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Methodological guide for implementation of the AERMOD system with incomplete local data

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ABSTRACT

The state-of-the-art air quality modelling system AERMOD includes an updated treatment of turbulence and dispersion in the planetary boundary layer for flow over the flat and complex terrain, scaling concepts, and surface and elevated sources. However, the data requirements are higher than for the screening and the ISCST3 models, in particular meteorological, topography and land use data for the modelling domain.

This work presents a methodology for implementation of the AERMOD modelling system when local data is incomplete and is not in the format required by the model, which is a typical situation in many countries, particularly in developing ones. In addition, the main computational tools developed to achieve this objective were presented: *LandUse.xls*, which takes the place of AERSURFACE; *AERMET+*, a version of AERMET that runs without upper air sounding meteorological data; and *SD_Aermet*, which converts the surface meteorological data to a format accepted by AERMET.

Three representative case studies were also presented, and the modelling results of a case study were compared to measurement data. The work concludes with a discussion of the possibility of using the AERMOD model in Cuba and in other countries, even when some input data is absent and climatological conditions differ from the medium latitudes for which the model was developed for.

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1. Introduction

Air quality assessment by integrating measurement techniques and modelling tools is a crucial element in pollution mitigation. However, in many countries systematic measurements for monitoring and evaluation of air quality are not available, mainly due to lack of resources.

Additionally, modelling works are not an effective management tools in many countries due to lack of regulations. In developing countries like Cuba, the regulatory framework is based on screening models, which are many years behind the state-of-the-art dispersion models and they generally yield inaccurate predictions.

The implementation of high–resolution models at the local scale, such as AERMOD (American Meteorological Society–AMS/ Environmental Protection Agency–EPA Regulatory MODel), improves the accuracy of predictions, which translates directly into a better understanding of the risks at involved receptors and an improved assessment of compliance with air quality standards, enabling more informed decisions. However, data requirement for high–resolution models is higher than for screening models, therefore their use is limited in developing countries.

The U.S. EPA established AERMOD as the regulatory model in 2005 (EPA, 2005), to replace ISCST3 (Industrial Source Complex model for Short Terms, version 3). AERMOD is an advanced plume model that incorporates updated treatments of turbulence and dispersion in the planetary boundary layer for flow over the flat and complex terrain.

AERMOD adopts the ISCST3's input/output architecture, ensuring that the sources and atmospheric processes modelled by the ISCST3 can still be handled. Therefore, all the work done to implement ISCST3 (Turtos et al., 2007a) is a starting point for the implementation of AERMOD.

AERMOD, like its predecessor ISCST3, is open–source software. The source code, user manuals, model formulation, and test cases are available for public access as anonymous user at http://www.epa.gov/scram001/dispersion_prefrec.htm and dispersion_alt.htm respectively. Being open–source has facilitated its steady improvement and ensured that it can be used in developing countries at no additional cost, after making the necessary adjustments.

2. Methodology

The AERMOD modelling system includes the AERMOD dispersion model (EPA, 2004a) and two input data processors that are regulatory components: AERMET (EPA, 2004b), a meteorological data processor, and AERMAP (EPA, 2004c), a terrain data processor. Other non–regulatory components of this system are AERSURFACE (EPA, 2008), a surface characteristics processor, and BPIP–PRIME (EPA, 2004d) for processing data from buildings and obstacles near emission points to determine their

interference with plume rise and to estimate the variables needed by AERMOD to evaluate building downwash effect.

2.1. AERMAP

One of the main limitations for the use of AERMAP in Cuba and other developing countries is the availability of a digital elevation model (DEM) containing topographical data of the modelling domain with an adequate resolution that can be acquired quickly and inexpensively. There are online free DEM sources that can be used to run AERMAP when a local one is not available. The following data sets were evaluated:

GTOPO30. A DEM with sample spacing of 30 arc–seconds (~ 900 m) (GTOPO30, 1996), using the Latitude/Longitude WGS84 projection. In the case of Cuba, Central America, Mexico and the Caribbean, the files *w100n40.dem* and *w140n40.dem* are required.

SRTM (Shuttle Radar Topography Mission). A DEM with sample spacing of 3 arc–seconds (~ 90 m), using the Latitude/Longitude projection. Each file corresponds to one degree of latitude and longitude. The largest local domain (100 x 100 km) could require up to nine files. The names of the files, e.g. *N23W075.hgt*, contain the latitude (North or South) and longitude (West or East) corresponding to the lower left corner of the grid system.

SRTM is an international project spearheaded by the National Geospatial–Intelligence Agency (NGA) and the National Aeronautics and Space Administration (NASA). Elevation data on a near–global scale was obtained to generate the most complete high–resolution digital topographical database of Earth (Rodriguez et al., 2005; Farr et al., 2007).

The resolution of this data set is 10 times higher than GTOPO30. Recently, version 2 of the SRTM was released. Version 2 is the result of a substantial editing effort by the NGA and exhibits well–defined water bodies and coastlines and the absence of spikes and wells (single pixel errors), although some areas of missing data ("voids") are still present. Both are available using anonymous ftp at e0srp01u.ecs.nasa.gov/srtm.

2.2. Land use

AERSURFACE, designed to aid in obtaining realistic and reproducible surface characteristic values for the AERMOD modelling system, is available from early 2008 (version 08009) and requires the input of land cover data from the U.S. Geological Survey (USGS) National Land Cover Data 1992 archives (NLCD92), at a spatial resolution of 30 meters. This information is available at no charge only for users from the United States. This methodology proposes to replace AERSURFACE combining the use of the following tools:

1) A Geographical Information System (GIS), for the processing of the available land use layer is used to integrate it with the layer that represents the modelling domain in order to estimate the percentage corresponding to each land use category for each sector. In order to satisfy both AERMET and AERMOD requirements, the modelling domain must be composed of 72 radial sectors of five degrees each.

2) The MSExcel application, *LandUse.xls*, is used to calculate a weighted average of the Albedo and Bowen ratio at midday and an arithmetic average for the surface roughness length as inputs to AERMET (see Supporting Material). The estimation is based on the land use cover of each category for each sector and the default values of these three surface characteristics for each season/land use category are adjusted depending on the study area.

For Cuba, the following adjustments to the default values defined by AERMET's user guide for different seasons (defined by default for mid–latitude continental areas) are proposed:

- Values in summer equal to AERMET's defaults in summer,
- Values in winter equal to AERMET's defaults in autumn,
- Values in autumn equal to the average of the AERMET's default values for summer and autumn,
- Values in spring equal to the average of the AERMET's default values for spring and summer.

In all cases, the default values of the Bowen ratio must be used for average moisture conditions. In some areas of the country as the very dry regions of Guantanamo, these considerations may vary.

In Cuba, as in many other countries, there is a lack of updated digital land use layers. In this case, the layer contained in the International North America land cover database could be used. This layer is part of the Global Land Cover Characteristics Database (available in http://LPDAAC.usgs.gov/glcc/glcc.asp) from the USGS and includes all continents. Data share the same projections (Interrupted Goode Homolosine and Lambert Azimuthal Equal Areas) at a spatial resolution of ~1 000 m. The decision was made to use the data in the Lambert Azimuthal Equal Areas projection, which is supported directly in most GIS applications.

The data is presented as a raster image with the spatial resolution of 1 000 m. A land use value corresponds to a 24–category land use classification given in the first column in Table 1. In addition, Table 1 shows the correspondence proposed between the categories used in this database, in AERMET, and AERMOD.

If another source of data is used, the correspondence to the categories established for AERMET and AERMOD should be verified.

Table 1. *Land use categories in USGS and AERMET–AERMOD*

USGS categories	AERMET	AERMOD
Urban and Built-Up Land	Urban	Urban land, no vegetation
Dry-land, Cropland and Pasture	Cultivated Land	Agricultural land
Irrigated Cropland and Pasture		
Mixed Dry-land/Irrigated Cropland and Pasture		
Cropland/Grassland Mosaic		Rangeland
Cropland/Woodland Mosaic		
Grassland	Grassland	
Shrub-land	Desert Shrubland	Barren land, mostly desert
Mixed Shrub-land/Grassland	Grassland	Rangeland
Savannas		
Deciduous Broadleaf Forest	Deciduous Forest	Forest
Deciduous Needle-leaf Forest		
Evergreen Broadleaf Forest	Coniferous Forest	
Evergreen Needle-leaf Forest		
Mixed Forest		
Water Bodies	Water	Bodies of water
Herbaceous Wetland	Swamp	Non–forested wetlands
Wooded Wetland		Forest
Barren or Sparsely Vegetated	Desert Shrubland	Barren land, mostly desert

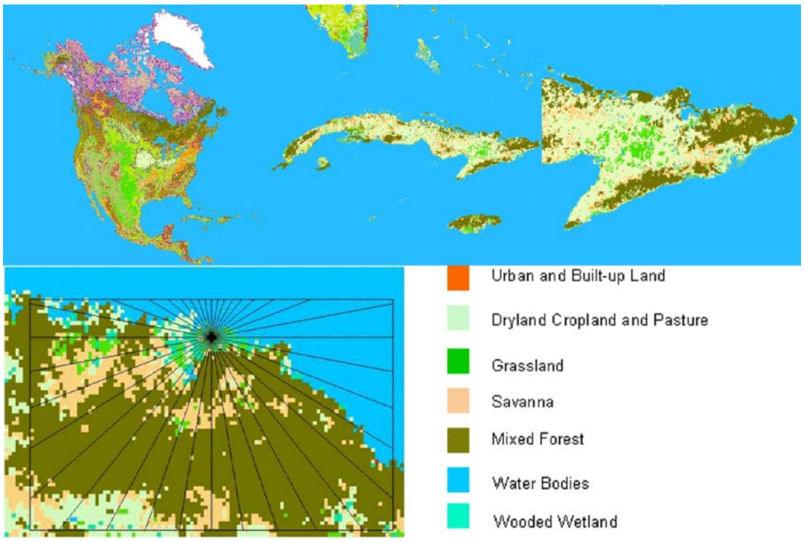

Figure 1. *Example of land use map processed by radial sectors.*

Figure 1 shows an example of a land use category map processed by radial sectors, as required by AERMOD–AERMET, for a modelling domain of 100 x 60 km.

2.3. AERMET

AERMET requires surface and upper air meteorological data. Since a version that supports a free format for surface data is still pending, the program *SD_Aermet* was developed to convert the national surface data into a format supported by AERMET.

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

• During the day, when the Monin–Obukhov Length is negative, it is estimated as the larger of the convective or the mechanical mixing height.

• During the night, when the Monin–Obukhov Length is positive, it is equal to the mechanical mixing height.

A problem emerges when trying to estimate the convective mixing height because upper air meteorological data are required. In Cuba and in other countries, upper air soundings are not available with the required frequency (twice daily) or they are never observed. Under these conditions, an upper air estimator (UAE) that can estimate the convective mixing heights is required. The simplest UAE could be based on surface meteo-rological data. Other more complicated estimators could be implemented using the results of 3D meteorological meso–scale models as MM5 (PSU/NCAR, 2005) or WRF–ARW (Advanced Research WRF) (PSU/NCAR, 2010).

To develop the required UAE two algorithms were added to the MPPBL module of AERMET and a new version was obtained (AERMET+). It does not require upper air meteorological data and estimates the vertical data (specifically the height of the convective mixed layer, the convective velocity scale, and the potential temperature gradient above the mixing height) from surface data.

The algorithms mentioned above are:

1. The equation proposed by Batchvarova and Gryning (1991),

$$\frac{dZ_C}{dt} = (1+2A)\frac{H}{\rho C_P \gamma_\theta Z_C} + 2B\frac{u_*^3 T}{g \gamma_\theta {Z_C}^2} \quad (1)$$

2. The equation originally proposed by Driedonks (1982), used in conjunction with the equation for the variation of the temperature jump across the top of the boundary layer. This model was adapted for use in ADMS 3.1 (CERC, 2001), as described by Thomson (1992), Thomson (2000) and also in Lakes Environ-mental AERMOD–ISC View (The et al., 2001).

$$\frac{dZ_C}{dt} = \frac{S_D}{\Delta\theta} \quad (2)$$

$$\frac{d\Delta\theta}{dt} = \frac{\gamma_\theta S_D}{\Delta\theta} - \frac{H}{\rho C_P Z_C} - \frac{S_D}{Z_C} \quad (3)$$

$$S_D = A\frac{H}{\rho C_P} + B\frac{u_*^3 T}{g Z_C} \quad (4)$$

where u_* *is the* friction velocity (m/s), *H is the* surface heat flux (Joule/s m^2), Z_{ic} is the convective mixing height for hour "*i*" (m), *t* is the time of calculation (s), Z_C is the convective mixing height for time "*t*" (m), *A and B* are constants, *ρ* is the density of air (kg/m^3), C_P *is the* specific heat of air at constant pressure (Joule/kg K), *g is* acceleration of gravity (m/s^2), γ_θ is the potential temperature gradient above the mixing height (K/m), *T is the* reference temperature (on ground surface) (K), $\Delta\theta$ *is the* temperature jump across the boundary layer top (K). The potential temperature gradient above the mixing height γ_θ was estimated using the expression proposed by Gill (1982):

$$\gamma_\theta = \frac{N_u^2 T}{g} \quad (5)$$

where Nu is the Brunt-Vaisala frequency above the boundary layer in (1/s). The default values are 0.013, as suggested by Thomson (2000), and 0.011, as implied by the U.S. Standard Atmosphere (Gill, 1982).

Both algorithms are given in Seibert et al. (2000). A combination of algorithms 1 and 2 was satisfactorily implemented

as described in Turtos et al. (2009a). The differential equation [1] was solved numerically, taking into account that for the small time intervals Δt = 360 seconds at which calculations were conducted, the rate of change with time of the dependent variable Z_C, estimated as the finite difference $\Delta Z_C / \Delta t$, can be satisfactorily approximated as the variable derivative dZ_C / dt in the corresponding time interval.

When this calculation method based on a finite differences scheme was used, 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.

$t_0 = 0$ was considered to be the specific moment of dawn for which the surface heat flux, and consequently the convective mixing height, began to grow, starting from the initial condition: $Z_C(0) = 0$; $\Delta\theta(0) = 0$; $H(0) = 0$.

The main problem was to estimate an accurate first non–zero value $Z_{C_1} = Z_C(\Delta t)$ to initialize the calculation. It was demonstrated that the algorithm to determine the first Z_C value is the same as for algorithms 1 and 2. It included an iterative scheme and the determination of the upper value limit in order to avoid non-convergence of the solution.

Although AERMOD does not evaluate the concentration at calm wind hours, the implementations of algorithms 1 and 2 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 preceding hours, even if the conditions were calm. The same analysis leads to the linear interpolation for estimating the missing meteorological data.

Sensitivity analysis and assessment of results. The results of several sensitivity analyses conducted with the implementation of these algorithms were presented in Turtos et al. (2009a). They were performed to evaluate the impact of certain parameters and the use of algorithms 1 or 2. Values considered for *Nu* were either 0.011 (as suggested by EPA) or 0.013 (as suggested by UK authorities), and two possible values were considered for the constant *B* in Equations (1) (Batchvarova and Gryning algorithm) and [4] (Driedonks algorithm).

The comparison of the convective mixing heights estimated from upper air data for all AERMET–EPA test cases (EX01–EX05), and the results of algorithms 1 and 2 for different values of *Nu* and *B*, shows that:

• The model is 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 *Nu*, *A* and *B*, provided that they are sufficiently representative.

• The results of algorithms 1 and 2 are very similar (Figure 2a) and the algorithms could be used interchangeably without significant changes in simulated air pollutant concentrations. Algorithm 2 generated results that are slightly more accurate if the parameters associated with the trend lines are compared, but the Batchvarova and Gryning algorithm, composed by just one differential equation, is very suitable for the present application due to its simplicity and accuracy.

• Very good correlations were achieved in all test cases. The slopes of the regression equation and the coefficients of determination R^2 were close to 1.0 (see for example in Figure 2b, y = 1.071x, R^2 = 0.921). On the average, the proposed methodology overestimated concentrations by approximately 5–7% for Nu = 0.011 and underestimated concentrations by 2–4% for Nu = 0.013 with respect to the values derived from upper air soundings.

2.4. AERMOD

The methodology for the implementation of the dispersion model AERMOD, in addition to the previous steps, involved:

1) Proposal of the control options:

   a) Estimation of concentrations and wet and dry deposition of pollutants (gases and particulates)
   b) Selection of the averaging periods (in Cuba, hourly, daily and annual) according to the pollutant and established standards for analyzing results
   c) Use of the following default output options:

      • Concentrations and depositions at each receptor due to emissions from each group of sources: the average during long periods (annual or whole period) and the maximum in each short averaging period (PLOTFILE option)
      • Concentrations higher than the threshold values due to emissions from each group of sources in each short averaging period (MAXIFILE option)
      • All concentrations at each receptor in each short averaging period (POSTFILE option); only for validation studies

2) Establishment of methodologies to generate the data required by the high–resolution models for characterization of emission sources, which is unavailable in the country:

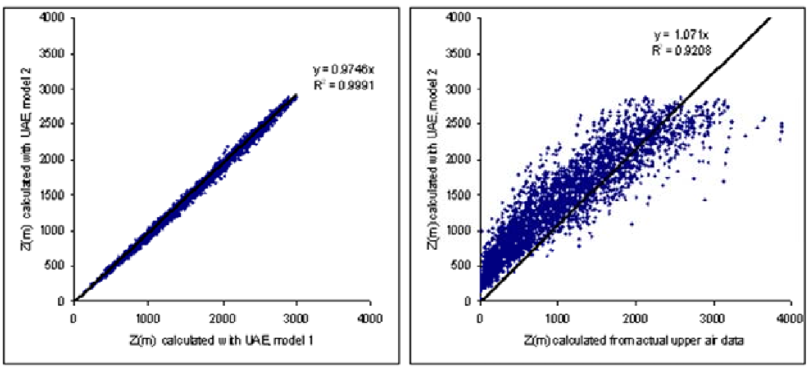

Figure 2. *Comparison of convective mixing heights estimated using algorithms 1 and 2. EPA test case EX03, Nu=0.013 and B=5.*

a) Particulate emissions and size distribution of particles (for each category, the mass fractions and density) from available international databases such as AP–42 (EPA, 1998). If the concentrations are half of the reference values, sensitivity studies must be conducted for the range of probable values.
b) Simulation of flares as point sources with the corresponding adjustment in equivalent emission height and diameter.

3) Approaches and algorithms for using variable emission patterns, even for real-time modelling.

4) Defining urban and rural conditions based on the Auer method or the population density procedure.

As in ISCST3, the modelling of each pollutant in AERMOD is independent and therefore necessary to build a control file for each pollutant. In order to avoid renaming the control and output files for each pollutant, a "*.bat*" file is used (*Aermodb.bat*). It is further recommended that a "*.bat*" file is created for each case study in order to consecutively simulate the considered pollutants.

Data for deposition algorithms. The deposition algorithms in AERMOD (EPA, 2004e; EPA, 2004f) are different from those used in ISCST3 (Wesely et al., 2002). The new deposition algorithms require the previously mentioned land use categories as well as some gas deposition resistance terms for five seasonal categories:

1) Midsummer with lush vegetation,
2) Autumn with unharvested cropland,
3) Late autumn after frost and harvest, or winter with no snow,
4) Winter with snow on ground, and
5) Transitional spring with partial green coverage or short annuals.

For Cuba, Category 2 is appropriate from November to March and Category 1 is applicable for the rest of the year.

Table 2 lists the chosen values of parameters needed for modelling sulphur and nitrogen oxides, H_2SO_4 and H_2S in AERMOD at 25 °C. The EPA proposes values to use for a long list of pollutants (Wesely et al., 2002).

Table 2. *Constants for gas deposition algorithms in AERMOD*

Parameters	**SO_2**	**NO_x**	**H_2S**	**H_2SO_4**
Diffusivity in air, D_a (cm^2/s)	0.1509[a]	0.1656[a]	0.1623[b]	0.986[c]
Diffusivity in water, D_w (cm^2/s)	$1.83x10^{-5}$ [d]	$1.4x10^{-5}$ [d]	$1.36x10^{-5}$ [e]	$1.28x10^{-5}$ [c]
Cuticular resistance, r_c (s/cm)	80[f]	200[f]	-	-
Henry's Law constant, H_C (Pa-m^3/mol)	72.37[g]	$84.43x10^3$ [g]	$1.01x10^3$ [g]	$5.08x10^{-10}$ [c]

[a](Scire et al., 2000), [b](GasSim 2, 2005), [c](Dortch et al., 2005), [d](Boerboom et al., 1969), [e](Himmelblau, 1964), [f](Currie and Bass, 2005), [g](Sander, 1999)

An adequate value was not found for the cuticular resistance to H_2SO_4 and H_2S, therefore, sensitivity studies were conducted to evaluate the influence of the chosen values. Three AERMOD simulations were conducted for H_2S; the first simulation, identified as D_1, used the default proposed (r_c = 80 s/cm), the second (D_2) used the values selected for SO_2 (r_c = $1.36x10^{-5}$ s/cm), and the third (D_n) did not consider deposition.

To compare the results, the relative differences (dr) between the calculated concentrations and depositions at each receptor in the simulations D_1, D_2 and D_n were calculated using the following expression:

$$dr = \left(1 - \frac{m_i}{m_j}\right)100, \qquad (\%) \qquad (6)$$

where m represents the concentration or deposition values and *i, j* indicate the simulations being compared.

The maximum, minimum and mean values of dr for one hour, 24 hours and the whole period show that the relative difference is small, on average 5.6% for 1 hour, 4.7% for 24 hours, and 1.4% for the whole period. Consequently, the deposition increases on the average by 19% for the whole period and 28% for 1 hour. In general, the value selected for cuticular resistance does not significantly influence the results.

3. Case Studies

3.1. CASE 1 - Validation of AERMET+

A study was conducted in order to compare the surface concentrations calculated by AERMOD, using mixing heights obtained from upper air meteorological soundings and mixing heights derived from the UAE using algorithms 1 and 2 (C1 and C2, respectively). This case study included hourly, daily, and annual estimates of SO_2 concentrations and deposition rates, with emissions from 6 point sources located in the domain of the EPA's Test Case 3 for AERMET (EPA, 2007). The concentrations were estimated at three discrete receptors and at 720 receptors included in two Cartesian grids centred on the sources. The first grid includes 240 receptors, has a horizontal resolution of 5 km and covers an area of 60 x 100 km, from south to north and west to east, respectively. The second grid includes 480 receptors and has a horizontal resolution of 0.5 km on a rectangular domain of 12 x 10 km.

Table 3 shows the maximum hourly and daily concentrations and the highest average concentrations at all receptors, with initial mixing heights calculated with different algorithms. The maximum values were used in the comparison because the maximum concentrations are the focus of regulations. The changes in the concentrations with respect to C_0 are calculated as a percentage ($(C_1–C_0)/C_0$ x 100) and as a fractional bias (FB) when UAE are used.

The fractional bias was selected as the basic measure of performance in this evaluation because it is symmetrical and bounded. Its values range between -2.0 (extreme over–prediction) and +2.0 (extreme under–prediction). The fractional bias between C_1 and C_0 is estimated as $2(C_1–C_0)/(C_1+C_0)$.

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 all averaging periods (hourly, daily, and annual). The maximum hourly and daily concentrations were predicted at the same receptor independently of which mixing height estimation algorithm was used: at a receptor 2 237 m from the central source point for hourly concentrations and 1 275 m for daily concentrations.

The highest average annual concentration was estimated at a receptor located 313 m away from the central source when the mixing heights were obtained from the upper air meteorological soundings and the UAE using algorithm 2. When algorithm 1 is used, the maximum concentration of 146 $\mu g/m^3$ was found at a receptor located 829 m from the source centre, slightly higher than a concentration of 145 $\mu g/m^3$ calculated at a receptor located 313 m from the source.

Table 3. *Comparison of surface concentrations calculated by AERMOD using mixing heights obtained from upper air meteorological soundings (C_0) and derived from the UAE using algorithms 1 and 2 (C_1 and C_2 respectively)*

		Actual UA Data (C_0)	UAE, algorithm 1 (C_1)	ΔC_{1_0}, %	FB_{1_0}	UAE, algorithm 2 (C_2)	ΔC_{2_0}, %	FB_{2_0}
Annual Average	Max.	148	145	-2.04	-.0205	149	0.92	0.0092
	Average	12.7	12.4	-6.01	-.0640	12.6	-2.86	0.0292
Highest 1-hour	Max.	15 458	15 469	0.07	0.0007	15 469	0.07	0.0007
	Average	848	812	4.16	-.0292	824	-2.75	0.0279
Highest 1- day	Maximum	2 610	2 603	-0.25	-.0025	2 600	-0.36	0.0036
	Average	159	158	-2.50	-.0304	158	-1.49	0.0164

The deviations in average concentrations are bigger than deviations in maximum concentrations, but less than 6% for algorithm 1 and less than 3% for algorithm 2. These results corroborate the statement of the slight superiority of algorithm 2 over algorithm 1.

The criterion that the performance of a model can be regarded acceptable if FB is between -0.5 and 0.5 (Kumar et al., 2006) was used. Therefore, it can be concluded that the UAE is sufficiently accurate and is a viable approach to provide mixing heights for models such as AERMOD when upper air sounding data are not available.

3.2. CASE 2 – Comparing modelling results with measurement data

The developed methodology was successfully applied to a national case study (Turtos et al., 2007b) where local topography, land use and upper air meteorological data are not available. The AERMOD model was run with the POSTFILE output option for two receptors fixed at the exact location of two air quality monitoring stations (identified as MS–A and MS–B) in order to compare measurements and model results.

The comparison was mainly qualitative. It was not based on statistical techniques, since the study assumed average operating conditions for the whole assessment period and did not take into account variations in the operating management for any reason (e.g. maintenance periods or partial cleaning system failures). Additionally, fugitive emissions were not considered, which were expected to be important, but cannot be estimated.

A period of almost 4 years was simulated including the emissions of SO_2, H_2S, PM_{10} and $PM_{2.5}$ from all point sources and a river basin which was modelled as a complex polygonal area source.

Figure 3 shows the location of the MS relative to the sources and the wind rose for the 36 sectors in the region, which was obtained from the statistical processing of the hourly data used in the calculations.

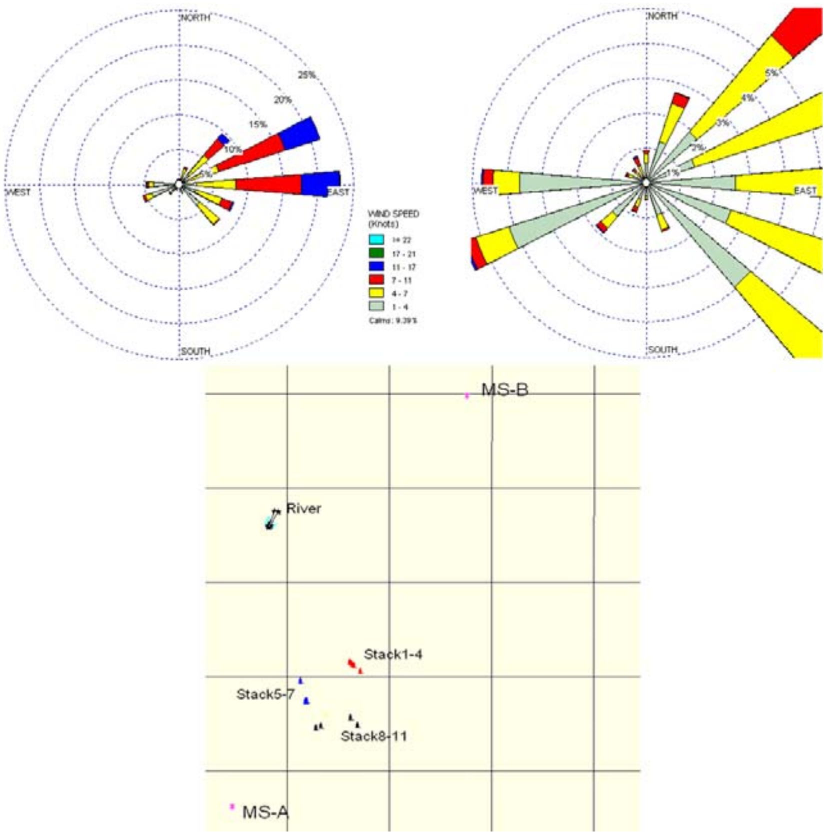

Figure 3. *Wind rose for the study zone and location of sources and MS.*

Predicted and measured concentrations were compared. In general, measured concentrations exceeded predicted values. For PM_{10} and $PM_{2.5}$, the average predicted concentration is less than 1% of the measured values at both MS, suggesting a low contribution of the modelled sources to particulate air pollution. This is in agreement with the analysis of existing sources in the modelling domain, and therefore a detailed comparison for this pollutant is not necessary.

For H_2S and SO_2, the most interesting finding is the following apparent contradiction in the results: the simulated and measured SO_2 concentrations at MS–A are larger than at MS–B, whereas the opposite occurs for H_2S. The isolines of average concentrations at all modelled receptors as shown in Figure 4 support this distinct behaviour, despite having been obtained by using the same meteorological, topographical and land use data.

For SO_2, the concentration isolines follow the prevailing wind direction (see the wind rose and the relative positions of the sources and the MS shown in Figure 3). For H_2S, although the prevailing winds come from the east–northeast and the east, the highest concentrations were found in the east–northeast, caused by an important component of the winds from the west–southwest at very low speeds (< 2 m/s). These winds cause very high concentrations because of the evaporative emissions from the river modelled as an area source. These results agreed with the measurements.

For both pollutants, the measured values exceeded the simulated values. This is an expected result for SO_2 because not all of its sources in the domain were modelled. For H_2S, the differences in the hourly and daily values account for the fact that the study assumed average operating conditions for the whole period. This does not take into account the variations in the operating regimen; i.e., the total emissions are uniformly distributed, but in reality there are emissions exceeding those considered. Differences in mean values were assumed to come from fugitive emissions, which were not considered in the modelling studies.

It is concluded that there is a reasonable match between the predicted and measured concentrations taking into account the simplifications introduced in the modelling, the absence of upper air meteorological data and other uncertainties. Typically, this correspondence can only be achieved by the use of high–resolution models. A simplified model could never explain the apparent contradiction between the concentrations at both MS for SO_2 and H_2S. The consistency of the model estimates in comparison with the pollutant concentration measurements indirectly validates the proposed methodology.

3.3. CASE 3 – Assessing the influence of meteorological conditions to support operational air pollution mitigation

The aim of this case study is to evaluate the influence of meteorological conditions on air quality deterioration in order to support operational mitigation procedures (Turtos et al., 2008; Turtos et al., 2009b).

In the framework of the distributed power generation program, groups of generator sets (GS, internal combustion engine for electric generation) are being installed in urban areas of the country to provide base and emergency power by burning fossil fuel. The operation of a GS could cause significant local air pollution due to emissions of sulphur dioxide, nitrogen oxides and particulate matter.

As air pollution depends on many factors, various mitigation strategies can be applied including proper selection of a GS location, design or operational alternatives. The selected mitigation type depends upon the status of the particular facility. Where GSs are already installed, design and location options are difficult to implement.

It is extremely difficult to assess all effects of meteorological conditions on air quality. Among the local meteorological variables, the wind pattern (primarily horizontal speed and direction) has the most pronounced influence on pollutant concentrations. Common practice is to locate facilities so that the prevailing winds do not transport contaminants to populated areas. However, the incremental concentrations of pollutants depend on the energy balance in the atmosphere, which determines the stability and turbulence (both thermal and mechanical), and the thickness of the mixing layer. The incremental concentrations are negatively correlated with wind speed and the mixing height. Other meteorological variables are cloudiness, ceiling height (because they alter the atmospheric energy balance and consequently the mixing height), temperature, precipitation, and relative humidity.

This case study uses the AERMOD modelling system to evaluate the incremental concentrations due to the emissions of a hypothetical power plant consisting of 4 groups of 4 engines of 1.7 MW each in a grid of polar receptors. The calculations were carried out assuming flat terrain to remove the influence of topography on the results.

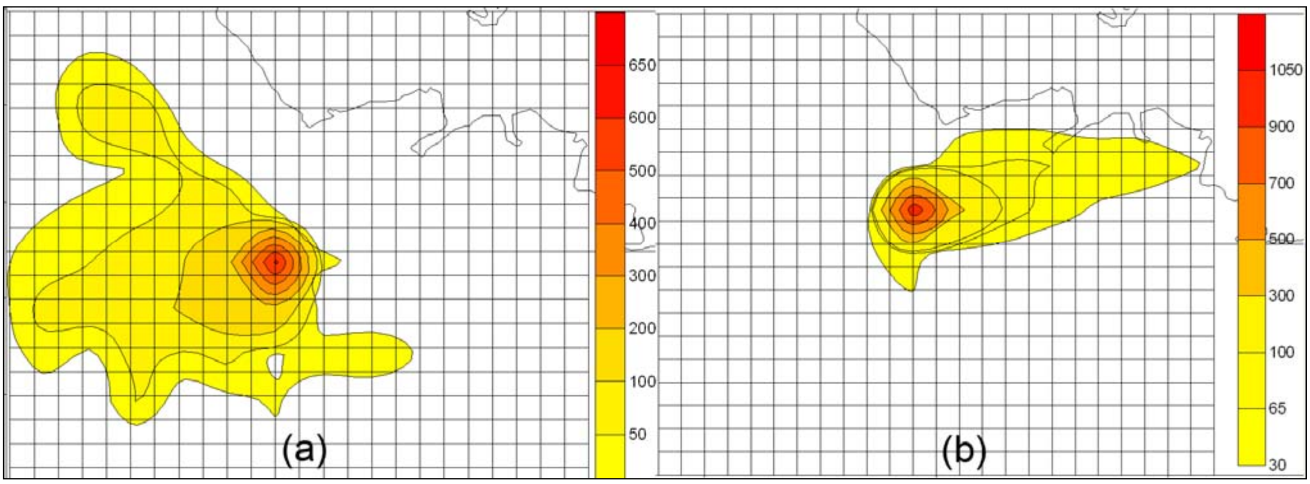

Figure 4. *Contours of average concentrations of (a) SO_2 and (b) H_2S.*

Figure 5 shows hourly incremental concentrations as a function of the distance from the source [up to 30 km in (a) and up to 5 km in (b)] for January 1, 2006, assuming that during the whole day the wind blew to the receptors. This assumption allows excluding the effect of wind direction on the results. For the actual meteorological data file for 2006, the correlation between incremental concentrations and wind direction is around 0.2 at any distance from the source.

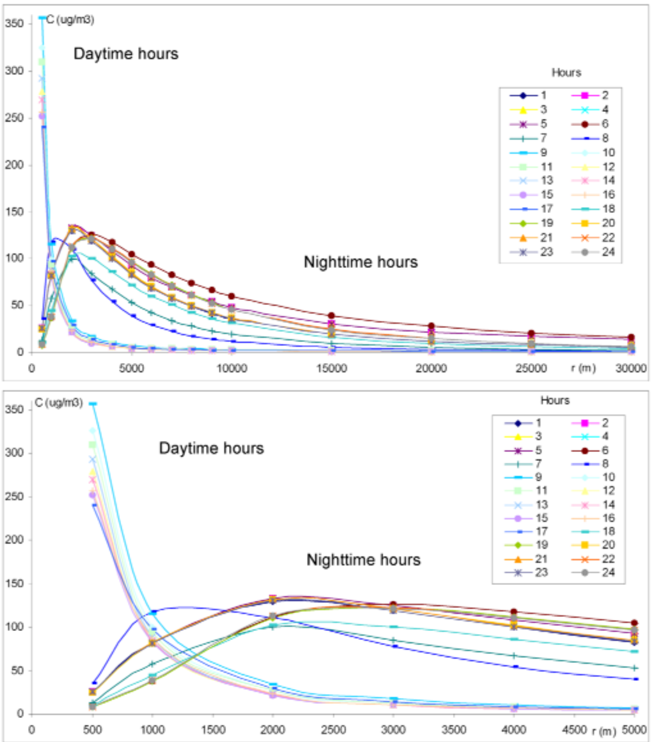

Figure 5. *Dependence of incremental concentrations at different hours on the distance from the source* ***(a)*** *up to 30 km and* ***(b)*** *up to 5 km, assuming a constant wind direction relative to the receptors.*

A distinctive behaviour was observed during daytime and nighttime hours, although in both cases the maximum concentration and the location where it is predicted were shown to depend crucially on the effective emission height. During the day, the concentrations are very high at the receptors close to the source and decay sharply (at 2 km from the source, concentrations have been reduced by an order of magnitude). At night, when stable conditions prevail, the peak concentrations were reached at receptors farther from the source, but the decay is softer, so that significant concentrations are maintained away from the source. Although the graph corresponds to one day of the year, this behaviour is representative of all days.

This distinctive behaviour allows making some suggestions regarding the operational management of the generator sets, and even about their location, i.e. to locate the generator sets at a greater distance from residential areas than the distance where the maximum concentration is reached at night. This exceeds the distance at which the maximum concentration is predicted during daytime hours and consequently it is guaranteed that the daytime concentrations will be significantly attenuated.

The plants should never be located downwind of other plants in the direction of prevailing winds, because the overlapping of the pollutant plumes is greatest in this case. The direction of prevailing winds in Cuba is NE (northeast), i.e. winds blowing from the northeast to the southwest.

Operational measures can be applied to reduce the impact of GS on air quality. It is proposed to adapt the operating regimen for each site according to the distance to areas with high population density:

1. During daytime hours, it is recommended that GSs located in densely populated areas operate at low capacity or they do not operate at all.

2. At night, it is encouraged that GS located in urban areas but more than 2 km from densely populated areas do not operate or operate at low capacity, since peak concentrations are encountered relatively far from the source and then decrease gradually with distance.

A real–time monitoring of both emissions and air quality through modelling could support dispatching of mitigation options. This is recommended even when air quality monitoring systems are operating, due to their inability to identify the contribution of a specific source.

4. Conclusions

The present work confirms the possibility of implementing high–resolution models such as AERMOD to simulate dispersion of local pollutants in Cuba and other countries, despite the absence of some required input data and different meteorological and climatological conditions with respect to the region where the model was developed. This assertion is based on the validation of the developed methodological solutions and their corresponding computer tools. The implementation allows us to conclude that:

1. The methods proposed to complete the data required by the high–resolution models for the emission sources characterization, which are unavailable in the country, are at the level of international practices.

2. The lack of required upper air meteorological data was resolved. The major efforts were concentrated on developing of alternative methodologies for estimating the mixing height from surface data only. Regarding these methodologies, it was concluded that:

a) The influence of the parameters *Nu*, *A* and *B* used in the algorithms is not significant in the results in the range of assumed values for these parameters, although the best results are achieved with Nu = 0.013, A = 2.5 and B = 5.
b) The results of both algorithms are very similar and can be used with no significant variation in the concentrations later calculated by AERMOD.
c) The implementation was validated through:
   - The correlation of the mixing heights calculated with AERMET+ using surface and upper air meteorological data, for all test cases of the original model.
   - The comparison of the incremental concentrations estimated by AERMOD using AERMET (with surface and upper air data) and AERMET+ (using only surface data).

3. The lack of a DEM with the appropriate resolution for the model domain does not prevent the use of high–resolution models, as there are free online data sets that fulfil these requirements. It is proposed to combine the SRTM2 data set (spatial resolution of 3'') with GTOPO30 (spatial resolution 30'').

4. The availability of updated land use digital layers of the model domain with the proper resolution is also not a limitation.

The "North America land cover database" in Lambert Azimuthal projection of equal areas can be used. It is proposed to replace AERSURFACE by the combined use of GIS and a land use layer of the model domain processed with the application *LandUse.xls*, developed specifically for this purpose.

5. A comparison of AERMOD results using the proposed methodology with values measured at two continuous monitoring stations, although primarily qualitative because statistical techniques were not used, showed good agreement and it was presented as an indirect validation of the methodology, reinforcing the need to introduce high–resolution modelling.

This validation allows us to propose the inclusion of AERMOD in the national modelling framework at the local scale, despite its relative complexity in data and large computation time when multiple sources and receptors are modelled.

This proposal is the base for solving the problem of insufficient capacity of modelling tools in the country for assessing and monitoring local air pollution. Such models are an indispensable complement to measurements in any context, but most importantly in Cuba and other developing countries, due to lack of resources for installation of an adequate air quality monitoring network.

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Supporting Material Available

The MSExcel application (*LandUse.xls)* that was used to calculate a weighted average of the Albedo and Bowen ratio at midday and an arithmetic average for the surface roughness length as inputs to AERMET. This information is available free of charge via the Internet at http://www.atmospolres.com.

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