Comparative analysis between results of Lagrangian and Gaussian Atmospheric Models.

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ABSTRACT

The atmospheric modeling has simple fast-running models with little data demands, which require some academic preparation from users, but the accuracy of their results is questionable and they are recommended only for screening to determine if a complex modeling is necessary or not. SCREEN3 was the screening model used in this research. The use of more complex modeling will depend on the atmospheric conditions in the study area, the complexity of the topography and the variability in terrestrial coverage. The Panama Canal being a complex area, with undulating topography, the presence of the change in water-soil cover that contributes to a three-dimensional variability of the meteorological conditions and the phenomena of fumigation, it was proposed to use the Lagrangian model CALPUFF. However, it was important to consider the evaluation, through a correlational analysis of the results, of the advantage of using CALPUFF instead of SCREEN3. The results of both models yielded Pearson coefficients for the three modeled pollutants (PM_{10}, NO_2, SO_2) in a range of 0.7 to 0.84, indicating a considerable correlation; however, the values of CALPUFF hourly concentrations were greater than the SCREEN3 values up to a factor of 5, which would suggest the use of CALPUFF.

Keyword: Atmospheric Contamination, atmospheric modeling, CALPUFF, Panama Canal, SCREEN3, Thermoelectric Plant.

I. INTRODUCTION

In the modeling of dispersion and transport of air pollutants there are currently a variety of options. Some of less complex and demand for input data, whose results are adjusted to small areas of land with little topographical variation with a single type of land cover and homogeneous meteorological conditions.

In the other hand, there are more complex options that require better training of the user, greater temporal and spatial variation of input data and that are better suited to long dispersion routes, considering a three-dimensional meteorology.

The following questions arise: for a modeling domain selected for this investigation in the vicinity of the Miraflores Thermoelectric Plant located in the Pacific Sector of the Panama Canal, where the area is small, the terrain can be considered flat and the meteorology as homogeneous, based on which the Gaussian model SCREEN3 seems to be the most appropriate, it will be important or not to consider the effects on the variation of land cover, since in the modeling domain there are water-soil interfaces? It will be enough to consider homogeneous meteorological conditions or the three-dimensional variation should be included?

To answer these questions, first it was used the Eulerian Gaussian Model: SCREEN3, version for screening of the dispersion model for Complex Industrial Source (ISC3) [1]. The SCREEN3 is a stable Gaussian plume model from a single source: point with or without flame, area or volume; calculates the maximum concentrations at ground level, after evaluating all possible meteorological conditions. It also includes the calculation of concentrations by fumigation in water-soil interfaces within 3 km of the source. It is recommended for distances up to 100 km,[2]

And then, as Lagrangian Model it was used: CALPUFF of dispersion in packages (*poof's*) recommended for distances up to 300 km from the source,[3] It includes the meteorological modeler CALMET, which constructs a wind field of three-dimensional variation from measurements in superficial meteorological stations and radiosondes in balloons; or from predictions of global meteorological models such as the Weather Research and Forecasting Model (WRF). This three-dimensional meteorology was georeferenced on a grid that included the topographic variation, land use and coverage.[4]

II. MATERIALS AND METHODS

In this research, the following models were used: Gaussian SCREEN3 [5] and Lagrangian CALPUFF v. 5,8,5 [6] both free-licensed and approved by the United States Environmental Protection Agency (EPA), with their respective input data that are detailed later.

2.1 Fixed source of emission and contaminants to modelling

The fixed source of emission chosen was the Miraflores Thermoelectric Plant, which at the time of this investigation had three bunker engines whose emissions were measured and supplied by the call at that time: *Division of Environment, Water and Energy of the Panama Canal Authority* (ACP), during an internship of January to April 2014.[7]

The three characteristic pollutants of fossil fuel combustion in Thermoelectric Plants were modeled: the particulate material with a diameter equal to or smaller than 10 µm (PM_{10}), the nitrogen dioxide (NO_2) and the sulfur dioxide (SO_2).

The three chimneys from each engine were replaced by an equivalent chimney of equal diameter and height, located in the centroid of the triangle formed by the three real chimneys, since the models used only allow a single source of each type. The weighted emissions of the equivalent chimney were calculated for each modeling pollutant as established in Executive Decree No.5 of February 4, 2009, Republic of Panama: "Whereby environmental regulations are issued for emissions from fixed sources".[8]

2.2 Modeling with SCREEN3

Two runs of SCREEN3 were made: one without taking into account the fumigation effect caused by the water-soil interaction of the Miraflores Lock, in the path of the plume coming from the Thermoelectric Plant of the same name and another run taking into account this effect. It was used the meteorological data of the Balboa Station (FAA) located at the coordinates: 8°58'08" N, 79°32'58" W and at 10 m elevation with respect to the Mean Sea Level (MSL), operated by the Panama Canal Authority (ACP). The meteorological data of this Station for 2014 were obtained from the Integrated Surface Data Base (ISD) of the National Atmospheric and Oceanic Administration of the United States (NOAA),[9]

With this meteorological data, the Rose of the Winds was prepared for 2014 using the Wind Rose Plotter (WRPLOT) program,[10] The predominant direction of winds was determined by the rose plotted and using a base reference map it was possible to calculate the distance to the water-soil interface to be used in the second run of SCREEN3.

For both runs, the input data were the following:

- Type of source: point source.
- Dispersion coefficient: rural.
- Receiver height: 0 m (at ground level).
- Emission rate: 2.315 g/s for PM_{10}, 4.514 g/s for NO_2, 23.84 g /s for SO_2.
- Chimney height: 30 m.
- Internal diameter of the chimney: 1.61 m.
- Gas outlet speed: 29.72 m/s.
- Gas outlet temperature: 605.32 K.
- Ambient temperature: 293 K.
- Simple and flat land (same elevation as the base of the chimney).
- Complete meteorology (all kinds of atmospheric stability and possible wind speeds).
- Anemometer height: 10 m (standard for surface measurements in meteorological stations).
- Mixing height Brode2: No.
- Automated distances: mínimum of 100 m and maximum 50 000 m of the chimney.
- Discrete distance: 5 718.5 m (to compare the concentration value SCREEN3 with the calculated by CALPUFF for this receiver as the point with the highest hourly concentration).
- Building Downwash: No.
- Fumigation: No for the first run.
- Shoreline fumigation: within 300 m of the chimney, for the run where fumigation is taken into account.

The program was run and the results were obtained in graphs and in text format for its comparative analysis.

2.3 Modeling with CALPUFF

To determine the influence of the 3D variation of the meteorological conditions, the CALPUFF run required WRF data [11]. Since the measurements of surface meteorological stations and radiosonde probes did not have the necessary spatial coverage.

WRF data were used for the year 2014 in a domain of 50x50 km^2 with a resolution of 4x4 km^2 and 35 vertical levels over 20 m above ground. This data was georeferenced in a grid of 1x1km^2, resolution managed by CALPUF.

The terrain configuration data added to this grid was provided by the Global Coverage Model of the Topographic Mission with Radar on Board (SRTM1),[12] In addition, the land cover use and coverage data was added by the Global Soil Coverage Characterization Model (GLCC),[13] CALMET, the meteorological model of CALPUFF, was run to build the 3D variation field.

Once CALMET was completed, the CALPUFF pollutant dispersion and transport model was run, which required the following input data:

- Coordinates of the chimney: 654 895.7 mE, 995 199.5 mN.
- Elevation of the base of the chimney with respect to the MSL: 19.60 m (calculated by CALPUFF using the SRTM1 Model).
- Height of the chimney: 30 m.
- Average gas temperature: 605.32 K.
- Inside diameter of the chimney: 1.61 m.
- Gas velocity at the outlet: 29.72 m/s.
- Emissions in ton/year: 79.83 for PM_{10}, 147.21 for NO_2, 755.80 ton/year for SO_2.

For more details of the CALPUFF modeling performed, you can consult our article: *Modeling CALPUFF-WRF of dispersion of PMx, NOx and SO_2 emitted by the Miraflores Thermoelectric Plant in the Panama Canal*.[14]

2.4 Comparative Analysis of Results

Maps were made with the results of the models showing the spatial variation of the maximum hourly concentrations of each modeled pollutant. For this, ARCMap v.10.5 with an academic license was used.[15]

For the comparative analysis of the numerical results obtained by each model, Pearson correlation analyzes were performed using Microsoft Excel as a computational tool.[16,17].

III. THEORY/CALCULATION

The distribution of the winds by speeds and frequencies of occurrence, based on the hourly measurements of the FAA surface meteorological station of Albrook, Panama City, are shown in Figure 1. For 2014, the most frequent winds were in a range of 2.10 m/s to 3.60 m/s (7.56 km/h to 12.96 km/s) with an occurrence of 34.2%.

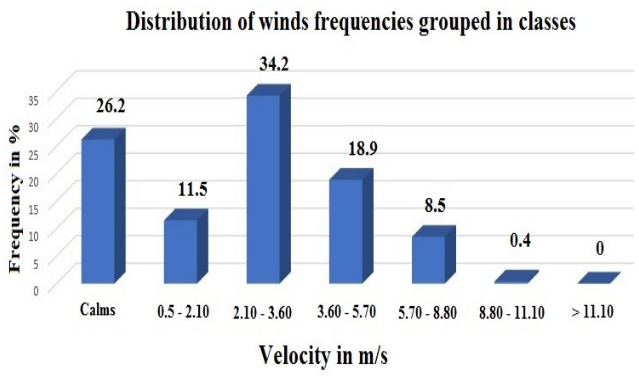

Figure 1

Figure 1. Distribution of measured wind frequencies at the Albrook FAA Station during 2014, grouped into speed ranges. Source: Time data, NOAA, ISD. https://www.ncdc.noaa.gov/data-access/land-based-station-data.

According to the spatial distribution of the winds, based in a homogeneous atmosphere with data from this unique meteorological station, the average direction of the winds, with a frequency of 71%, was at an Azimut 157° N (heading S 23° E), see Figure 2.

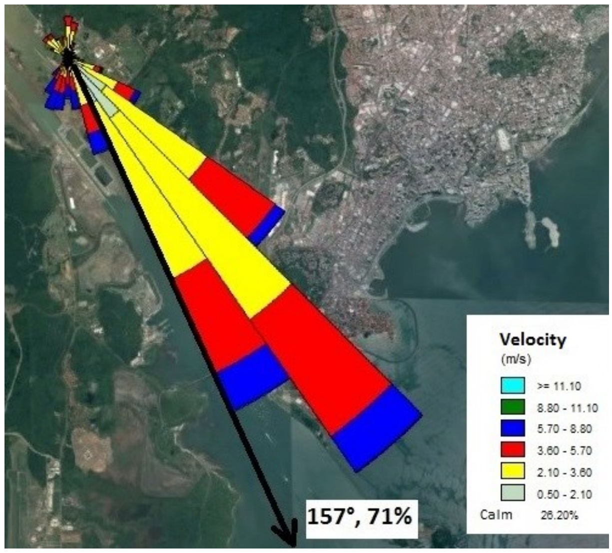

Figure 2

Figure 2. Wind rose based on the data measured at the FAA station in Albrook during the year 2014, grouped at speed intervals. It shows the average velocity vector, its direction and frequency. Picture of Google Earth. Rose of the winds drawn up with the Wind Rose Plotter Program (WRPLOT V. 8.0.2 of Lakes Enviromental Software).

In this average direction of the wind, SCREEN3 modeled the distribution of hourly concentrations of each pollutant at ground level, taking into account the fumigation effect given that the chimney exceeds 10 m in height and the area is rural in that path of the plume.

This phenomenon of fumigation is nothing more than the rapid fall of the plume towards the ground due to having reached the atmospheric layer of thermal inversion, barrier of dispersion. It occurs at a distance from the source, in the direction of the wind, called *inversion breakup*. The respective fumigation is known as *inversion breakdown fumigation*.

The maximum hourly concentrations of 5.13 $\mu g/m^3$, 9.99 $\mu g/m^3$ and 52.79 $\mu g/m^3$ for PM_{10}, NO_2 and SO_2, respectively, at a distance of 1 100 m from the equivalent chimney, can be seen in Table 1 for the run without taking into account the fumigation.

Table 1. Points of maximum time concentration SCREEN3 according to the type of run performed

Distance (m)	Maximum Hourly Concentrations ($\mu g/m^3$)			Type of run of the model
	PM_{10}	NO_2	SO_2	
445	52.39	102.2	539.5	Shoreline Fumigation
1100	5.13	9.99	52.79	No fumigation
8312	7.11	13.86	73.23	Inversion breakdown Fumigation

Taking into account only the inversion breakdown fumigation, SCREEN3 calculated hourly maximum concentrations of 7.11 $\mu g/m^3$, 13.86 $\mu g/m^3$ and 73.23 $\mu g/m^3$ for PM_{10}, NO_2 and SO_2, respectively, at an inversion breakdown distance of 8 312 m from the equivalent chimney, in the average wind direction path (see Table 1).

With the help of the rose of winds, it could be determined that the equivalent chimney is at a distance exceeding 300 m to the nearest water-soil interaction line (see Figure 3).

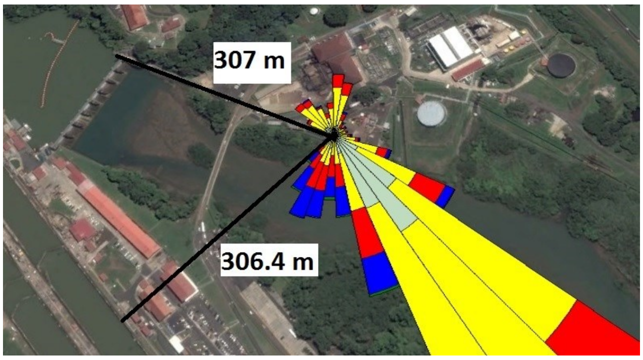

Figure 3

Figure 3. Distance from the equivalent chimney at Miraflores Thermoelectric Plant to the nearest water-soil interaction line for the evaluation of shoreline fumigation with SCREEN3. Picture of Google Earth.

When the wind blows in the direction of each path to the body of water, indicated by the black lines in Figure 3, the plume is pushed back by the mass of air that is located over the water (*thermal internal boundary layer*, TIBL), in the opposite direction and falls to the ground at a short distance from the source. This effect is known as *shoreline fumigation*.

SCREEN3 calculated the shoreline fumigation assuming that the body of water is located at 300 m from the equivalent chimney. The hourly maximum concentrations of 52.39 µg/m^3, 102.2 µg/m^3 and 539.5 µg/m^3 for PM_{10}, NO_2 and SO_2, respectively, at a distance of fumigation of 445 m from the equivalent chimney, in the opposite direction to the wind, were obtained (see Table 1).

It should be noted that the shoreline fumigation only occurs when the wind blows towards the body of water in the trajectories indicated with black lines in Figure 3, being winds of low frequency of occurrence.

For the other trajectories, the body of water is farther away and the calculations of SCREEN3 showed that the height of the plume is superior to the TIBL not presenting shoreline fumigation. This was the result, when the coastal fumigation was evaluated for the average wind direction indicated in Figure 2. In this case the body of water is located 767.61 m from the equivalent chimney.

The maximum hourly concentrations, for each pollutant, calculated by SCREEN3 along the average wind direction for 2014 are shown in Figure 4.

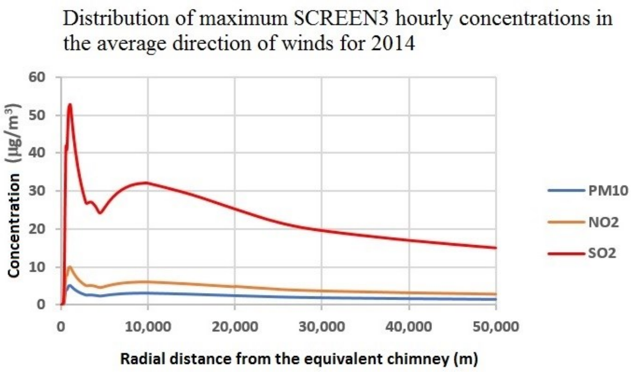

Figure 4

Figure 4. Distribution of PM maximum hourly concentrations of PM_{10}, NO_2 and SO_2 modeled by SCREEN3.These values are given for different wind velocities and atmospheric stability classes of Pasquill-Glifford.

In Figure 4 it can be observed that the maximum hourly concentrations, without taking into account fumigation, are given for receptors at 1 100 m from the equivalent chimney. For shorter distances, the concentration values were increased for a class E stability (*slightly stable*) and winds of 1.0 m/s (3.6 km/h) before 300 m. At 300 m, the concentration shown was given for a class C stability (*slightly unstable*) and winds of 10 m/s (36 km/h). From 400 m to 2900 m the concentrations shown are given for a class A stability (*very unstable*), with winds of 3 m/s (10.8 km/h) up to 700 m, 1.5 m/s (5.4 km/h) up to 900 m and 1.0 m/s (3.6 km/h) the rest. From 3 000 m to 4 500 m the concentration values shown are given for class B stability (*unstable*) and winds of 1.0 m/s (3.6 km/h). From 5 000 m to the 25 000 m the concentrations shown are given for a class E stability and winds of 1.0 m/s (3.6 km/h) and, finally, from 30 000 m to 50 000m the concentrations shown are given for a class F stability (*stable*) and winds of 1.0 m/s (3.6 km/h).

The spatial distribution of PM_{10}, NO_2 and SO_2 hourly maximum concentrations modeled by SCREEN3, considering a homogeneous atmosphere, are shown in Figure 5.

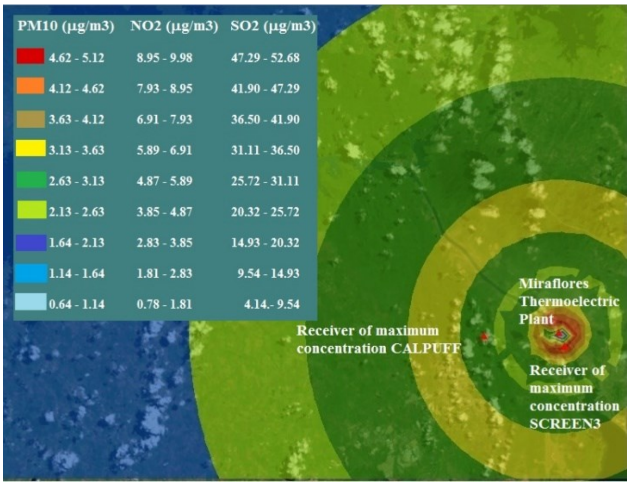

Figure 5

Figure 5. Spatial distribution of PM_{10}, NO_2 and SO_2 maximum hourly concentrations modeled by SCREEN3. Picture of World imagery, ArcGIS online, ESRI.

In these distributions, the maximum hourly concentrations of the three modeled contaminants, without taking into account fumigation, were given at a radial distance of 1 100 m from the source, a wind velocity of 1.0 m/s (3.6 km/h) at 10 m over the terrain surface and a very unstable Class A (*turbulent*) stability atmosphere of Pasquill-Glifford.

The spatial distribution of PM_{10}, NO_2 and SO_2 hourly concentrations modeled by CALPUFF, considering the 3D atmospheric variability, are shown in Figure 6.

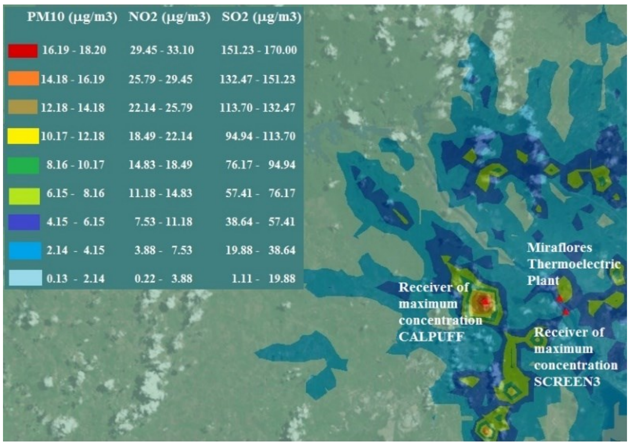

Figure 6

Figure 6. Spatial distribution of PM_{10}, NO_2 and SO_2 maximum hourly concentrations modeled by CALPUFF. Picture of World imagery, ArcGIS online, ESRI.

CALPUFF shows greater spatial variability of the dispersion where the values of hourly concentrations, in general, are higher than those shown by SCREEN3 in a factor of 5 for PM_{10} and 3 for NO_2 and SO_2.

Similarly, to SCREEN3, the maximum hourly concentration values tend to be concentrated near the source. However, due to the atmospheric variability during the year 2014, the maximum hourly concentrations for the three modeled contaminants were given to 5 718 m from the equivalent chimney, on October 12, 2014 at 4:00 am (see Figure 7 and Table 2).

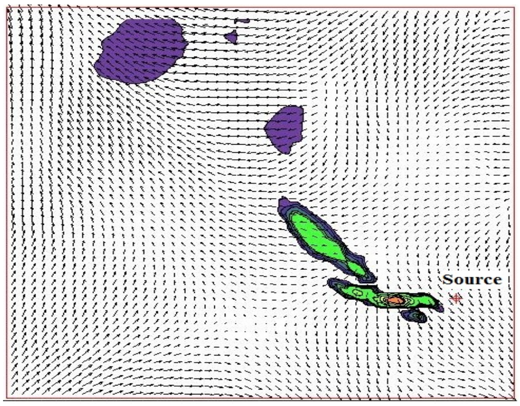

Figure 7

Figure 7. Spatial variation of winds based on WRF data and plume simulation for October 12, 4 a.m., hour of maximum hourly concentrations were given to 5 718 from the source. Picture of CALPUFF View v. 8.4.0.

Table 2. CALPUFF and SCREEN3 values given for the point of highest hourly concentrations CALPUFF

Coordinates UTM WGS84 (m)		Distance (m)	Maximum hourly concentrations (µg/m³)			Model
X	Y		PM_{10}	NO_2	SO_2	
649 181	994 991	5718	18.19	33.1	169.95	CALPUFF
			2.69	5.25	27.72	SCREEN3

This receptor is not in the path of most frequent direction of the winds. However, if the plume were to pass through that receptor sometime, the maximum hourly concentration values would be shown in Table 2, calculated by SCREEN3. Note that these values are very below those calculated by CALPUFF.

IV. RESULTS AND DISCUSSION

It was complemented the graphical and point data comparisons with the results of the correlation analysis between the CALPUFF values and their corresponding SCREEN3 values for the 1x1 km^2 cell centers in the modeling domain of 50x50 km^2. Of the 2 500 centers, were discarded those whose distance to the source was greater than 50 km (limit of SCREEN3) leaving 2 310 receptors with values of hourly concentrations CALPUFF and SCREEN3 for each contaminant modeled.

In Figure 8 you can see the distribution of SCREEN3 values with respect to the radial distance (in meters) from the source to each 2 310 receptors. Since SCREEN3 assumes a homogeneous atmosphere, each concentration value will be given for the only radial distance to the source. However, for CALPUFF the same concentration can be given for several receptors at different radial distances from the equivalent chimney, due to the non-homogeneous atmosphere. For CALPUFF concentrations equal to or less than: 2 µg/m³ of PM_{10}, 5 µg/m³ of NO_2 and 20 µg/m³ of SO_2 the greatest variation in receptor-source distance is given.

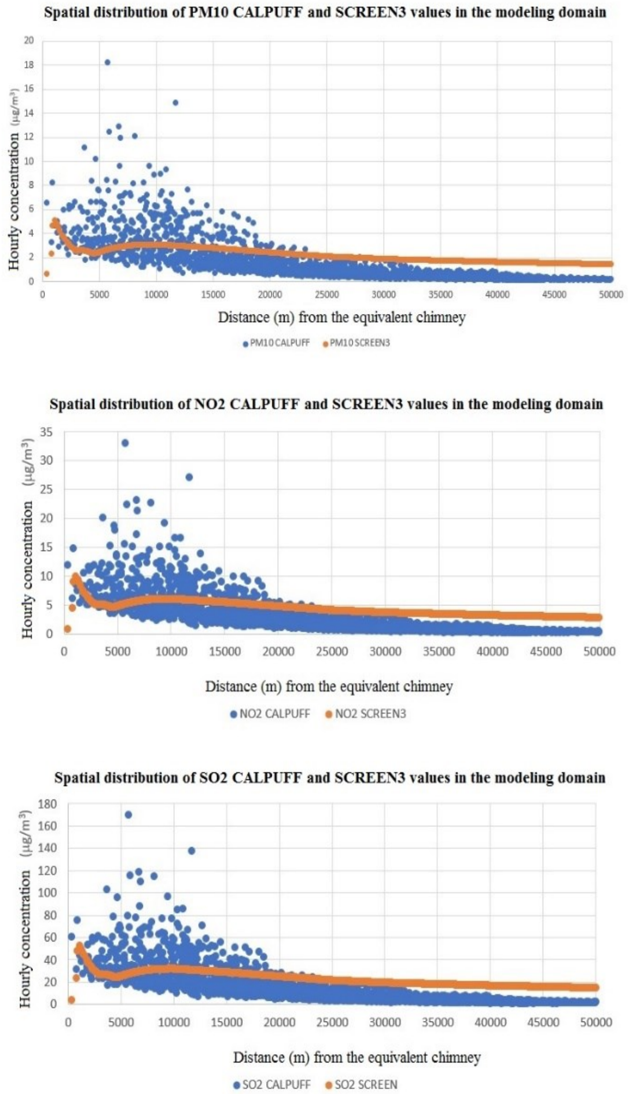

Figure 8

Figure 8. Space distribution of PM_{10}, NO_2 and SO_2 hourly concentrations modeled by CALPUFF and SCREEN3.

If the CALPUFF concentrations are higher than those indicated above, the variation of receptor-source distance is lower and they are presented just for those receptors that are less than 15 000 m from the equivalent chimney (see Figure 8).

The Pearson (***r***) coefficients calculated by Microsoft Excel were 0.70 for the PM_{10} and SO_2 values. For the values of NO_2 the Pearson coefficient was 0.71 (see Figure 9), suggesting a considerable correlation between the values calculated by both models for each pollutant.

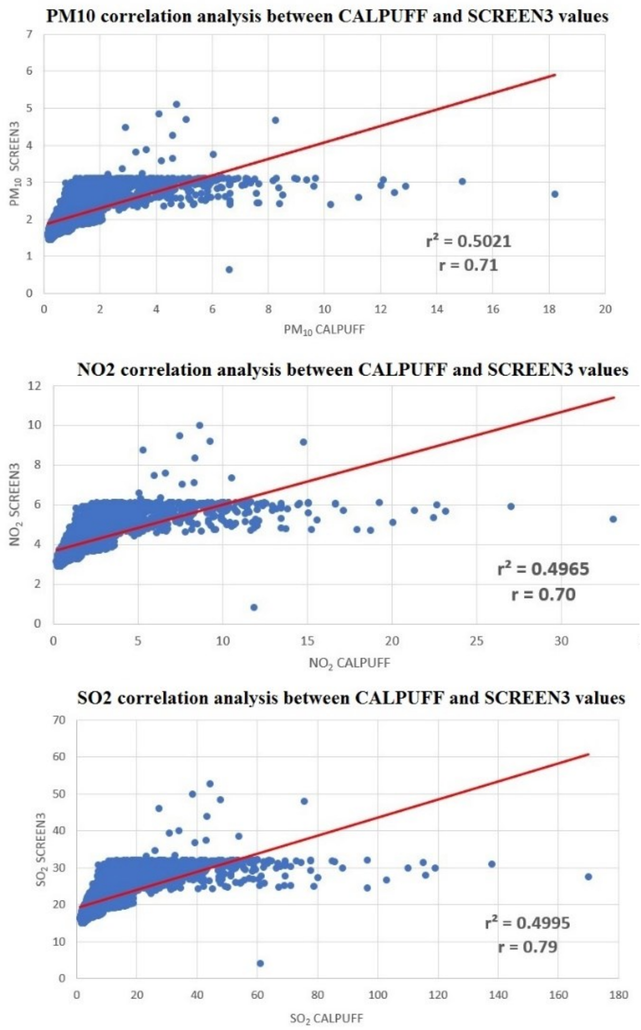

Figure 9

Figure 9. Correlation analysis results of hourly concentrations of PM_{10}, NO_2 and SO_2 calculated by CALPUFF and SCREEN3. The red line represents the line of best fit (correlation 1: 1) and the blue points the realcorrelation of the values thrown by SCREEN3 and CALPUFF. Observe the values of r and r^2 for each case.

However, when evaluating r^2, it was observed that for the three contaminants it is approximately 0.5, which indicates that for 50% of the data there is correlation (considerable) and for the other 50% there is no correlation. This can be seen in Figure 9, for the graphics of the three modeled contaminants, where for the first half of the adjustment line the dots approach it. These Points correspond to all receptors located more than 15 km from the source and most of the receptors located less than 15 km from the source. For the last stretch, the dots are completely away from the adjustment line. These points correspond to those receptors located within 15 km of the source whose CALPUFF concentration exceeds 8 μg/m³ of PM_{10}, 15 μg/m³ of NO_2 and 80 μg/m³ of SO_2.

V. CONCLUSIONS

Based on the results, we conclude the following:

- In atmospheric modeling it is important to include the meteorological 3D variability, the variation in topography and coverage, as well as the fumigation phenomena which reveals points where the concentrations of the modeled contaminants are much higher than those of the point of maximum concentrations determined with a basic Gaussian modeling.
- The research showed that SCREEN3 values are much lower than those calculated with CALPUFF, due to the simplicity of modeling.
- Despite the above, correlational analysis showed Pearson coefficients in the range from 0.7 to 0.84, which translates into a considerable correlation between the SCREEN3 and CALPUFF values for receptors whose hourly concentrations were below 8 μg/m³ of PM_{10}, 15 μg/m³ of NO_2 and 80 μg/m³ of SO_2, regardless of its distance to the source.
- For these receptors the CALPUFF values were slightly higher, differing in the decimals.
- This means that the dispersal behavior given by the Gaussian basic model and the Lagrangian model is similar, although the values do not match exactly.
- However, for those receivers less than 15 km from the source, where concentrations were higher than indicated, there was no correlation between the models. This could justify the use of the CALPUFF model in the study area, although the current literature recommends it for distances equal or greater than 50 km.
- It is advisable to make measurements in the field of the hourly concentrations of PM_{10}, NO_2 and SO_2 to determine whether or not correlation exists between the measured values and those calculated by CALPUFF, considering that there are contributions from other fixed and mobile sources in the study area.

VI. ACKNOWLEDGEMENTS

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