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METHOD FOR THE ESTIMATION OF THE CONVECTIVE MIXING HEIGHT AIMED TO ATMOSPHERIC LOCAL DISPERSION MODELING

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ABSTRACT

The atmospheric local dispersion modeling is a very important step involved with the atmospheric environmental impact assessment of many processes and facilities.

Since 2006, EPA established the AERMOD as regulatory for atmospheric pollutants local dispersion modeling. The AERMOD model utilizes as input data two files of meteorological variables prepared with the meteorological pre-processor AERMET. In order to prepare these files, AERMET requires meteorological data from an upper air station. In Cuba and in other developing countries, upper air soundings are not performed at all or they are not available with the necessary frequency. The application of the AERMOD model in those specific conditions requires the use of an upper air estimator (UAE) to assess convective mixing heights. The simplest UAE is based only on surface meteorological data. Other local dispersion models, such as ISCST3, have the same requirements.

This chapter describes two methodologies to estimate the convective mixing height based on the solution of the Batchvarova and Gryning, 1991 and the equation system presented by Driedonks, 1982. These methodologies were added to the meteorological pre-processor AERMET. The results of the new version (that is identified in this chapter as AERMET+) have been compared with the original AERMET from EPA, using its own test cases and also, with other UAE implemented in AERMOD-ISC View software from BREZEE and Lakes Environmental. The comparisons show an adequate correlation with EPA's results calculated from actual upper air data and a better adjustment than the above-mentioned UAE tools. These achievements are the result of a rigorous estimation of the initial conditions; the implemented solutions for the evaluation of the hours with calm winds and missing meteorological data; and the sensitivity studies in order to select several constants involved in the algorithms.

The comparative assessment of the local modeling with AERMOD, starting from upper air sounding and using the AERMET+ is presented. The developed methodology was successfully applied as part of a contract for the local dispersion assessment of pollutant gases emitted by MOA NICKEL S.A in 2007, and the estimated pollutants concentrations in two receptors were compared with the measurements from air quality monitoring stations.

INTRODUCTION

Since 2006, EPA established the AERMOD as the regulatory model for atmospheric pollutants local dispersion modeling (USEPA, 2005) [1]. The AERMOD model utilizes as input data two files of meteorological variables calculated with the meteorological pre-processor AERMET (Cimorelli, A. J., et al., 2004 [2] and 2005) [3]. In order to prepare these files, AERMET requires meteorological data from an upper air station. (USEPA, 2004) [4]. Other local dispersion models, such as ISCST3, have the same requirements (USEPA, 1995a [5], USEPA, 1995b) [6].

AERMET estimates the mixing height in the Convective Boundary Layer, taking into account its dependency on both mechanical and convective processes. The mixing height is then calculated based on the following criteria:

- During the day, when the Monin- Obukhov Length is negative, it is estimated as the larger value of the convective and the mechanical mixing height
- During the night, when the Monin- Obukhov Length is positive, it is equal to the mechanical mixing height

The problem emerges when trying to estimate the convective mixing height without the upper air station meteorological data required by AERMET. In Cuba and other developing countries, upper air soundings are not performed at all or they are not available with the necessary frequency. The application of the AERMOD model in those specific conditions requires the use of an upper air estimator to assess convective mixing heights. The simplest UAE is based only on surface meteorological data. Other solutions that are more complicated could be implemented using the results of meteorological mesoscale 3D models such as MM5 (Grell, G. A., et. al., 1994) [7] and WRF (Skamarock, W. C., et al., 2005) [8].

Three possible algorithms where considered to develop the required upper air estimator for AERMOD applications in Cuba:

1. The option implemented in module PBLAER of software BREZEE Air, AERMOD ISC, 2004 (Trinity Consultants, 2004b) [9].
2. The equation proposed by Batchvarova, E.; Gryning, S. E. 1991 [10], included as equation (8) in Seibert, P. et al., 2000 [11].
3. The equation originally proposed by Driedonks, A. G. M., 1982 [12], included as equation (7) in Seibert, P. et al., 2000, used in conjunction with the equation for the variation of the temperature jump across the boundary layer top. This model is adapted for use in ADMS 3.1 (CERC, 2001) [13], as described by Thomson D. J.,

1992 [14] and 2000 [15] and also in Lakes Environmental AERMOD-ISC View (Thé, J. L., Lee, R., Brode, R. W., 2001) [16].

These methodologies were added to the MPPBL module of meteorological pre-processor AERMET and a new version AERMET+, was obtained. AERMET+ included an UAE with three algorithms. The chapter describes, specifically, the methodology and results obtained by the application of the last two algorithms, leading to convective mixing heights values that could be adequately correlated with EPA test cases (EX01-EX05). The results of the AERMET+ are compared with similar tools implemented in AERMOD-ISC View software from BREZEE [17] and Lakes Environmental [18].

METHODOLOGY FOR THE ESTIMATION OF THE CONVECTIVE MIXING HEIGHT

The basic equations for the estimation of the convective mixing height, according to the three above-mentioned algorithms, are shown in Table 1.

Table 1. Basic Equations of the considered algorithms

Algorithm	Basic Equations	
Module PBLAER of BREZEE	$Z_{ic} = \sqrt{{Z_{ie}}^2 + 1400\sum_0^i H}, \quad Z_{ie} = \frac{u_*}{4f}$	(1)
Batchvarova and Gryning, 1991	$\frac{dZ_C}{dt} = (1+2A)\frac{H}{\rho C_P \gamma_\theta Z_C} + 2B\frac{u_*^3 T}{g\gamma_\theta {Z_C}^2}$	(2)
Driedonks, 1982	$\frac{dZ_C}{dt} = \frac{S_D}{\Delta\theta}$	(3)
	$\frac{d\Delta\theta}{dt} = \frac{\gamma_\theta S_D}{\Delta\theta} - \frac{H}{\rho C_P Z_C} - \frac{S_D}{Z_C}$	(4)
	$S_D = A\frac{H}{\rho C_P} + B\frac{u_*^3 T}{gZ_C}$	(5)

Where:
u_*, friction velocity, m/sec
f, Coriolis parameter, sec^{-1}
Z_{ie}, equilibrium mechanical mixing height for hour "i", m
H, surface heat flux, Joule/(sec-m^2)
Z_{ic}, convective mixing height for hour "i", m
t, time of calculation, sec
Z_C, convective mixing height for time "t", m
A, B constants

ρ , density of air, kg/m^3

C_P, specific heat of air at constant pressure, Joule/(kg-K)

g, acceleration of gravity, m/sec^2

γ_θ, potential temperature gradient above the mixing height, K/m

T, reference temperature (on ground surface), K

$\Delta\theta$, temperature jump across the boundary layer top, K

Potential temperature gradient above the mixing height γ_θ was estimated using the expression proposed in Gill, 1982 [19], p54.

$$\gamma_\theta = \frac{N_u^2 T}{g} \tag{6}$$

Where N_u is the Brunt-Väisälä frequency above the boundary layer in sec^{-1}. The default values used are 0.013; suggested by Thomson, D. J., 2000; and 0.011 implied by the U.S. Standard Atmosphere, Gill, 1982, p49.

When using the algorithm implemented in module PBLAER of software BREZEE, the convective mixing height can be estimated by the direct evaluation of the algebraic equation (1).

This approach is very simple and easy to implement but unfortunately it did not lead to good results when compared with the ones reported for the EPA test cases, (as it is shown in Figure 3. and, consequently, no further attention will be dedicated to it in the present chapter.

On the other hand, a combined implementation of algorithms 2 (Batchvarova, E.; Gryning, S. E. 1991) and 3 (Driedonks, A. G. M., 1982) was completed satisfactorily. In the Batchvarova and Gryning algorithm, one differential equation, (2), describes the time dependency of convective mixing height Z_C, while in the Driedonks algorithm the solution of the differential equations system, composed by equations (3) and (4), allows calculating simultaneously the time dependency of convective mixing height Z_C and the temperature jump across the boundary layer top $\Delta\theta$.

Batchvarova and Gryning algorithm, composed by just one differential equation, was considered very suitable for the present application due to its simplicity and accuracy. The differential equation (2) was solved numerically, taking into account that for the small time intervals Δ t = 360 seconds, for which calculations were conducted, the rate of change of the dependent variable Z_C with time, estimated as the finite difference $\frac{\Delta Z_C}{\Delta t}$, satisfactorily approximates the variable derivative $\frac{dZ_C}{dt}$ in the corresponding time interval.

Hence, equation (2) was approximated to estimate the convective mixing height $Z_{C_n} = Z_C(n.\Delta t)$ as a function of its precedent value $Z_{C(n-1)} = Z_C[(n-1).\Delta t]$ for n = 2, 3, 4..., by means of expression (7):

$$Z_{C_n} = Z_{C(n-1)} + \left[(1+2A)\frac{H_{(n-1)}}{\rho_{(n-1)} C_P \gamma_{\theta_{(n-1)}} Z_{C(n-1)}} + 2B\frac{u^3_{*(n-1)} T_{(n-1)}}{g\gamma_{\theta_{(n-1)}} Z^2_{C(n-1)}} \right].\Delta t; \quad \text{n = 2, 3, 4…} \tag{7}$$

Where $H_{(n-1)}, u_{*(n-1)}, T_{(n-1)}, \rho_{(n-1)}, \gamma_{\theta_{(n-1)}}$ are the values of the specified variables, corresponding to the time $t = (n-1).\Delta t$.

The same procedure was implemented to solve the equation system of the algorithm 3. When using this calculation method based on a finite differences scheme, the estimated values for all convective mixing heights at the different hours of the day were found to be strongly dependent on the accuracy of the convective mixing height estimated for the first convective hour.

Consider t_0 =0 as the specific moment of dawn for which the surface heat flux and, consequently, the convective mixing height, begin to grow, starting from the initial condition:

Z_C (0) = 0; $\Delta\theta$ (0) = 0; H (0) = 0 (8)

The main problem was to estimate an accurate first non-zero value $Z_{C1} = Z_C(\Delta t)$ to feed the calculating process of equation (7). It was demonstrated that the algorithm to determinate the first Z_C value is common for algorithms 2 and 3. The approximate solution of the Driedonks algorithm (equations (3), (4) and (5)), specifically oriented to the calculation of Z_{C1}, based in the finite difference scheme corresponding to this equations system, particularized for $t_1 = \Delta t$; $Z_{C1} = Z_C(\Delta t)$ and $\Delta\theta_1 = \Delta\theta(\Delta t)$ is the following:

$$\frac{Z_{C_1}}{\Delta t} = \frac{S_1}{\Delta\theta_1} \tag{9}$$

$$\frac{\Delta\theta_1}{\Delta t} = \frac{\gamma_{\theta_1} S_1}{\Delta\theta_1} - \frac{H_1}{\rho_1 C_P Z_{C_1}} - \frac{S_1}{Z_{C_1}} \tag{10}$$

$$S_{D1} = A\frac{H_1}{\rho_1 C_P} + B\frac{u_{*1}^3 T_1}{g Z_{C_1}} \tag{11}$$

Substituting $\Delta\theta_1$ from equation (9) into equation (10), the following expression for Z_{C1} as a function of S_{D1} was obtained:

$$Z_{C_1} = \sqrt{\frac{2S_1 + \frac{H_1}{\rho_1 C_P}}{\gamma_{\theta_1}}\Delta t} \tag{12}$$

An iterative scheme was implemented to determine Z_{C1} from expressions (11) and (12):

$$S_{D1}^{(k+1)} = A\frac{H_1}{\rho_1 C_P} + B\frac{u_{*1}^3 T_1}{gZ_{C_1}^{(k)}}; \qquad \text{k = 1, 2, 3...} \tag{13}$$

$$Z_{C_1}^{(k+1)} = \sqrt{\frac{2S_{D1}^{(k+1)} + \dfrac{H_1}{\rho_1 C_P}}{\gamma_{\theta_1}}\Delta t} \qquad \text{k = 1, 2, 3...} \tag{14}$$

The first Z_{C1} value, $Z_{C_1}^{(1)}$, was estimated evaluating expressions (11) and (12) for the particular condition $H_1 = 0$, assumed as a starting point, which leads to:

$$Z_{C_1}^{(1)} = \left(\frac{2BT_1\Delta t}{g\gamma_{\theta_1}}\right)^{\frac{1}{3}} u_{*_1} \tag{15}$$

In order to avoid the non-convergence of the solution, this value is limited by:

$$Z_{C_1}^{(1)} < \frac{Bu_{*1}^3 T_1 \rho_1 C_P}{gH|A-1|} \tag{16}$$

It is very simple to obtain the same expressions for algorithm 2, if the main equation is expressed as:

$$\frac{dZ_C}{dt} = \frac{S_B}{\gamma_\theta Z_C} \tag{17}$$

$$S_B = (1+2A)\frac{H}{\rho C_P} + 2B\frac{u_*^3 T}{gZ_C} \tag{18}$$

For algorithm 3, the starting value for $\Delta\theta$ was also estimated, considering H (0) = 0:

$$\Delta\theta_1^{(1)} = \frac{\gamma_\theta Z_C}{2} \tag{19}$$

Calm Wind Conditions

Although the AERMOD does not evaluate the concentration at calm wind hours, the implementations of the algorithms 2 and 3 in AERMET considered the estimation of the increment of convective mixing height during these hours because the mixing height always

depends on the increment in precedents hours, even if was calm. The same analysis leads to the linear interpolation for assessing the missing meteorological data.

As expression (15) can not be used for a calm condition ($u_{*_1} = 0$), expression (11) was particularized for this special case and the obtained S_1 value substituted in (12), which leads to a different expression for Z_{C1}, providing a first Z_C value, which can be used directly in n = 2, 3, 4… (7), without an iteration process:

$$Z_{C_1} = \sqrt{\frac{(2A+1)H_1}{\rho_1 C_P \gamma_{\theta_1}} \Delta t} \text{ ; Valid for } u_{*_1} = 0 \tag{20}$$

$$\Delta\theta_1^{(1)} = \frac{A}{1+2A} \gamma_\theta Z_C \tag{21}$$

SENSITIVITY ANALYSIS AND ASSESSMENT OF THE RESULTS

Several sensitivity analyses were performed to evaluate the influence on the results of: 1) using the algorithms 2 or 3; and 2) some parameters, specifically, the effects of using for N_u a value of 0.011 (as suggested by EPA) or a value of 0.013 (as suggested by UK authorities) and two possible values for the constant *B* of the equations (2) (Batchvarova and Gryning algorithm) and (5) (Driedonks algorithm).

Figure 1 shows the comparison between the convective mixing heights estimated from upper air data (in axis X) for the EPA Test Case 3 (EX03) and the results of the algorithm 2 (in axis Y) for different values of *Nu* and *B*. It can be observed, they are not significantly sensitive to the variation of the analyzed parameters within their usual ranges. Therefore, it can be concluded that the proposed methodology can predict satisfactorily the convective mixing heights based on surface meteorological data, with relative independence of the values selected for the algorithm parameters N_u, *A* and *B*.

As can be seen, a very good correlation was achieved, with R^2 around 0.9. An average overestimation of the proposed methodology, with respect to the values derived from upper air soundings, of approximately 5-7% for Nu=0.011 and light underestimation from 2-4% for Nu=0.013 is observed. Table 2 shows the results for all AERMET-EPA test cases (EX01-EX05), using Nu=0.011 and B=5 (the worst adjust of the options above presented), confirming the validity of the proposed methodology for this range of data, considered sufficiently representative.

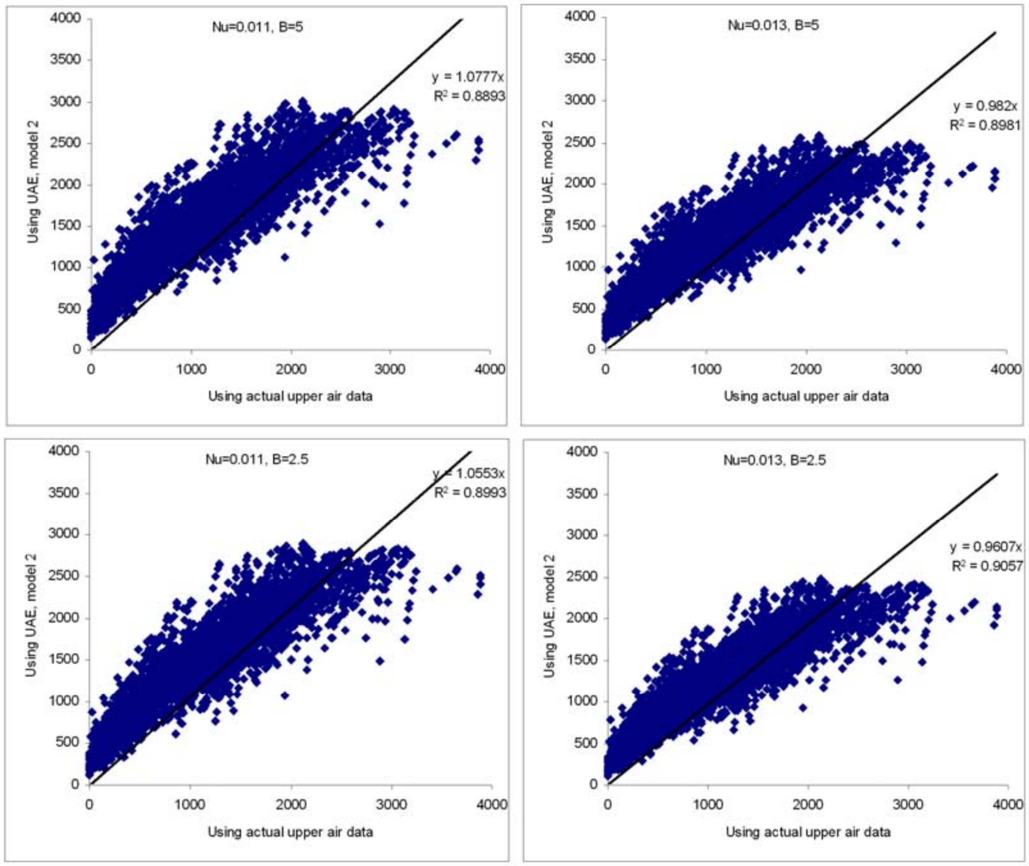

Figure 1. Comparative results of estimated convective mixing heights for EX03, using actual sounding data and UAE corresponding to algorithm 2, for different values of *Nu* and *B*

Table 2. Comparison results of the proposed methodology with EPA test cases (EX01-EX05)

Test Case Name	Test case description	Coefficient of Determination (R^2)	Regression equation
EX01	96 hours (4 days) of meteorological data	0.9015	y = 1.2002x
EX02	96 hours (4 days) of meteorological data, including on site data	0.765	y = 1.0399x
EX03	1 year of meteorological data	0.8893	y = 1.0777x
EX04	1 year of meteorological data	0.7654	y = 1.0363x
EX05	744 hours (1 month) of meteorological data	0.5969	y = 0.8959x

As can be observed in Figure 2a, the results of algorithms (or models) 2 and 3 are very close, and they could be used be used indistinctly without significant changes in the air pollutant concentrations. Actually the algorithm 3 generate lightly more accurate results if the

parameters associated to the trendline for this algorithm (Figure 2b, y = 1.071x, R^2=0.9208) are compared with the corresponding to algorithm 2 (y = 1.0777x, R^2=0.8893)

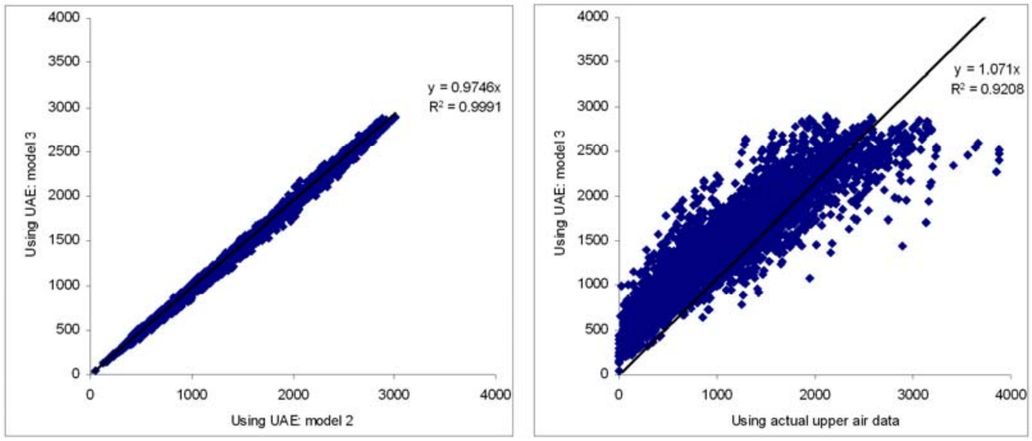

Figure 2. Comparative results of estimated convective mixing heights using the algorithms 2 and 3. EPA test case EX03, Nu=0.013 and B=5.

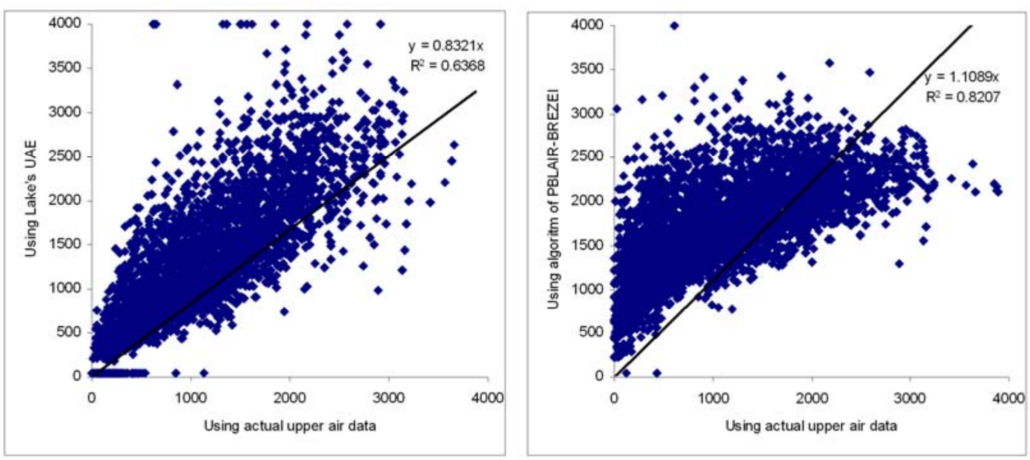

Figure 3. Comparative results of estimated convective mixing heights using Lakes Environmental Tool and sounding data.

On the other hand, Figure 3 shows the comparison of convective mixing heights corresponding to the EPA Test Case 3 (EX03) calculated by AERMET using upper air soundings (in axis X) and estimated by: a) Lakes Environmental Parameterization Tool (Upper Air Estimation Tool) from surface meteorological data (in axis Y) and b) algorithm 1 considered (module PBLAER of BREZEE Air AERMOD ISC version 5.0).

The visual inspection of the Figure 3 shows higher scatter than Figure 2. The numerical parameters associated to trendline confirm the assessment. As much the slope of the adjust equation (y=0.8321x and y=1.1089x respectively) as the R-squared value (R^2=0.6368 and 0.8207) of the lineal trendline are less close to 1.

APPLICATION TO THE LOCAL DISPERSION MODELING

This section presents the comparisons between ground concentration calculations by AERMOD using mixing heights obtained from upper air meteorological soundings (C_1) and mixing heights derived from the UAE using algorithms 2 and 3 (C_2 and C_3 respectively). The study case used for comparison included annual, daily and hourly estimations of concentrations and depositions of SO_2 emissions from 6 hypothetical point sources located in the domain of the EPA´s test case 3 for AERMET. The concentrations were estimated in 723 receptors including in two cartesian grids plus three discrete receptors located very near the sources. One grid of 240 receptors covers 60 x 100 km from south to north and west to east, center on the sources with step of 5 km and the second grid includes 480 receptors in a rectangular domain of 12 x 10 km, also center in the sources with step of 0.5 km.

Table 3 shows the effects of the mixing heights derived from different algorithms on the highest (among all receptors) hourly and daily concentration and on the highest annual average concentration because maximum concentrations are the focus in regulatory modeling. Also the respective average concentrations and deviations are presented. The changes in the concentrations when UAE are used, respect to C_1, are calculated as percent (ej. $(C_2\text{-}C_1)/C_1$ x 100 and as fractional bias (FB).

The fractional bias is often used because it has two desirable features. First, it is symmetrical and bounded: its values range between -2.0 (extreme over-prediction) and +2.0 (extreme under-prediction). Second, the fractional bias is a dimensionless number which is convenient for comparing the results from studies involving different concentration levels or even different pollutants. The fractional bias between C_2 and C_1 is estimated as $2(C_2\text{-}C_1)/(C_1+C_2)$. The fractional bias of the average is computed using the same equation where C_2 and C_1 refer to the averages of the respective data sets.

As can be observed from Table 3, maximum concentrations are not highly sensitive to the algorithm used in mixing height estimation because the differences are less than 3 % for three average periods; annual, hourly and daily. The deviations in average concentrations are bigger than for maximum concentrations but less than 6% for algorithm 2 and less than 3 for algorithm 3. These results corroborate the statement about the light superiority of the algorithm 3 with respect to 2.

The comparisons presented indicate that the UAE is sufficiently accurate to be a viable approach to providing mixing heights for modeling purposes using models such as AERMOD when upper air sounding data are not available.

Table 3. Comparisons between ground concentration calculations by AERMOD using mixing heights obtained from upper air meteorological soundings (C1) and mixing heights derived from the UAE using algorithms 2 and 3 (C2 and C3 respectively).

		Actual UA Data (C_1)	UAE, algorithm 2 (C_2)	ΔC_{1_2}, %	FB_{1_2}	UAE, algorithm 3 (C_3)	ΔC_{1_3}, %	FB_{1_3}
Annual	Maximum	148.00	144.98	-2.04	-0.0205	149.36	0.92	0.0092
Average	Average	12.72	12.41	-6.01	-0.0640	12.57	-2.86	-0.0292
Highest	Maximum	15457.9	15468.7	0.07	0.0007	15468.7	0.07	0.0007
1-hour	Average	847.70	812.41	4.16	-0.0292	824.40	-2.75	-0.0279
Highest	Maximum	2609.78	2603.15	-0.25	-0.0025	2600.31	-0.36	-0.0036
1- day	Average	158.93	157.55	-2.50	-0.0304	158.28	-1.49	-0.0164

The developed methodology was successfully applied as part of a contract for the local dispersion assessment of pollutant gases emitted by MOA NICKEL S.A in 2007 [20]. The pollutants concentration estimations were validated for two air quality monitoring stations. The AERMOD model was executed with POSTFILE output option activates for two receptors located exactly in the coordinates of the air quality monitoring stations. The pollutant concentrations predicted by the model and measured in these points were compared and a high degree of concordance could be observed.

The consistency of the model estimations in comparison with the pollutants concentration measurements constitutes an indirect validation of the proposed algorithms, due to the crucial importance of accurate convective mixing height estimations to achieve a precise modeling of the pollutants atmospheric diffusion processes during the daily hours.

Conclusion

An upper air estimator with two options to assess convective mixing heights was developed and implemented. It was based on the Batchvarova and Gryning algorithm, and the equation system presented by Driedonks in 1982 and applied in ADMS, as described by Thomson D.J., 2000, complemented with the rigorous estimation of the convective mixing height for the first convective hour and solutions to evaluate the hours with calm winds and missing meteorological data.

The implemented methodology, based on surface meteorological data, shows a very good correlation with the convective mixing heights determined by AERMET for the EPA Test Cases using upper air soundings.

The sensitivity analysis performed indicates that the proposed methodology can predict satisfactorily the convective mixing heights, with relative independence of the values selected for the algorithm parameters N_u, A and B.

The comparisons between ground concentration calculations by AERMOD using mixing heights obtained from upper air meteorological soundings and mixing heights derived from the UAE using algorithms 2 and 3 indicate that the developed UAE is sufficiently accurate to be a viable approach to providing mixing heights for modeling purposes using models such as AERMOD when upper air sounding data are not available, as much for maximum concentrations as for average concentrations.

The developed Upper Air Estimator allowed the application of AERMOD to the local dispersion assessment of pollutant gases emitted by MOA NICKEL S.A in 2007. The model results validated satisfactorily when compared with the actual values of pollutants concentrations in the air, measured for two air quality monitoring stations.

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