IMPACT OF HEIGHT AND LOCATION OF STACKS IN A LAGRANGIAN PARTICLE MODEL: INDUSTRIAL COMPLEX IN VENEZUELA, CASE STUDY.

IMPACTO DE LA ALTURA Y LOCALIZACIÓN DE CHIMENEAS USANDO UN MODELO LAGRANGIANO DE PARTÍCULAS: CASO DE ESTUDIO; COMPLEJO INDUSTRIAL EN VENEZUELA.

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ABSTRACT

In absence of information about the system to be simulated, it is important to know the uncertainties associated with the assumptions made. The present work is a comparative study of the effect of the height and location of stacks on the spatial distribution of pollutants in the air and the pollutant concentration on the surface using the Lagrangian particle dispersion model (LADISMO). The study was applied to the dispersion of total suspended particles (TSP) from 27 stacks located in an industrial center in Venezuela. The criterion for comparing Lagrangian particle paths has proved to be stricter than the criterion for comparing TSP-24h concentrations. Furthermore, the effect of the height of emission sources seems to be not important if just a maximum of 25% of the stack heights are modified and the effect of the location of emission sources on the trajectory of pollutants seems to be not relevant.

KEY WORDS: Lagrangian particle dispersion model, air pollutant concentration, Lagrangian-particles trajectory, impact of height and location of stacks.

RESUMEN

Cuando no se dispone de información completa sobre los datos de entrada para hacer una simulación, se hace necesario conocer la incertidumbre asociada a las suposiciones hechas. En el presente trabajo se hace un estudio comparativo del efecto de la altura y localización espacial de las chimeneas, sobre la trayectoria de los contaminantes emitidos por las mismas, haciendo uso del Modelo Lagrangiano de dispersión de partículas (LADISMOS). Este estudio fue aplicado para la dispersión del total de partículas suspendidas (TSP) desde 27 chimeneas localizadas en un complejo industrial en Venezuela. Se demostró que el criterio de comparación de la trayectoria de las partículas Lagrandianas resultó ser más estricto que el de comparación de la concentración de TSP -24h. Así mismo, el efecto de la altura de la fuente de emisión pareciera no ser significativo siempre y cuando se desconozca el 25% del total de las alturas de las chimeneas.

PALABRAS CLAVES: Modelo de dispersión de partículas Lagrangian, Concentración de contaminantes en el aire, Trayectoria de partículas Lagrangian, Altura de impacto y ubicación de aglomeraciones.

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INTRODUCTION

The results of the mathematical simulation of a phenomenon as complex as the atmospheric diffusion of pollutants is, although not accurate, the most valid tool for planning and implementation of remedial measures, as they attempt to identify those areas affected by air pollution and those sources responsible for it. In the absence of detailed information about the system to be simulated, it is important to know the uncertainties associated with the assumptions made, in order to establish the degree of confidence in the results.

Using an air emissions inventory to nine industries located in an industrial complex - IC in Venezuela (Cremades and Rincón, 2011), were identified 55 point sources that emit at least one ton per year of TSP (total suspended particles) from IC. However, in this emissions inventory, the exact height and coordinates of all the stacks are not known. It is then necessary to assume their height using guidelines proposed by several authors (Walas 1988; Perry et al, 1985), previous experience and equipment vendors quotations.

The aim of this study is to know the influence of the height and location of the stacks on the pollutant path in the air and its concentration at some immission volumes on the surface, by means of the LADISMO Lagrangian particle dispersion model. This study was developed through a case study in an industrial complex on the northeast coast of Venezuela.

Table 1. *Main input data of LADISMO.*

Datatype	Function	Input data
Configuration	Basic data and data for the diagnostic sub-model	Time step[1]. Number of Langrangian particles per minutes emitted by each source. Duration of simulation. Pollutant type Interval of simulation[2]. Seed for generating random numbers. Deposition of particles[3].
Domain	Terrain orography	UTM coordinates of the SW corner in the domain. Cell size in the XY plane. Number of points in the W-E direction and in the S-N direction. Number of vertical layers. Height of each vertical layer. Top height of the domain, Grid type. Land uses at each grid cell.
Meteorology	3D wind field	Height of boundary layer. Height of surface layer. Monin-Obukov's length. Surface meteo stations: Number. Wind speed and direction. Temperature, solar radiation and pressure at surface. Relative humidity. Pasquill's stability. Upper meteo stations: Number. Height of mixing layer and number of layers. For each layer: wind speed components, temperature lapse rate, Pasquill's stability.
Emission	Pollutant path and concentration	UTM coordinates of emission sources. Height and diameter of each source. Exit temperature, emission rate, and pollutant concentration for each interval of simulation.
Inmission	Information about inmission points	UTM coordinates of inmission points. Pollutant concentration measured for each interval of simulation.

Source: *Own elaboration*

[1]At each time step, positions of the Lagrangian particles are updated. This should be small enough so that the displacement of particles be smaller than the length scale variation of meteorological data.
[2]Simulation interval between two requests for emission and meteorological data.
[3]Deposition of particles occurs when a particle leaves the domain or when it goes below the ground. In both cases the particle is discarded.

The model

The Lagrangian particle dispersion model LADISMO, developed at the Universitat Politécnica de Catalunya (Hernández 1995), simulates the dispersion of air pollutants coming from one or more point sources (stacks) and is specially suited for the diagnosis within short time periods at local-regional scale, taking into account the terrain and the three components of wind speed. It includes:

(1) one sub-model of diagnostic type for generating wind fields and,

(2) one sub-model of Lagrangian particle type for dispersion.

The diagnostic model for generating 3D wind fields follows Sasaki (1970a,b), Achtemeier (1975) and Sherman (1978) approaches, and incorporates Endlich et al (1982) and mainly Mathur and Peters (1990) updates. On the other hand, the Lagrangian particle model simulates the transport and dispersion of an atmospheric passive pollutant, tracking the trajectories of many Lagrangian-particles (computational) to build up a representation of the concentration distribution.

The theory and principles behind the Lagrangian model are well documented in technical literature like Zannetti and Al-Madani (1983), Zannetti (1986, 1990), Reid (1979), Thomson (1984, 1986), de Baas et al. (1986), Hanna (1979; 1981), and Lamb (1979). For more details on LADISMO, see Hernández et al (1994), Hernández (1995). The input data required by LADISMO are organized in several input files. Table 1 shows a summary of the main input data required by both sub-models of LADISMO.

LADISMO was validated successfully in three cases:

1) Castellón power plant located at the Spanish Mediterranean coast (Hernández et al, 1994) where emissions of SO_2 came from two 150 m height stacks, whose releases varied from 1000 to 6500 $g.s^{-1}$, and,

2) and 3) Guardo power plant located at the mountain of Palencia province, north central Spain (Hernández and Cremades 1997). Case 2 refers to an elevated release of SF6 gas tracer (185 m a.g.l.). During this experiment a strong inversion and a dense cloud cover with a natural stability prevailed. The release rate was about 9.2 g s^{-1}. Case 3 refers to a release of SF_6 gas tracer from the valley floor during drainage flow. The emission location was at the Vivero site, at 3.5 km to the northeast of Guardo Power Plant. The release rate was about 8.3 g 5-1 during the experiment. The results of these two cases were compared with results obtained using the MATHEW/ADPIC system (Lange, 1978).

Study area

The study area is located on the northeastern coast of Venezuela, bounded on the southeast by the Coordillera de la Costa. The types of industries located in the IC are: one gas processing, four petrochemical industries, and four extra heavy crude upgrading industries. Those industries emit around 238 kg:h-1 of TSP (from 55 stacks).

For diagnostic sub-model, the study area has been discretized in 80 x 90 cells-grids. Its south-west corner has the following UTM coordinates: X = 266 433 m, Y = 1 064 771 m. The horizontal cell size is 1000 x 1000 m^2.

The vertical spacing is variable and consists of 1 terrain-following layers with a top height of 10 000 m (0, 6, 12, 50, 100, 200, 400, 800, 1500, 5 000, 10 000 m). Therefore, the domain size is 80 000 x 90 000 x 10 000 m^3.

At 30 km away from IC in the East direction, there are four little cities: Barcelona (Ben), Lecheria (Lec), Puerto La Cruz (Plc), and Guanta (Gnt), while at about 15 km from IC in the West direction there are Píritu (Pir) and Puerto Píritu (PPI) cities.

The study area has one TSP sampling station at Bcn city and other at Plc city. These stations collect TSP values of 24 hours (TSP-24 h) every six days. It also has three surface meteorological stations: Urucual, Panamayal, and Criogénico, whose data are reported every hour. Of a total of 8 760 records expected in a year, 7 512 were available for 2006. It was impossible to obtain experimental data for vertical soundings of temperature and wind speed for the study area. This information was obtained every six hours (01:30, 07:30, 13:30, 19:30, LST, Local Standard Time) from NOAA website (ARL, 2010) for one location (UTM coordinates: X: 317 092; Y=1 113 000 m).
Fig. 1 shows the horizontal plane of the study area.

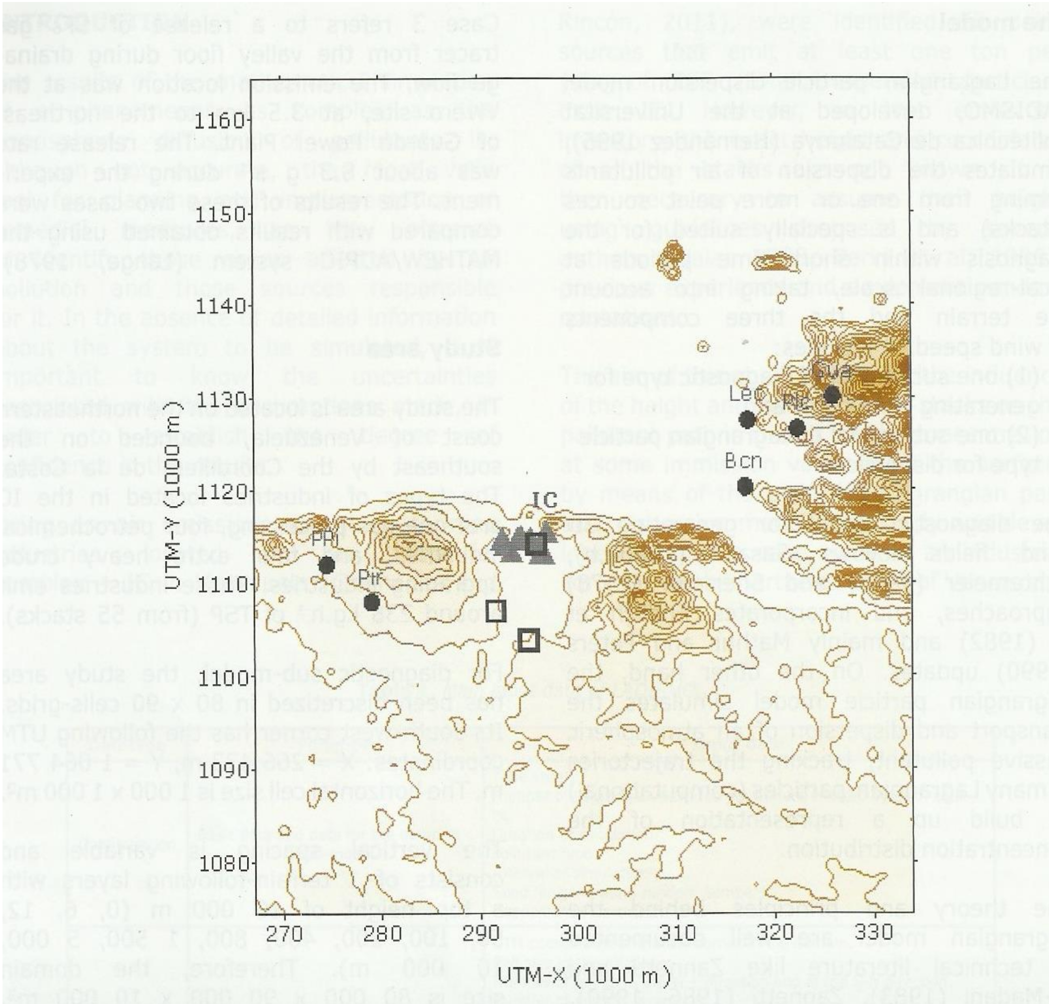

Figure 1. *Horizontal view of the study area*
The following locations are identified: the stacks with grey triangles; main cities with black dots; meteorological towers and upper wind (sounding) with empty black squares.
Source: Own elaboration

Selection of periods

The study area is located in an inter-tropical area with a rainy season and other drought season. The average monthly temperature is constant throughout the year, variations of 2 °C (see Fig. 2). Daily temperature ranges go from 18 to 39 °C. Solar radiation on the region maintains a similar pattern during the year, with a maximum between 12:30 and 13:30 LST, depending on the season.

In this region are observed surface winds from the NE, NW and S (Goldbrunner, 1983). Upper thermal gradient has a pattern of similar behavior during the year. Between 200 and 300 m agl (above ground level), the vertical gradient of temperature presents condition slightly stable or neutral. In the 2006, winds at the station Criogénico showed three trends (NE, S, WE), clearly distributed throughout the year: NE from January to May, S from May to September, and a combination of NW and NE winds between September to January. Wind speed at that station is less than 6.5 m.s-1. Three periods which complete meteorological information for six consecutive days were selected: period #1, February 6-11, 2006; period #2, June 5-10, 2006, and period #3, October 23-28, 2006. Fig. 3 presents the wind roses for selected periods in Cryogenic station. The three periods had low rainfall. During those periods only rained 0.4 mm between days 6 and 8 June, and on 23 October. The three periods selected are also representative of the temperature, relative humidity, solar radiation and rainfalls in the study area.

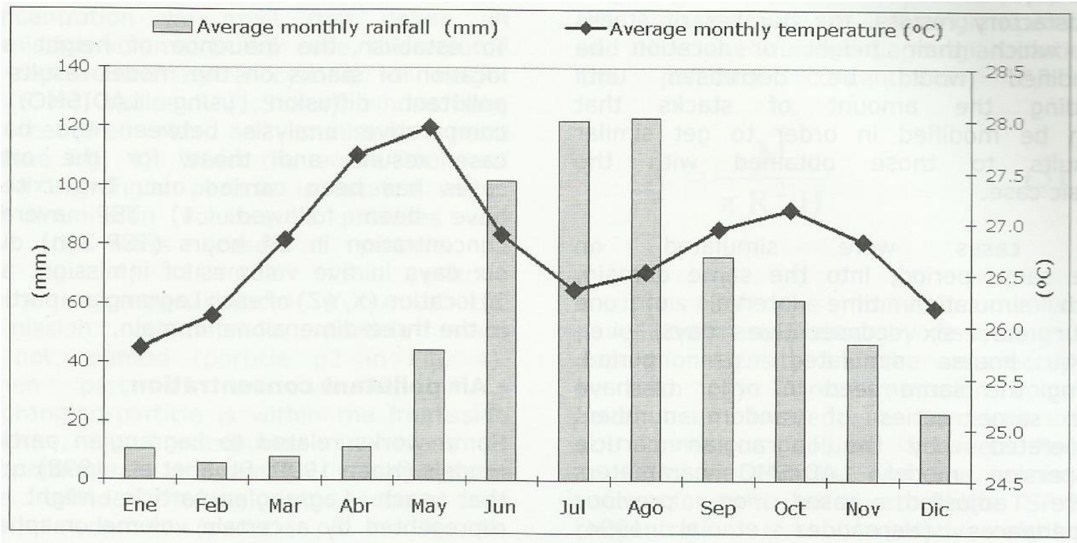

Figure 2. *Average monthly rainfall and average monthly temperature for 1955-2008*

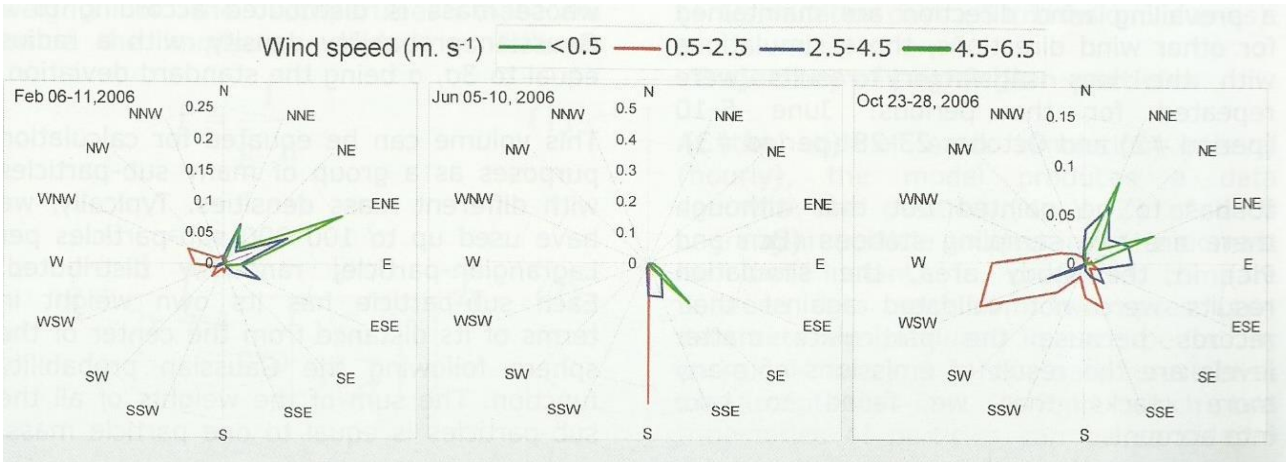

Figure 3. *Wind rose at the meteorological Cryogenic Station*
Source: Own elaboration

Case Studies

The universe of this study is limited to 27 stacks which the information about their height and location is known. These stacks belong to seven out of the nine plants operating in the IC and these stacks are located in an area of about 20 km2, whose Southwest corner is: UTM-X = 293 000 m, UTM-Y = 1 112 000 m. The following case studies have been simulated for the period February 6-11 (period #1):

- Basic case, which represents the actual height and location of the 27 stacks inside the IC. This case is considered as reference or "reality".

- Height cases, where the height of the 27 stacks are modified with respect to the basic case. Two simulations are carried out by changing the heights of all stacks.

  • hmax case. All the heights are considered equal to that highest stack in the basic case (67.1 m).
  • hmin case. All the heights are considered equal to that the lowest stack in the basic case (5.5 m).

- Location cases, where the locations of the 27 stacks inside the IC are changed with respect to the basic case. The new location must be within the battery limits of each industry. The process area of each industry is less than 1.5 km2. Two new simulations are studied:

  • row case. The stacks are placed in rows in the middle of the battery limits of the plant to which they belong.
  • random case. The stacks are placed at random within their plant battery limits.

If any of these cases did not give satisfactory results, the number of stacks to which their height or location be modified would be decreased until finding the amount of stacks that can be modified in order to get similar results to those obtained with the basic case.

All cases were simulated on the same period, into the same domain, with simulation time intervals of one hour for six consecutive days, i.e., 144 hours simulated per period, using the same seed in order to have the same series of random numbers generated by the Lagrangian particle dispersion model. LADISMO parameters were adjusted based on previous experiences (Hernández et al 1994; Hernández and Cremades, 1997).

To check whether the results obtained for a prevailing wind direction are maintained for other wind directions, those simulations with the less satisfactory results were repeated for the periods: June 5-10 (period #2) and October 23-28 (period #3).

It has to be pointed out that although there are two sampling stations (Bcn and Plc) in the study area, the simulation results were not validated against their records because the particulate matter levels are the result of emissions of many more stacks that we failed to take into account.

Comparative analysis

To establish the influence of height and location of stacks on the model results of pollutant diffusion using LADISMO, a comparative analysis between the basic case results and those for the other cases has been carried out. Two criteria have been followed: 1) TSP. average concentration in 24 hours (TSP-24h) over six days in five volumes of inmission, and 2) location (X,Y,Z) of each Lagrangian-particle in the three-dimensional domain.

- Air pollutant concentration

Some works related to Lagrangian particle models (Haan 1999, Stohl et al., 1998) refer that each Lagrangian-particle might be represented by a certain volume or sphere of uniform or variable density. In our case, we have assumed that each particle is a sphere of variable density whose mass is distributed according to a Gaussian probability density, with a radius equal to 3σ, σ being the standard deviation.

This volume can be equated for calculation purposes as a group of many sub-particles with different mass densities. Typically, we have used up to 100 000 sub-particles per Lagrangian-particle, randomly distributed. Each sub-particle has its own weight in terms of its distance from the center of the sphere following the Gaussian probability function. The sum of the weights of all the sub-particles is equal to one particle mass.

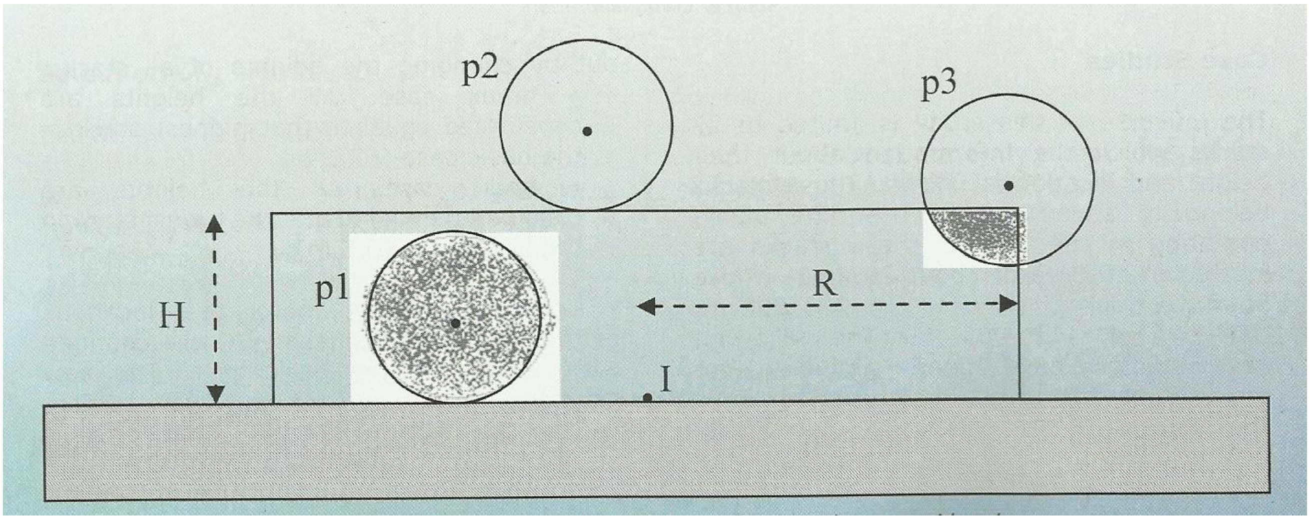

Figure 4. *Schematic 2D view of the inmission volume considered for computing pollutant concentrations*
Source: Own elaboration

For computing the air pollutant concentration we must first define an immission volume. In our case, this volume is represented by a cylinder of height H (6 m), radius R (1.5 km), whose base is centered at an immission point I (see Fig. 4). When the entire "volume" of a Lagrangian-particle is located within the immission volume, it provides one unit of mass (case of particle p1 in Fig. 4). If the whole volume of a Lagrangian-particle is out of the immission volume, its particle mass is not counted (particle p2 in Fig. 4). When part of the volume of a Lagrangian-particle is within the immission volume, its contribution in mass is proportional to the particle volume inside the cylinder, taking into account its variable density (particle p3 in Fig. 4).

In this last case, its contribution in mass can be approximated as the sum of weights of the sub-particles that are inside the immission volume, as follows:

$$f = \frac{1}{\bar{g}\ n} \qquad (1)$$

$$g = \frac{1}{2r}\int_{x=0}^{x=r} \frac{1}{\exp\left[\frac{1}{2}\left(\frac{x}{\sigma}\right)^2\right]}\,dx \qquad (2)$$

$$w = \sum_{i=1}^{n} \frac{f}{\exp\left[\frac{1}{2}\left(\frac{d_i}{\sigma}\right)^2\right]} \qquad (3)$$

where n is the number of sub-particles in one Lagrangian-particle, r is the radiusof Lagrangian-particle sphere (=3σ), d_i is the distance between a sub-particle i and a immission point, and w is the weight fraction of one Lagrangian-particle partially inside the immission volume. Then, total equivalent mass of particles, M, inside the cylinder can be calculated as:

$$M = \frac{Q}{L}\sum_{j=1}^{N} w_j \qquad (4)$$

where Q is the pollutant emission rate, L is the emission rate of Lagrangian-particle, and N is the number Lagrangian-particle. The pollutant concentration, C, is:

$$C = \frac{M}{\pi R^2 H} \qquad (5)$$

Locations of the immission volumes have been established by assessing the population density and the area occupied by each city. Three immission volumes have been located in Barcelona city, one immission volume between Puerto La Cruz and Guanta, and one immission volume for Píritu and Puerto Píritu. TSP-24h concentration is subsequently calculated as a simple average of the concentration of particles in each hour at each immission volume. Therefore, there are 30 records (= 6 simulation days x 5 immission volumes).

-Trajectory of Lagrangian-particles

At the end of each simulation interval (hourly), the model produces a data set with the position (X, Y, Z) of each Lagrangian-particle located into the domain for that instant. In order to compare between data sets from two cases (144 data sets are produced in each period for one single case), it is necessary to establish an acceptance limit beyond which two trajectories of particles can be considered similar one each other. Whereas some particles are lost when they go outside the domain, and there is no guarantee that the particles that were lost in one case paired up with their counterparts in the other cases, we have defined an acceptance limit of 80%, i.e., 116 out of 144 data sets should be no different.

Each Lagrangian-particle emitted from a stack is located at a point (X, Y, Z) within the 3D domain. Let d be the distance between the position of each Lagrangian-particle and the SW corner of the domain (266 430, 1 074 771, 0 in m). For each study case the set of distances d for each simulation interval (1 hour) was compared with the homologous set of distances d from the basic case. If the difference between these two data sets is zero or very small, it is considered that the path followed by particles is the same. In this approach, by using statistical tests that compare cloud data for the analysis of the differences between two sets (t-Student test for equal variances), we have considered that each particle is just represented by a point, i.e., volume equal to zero.

Results and discussion

In order to know whether TSP-24h concentrations for the basic case are not statistically different from those for the height and location cases, separately, a statistical analysis was done. Table 2 shows this statistical analysis for the period February 6-11. For all study cases t-Student test indicates that there are not any statistically significant difference (> 5%) between the TSP-24h concentration for basic case and the other cases. Variance has high values due to the large difference between the maximum and minimum, because during the first two days simulation did not generate enough background for detecting presence of pollutants at immission volume.

Concentration is null for 48 hours, because the Lagrangian-particles have not yet reached the immission volume, and it is assumed that the concentration of TSP is zero at the beginning of simulation (zero background).

As to the statistical analysis of Lagrangian-particle path, Table 3 presents as an example P-values of the t-Student test for d between the basic, row, random hmax, and hmin cases, for February 6-11 at 12:00 and 00:00 LST. P-values for the row and random cases are greater than 0.05 in 90 % of the intervals simulated (i.e., 130 and 132 out of 144 data sets, respectively), in full compliance with the limit of acceptance. This result confirms that there is no statistically significant difference (> 5 %) between the path of Lagrangian-particles for location cases and that for the basic case. This is probably related to the relative small area occupied by each process plant when compared to cell size (1 km2). So, in some cases the stacks are located inside the same grid cell and their emissions are dispersed by the same wind vector.

The analysis of the P-values for hmax and hmin cases shows that the trajectory of particles is not equal to the trajectory of the basic case, because it has P-value < 0.5 in more than 50 % of the time (see Table 3). This result contradicts those obtained by comparing the TSP-24h concentration, whose P-values indicate no difference between concentrations by modifying the height of all stacks. The reason for this lies in that the analysis of the trajectories is more stringent when comparing positions of all particles in the domain, and not of isolated points as is the case when comparing concentrations.

Table 2. *Statics for the analysis of TSP-24h concentration for study cases. t-Student test is significant at 0.05 level*

	Basic case	Row case	Random case	h max case	h min case
P-t value		0.97	0.49	0.93	0.88
Mean (µg/m^3)	7	7	4	8	9
Variance (µg/m^3)	731	535	147	749	815
Mediana (µg/m^3)	0	0	0	0	0
Min value (µg/m^3)	0	0	0	0	0
Max value (µg/m^3)	119	88	45	116	119

Note: P-t value = P-value of t-Student test between TSP-24h concentration for the basic case and that for the other cases (hmax, hmin, row, and random cases); Min value = Minimum value; Max value = Maximum value
Source: Own elaboration

Table 3. *P-value of the t-Student test for the analysis of d for basic case, row case, random case, hmax case, and hmin case t-Student test is significant at 0.05 level*

Study Cases	Feb 6°		Feb 7°		Feb 8		Feb 9		Feb 10		Feb 11	
	12:00 LST	00:00 LST	12:00 LST	00:00 LST	12:00 LST	00:00 LST	12:00 LST	00:00 LST	12:00 LST	00:00 LST	12:00 LST	00:00 LST
Row case	0.21	0.89	0.80	0.19	0.21	0.37	0.16	0.83	0.14	<u>0.00</u>	0.66	0.59
Random case	0.46	0.58	0.91	0.83	0.36	0.91	0.64	0.91	<u>0.00</u>	0.32	0.50	0.41
hmax case	0.96	0.89	0.16	0.66	<u>0.01</u>	<u>0.00</u>	<u>0.02</u>	<u>0.00</u>	<u>0.00</u>	<u>0.00</u>	<u>0.00</u>	<u>0.00</u>
hmin case	0.84	0.38	<u>0.00</u>	0.35	0.17	<u>0.02</u>	0.91	<u>0.00</u>	0.23	<u>0.00</u>	<u>0.00</u>	<u>0.00</u>

Note: LST = Local Standard Time.
P-values with values less than 0.05 are underline
Source: Own elaboration

The number of stacks with modified height was decreasing to find the number that met the proposed acceptance limit: we changed the height of 7 stacks out of 27 (3 stacks with height of 5.5 m and 4 stacks of 67.1 m). Thus, the acceptance limit was exceeded: 120 out of 144 data sets with P-values > 0.05 (84%).

Simulations of the basic, location and modified height cases (by changing up to 25% of the stack heights) were repeated successfully for Jun 5-10 and Oct 23-28, 2006. Fig. 5 shows as an example the distributions of Lagrangian-particles in the XY plane for the basic, random and modified height cases, obtained for the simulation of February 11 at 18:00 LST. Wind field for the first layer of the domain grid (6 m asl) is also depicted in the figure. On the other hand, Fig. 6 contains information equivalent to Fig. 5 for the XZ plane, showing the wind field up to the layer of 1 500 m agl.

From a qualitative point of view, global distribution and bulk trajectory of Lagrangian-particles are very similar in all cases represented. From this visual analysis it may be concluded that by using Lagrangian particle dispersion model LADISMO is not observed significant deviations between the trajectory of particles, due to changes in height or location of the stacks within a reasonable range.

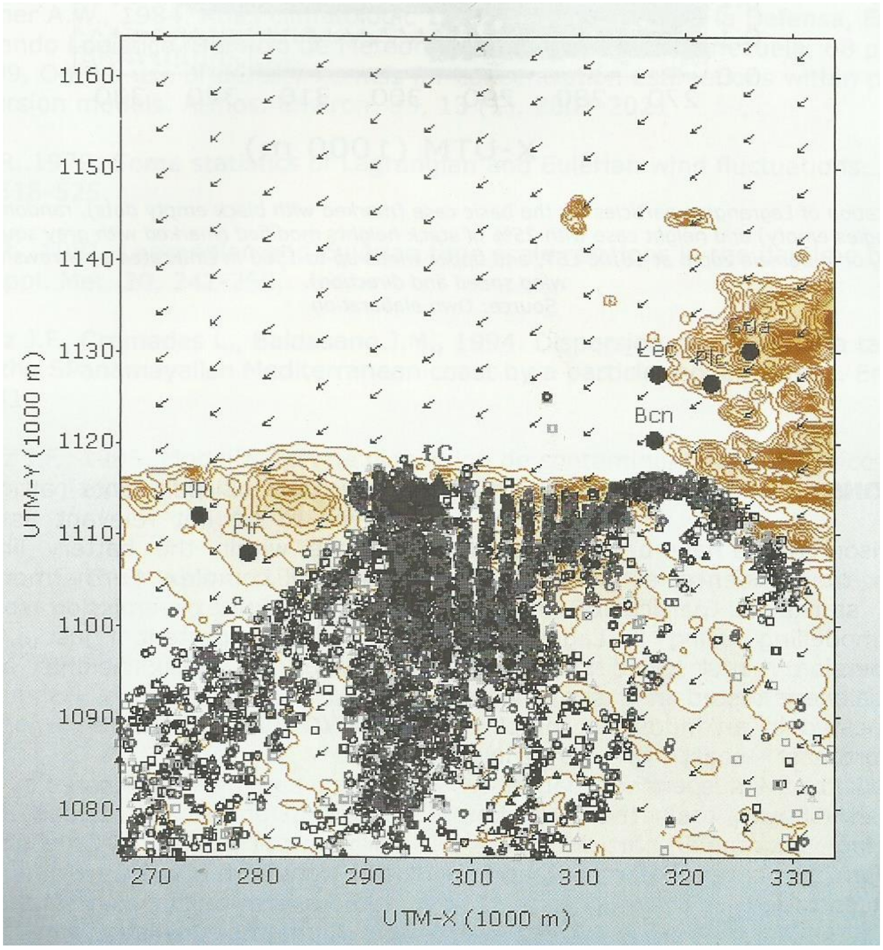

Figure 5. *Location of Lagrangian particles for the basic case (marked with black empty dots), random case (marked with dark gray triangles empty) and height case with 25% of stack heights modified (marked with gray squares empty) for the XY plane, on the domain on February 11, 2006 at 18:00 LST, and surface winds (indicated by arrows that represent wind speed and direction). Locations of major cities are indicated by black filled dots and the stacks are indicated by black filled triangles.*

Source: Own elaboration

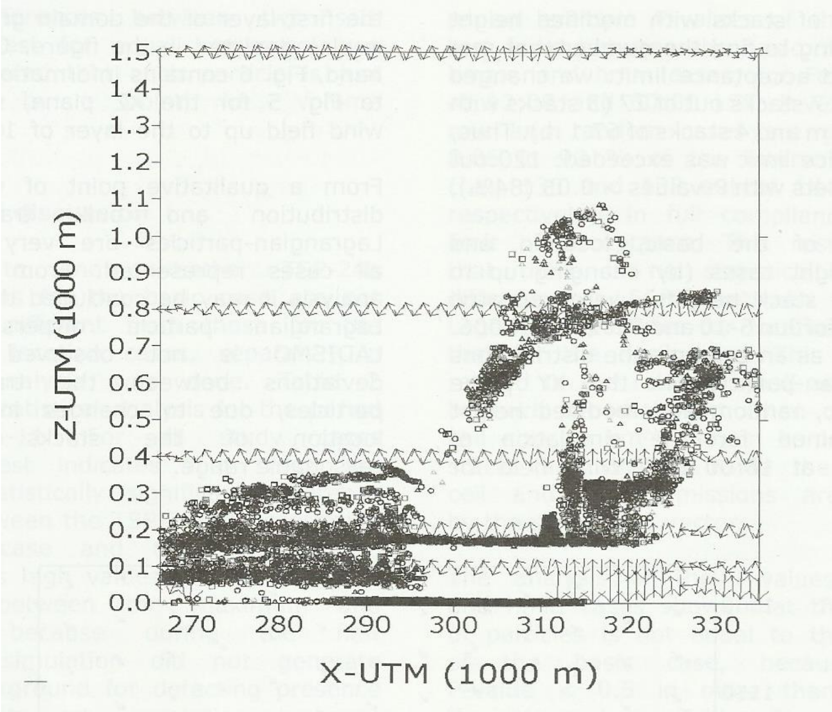

Figure 6: *Location of Lagrangian particles for the basic case (marked with black empty dots), random case (marked with gray triangles empty) and height case with 25% of stack heights modified (marked with gray squares empty) for the XZ plane, on a domain zoom at 18:00 LST, and upper winds up to 1500 m (indicated by arrows that represent wind speed and direction).*
Source: Own elaboration

CONCLUSIONS

Two comparison criteria have been proposed to establish the influence of height and location of stacks in particulate matter dispersion modelling using a Lagrangian particle dispersion model called LADISMO. These criteria were tested in a study with 27 stacks located in an industrial complex on the northeast coast of Venezuela that emitted total suspended particles. It has been shown that the criterion for comparing Lagrangian-particle paths is stricter than the criterion for comparing TSP-24h concentrations.

In the application of the Lagrangian particle dispersion model LADISMO, the effect of the location of emission sources on the trajectory of pollutants at the surface, seems to be not relevant as long as the PS are within the battery limits of their industrial complex. Furthermore, the effect of the height of emission sources seems to be not important if just a maximum of 25% of the stack heights are modified.

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