model is compared with that of the CTDMPLUS model (Perry, 1992), which includes the physics of dispersion in complex terrain in an explicit manner. The relative performance of the models at four complex terrain sites is described next.

The first data set considered here was collected in a field study designed to evaluate CTDMPLUS. The study was conducted in August 1984 near the **Tracy Power Plant** (Perry, 1992) located 27 kilometers east of Reno, Nevada, in the Truckee River valley, which is surrounded by mountainous terrain. Dispersion from the plant was simulated by releasing SF_6 through the 91-m stack. A total of 128 hours of data were collected over 14 experimental periods. 115 of these hours corresponded to stable atmospheric conditions.

Figure 1 shows a Q-Q plot for 1-hour averages for both AERMOD and CTDMPLUS. Both curves parallel the 1-1 line for the entire concentration domain, but AERMOD shows nearly unbiased results at the top end of the concentration range, while CTDMPLUS shows a small under prediction tendency at the upper end of the distribution.

The second data set was derived from the **Lovett Power Plant** study (Paumier et al., 1992), which consisted of a buoyant, continuous release of SO_2 from a 145-m tall stack. The site is located in complex terrain in a rural area. The data spans one year from December 1987 through December 1988. Data were collected from 12 monitoring sites (10 on terrain, 2 as background) located about 2 to 3 km from the plant. The important terrain features rise approximately 250 m to 330 m above stack base. The monitors on terrain are generally about 2 to 3 km downwind from the stack.

The Q-Q plot comparing results for AERMOD and CTDMPLUS is shown in Figures 2 (1-hour averages). Q-Q plots of AERMOD results are generally within a factor of two of the one-to-one line, although AERMOD tends to over predict the concentrations. On the other hand, concentration estimates from CTDMPLUS consistently over predict by more than a factor of two at the upper end of the distributions. At the low concentration end of the frequency distributions, both models under predict the observed values. This is related to background SO_2 concentrations that are not accounted for in the models. Evaluation of AERMOD with two other complex terrain databases also indicates that AERMOD performs at least as well as CTDMPLUS in describing observed distributions of concentrations.

Figure 1: Q-Q Plot for SF6 observations at the Tracy Power Plant Site

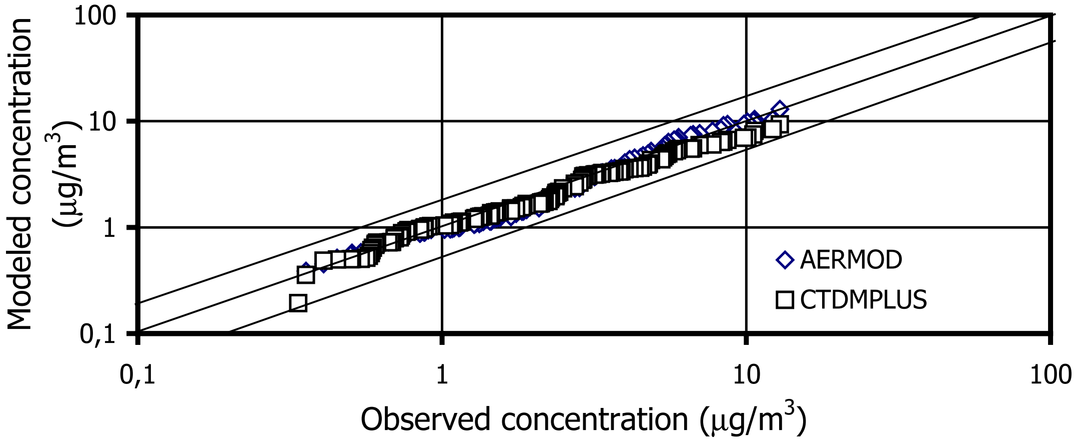
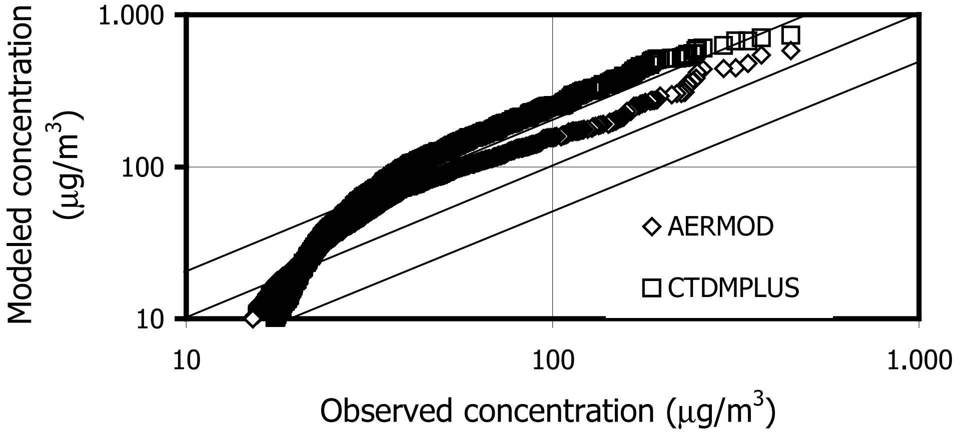


Figure 2: Q-Q Plot for SO2 observations at Lovett Power Plant Site



Summary and Conclusions

This paper suggests an approach to the development of an air quality model designed for regulatory applications. The model is not designed to describe the spatial and temporal distribution of concentrations. Rather, it is designed to meet a more limited objective, which is to simulate concentration frequency distributions observed under a variety of conditions. Knowledge of this frequency distribution is adequate for most regulatory decision-making. This approach to model development allows us to neglect model features that might be important in estimating concentrations at specific locations and times. The resulting model is relatively simple because it incorporates only those features that determine the magnitudes of the concentrations. The validity of this approach to developing a regulatory model has been demonstrated through a simple model for dispersion in complex terrain. We show that this model performs at least as well as a more complete model (CTDMPLUS, Perry, 1992) in simulating the distributions of concentrations observed at four complex terrain sites.

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