Environmental Technology

ISSN: 0959-3330 (Print) 1479-487X (Online) Journal homepage: http://www.tandfonline.com/loi/tent20

An analysis of error propagation in AERMOD lateral dispersion using Round Hill II and Utenweiller experiments in reduced averaging times

Professor Leonardo Hoinaski PhD, Professor Davide Franco PhD & Professor Henrique de Melo Lisboa PhD

To cite this article: Professor Leonardo Hoinaski PhD, Professor Davide Franco PhD & Professor Henrique de Melo Lisboa PhD (2016): An analysis of error propagation in AERMOD lateral dispersion using Round Hill II and Utenweiller experiments in reduced averaging times, Environmental Technology, DOI: 10.1080/09593330.2016.1205672

To link to this article: http://dx.doi.org/10.1080/09593330.2016.1205672

Accepted author version posted online: 27 Jun 2016.
Published online: 27 Jun 2016.

Publisher: Taylor & Francis & Informa UK Limited, trading as Taylor & Francis Group
Journal: *Environmental Technology*
DOI: 10.1080/09593330.2016.1205672

An analysis of error propagation in AERMOD lateral dispersion using Round Hill II and Utenweiller experiments in reduced averaging times.

Professor. Leonardo Hoinaski PhD [a,b*] E-mail: hoinaski@ifc-camboriu.edu.br

Professor. Davide Franco PhD [a] E-mail: d.franco.ocean@gmail.com

Professor. Henrique de Melo Lisboa PhD [a] E-mail: h.lisboa@ufsc.br

*Corresponding author: Phone: +55 48 99818227

Addresses

[a]Departamento de Engenharia Sanitária e Ambiental, Centro Tecnológico, Universidade Federal de Santa Catarina, Campus Universitário-Trindade, 88.010-970 Florianópolis-SC, Brazil

[b]Instituto Federal Catarinense, Rua Joaquim Garcia S/N, 88340-055 Camboriú-SC, Brazil

ACKNOWLEDGMENTS

The research presented here was performed with the financial support of Coordenação de Aperfeiçoamento de Pessoal de Nível Superior (CAPES). The authors wish to thank the Programa de Pós Graduação em Engenharia Ambiental (PPGEA) of Universidade Federal de Santa Catarina (UFSC). Special thanks to Vicente Camara for his help with figure preparation and to Filipe Fernandes de Souza Carvalho for help with the database.

ABSTRACT

Dispersion modeling is extensively used as a decision tool for estimating the impact of atmospheric emissions. However, it was proved by researchers that most part of the models, including the regulatory models recommended by US EPA (AERMOD and CALPUFF), do not have the ability to predict under complex situations. This inability arises from the errors in the lateral and vertical dispersion estimates, which are reliable only to predict 10 minute or longer average concentrations. In the knowledge of the possible issues on the models predictability, this article presents a novel evaluation of the propagation of errors in lateral dispersion coefficient of AERMOD with emphasis on estimate of average times under 10 minutes. The sources of uncertainty evaluated were parameterizations of lateral dispersion (σ_y), standard deviation of lateral wind speed (σ_v) and processing of obstacle effect. The model's performance was tested in two field tracer experiments: Round Hill II and Uttenweiller. The results show that error propagation from the estimate of σ_v directly affects the determination of σ_y, especially in Round Hill II experiment conditions. After average times are reduced, errors arise in the parameterization of σ_y, even after observation assimilations of σ_v, exposing errors on Lagrangian Time Scale parameterization . The assessment of the model in the presence of obstacles shows that the implementation of a PRIME algorithm can improve the performance of the AERMOD model. However, these improvements are small because of the limitations of the algorithm when the obstacles have a complex geometry, such as Uttenweiller.

Keywords: Dispersion models, AERMOD, PRIME, turbulent velocity, odor.

1. INTRODUCTION

Dispersion models play an important role in impact assessments of the air quality when pollutants are emitted by industry. In the model used here, the physical and chemical aspects of transportation, dispersion and processing of pollutants in the atmosphere are simulated [1]. It is therefore possible to predict a pollutant concentration in a given site or region and in a desired period even before emission occurs. However, application of the model has many limitations because of the complexity associated with the dispersion of pollutants.

According to Irwin and coauthors [2], the dispersion of pollutants in the air has a deterministic part and a stochastic part. Dispersion models such as AERMOD and CALPUFF, recommended by the Environmental Protection Agency of the United States (US-EPA), represent only the deterministic part of the process (ensemble averages). The stochastic part is treated as a deviation or an error of the ensemble average. However, even the plot represented by the model is subject to errors [2]. Because of the imperfection of input data (e.g., meteorological conditions, emissions, terrain, land use, etc.) and the difficulty of parameterizing dispersion of pollutants, the models can generate discrepant results [2].

The limitations of the models are aggravated when they are used to represent reduced timescales [3] and are applied in the presence of obstacles[4]. In the first case, the stochastic part, not treated by the model, becomes more evident. In the second, there is a change of turbulence in the area of influence of the obstacle which is not properly explained by the models. Irwin et al. [2] reported the influence of averaging time on atmospheric transport and diffusion. Analyzing data from the Round Hill II field experiment, the concentrations measured at 30 s are around 1.66 times higher than those measured at 10 min. In spite of this limitation, those methods have been extensively used to predict odor and toxic dispersion [4–9]. In this sense, more discussion appears to be needed on the communication of the magnitude of errors to decision makers [10].

Common practice consists of converting model predicted estimates to shorter time periods using Peak-to-Mean (P-M) formula, developed by Gifford [11]. However, according to Dourado et al. [12], a comparison of the model results with wind tunnel data showed that AERMOD fails to predict the peak concentrations using P-M equation. Additionally, Guo, Yu, and Lague and [13] Venkatram [14] have noted some limitations to the use of P-M equation to adjust the modelled concentrations.

More sophisticated techniques such as Large Eddy Simulation (LES) [12], and one-particle Lagrangian models, such as developed by Thomson [15], Franzese [16], Mortarini et al. [17] and Manor [18], should render better performance than AERMOD in complex situations, like reduced timescales and in the presence of obstacles. However, none of than is extensivelly used and worldwid knwon as AERMOD for regulatory propouses. On the other hand, only few studies have been conduced to evaluate the source of the errors [19,20] and adjust the regulatory models AERMOD. More stydies should be done to improve the predictability of this model in real cases under averaging times shorter than 10 minutes and in the presence of obstacles.

This study aims to evaluate the propagation errors in lateral dispersion coefficient of AERMOD in reduced timescales and in the presence of obstacles. Evaluations were made with the USA's Round Hill II [21] and Germany's Uttenweiller [22] experiment databases. To this end, the effects of a PRIME algorithm and the parameterization of lateral wind speed deviation (σ_v) were investigated after determination of lateral dispersion (σ_y) by AERMOD. The performance of AERMOD was compared by means of measured and estimated σ_v. The implementation of the PRIME algorithm was tested in AERMOD in an attempt to estimate σ_y in the presence of obstacles at different average times.

2. BACKGROUND

Among the most frequently used analytical formulations for calculating the dispersion of pollutants in the air is the traditional Gaussian (Equation 1), which in turn is the calculation basis for the AERMOD model:

$$C_{(x,y,z)} = \frac{Q_s}{2\pi\sigma_y\sigma_z u} . \exp\left(\frac{-y^2}{2\sigma_y{}^2}\right) . \left(\exp\left(\frac{-(z-H)^2}{2\sigma_z{}^2}\right) + \exp\left(\frac{-(z+H)^2}{2\sigma_z{}^2}\right)\right) \qquad (1)$$

where x, y and z are the positions where the concentration of contaminants (m) is estimated; $C_{(x,y,z)}$ is the expected contaminant concentration at x, y and z (g.m^{-3}); Q_s is the emission rate (g.s^{-1}); H is the effective height of release of pollutants; u is the average wind speed at the top of the chimney in the direction of flow (m.s^{-1}); $\sigma_y$and σ_z are the mean deviations of the distribution of concentration in the directions y and z (m).

In this model, one of the critical points in the estimation of concentrations is the determination of the term σ_y, which represents the lateral spread of the plume. The lateral dispersion in AERMOD is based on a formulation prepared by Pasquill [23], consistent with the theory of Taylor [24], given by Equation 2:

$$\sigma_y = \sigma_v T f \left({}^{T}\!/_{t_L} \right) \tag{2}$$

where σ_v is the standard deviation of lateral velocity to the average wind direction, f is a function based in T (source travel time to the receiver) and the Lagrangian time scale (t_L) [25].

Considering that the formula developed by Pasquill properly represents reality, the sources of uncertainty in estimating σ_y reside in the determinations of σ_v , T and $f\left({}^{T}\!/_{t_L} \right)$. The value of T can be easily obtained by dividing the distance between the source and the receptor by wind speed.

2.1 Estimating the standard deviation of lateral velocity (σ_v)

Variations in the lateral wind speed (σ_v) can be obtained by measurements. However, these measurements are not routinely made by weather stations, and thus it is still necessary to estimate the values of σ_v [26]. AERMOD has a specific formulation for estimating such parameters, which is one of the sources of uncertainty in determining σ_y [25]. According to Venkatram and coauthors [27,28] and Irwin and coauthors [2], σ_v explains much of the variability of lateral dispersion of pollutants in the air. These researchers also reported that estimates of the models are optimized when measurements of lateral wind variations are incorporated. In the AERMOD model, the σ_v is estimated by Equation 3 (Cimorelli et al. 2005):

$$\sigma_v^2 = \sigma_{vm}^2 + \sigma_{vc}^2 \tag{3}$$

where σ_{vm} and σ_{vc} are lateral wind fluctuations occasioned by mechanical and convective mechanisms. In the mixed layer σ_{vc} is related to convective velocity scale (w_*) as follows:

$$\sigma_{vc}^2 = 0.35 w_*^2 \tag{4}$$

A minimum value of 0.5 m.s^{-1} is assumed for σ_{vc} above the total mixing depth (z_i).

According to Cimorelli and coauthors [25], AERMOD assumes that σ_{vm} varies linearly with height between its value at the surface and an assumed residual value at the mechanical mixing height (z_{im}):

$$\sigma_{vm}^2 = \left(\frac{\sigma_{vm}^2\{z_{im}\} - \sigma_{vo}^2}{z_{im}}\right) z + \sigma_{vo}^2 \quad \text{for } z \le z_{im};$$

$$\sigma_{vm}^2 = \sigma_{vm}^2\{z_{im}\} \quad \text{for } z > z_{im} \tag{5}$$

where $\sigma_{vm}^2\{z_{im}\}$ = min (σ_{vo}^2, 0.25m^2.s^{-2}) and σ_{vo}^2 is equal to $3.6{u_*}^2$. In the stable boundary layer (SBL), the turbulence is exclusively mechanical. In the convective boundary layer (CBL), σ_v has both convective and mechanical contributions. While σ_{vm} is strongly influenced by u_* estimates, σ_{vc} is affected by w_* estimates.

2.2 Estimating the function $\mathbf{f}\left({}^{\mathbf{T}}/_{\mathbf{t_L}}\right)$

In order to allow the application of Equation 2, in AERMOD, the function $f\left({}^{T}/_{t_L}\right)$ is found empirically from field experiments performed on average times over 10 minutes. The lateral dispersion function is based on the theory of Taylor [24] and is defined as [25]:

$$\sigma_y = {}^{(\sigma_v T)}/_{(1+\alpha X)^p} \tag{6}$$

where $X = {}^{\sigma_v x}/_{\tilde{u} z_i}$, $T_{Ly} = l/\sigma_v$ and $\alpha = {}^{z_i}/_{l}$.

l represents the lateral turbulent scale, T_{Ly} is the Lagrangian time scale, x is the downwind distance. In this case, $f\left({}^{T}/_{t_L}\right)$ is given by Equation 7:

$$f\left({}^{T}/_{t_L}\right) = {}^{1}/_{(1+\alpha X)^p} \tag{7}$$

According to Cimorelli and coauthors [25], in AERMOD the $f\left({}^{T}/_{t_L}\right)$ expression was formulated to better fit the data from the Prairie Grass Experiment (Barad and Haugen 1958). A better agreement between Equation 6 and a subset of stable and convective cases from the Prairie Grass Experiment (Barad and Haugen, 1958) appeared when p and α were set equal to 0.3 and 78, respectively. In the respective tracer database, plume samples were collected over 10-min averages. As a consequence of averaging plume properties, fluctuations arising from plume meandering are smoothed after 10 minutes and short-term peak concentrations can no longer be observed. According to Irwin and coauthors [2], as average times increase, there is an increase in the lateral dispersion of the plume. For this reason, dispersion coefficients are valid only for timescales for which they were designed. For cases in which the impact occurs in the order of seconds, such as dispersion of pollutants with high toxicity and odor perception, it is known that conventional dispersion coefficients (valid for periods exceeding 10 minutes) are not adequate. With average times of over 10 minutes, the effects of dispersion and change in the axis of the plume, caused by different turbulent scales, are virtually indistinguishable, except that only the former is responsible for the effective dilution of pollutants. Therefore, the dispersion estimated by the models is usually greater than that which effectively occurs at average times shorter than 10 minutes.

2.3 Effect of obstacles

Besides the aforementioned uncertainty sources, lateral dispersion (σ_y) is also influenced by the presence of obstacles. To include the effect caused by the presence of obstacles in calculating the dispersion of pollutants, AERMOD uses the plume rise model enhancements (PRIME) algorithm. Among the benefits of PRIME are the correction of dispersion coefficients and the elevation of the plume [4]

3. METHODOLOGY

AERMOD performance was tested against Round Hill II (sulphur dioxide release from a source close to the ground under unstable and stable conditions) and Uttenweiler field tracer data (odorant gas released from a stack located on the top of a building under stable conditions). Despite some issues related to heavy gas tracer as sulfur dioxide (Round Hill II) and odor measurements (Utteinweiler), it was not found other field experiment databases available in the literature, which employs measurements under 10 minutes averages. Another important feature of the Round Hill II and Utteinweiler databases was the measurement of the standard deviation of the lateral wind velocity (σ_v), allowing the evaluation of the error propagation through the parameterizations of AERMOD. As mentioned, σ_v is not routinely measured in meteorological stations, consequently, it is generally estimated by the models. The first evaluation conducted in the present work was the comparison of observed and estimated values of σ_v by AERMOD. After that, the model was tested using the same observed and estimated values of σ_v to quantify the propagation of the errors on estimation of σ_y in comparison with observed lateral dispersion of the plume. Assuming that the measurements of σ_v were perfect, the residual differences between observed and estimated values of σ_y has its origins in AERMOD σ_y parameterization (Lagrangian time scale - T_{Ly}).

3.1 Round Hill II experiment

The quality of AERMOD estimates was tested by comparison with the Round Hill II experiment conducted in 1957 [21]. This experiment was conducted with the purpose of studying the diffusion of pollutants in the atmosphere at different average times. A tracer gas (SO_2) was issued constantly by a chimney 1.5 meters high with a horizontal opening. Measurements of the concentration of leeward SO_2 were performed in three concentric arcs from the source, located at 50, 100 and 200 meters. SO_2 samples were collected within the first 30 seconds, 3 minutes and 10 minutes. Thus, the database allowed evaluation of the difference between the concentrations at the above-mentioned average times. This experiment also included meteorological measurements of wind speed, wind direction and temperature. Wind direction standard deviation measurements during the Round Hill II experiment sample period were also made available by Cramer and Record (1957).

The Round Hill II experiment also provides wind direction standard deviation data every 10 minutes. Thus, it was possible to obtain the standard deviation of the horizontal speed of the wind by applying Equation 3:

$$\sigma_v = \bar{u}.sin(\sigma_\theta) \quad (3)$$

where σ_v is the standard deviation of horizontal wind speed, $\bar{u}$ is the average wind speed and σ_θ is the standard deviation of wind direction.

The standard deviation of wind speed is a parameter that can be included as an input in AERMOD. When measured values of σ_v are implemented in AEROMOD, the use of equations to estimate it can be avoided, and consequently error propagation in determining σ_y, found by estimating σ_v from the parameterization of AERMOD, is reduced.

In order to make it possible to run AERMOD, it was necessary to complement meteorological measurements of the Round Hill II experiment with data provided by Taunton[1] surface weather station, Massachusetts, NOAA domain,

[1]Available at http://www.ncdc.noaa.gov/most-popular-data#dsi-3505

located less than 50 km from the experimental site.[2] These measurements were used because of the lack of meteorological stations near the site during the period in which the experiment was performed and the need for temperature profile measurements at high levels of humidity, and pressure, among others. These stations were located in a grassy and flat terrain (17 meters altitude) with a low roughness length, surrounded by small suburbs and trees. Prospecting data from Nantucket Island,[3] Massachusetts, were used to characterize the height of the boundary layer. The Nantucket sounding station (4 meters in altitude) was located approximately 500 meters from the ocean, with vegetation and terrain similar to the experimental site. These supplementary data far away from the experimental site were used to fill in the missing model input data.

The Monin-Obukov length during unstable conditions by the time that the experiment was conducted varied from -771 to -3762 metres and from 93 to 580 metres under stable conditions. In general, the conditions of the atmosphere varied from slightly unstable to stable. The measurements of the wind velocity were in the range of 3.4 ± 1.1 ms^{-1}, which indicates the absence of low wind speed. To perform this step, version 13350 of AERMOD and AERMET (AERMOD weather processor) were used.

3.2 Uttenweiller experiment

The experiment took place in the rural zone of the municipality of Uttenweiller, Germany. The farm and its surroundings are primarily cultivated fields (Bächlin et al. 2002). The Uttenweiller database was developed by measurements of the intensity of odors emitted by a pig-breeding farm. This breeding farm consists of two buildings 7.65 and 10.65 meters high. The smallest has two chimneys 8.5 meters high, connected to internal ventilation systems (Bächlin et al. 2002). Only one of the chimneys was used in the experiment. The chimney used had three compartments, totaling 3.6 square meters. This procedure is analogous to that already performed by Souza and coauthors [6].

The set of 15 assays was conducted in two periods: from 12 to 13 October 2000 and on 31 October 2001. During all of the experiments, the cloud coverage was sufficient to prevent strong convective conditions, and the wind was not classified as calm (it was in the range 1.7 ms^{-1} ± 4.9) [22]. The Monin-Obukov varied between 35 (slightly stable) and 500 (stable conditions).In general, the conditions of the atmosphere were stable during data collection.

---

[2] Round Hill, Massachusetts.
[3] Nantucket is less than 130 km from the place where the experiment was conducted.

Another important feature was the absence of lulls during the evaluation period. Only two experiments (I and L) were selected because of the higher spatial resolutions of their receiver arches.

The odors were measured by 11 trained judges, positioned in line and leeward of the chimney. In this case, the intensity of the odor on a scale ranging from zero (neutral/odorless) to five (very strong) was measured. The judges responded on the intensity of odor perceived every 10 seconds during the 10 minutes of the experiment. Overall, in experiments I and L, approximately 120 10-second measurement tests were recorded. The experiment was also provided with two weather stations, one with a cup anemometer and one with a sonic anemometer.

Measurements of upper air were obtained by soundings of Schnarrenberg airport, about 84 km northwest of the experiment site. Atmospheric pressure and cloud cover data from the Laupheim weather station, 22 km northeast of Uttenweiller, were also used. In the present study, wind speed and direction data measured by the sonic anemometer installed on-site, with a resolution less than 10 seconds, were used. This meter also provided standard deviation data of horizontal and vertical wind speed and friction velocity, which were used as input data in AERMOD. As in Round Hill II, the availability of observations of σ_v allowed the performance of AERMOD to be evaluated with and without the implementation of these measures.

In Uttenweiller, there were two obstacles, one of which was the fireplace used in the experiments. Thus, it was necessary to simulate the building downwash effect caused by these obstacles of a change of turbulence and plume shape. AERMOD performs the treatment of flow with the presence of shields through the plume rise model enhancements (PRIME) algorithm. This model has been developed to incorporate key aspects associated with obstacle effects. Among these effects are the increase in plume dispersion coefficients caused by turbulence drag and a reduction in plume elevation. The latter is owed to the combined effects of downdraft lines at the back of the obstacle and to the capture of the plume by turbulence drag. Therefore, the model takes into account the position of the source in relation to the building, and calculates the intensity of flow velocity, turbulent wind intensity and inclination of current lines as a function of the projected shape of the obstacle.

<Approximate location of Figure 1>

3.3 Determination of lateral dispersion and maximum concentrations observed

The lateral dispersion observed in each experiment was obtained from the best adjustment between measurements and the Gaussian model shown in Equation 4:

$$C_{(x,y,z,H)} = C_{max}.\, exp\left(\frac{-y^2}{2\sigma_y{}^2}\right) \quad (4)$$

where x, y and z are the transverse and vertical distance to the average wind direction; C_{max} is the maximum concentration in the distance x; σ_y is the lateral dispersion and H is the height of the plume.

Given the above considerations, it was therefore assumed that the observed concentrations of the plume in each arc followed a Gaussian distribution. To find the best adjustment between the Gaussian curve of Equation 4 and the observations, a computational algorithm based on the nonlinear least squares method from Matlab® software was used. The convergence criterion used was achieved when the change in the parameters was less than 10^{-8}. σ_y and C_{max} data, from the experiment that did not meet the criterion, were excluded from the analysis. The restriction of values of σ_y within receiver arc limits were also part of the quality control of data.

The main difference between the bases of Round Hill II and Uttenweiller data is in the measurement of concentrations in the former and in odorant intensities in the latter. The hypothesis that the odorant intensity felt by the judges was proportional to the concentration of odors was assumed. However, it is known that the relationship between odor intensity and odor concentration is not linear [30]. Better agreements are found by a power law or logarithm expressions. This limitation of the present work is shared by other studies of odor dispersion. In order to reduce the errors, for this experiment was not evaluated the arc maximum concentration. It is expected that the lateral dispersion of odor concentration and intensity do not vary importantly.

Because of the lack of environmental odor concentration measurements, it was not possible to assess AERMOD performance in determining maximum concentrations. It is worth noting that, in Uttenweiller, the intensities of odors in the environment were measured, and this is a different concentration measurement. The conversion of intensity to odorant concentration requires an empirical equation that would result in a significant increase in uncertainty.

In addition to convergence criteria adopted in Round Hill II, 200 meters and 5 (maximum intensity) ceilings were set for σ_y and C_{max}, respectively. This procedure was necessary because Uttenweiller observations were performed on time scales and spatial resolutions of receptors lower than Round Hill's, therefore they were less stable than those of the Round Hill II experiment. The resolution in Uttenweiller allowed the plume's lateral dispersion data to be obtained every 10 seconds (judges' response time). Averages at every minute of observation of σ_v and perceived intensities were also evaluated, totaling 20 values. After the odor intensities on each receptor were averaged (for one minute), the value of σ_y was determined with the above-mentioned methodology. This procedure was designed to evaluate the effect of average times on the observations of σ_y and their respective impact on the performance of AERMOD in Uttenweiller experimental conditions.

3.4 Statistical indexes

The effectiveness in determining lateral dispersion (σ_y) and maximum concentrations (C_{max}) by AERMOD using measured and estimated standard deviation of lateral wind speed (σ_v) was assessed by comparing observed and modeled values. Statistical index bias, fractional bias (FB), normalized mean square error (NMSE), Spearman's correlation coefficient (ρ), factor of two (FACT2) and mean absolute error (MAE) were used. The estimated values of σ_y and also σ_v were directly extracted from AERMOD outputs.

4. RESULTS

4.1 AERMOD performance in Round Hill II experiment

Table 1 presents the means of statistical indexes used to compare measured and modeled σ_v. The Spearman's correlation coefficient (ρ) shows that the variability of σ_v observations in Round Hill II is well represented by parameterizations. However, bias (0.53 m/s) and FB (56% or 0.56) indexes suggest the presence of systematic errors. FACT2 also shows that 70% (0.7) of the data is within the range of half to twice the value of the observations.

<Approximate location of Table 1>

Table 2 shows the effect of errors in the parameterization of σ_v in the estimates of σ_y by the model. In this table, the comparison of AERMOD efficiency using measured and estimated σ_v is shown. It is possible to verify that all statistical indexes are optimized when the model uses the observations of σ_v. From the average values of fractional bias (FB), it is possible to state that the implementation of these latest observations in AERMOD may result in an improvement of around 40% (from 67% to 22% in an average time of 10 minutes) in the estimates of the lateral coefficients and of 30% of maximum concentrations. There is also a 30% improvement in the percentage of the values that lie within the range established in FACT2. NMSE values also show a reduction of random and systematic errors in estimates of σ_y and C_{max} when the model uses observations of σ_v.

In the absence of measurements of σ_v, an increment of bias values was found ion σ_y estimates, partly because of the bias in estimating σ_v. On the other hand, the high correlation between observations and estimates of σ_v (ρ = 0.98) provided a strong correlation between σ_y observed and modeled by AERMOD (ρ = 0.69), without implementing σ_v measurements.

Despite some improvement in the lateral dispersion estimates provided by the observed values of σ_v. it is still possible to verify large bias in maximum concentration estimates, (mainly) owed to errors in the parameterization of the vertical dispersion (σ_z). This can be seen in the FACT2 values, in which there is no significant difference from the estimates of C_{max} by AERMOD using observations and predictions of σ_v.

Using measurements of σ_v by AERMOD, we see that the simulated plume disperses less and it becomes closer to the observations of Round Hill II. However, even after the implementation of observations of σ_v, the model overestimates, in ascending order, the lateral spread of the plume as the average time is reduced. Hence, the maximum concentrations are underestimated as the averaging time is reduced. The error in the σ_y estimates increases from 22% to 71% when the average time is reduced from 10 minutes to 30 seconds. This suggests an error propagation in the $f\left({}^{T}/_{t_L}\right)$ parameterization. It can be seen that observed values of σ_y are smaller for averaging times of 30 seconds than for 10-minute averages. The more the averaging time increases, the more important the effect of non-dispersing eddies on the lateral dispersion is. Therefore, it is typical of observed plumes that the lateral and vertical instantaneous dispersion is smaller than the average and consequently the instantaneous concentrations are at least as large as the mean [3]. AERMOD does not consider the effect of averaging time, because the model was designed and calibrated to calculate 10-minute or longer averages.

<Approximate location of Table 2>

The results for the three downwind distance ranges were used to assess the variation in the models' performances as a function of the distance traveled by the plume and also as a function of AT. The dependence of the distance and AT in the comparison resulted in the lateral dispersion parameter estimates illustrated in Figure 2.

<Approximate location of Figure 2>

From Figure 2, it is clear that the assimilation of measurements of σ_v substantially improves the performance of AERMOD, reducing model errors in all evaluated distances. However, the improvement provided by the implementation of σ_v is not uniform because AERMOD increases the errors at further downwind distances and the reduction in average times. This indicates the persistence of systematic errors in AERMOD parameterizations of σ_v and $f\left({}^{T}/_{t_L}\right)$. The meandering effect grows as a function of distance and this is one of the possible reasons for the worse AERMOD results at the farthest downwind distances. Regarding the averaging time, AERMOD is insensitive to this effect. As can be seen from the FE values and the fraction of data within the factor 2 range in Figure 2, the model shows improved performance at longer averaging times.

The variation of FE is smaller at shorter distances and shorter averaging times, as also reported by Irwin [31]. This suggests that variation of the horizontal wind direction contributes significantly to the lateral dispersion at greater transport distances. According to Irwin [31], the dispersion estimation schemes assume steady-state meteorological conditions during transport downwind. Therefore, it is possible that variation in the transport direction may result in unexpectedly large values of lateral dispersion. Additionally, the effect of fluctuation of the wind direction on plume spreading is stronger for longer distances and longer averaging times. Hence, the standard deviations of FE (represented by the bars in Figure 2) are higher in these conditions. Cimorelli and coauthors [25] note that AERMOD considers the fluctuation of the plume center. According to them, for time-averaged concentrations, meander has the effect of increasing the lateral spread of the actual plume's distribution. As this fluctuation has little influence in terms of reducing average times, it is possible that the addition of this effect by AERMOD increased the value of σ_y and was the reason for overestimations at 30-second averaging time (Table 2). A further investigation of discrepancies increase with distance can be found in Hoinaski et al. [32]

4.2 AERMOD performance in Uttenweiller's experiment in the presence of obstacles

Table 3 shows the performance of AERMOD in the estimation of σ_v in average times of 10 seconds and one minute compared to observations of sonic anemometer. Table 4 shows statistical indexes from the comparison among observations and estimates of σ_y. It is worth to emphazise that estimated values of σ_v were obtained in AERMOD outputs.

<Approximate location of Table 3>

In Table 3 the model underestimates the observed values of σ_v, unlike what happened when AERMOD was tested with the Round Hill II database. The magnitude of systematic errors in estimating σ_v (evidenced by bias and FB) was lower when AERMOD was tested in Uttenweiller (Table 3) than in Round Hill II. This culminated in minor differences between bias estimates of σ_y with and without the use of σ_v measurements (Table 4). On the other hand, there is a lower correlation between observations and estimates of σ_v according to ρ values in Table 3. The comparisons related to 10-second (ρ = 0.23) and one-minute averages (ρ = 0.60) in Uttenweiller. Observations in Uttenweiller were difficult to describe when we compared the 10-minute averages used in Round Hill II (ρ = 0.98). This explains the poor correlation among observations and estimates of σ_y in 10-second average times. However, the respective field experiment is useful to represent the deterministic part of the dispersion process (ensemble averages), evaluating the bias of the model's estimations.

When the averaging time was increased from 10 seconds to one minute, the correlation between observation and predictions of σ_y intensified, although these relations were still weak. Also, both systematic and random errors decreased, according to bias and MAE values. The removal of outliers and discrepant values after averaging of the observations of σ_v and σ_y, reduced the stochastic parcel and variance of their values. This improved AERMOD's performance in estimating σ_y averaged in one minute.

<Approximate location of Table 4>

The PRIME algorithm accounted for a slight improvement in AERMOD performance in estimating σ_y. An FB reduction of 8% and 2% was found with measured values of σ_v and PRIME in AERMOD, for averaging times of 10 seconds and one minute. Vieira de Melo and coauthors (2012) have previously reported that PRIME improves AERMOD's performance. However, evaluations conducted on a pilot scale in the Uttenweiller experiment, which took place in a wind tunnel, showed that PRIME has shortcomings when used in buildings with complex geometry such as in this case (Figure 1). PRIME considers the Uttenweiller constructions as a single rectangular flat obstacle, since this algorithm uses only the projected height and width. It is likely that these are the reasons why substantial improvements were not observed with the use of PRIME in AERMOD in the Uttenweiller test.

Unlike what was observed in tests using the Round Hill II database, the implementation of σ_v did not show a positive effect on the estimates of σ_y in Uttenweiller. It is clear that statistical indexes for estimating σ_y, mainly bias and FB, are better when measurements of σ_v are not assimilated. In this case, it is likely to be a compensation of errors in the estimates of σ_v and σ_y by AERMOD. According to Table 3, AERMOD underestimates σ_v by about 18% and 13% for 10-second and one-minute average times, respectively. On the other hand, AERMOD has a tendency to overestimate observations because of the reduction of averaging times, as mentioned in Section 4.1. That is, the underestimation of σ_v by AERMOD compensates the amount by the model often overestimates σ_y for averaging times shorter than 10 minutes. The bias reduction in AERMOD while estimating observed one-minute averages of σ_y (6.68 meters) in relation to 10-second observations (1.63 meters) reinforces the above-mentioned premise.

Figure 3 shows an example of vertical concentration profile of the simulations using AERMOD in Uttenweiller, A) with estimated standard deviation of wind velocity and without PRIME, B) with estimated standard deviation of wind velocity and with PRIME, C) with measured standard deviation of wind velocity and without PRIME, D) with measured standard deviation of wind velocity and with PRIME. In this illustrative example, the estimated values of σ_v is smaller than the measured, providing greater concentrations due to the subestimation of σ_y values. With the implementation of the PRIME algorithm, a small change on plume shape is visualized. Greater ground concentrations were reproduced due to the influence of the obstacles, considered by the PRIME. As represented in Figure 4, similar results were found on the horizontal profile of the plume simulated by the AERMOD in respect of the same conditions mentioned before. Due to the subestimation of the σ_y (in consequence of the subestimation of

σ_v), the plume reached greater distances and reduced spread. With PRIME, the plume gets even larger distances and smaller spread, probably due to the cavity zone effect considered by the model.

<Approximate location of Figure 3>

<Approximate location of Figure 4>

5. CONCLUSION

The use of turbulence observations as input data in AERMOD promoted a substantial improvement in the estimates of that model. Deviations of lateral wind speed (σ_v) were overestimated by AERMOD in the Round Hill II experiment because of errors in input data and/or turbulence parameterizations. For this reason, the bias value relative to the 10-minute average σ_y was reduced from 15.47 to 2.74 meters by incorporating measurements of σ_v. The propagation of errors in the estimation of σ_v led to a substantial increase in systematic errors of the measurements of σ_y and C_{max}.

Even with the benefits afforded by observations of σ_v, the model overestimated lateral spread by 70% and underestimated maximum arc concentrations for 30-second averages by 126%. This discrepancy is attributed to the difficulty of predicting the plume spread in short average times, since AERMOD was developed to produce estimates with average times over 10 minutes.

This assessment also showed that errors in estimating σ_y also emerged as a function of distance from the source. These errors may have originated from the parameterization of σ_y, as well as from the way in which AERMOD includes the meandering effect of the plume's center. This result highlights the need for adjustment of the dispersion coefficients and removal of the bias. In AERMOD the meandering effect is added to lateral dispersion. Therefore, turning off the plume meandering treatment in odor and toxic dispersion situations could be envisioned as a possibility to reduce the bias.

When the model was tested under Uttenweiller experimental conditions, compensation of errors was verified by AERMOD's parameterizations of σ_v and σ_y. This compensation provided a better model performance without the assimilation of measured values of σ_v. Analysis confirmed that the quality of estimates of σ_v directly influences the determination of σ_y. In Uttenweiller, whereas σ_v was underestimated by the model, the function $f\left(T/t_L\right)$ probably overestimated the observations, compensating the errors in σ_y estimates.

The use of the PRIME algorithm produced a small improvement in the AERMOD under Uttenweiller experiment conditions. According to Vieira de Melo et al. [4], the complex geometry of the Uttenweiller building (Figure 1) is not perfectly handled by the model, which deteriorated the performance of the AERMOD-PRIME configuration.

The results presented by this work can be useful to analyze the CALPUFF model results which have a similar approach to AERMOD to calculate the lateral and vertical dispersion of the plume. AERMOD and CALPUFF dispersion coefficients (σ_y e σ_z) were designed and calibrated to calculate hourly concentrations. Therefore, both models share a weakness: the inability to calculate short-term time averages, as in the case of flammability, malodour nuisance and, often, toxicity [4,5]. According to Hoinaski et al. [32], the methods of lateral dispersion coefficients employed on AERMOD and CALPUFF reached a strong correlation with observed maximum concentrations and lateral dispersion. However, their estimates are biased and the magnitude of systematic errors tend to grow as the averaging time decreases.

The results presented by this work can be useful to analyze the CALPUFF estimates, because this model has a similar approach to AERMOD to calculate the lateral and vertical dispersion of the plume. AERMOD and CALPUFF dispersion coefficients (σ_y e σ_z) were designed and calibrated to calculate hourly concentrations. Therefore, both models share a weakness: the inability to calculate short-term time averages, as in the case of flammability, malodour nuisance and, often, toxicity [4,5]. According to Hoinaski et al. [32], the methods of lateral dispersion coefficients employed on AERMOD and CALPUFF reached a strong correlation with observed maximum concentrations and lateral dispersion. However, their estimates are biased and the magnitude of systematic errors tend to grow as the averaging time decreases.

In order to achieve good results in averaging times of less than 10 minutes, it is necessary to make adjustments in parameterizations of σ_y and the effect of plume meandering in AERMOD. These adjustments could assist the model's performance optimization, when it is necessary to anticipate concentrations in short periods (seconds), as in the case of toxic pollutants and odorous emissions.

Despite of important findings found by this work, there are some concerns about the present evaluation, due to the limited databases that are available for investigating the effects of AT. The development of a more robust dataset that comprises various atmospheric conditions, distances and ATs would allow for finding a more consistent analysis.

REFERENCES

1. De Melo Lisboa H, Guillot JM, Fanlo JL, Le Cloirec P. Dispersion of odorous gases in the atmosphere - Part I: Modeling approaches to the phenomenon. Sci. Total Environ. 2006;361:220–228. .
2. Irwin JS, Petersen WB, Howard SC. Probabilistic Characterization of Atmospheric Transport and Diffusion. J. Appl. Meteorol. Climatol. [Internet]. American Meteorological Society; 2007 Jul;46:980–993. Available from: http://dx.doi.org/10.1175/JAM2515.1.
3. Hanna SR. Concentration fluctuations in a smoke plume. Atmos. Environ. [Internet]. 1967;18:1091–1106. Available from: http://www.sciencedirect.com/science/article/pii/0004698184901410.
4. Vieira de Melo AM, Santos JM, Mavroidis I, Reis Junior NC. Modelling of odour dispersion around a pig farm building complex using AERMOD and CALPUFF. Comparison with wind tunnel results. Build. Environ. [Internet]. 2012 Oct;56:8–20. Available from: http://www.sciencedirect.com/science/article/pii/S036013231200056X.
5. Dourado H, Santos JM, Reis NC, Mavroidis I. Development of a fluctuating plume model for odour dispersion around buildings. Atmos. Environ. 2014;89:148–157. .
6. Souza FFC, Hoinaski L, De Melo Lisboa H. Comparison of AERMOD and SYMOS'97 models for calculating odor dispersion: A study case in Uttenweiller. Ist Int. Semin. Odours Environ. Santiago, Chile; 2014. p. 7. .
7. Turner DB. The Long Lifetime of the Dispersion Methods of Pasquill in U.S. Regulatory Air Modeling. J. Appl. Meteorol. 1997. p. 1016–1020. .
8. Schiavon M, Ragazzi M, Torretta V, Rada EC. Comparison between conventional biofilters and biotrickling filters applied to waste bio-drying in terms of atmospheric dispersion and air quality. Environ. Technol. [Internet]. Taylor & Francis; 2016 Apr;37:975–982. Available from: http://dx.doi.org/10.1080/09593330.2015.1095246.
9. Gutiérrez MC, Martín MA, Chica AF. Usual variables and odour concentration to evaluate composting process and odour impact. Environ. Technol. [Internet]. Taylor & Francis; 2014 Mar;35:709–718. Available from: http://dx.doi.org/10.1080/09593330.2013.846941.
10. Hoinaski L, Franco D, de Melo Lisboa H. Comparison of plume lateral dispersion coefficients schemes: Effect of averaging time. Atmos. Pollut. Res. [Internet]. Available from: http://www.sciencedirect.com/science/article/pii/S1309104215000422.
11. Gifford Jr. F. Statistical Properties of A Fluctuating Plume Dispersion Model. In: Advances in Geophysics, editor. Elsevier; 1959. p. 117–137. Available from: http://www.sciencedirect.com/science/article/pii/S0065268708600990.
12. Dourado H, Santos J, Reis Junior N, Melo AM V. The Effects of Atmospheric Turbulence on Peak-to-Mean Concentration Ratio and its Consequence on the Odour Impact Assessment Using Dispersion Models. Chem. Eng. Trans. 2012. p. 163–168. .
13. Guo H, Yu Z, Lague C. Livestock Odour Dispersion Modeling : A Review. CSBE/SCGAB 2006 Annu. Conf. 2006. .
14. Venkatram A. Accounting for averaging time in air pollution modeling. Atmos. Environ. [Internet]. 2002 May;36:2165–2170. Available from: http://www.sciencedirect.com/science/article/pii/S1352231002002005.
15. Thomson DJ. A stochastic model for the motion of particle pairs in isotropic high-Reynolds-number turbulence, and its application to the problem of concentration variance. J. Fluid Mech. 1990. p. 113. .
16. Franzese P. Lagrangian stochastic modeling of a fluctuating plume in the convective boundary layer. Atmos. Environ. 2003;37:1691–1701. .
17. Mortarini L, Franzese P, Ferrero E. A fluctuating plume model for concentration fluctuations in a plant canopy. Atmos. Environ. 2009;43:921–927. .
18. Manor A. A Stochastic Single-Particle Lagrangian Model for the Concentration Fluctuations in a Plume Dispersing Inside an Urban Canopy. Boundary-Layer Meteorol. [Internet]. Springer Netherlands; 2014;150:327–340. Available from: http://dx.doi.org/10.1007/s10546-013-9871-5.
19. Gschwandtner G, Eldridge K, Zerbonia R. Sensitivity Analysis of Dispersion Models for Point and Area Sources. J. Air Pollut. Control Assoc. [Internet]. Taylor & Francis; 1982 Oct;32:1024–1028. Available from: http://dx.doi.org/10.1080/00022470.1982.10465506.
20. Irwin JS, Rao ST, Petersen WB, Turner DB. Relating error bounds for maximum concentration estimates to diffusion meteorology uncertainty. Atmos. Environ. 1987;21:1927–1937. .
21. Cramer HE, Record FA. Field Studies of Atmospheric Diffusion and the Structure of Turbulence. Am. Ind. Hyg. Assoc. Q. [Internet]. Taylor & Francis; 1957 Jun;18:126–131. Available from: http://dx.doi.org/10.1080/00968205709343479.
22. Bächlin W, Rühling A, Lohmeyer A. Bereitstellung von validierungs-daten für geruchsausbreitungs-modelle-naturmessungen. Baden-Württemberg, Germany; 2002. .

23. Pasquill F. Atmospheric dispersion of pollution. Q. J. R. Meteorol. Soc. [Internet]. John Wiley & Sons, Ltd; 1971 Oct;97:369–395. Available from: http://dx.doi.org/10.1002/qj.49709741402.
24. Taylor. Diffusion by continuous movements. Proc. London Math. Soc. 1921;Ser.2(20),. .
25. Cimorelli AJ, Perry SG, Venkatram A, Weil JC, Paine RJ, Wilson RB, Lee RF, Peters WD, Brode RW. AERMOD: A Dispersion Model for Industrial Source Applications. Part I: General Model Formulation and Boundary Layer Characterization. J. Appl. Meteorol. [Internet]. American Meteorological Society; 2005 May;44:682–693. Available from: http://dx.doi.org/10.1175/JAM2227.1.
26. Weber RO. Estimators for the Standard Deviation of Horizontal Wind Direction. J. Appl. Meteorol. 1997. p. 1403–1415. .
27. Venkatram A, Princevac M. Using measurements in urban areas to estimate turbulent velocities for modeling dispersion. Atmos. Environ. 2008;42:3833–3841. .
28. Venkatram A, Isakov V, Yuan J, Pankratz D. Modeling dispersion at distances of meters from urban sources. Atmos. Environ. 2004;38:4633–4641. .
29. Barad ML, Haugen DA, Directorate USAFCRCGR. Project Prairie Grass, a Field Program in Diffusion [Internet]. United States Air Force, Air Research and Development Command, Air Force Cambridge Research Center, Geophysical Research Directorate, Atmospheric Analysis Laboratory; 1958. Available from: http://books.google.com.br/books?id=jiXnQgAACAAJ.
30. Harden AK, Hood RA. Odour measuring techniques. Environ. Technol. Lett. [Internet]. Taylor & Francis; 1984 Jan;5:163–170. Available from: http://dx.doi.org/10.1080/09593338409384264.
31. Irwin JS. Estimating Plume Dispersion-A Comparison of Several Sigma Schemes. J. Clim. Appl. Meteorol. [Internet]. American Meteorological Society; 1983 Jan;22:92–114. Available from: http://dx.doi.org/10.1175/1520-0450(1983)022<0092:EPDACO>2.0.CO.
32. Hoinaski L, Franco D, de Melo Lisboa H. Comparison of plume lateral dispersion coefficients schemes: Effect of averaging time. Atmos. Pollut. Res. [Internet]. 2015;-. Available from: http://www.sciencedirect.com/science/article/pii/S1309104215000422.

TABLES

Table 1: Mean statistical indexes between observations and estimates of σ_v for the Round Hill II experiment.

Index	**Value**
BIAS (m.s^{-1})	0.53
FB	0.56
NMSE	0.25
ρ	0.98
FACT2	0.70
MAE	0.53
n	10

Table 2: Statistical indexes of the comparison among observations at different average times in Round Hill II and simulations with AERMOD using estimated and measured σ_v in the respective experiments.

Index	**Average time**	**AERMOD σ_y**	**AERMOD C_{max}**

		σ_v measured	σ_v modeled	σ_v measured	σ_v modeled
BIAS (m)	10 min	2.7	15.5	-96.9	-114.3
	3 min	7.2	20.0	-129.0	-147.3
	0.5 min	11.0	23.7	-151.1	-169.0
FB	10 min	0.22	0.67	-1.15	-1.51
	3 min	0.45	0.88	-1.26	-1.59
	0.5 min	0.71	1.10	-1.26	-1.59
NMSE	10 min	0.02	0.40	2.52	8.08
	3 min	0.20	0.94	3.14	9.42
	0.5 min	0.59	1.68	3.88	11.11
ρ	10 min	0.81	0.69	0.93	0.86
	3 min	0.84	0.79	0.94	0.89
	0.5 min	0.74	0.78	0.90	0.85
FACT2	10 min	0.77	0.40	0.07	0.03
	3 min	0.70	0.20	0.03	0.00
	0.5 min	0.40	0.03	0.10	0.00
MAE	10 min	6.8	17.4	96.95	114.31
	3 min	7.7	20.0	128.99	147.33
	0.5 min	11.0	23.7	151.12	169.04

Table 3: Statistical indexes of the comparison of observed and estimated σ_v values by AERMOD in average times of 10 seconds and one minute.

Index	**σ_v 10 seconds**	**σ_v 1 minute**
Bias	-0.09	-0.07
FB	-0.18	-0.13

NMSE	0.02	0.01
ρ	0.23	0.60
FACT2	0.83	1.00
MAE	0.26	0.15
n	120	20

Table 4: Statistical indexes among observations of lateral dispersion in Uttenweiller every 10 seconds and one minute.

Index	**10-second average**				**1-minute average**			
	σ_y		**σ_y+ PRIME**		**σ_y**		**σ_y+ PRIME**	
	Measured σ_v	**Estimated σ_v**	**Measured σ_v**	**Estimated σ_v**	**Measured σ_v**	**Estimated σ_v**	**Measured σ_v**	**Estimated σ_v**
BIAS (m)	6.68	5.92	6.43	5.31	1.63	-1.34	4.09	0.62
FB	0.42	0.30	0.34	0.24	0.17	-0.01	0.15	-0.01
NMSE	0.15	0.12	0.14	0.11	0.01	0.01	0.05	0.00
ρ	-0.17	-0.04	0.01	0.07	0.08	0.13	0.16	0.27
FACT2	0.61	0.54	0.60	0.60	0.85	0.85	0.69	0.85
MAE	9.49	10.59	10.06	10.64	6.34	5.67	10.31	8.80

FIGURE CAPTIONS

Fig 1: Obstacles in Uttenweiller experiment. Position of the buildings in relation to the geographic north (centered in the chimney), plan view and cuts. Source: adapted from Vieira de Melo et al. (2012).

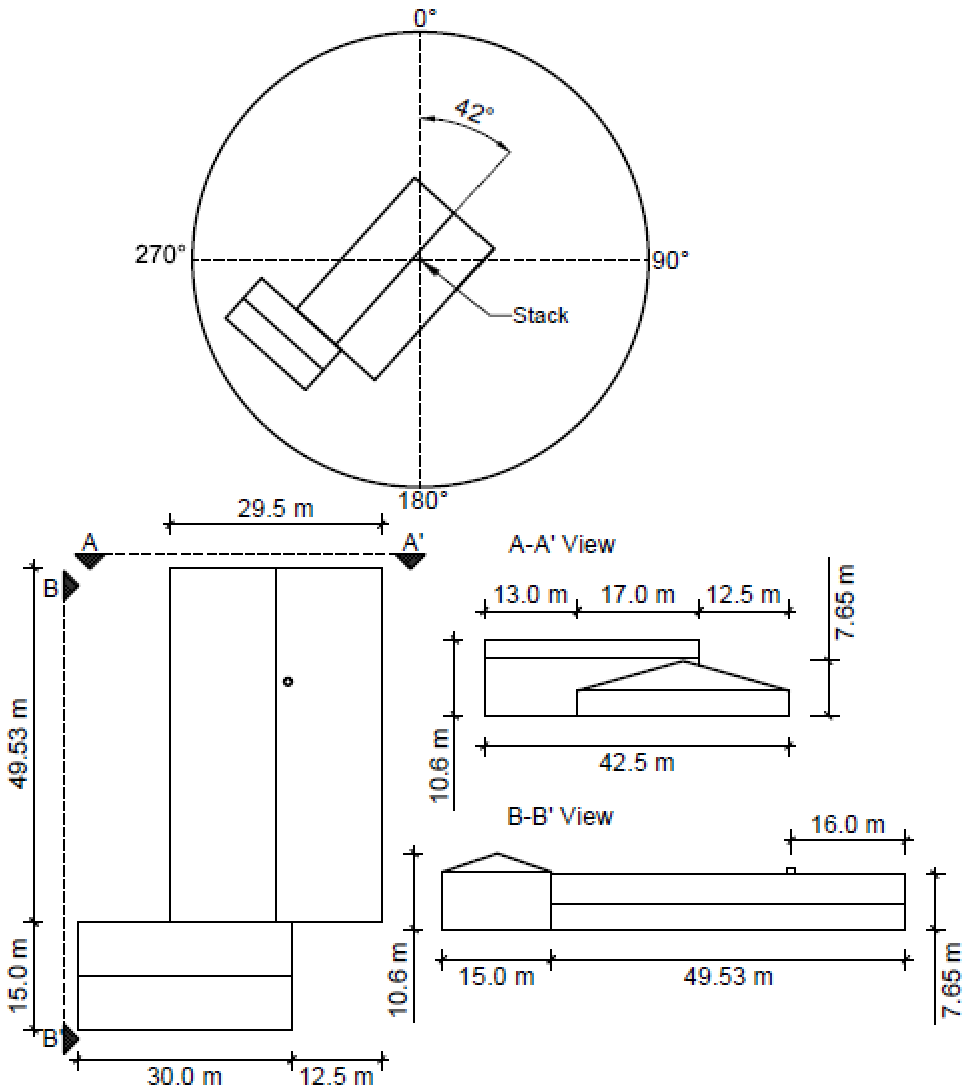


Fig 2: Fractional bias (FB) among observations and estimates of lateral dispersion 50, 100 and 200 meters for Round Hill II experiment in 0.5, 3 and 10-minute average times. The bars indicate the standard deviation of FB and the values in red indicate FACT2.

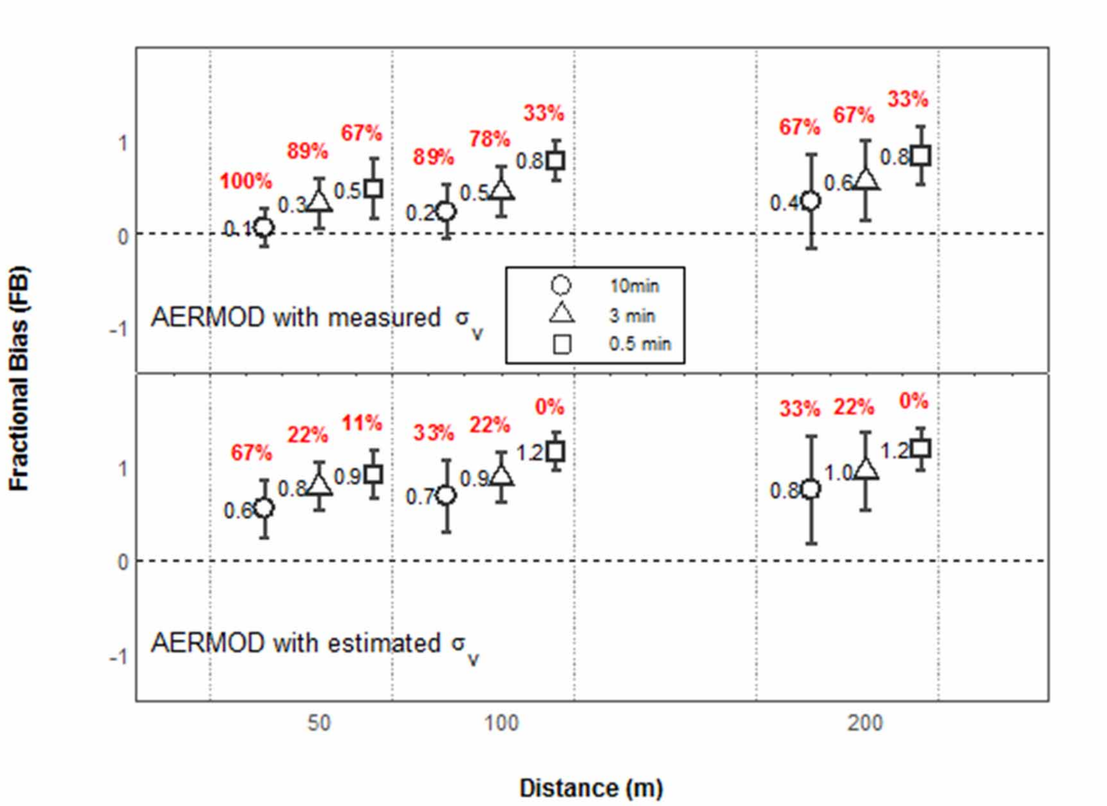


Fig 3: Vertical profile of the AERMOD simulation using estimated and measured values of σ_v, with and without implementation of PRIME.

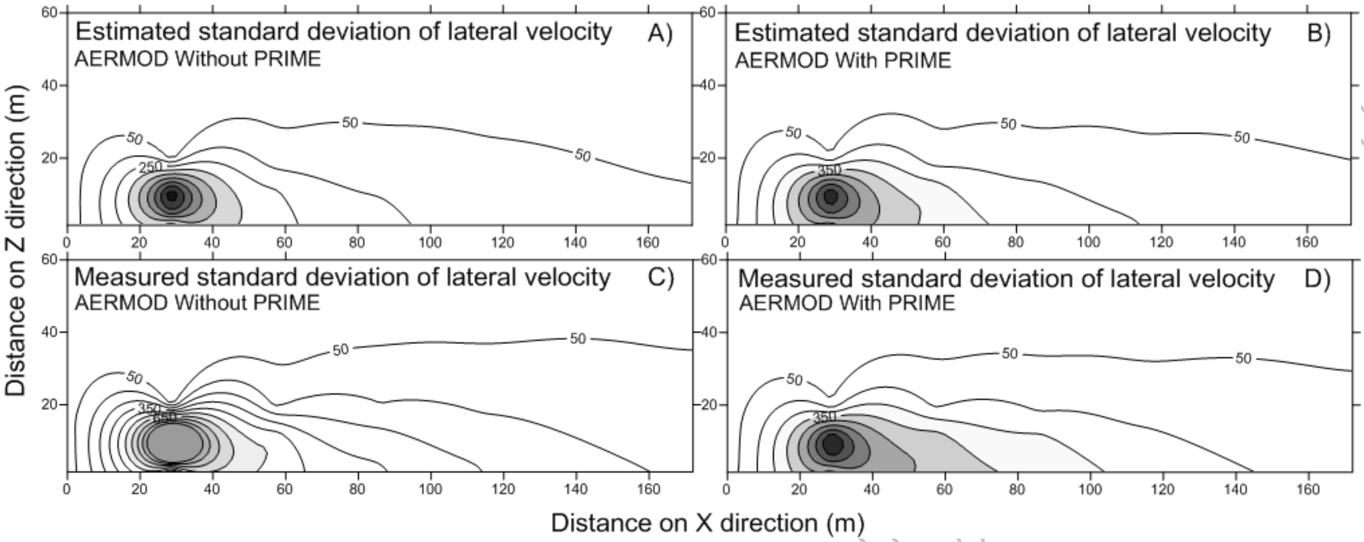
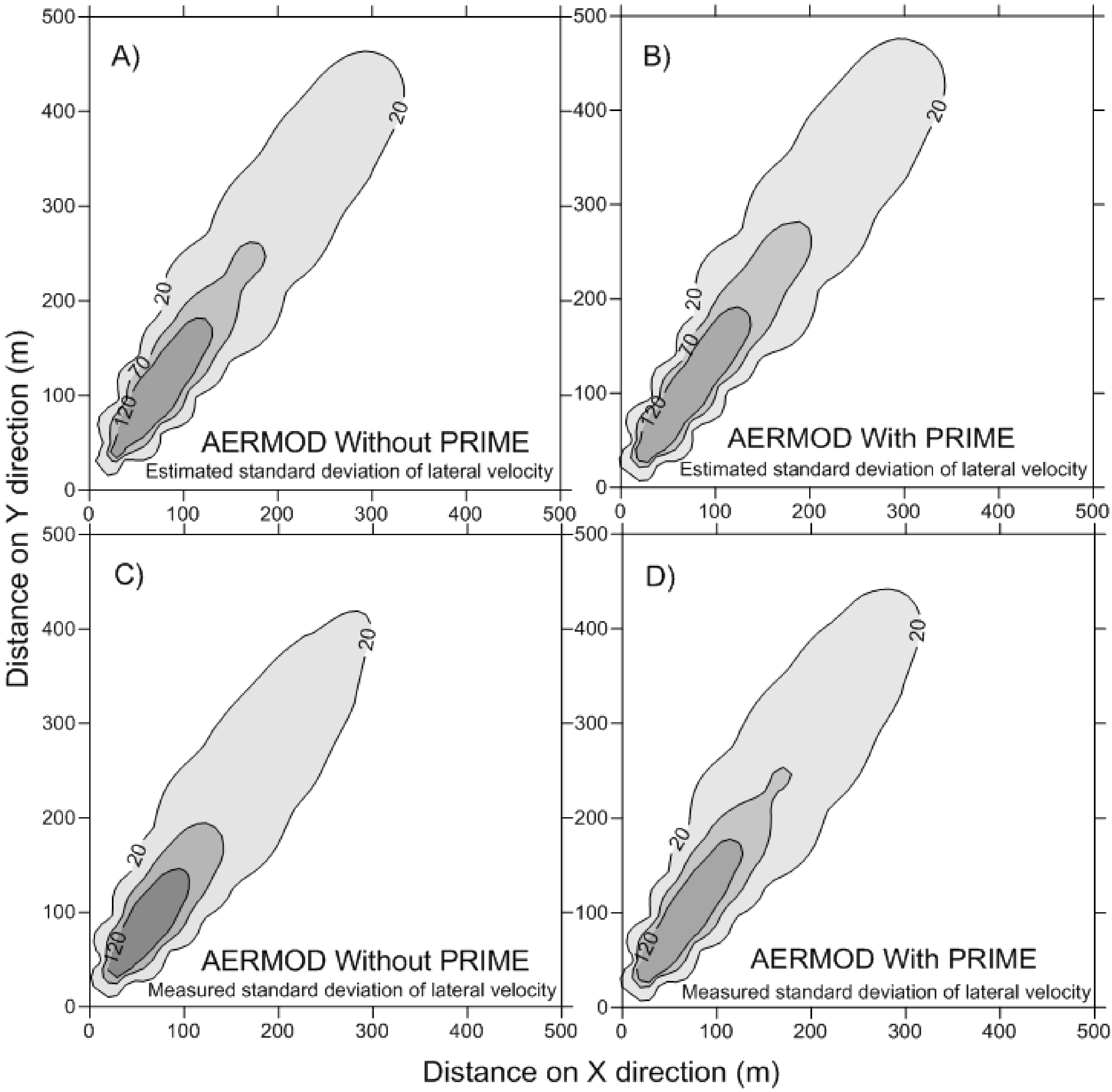
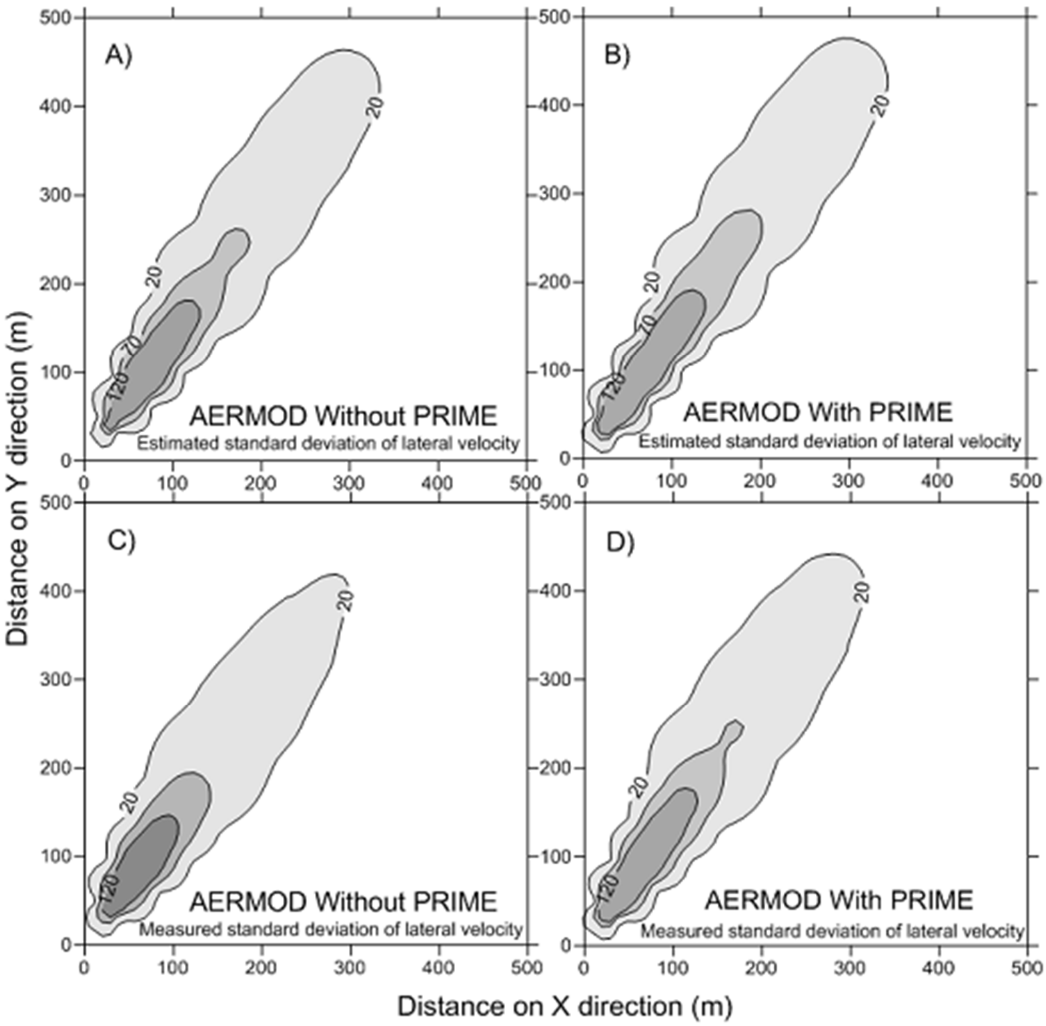


Fig 4: Horizontal profile of the AERMOD simulation using estimated and measured values of σ_v, with and without implementation of PRIME.



GRAPHICAL ABSTRACT:


A)
AERMOD Without PRIME
Estimated standard deviation of lateral velocity
B)
AERMOD With PRIME
Estimated standard deviation of lateral velocity
C)
AERMOD Without PRIME
Measured standard deviation of lateral velocity
D)
AERMOD With PRIME
Measured standard deviation of lateral velocity
Distance on Y direction (m)
Distance on X direction (m)