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Original Research

Concentrations modeling of sulfur dioxide pollutant emitted by two industrial boilers in Santiago de Cali (Colombia)

Modelación de las concentraciones del contaminante dióxido de azufre emitido por dos calderas industriales en Santiago de Cali (Colombia)

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Abstract

This article deals with modeling sulfur dioxide (SO2) concentrations emitted by two industries in Santiago de Cali. These industries use different fuel types in their boilers: Boiler 1 uses Fuel Oil, and Boiler 2 uses Diesel. To evaluate and compare the behavior of SO2 concentrations, the substitution of these fuels by natural gas is proposed. Using Aermod View, this pollutant's dispersion was modeled and obtained that the maximum SO2 concentration from the boilers with Fuel Oil and Diesel was 1440.32 µg/m3 for an exposure time of one hour. For a 24-hour exposure time, the SO2 concentration reached 178.56 µg/m3. These levels exceed the limits established in resolution 2254 of 2017, where the maximum permissible value for one hour is 100 µg/m3, and for 24 hours is 50 µg/m3. In contrast, when using Natural Gas as fuel, it is observed that the concentrations are considerably lower. The maximum concentration is 0.74 µg/m3 for a one-hour exposure time, and for a 24-hour exposure time, 0.04 µg/m3. These results comply with current regulations. It can be concluded that natural gas is a more favorable alternative, generating significantly lower SO2 concentrations. This change in the fuel type will favor compliance with environmental regulations and effectively contribute to reducing SO2 concentration in the air.

Resumen

En el presente artículo aborda la modelación de las concentraciones de Dióxido de Azufre (SO2) emitidas por dos industrias ubicadas en la ciudad Santiago de Cali. Estas industrias emplean distintos tipos de combustible en sus calderas: la caldera 1 utiliza Fuel Oil y la caldera 2 utiliza Diésel. Con el objetivo de evaluar y comparar el comportamiento de las concentraciones de SO2, se propone la sustitución de estos combustibles por Gas natural. Mediante el uso de Aermod View se realizó la modelación de la dispersión de este contaminante y se obtuvo que para un tiempo de exposición de una hora la concentración máxima SO2 proveniente de las calderas con Fuel Oil y Diésel fue de 1440.32 µg/m3. Para un tiempo de exposición de 24 horas se alcanzó una concentración de SO2 de 178.56 µg/m3. Estos niveles, exceden los límites establecidos en la resolución 2254 de 2017, donde el valor máximo permisible para una hora es 100 µg/m3 y para 24 horas es 50 µg/m3. En contraste al usar Gas natural como combustible se observa que las concentraciones son considerablemente más bajas. Para un tiempo de exposición de una hora la máxima concentración es de 0.74 µg/m3 y para un tiempo de exposición de 24 horas, de 0.04 µg/m3. Estos resultados cumplen con la normatividad vigente. Se puede concluir que el Gas natural se presenta como una alternativa más favorable, generando concentraciones significativamente menores de SO2. Este cambio en el tipo de combustible no solo favorecerá el cumplimiento de las normativas ambientales, sino que también contribuirá de manera efectiva a la reducción de la concentración de SO2 en el aire.

Keywords: air quality, Air pollution, Dispersion, Emission spatialization, Aermod View.

Palabras clave: calidad del aire, Contaminación atmosférica, Dispersión, Espacialización de las emisiones, Aermod View.

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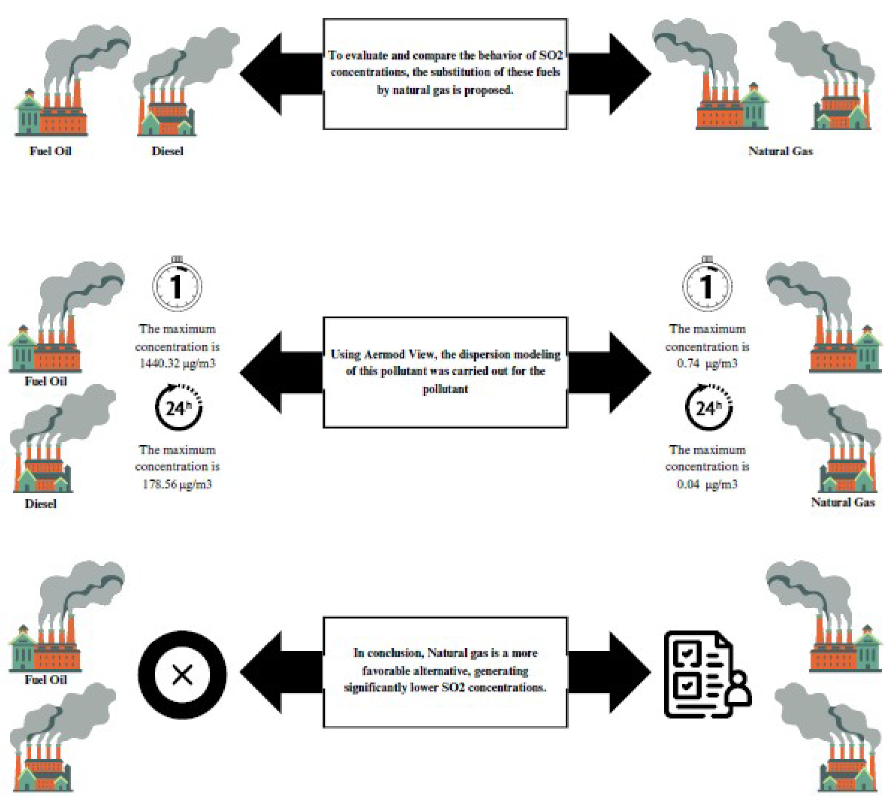
Why was it carried out?
To determine the most suitable fuel for implementation in industries, with the objective of contributing positively to the reduction of atmospheric emissions and minimizing environmental impact.

What were the most relevant results?
It has been shown that Fuel Oil and Diesel fuels generate a higher concentration of Sulfur Dioxide (SO2) reaching a maximum concentration of 1440.32 μg/m3 for an exposure time of one hour. Likewise, its maximum concentration for a 24-hour exposure time is 178.56 μg/m3. However, when the fuel is changed to Natural Gas, these concentrations decrease significantly. For a one-hour exposure time the maximum concentration is 0.74 μg/m3 and for a 24-hour exposure time it reaches a maximum concentration of 0.04 μg/m3.

What do these results provide?
Its contribution is of great significance because it is evident that fuels contain a high percentage of sulfur, which generates SO2 emissions, affecting both the environment and people's health. In addition, it is highlighted that the change of fuel to Natural Gas is ideal to be implemented by the industries, contributing in this way to the reduction of SO2 emissions.

Graphical Abstract



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Introduction

Air pollution has a high environmental impact (1) and severe consequences for ecosystems (1) and human health (1). It can cause cerebrovascular diseases, respiratory infections, allergies, and lung cancer (1). Many diseases can cause premature death due to exposure to this pollution, even at low concentrations (1).
The sources of pollution that cause these problems are diverse. One of the main ones is the burning of fossil fuels that are used as a source of energy for the industrial, transportation, and construction sectors (1). All this has led to increased emissions, a major problem that demands society's attention (1). Globally, it has caused around 7 million deaths each year (2). In addition, according to the National Planning Department (DNP), the costs of deaths and diseases related to air quality amounted to 12.3 billion pesos, representing 1.5% of the Gross Domestic Product (GDP) in 2015, associated with about 8,000 deaths (2).

Among the primary air pollutants are gases such as sulfur dioxide (SO_2), nitrogen oxides (NOx), ozone (O_3), and carbon monoxide, in addition to particulate matter ($PM_{2.5}$, PM_{10}, and PST) (3). These pollutants are transported (4) and carried by winds over long distances (5), mainly due to atmospheric stability, which depends on the radiative balance and wind speed in the area (4). Several studies have considered the relationship between increased immission levels and the incidence of respiratory diseases (6).
In Colombia, Resolution 2254 of 2017 establishes air quality standards to ensure the population's well-being and reduce the risk to human health due to the degree of exposure present (7).

Colombia's highest air pollution levels occur in urban areas and major industrial sectors, where approximately 74% of the population lives. These pollutants come mainly from fossil fuels used by mobile, stationary, or area sources. Forty-one percent of Colombia's total emissions are located in Bogotá, Medellín, and Cali (8).

Santiago de Cali is one of the main cities in the country and has several industries that contribute to generating atmospheric emissions. Some of the fuels commonly used in these industries emit sulfur dioxide (SO2), which reacts with photochemical oxidants in the atmosphere to form sulfur trioxide, which combines with water to form sulfuric acid and sulfate particles that contribute to the process of generating acid rain (9).

The present study focuses on the city of Santiago de Cali, considering four receptors to model the concentrations of the pollutant sulfur dioxide (SO_2) emitted by two industrial boilers. It compares the variation in concentrations due to the substitution of liquid fuels (Fuel Oil and Diesel) for natural gas. Boiler 1 belongs to an industry dedicated to manufacturing and dyeing textile garments, while boiler two is located in an industry that performs waste incineration processes (10).

Methodology

The study area, the scenarios considered, the location of the receptors, and the parameters used for modeling the dispersion of the pollutant are detailed below.

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Study area

Cali, the capital of the Valle del Cauca department, is in the country's southwestern corner. It comprises 22 municipalities and 15 districts, has an average altitude of 1,000 meters above sea level, and covers an area of 619 km^2 (11). The air quality monitoring system of Santiago de Cali has nine fixed monitoring stations that measure criteria pollutants, three fixed stations, and one mobile unit for measuring environmental noise (12).

Resolution 2254 of 2017 establishes the maximum permissible values for the concentration of criteria pollutants, as detailed in Table 1.

Table 1. Maximum allowable criteria pollutants.

Pollutant	Maximum permissible level µg.m^3	Exposure time
PM_{10}	50	Annual
	75	24 hours
$PM_{2.5}$	25	Annual
	37	24 hours
SO_2	50	24 hours
	100	1 hour
NO_2	60	Annual
	200	1 hour

Source: Adapted from (7).

Table 2 describes the three fuels of interest: Fuel Oil, Diesel, and Natural Gas.

Table 2. Characteristics of the different fuels.

Fuel	Description	Calorific Power	Sulfur Content (S)
Fuel Oil	It is produced in the fractionated refining of petroleum. This fuel is very dark and black. It is mainly used in power plants, furnaces, and boilers; it can be refined to produce asphalt and lubricants (13).	150204 BTU/Gal	1.8%
Diesel	A hydrocarbon is composed of paraffins and is mainly used in diesel engines and as boiler fuel (13). It generates high heat temperatures; this fuel cannot be exposed to low temperatures because the paraffins could solidify (13).	140000 BTU/Gal	0.0015%

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Natural Gas	Natural gas is a gaseous mixture of light hydrocarbons whose main components are methane, ethane, and, to a lesser extent, propane, butane, pentane, and various heavy hydrocarbons (14).	136.35 BTU/Gal	1.4364E-6 Lb/ft^3

Source: Adapted from (14).

Annex 1 Modeling domain, receiver locations, and modeling sources details.

Scenarios

This study has two scenarios. Scenario 1 considers the two industrial boilers of interest with their respective fuels: fuel oil in boiler 1 and diesel in boiler 2. In scenario 2, the fuel is changed to Natural Gas. Table 3 shows the chimney characteristics of each selected stationary point source. If the sources exist, these parameters are obtained through isokinetic sampling; if they are projected, they are established in the design of the stacks.

Table 3. Characteristics of the two fixed point sources.

Parameters	Boiler 1	Boiler 2
Fuel	Fuel Oil	Diesel
Location	Carrera 1 No. 39 – 55 Comuna 4	Av. 4N #7N-81 Comuna2
UTM Location	X: 331909.52 m Y: 383386.48 m	X: 329243.78 m Y: 381987.57 m
Chimney diameter	0.60 m	0.30 m
Chimney height	15.0 m	44.8 m
Exit area	3.043 ft^2	0.761 ft^2
Boiler Power	350 BHP	150 psi
Boiler Capacity	17.700 lb/hr	----------
Average gas velocity in the chimney	19.06 ft/S	8.77 ft/S
Exhaust gas temperature	387.594 K	313.15 K

Source: Adapted from (15).

Location of the receptors

Four receptors were selected in the city of Santiago de Cali, considering the main factors: the points with a high influx of people or if there is a vulnerable population that is more likely to present health effects due to exposure to SO_2 pollutant emissions. Figure 1 shows the location of the two fixed point sources and the receptors.

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Figure 1. Location of sources and receptors, Santiago de Cali – Google Earth.

Table 4 shows the selected receptors with their respective geographic coordinates.

Table 4. Location of the receptors in UTM Zone 18N.

Points	Receptors	X (m)	Y (m)
1	San Juan de Dios Hospital	330288.84	381999.86
2	Versalles Neighborhood Park	330411.83	383040.39
3	La Caña Aquapark	332512.31	382040.27
4	ICBF Northeastern Zonal Center	331876.62	383500.37

Source: Google Earth.

Annex 1 shows the grid of receptors to estimate the field of concentrations.

Modeling using Aermod View

The AERMOD VIEW software is a stationary Gaussian plume model (16) used to determine the dispersion of pollutants from existing emission sources or to model the dispersion of pollutants (17).

The following must be taken into account for modeling:

Atmospheric emissions

The sulfur dioxide (SO_2) emissions inventory is carried out using the emission factors of the United States Environmental Protection Agency (AP-42) Chapter 1 for the different fuels of interest, such as fuel oil, diesel, and natural gas. Table 3 shows the parameters for the design of the stacks.

The SO_2 emission calculation uses the formula E = Emission, FE = Emission factor, and P = Boiler power.

E = FE $\times$ P (1)

The emission calculations for each of the scenarios are made.

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Scenario 1

The following is a detailed description of the calculations made to obtain the emission of each of the industrial boilers.

Boiler 1

Considering the SO_2 Emission Factor, according to AP-42 Fuel Oil Combustion Boilers <100 million BTU/h N°6. The calorific value is 150204 BTU/Gal, and Sulfur (S) is 1.8%.

$$FE:\ 157S\,\frac{Lb}{1000\ gal} = 157 \times 1.8\,\frac{Lb}{1000\ gal}$$

$$FE: 283\,\frac{Lb}{1000\ gal} \times \frac{gal}{150204\ BTU} \times \frac{3412.14\ BTU}{1\ Kw-h} \times \frac{1h}{3600\ S} \times \frac{453.592\ g}{1\,Lb}$$

$$FE: 8.1002\ \times 10\text{^} - 4\,\frac{g}{1Kw-s}$$

$$P: 3433.33\ Kw$$

The SO_2 emission is calculated.

$$E: FE\ \times P\ =\ 8.1002\ \times 10\text{^} - 4\,\frac{g}{1Kw-s} \times\ 3433.33\ Kw$$

$$E: 2.78\ \frac{g}{s}$$

In this way, each of the corresponding calculations for boiler 2 is performed, considering that the calorific value is 140000 BTU/Gal and the sulfur percentage is 0.0015% (18).

Scenario 2

In scenario 2, a mass balance is performed to determine the emission factor for the two industrial boilers operating with Natural Gas, considering that this fuel has a calorific value of 136.35 BTU/Gal and a sulfur content of 1.4364 x 10^{-6} Lb/ft^3.

Mass Balance

$$FE: Sulfur\ Content\ \times\ 2 \quad (2)$$

$$FE: 1.4364\ \times 10\text{^} - 6\,\frac{Lb}{ft3} \times\ 2\ =\ 2.87\ \times 10\text{^} - 6\,\frac{Lb}{ft3}$$

$$FE:\ 2.87\ \times 10\text{^} - 6\,\frac{Lb}{ft3} \times \frac{1\ ft3}{7.48\ Gal} \times \frac{1\ Gal}{136.35\ BTU} \times \frac{3412.14\ BTU}{1\ Kw-h} \times \frac{1h}{3600\ S} \times \frac{453.592\ g}{1\ Lb}$$

$$FE: 1.2108\ \times 10\text{^} - 6\,\frac{g}{1Kw-s}$$

As mentioned above, using equation (1), the SO_2 emission is calculated from the emission factor and the activity. Table 5 specifies the emission factors (g/KW-s), activity (kW), and SO_2 emission (g/s) for the boilers in the two scenarios.

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Table 5. SO_2 emissions for the two scenarios

Scenario	ID	Emission Factor (g/KW-s)	Activity (KW)	SO_2 (g/s)
1	CAL1	8.10E-04	3433.33	2.78E+00
	CAL2	6.91E-07	490.48	4.16E-03
2	CAL3	1.21E-06	3433.33	3.39E-04
	CAL4	1.21E-06	490.48	5.94E-04

Source: Authors.

Meteorology

For the present study, meteorology for the year 2022, obtained from WRF (18), is used from January 1 to December 31. Figure 2 shows the wind rose of the city of Santiago de Cali, where it is possible to observe winds with predominant directions towards the southeast, mainly due to the winds coming from the country's interior, with a speed between 0.50 to 2.10 m/s. Likewise, winds predominate towards the northwest due to the winds coming from the Pacific, with speeds of 3.60 to 5.70 m/s. Therefore, the wind direction is essential to estimate the dispersion of pollutants. Annex 2 shows the surface and height (profile) meteorological data for 2022 used in the modeling.

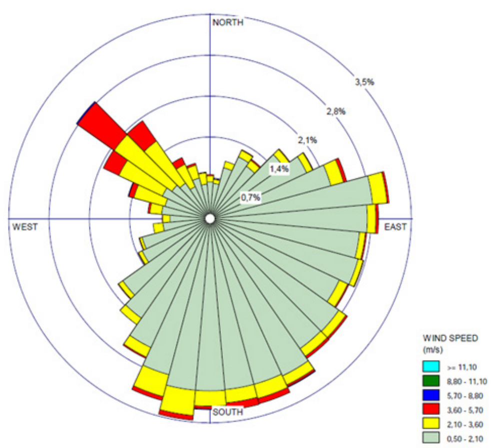

Figure 2. Wind rose

Topography

The Digital Elevation Model (DEM) dataset known as GTOPO30/ SRTM30, which was obtained by collecting information during the Shuttle Radar Topography Mission (SRTM) developed in February 2000 with the GTOPO30 dataset provided by the U.S. Geological Survey, is used. (19).

Results and discusión

Below are the modeling results for the two scenarios, for one hour and 24 hours, according to the Colombian air quality standard.

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Scenario 1

Figure 3 shows the results of the one-hour modeling; its highest concentration is 495.09 μg/m^3, which does not comply with the maximum permissible limit values established in resolution 2254 of 2017, given that for 1 hour the maximum permissible value is 100 μg/m^3. In Figure 4, the 24-hour modeling can reach a maximum concentration of 26.92 μg/m^3, complying with the current regulations establishing for 24 hours a maximum permissible value of 50 μg/m^3. For both models, the point of highest concentration is the residential areas of commune 4 (coordinates 383344.56N; 331663.4E). It should be noted that boiler 2 uses diesel as fuel; its SO_2 concentration is within the permissible values, mainly due to the lower percentage of sulfur compared to fuel oil. It should be mentioned that in the case of diesel, the reduction is 99.67% between 1999 and 2023 (20), contributing to the reduction of SO_2 emissions.

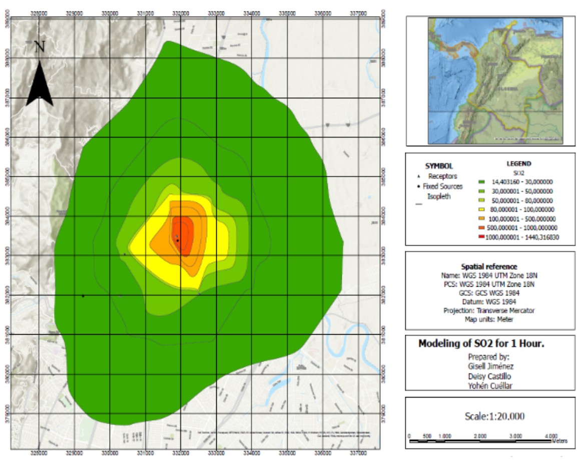

Figure 3. Modeling of SO_2 for 1 Hour.

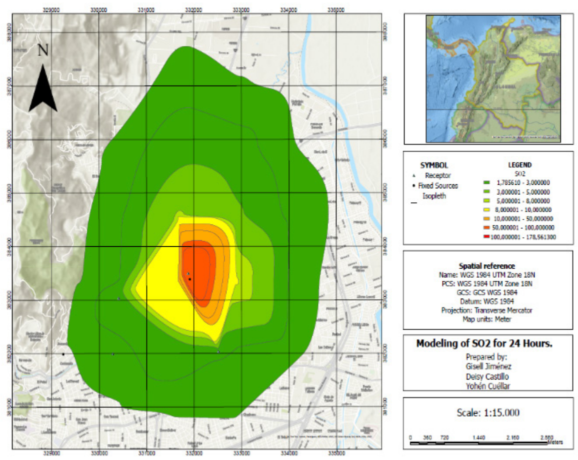

Figure 4 Modeling of SO_2 for 24 Hours.

Scenario 2

Figure 5 shows that the one-hour modeling reaches its highest concentration of 0.74 μg/m^3, and Figure 6 shows the 24-hour modeling, with a maximum concentration of 0.04 μg/m^3; this scenario complies with current regulations. For both modeling scenarios, the point of highest concentration is the residential areas of commune 4 (coordinates 383344.56N; 331663.4E).

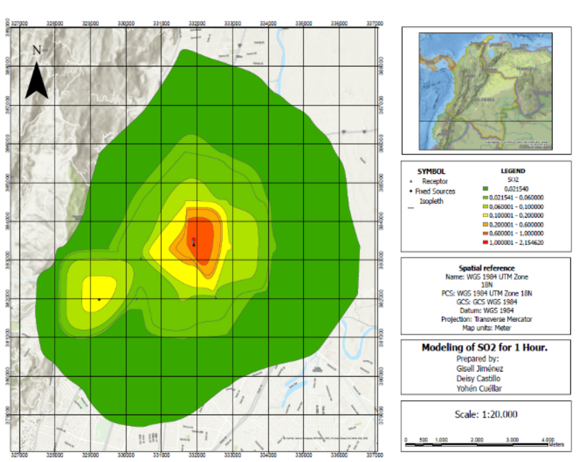

Figure 5. Modeling of SO_2 for 1 Hour.

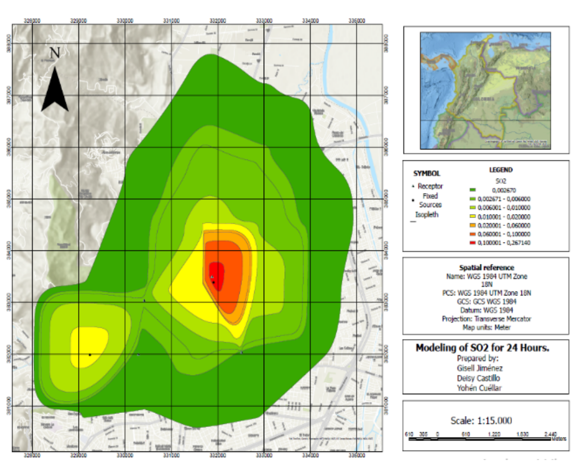

Figure 6. Modeling of SO_2 for 24 Hours.

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Comparison of the Receptors

Figures 7 and 8 compare the scenarios depending on the exposure time according to the receptors.

The receptor that presents the most significant impact due to SO_2 emissions is the Colombian Institute for Family Welfare (ICBF). In scenario 1, the maximum permissible limits are not met according to current regulations for both models; for 1 hour, it reaches a concentration of 1440.32 µg/m^3, and for 24 hours, it reaches a concentration of 178.56 µg/m^3. This result affects the sector's population because they are mainly children and are more affected by the harmful effects of exposure to high concentrations of SO_2 with certain respiratory diseases for the health of everyone. Scenario 2 complies with the maximum permissible limit values according to current regulations; for both models, for 1 hour, it reaches a concentration of 2.15 µg/m^3, and for 24 hours, it reaches a concentration of 0.27 µg/m^3. Therefore, industries must implement a fuel that generates lower emissions, such as natural gas, which reduces the concentration of SO_2 emissions, positively impacting the environment and the population's health.

Several studies indicate that natural gas is an ideal fuel for boilers and furnaces, among other uses. It contributes to efficient production processes compared to other types of fuels, varying according to the industrial sector. An example is the textile sector, in which energy consumption decreases, thus reducing production costs (21).

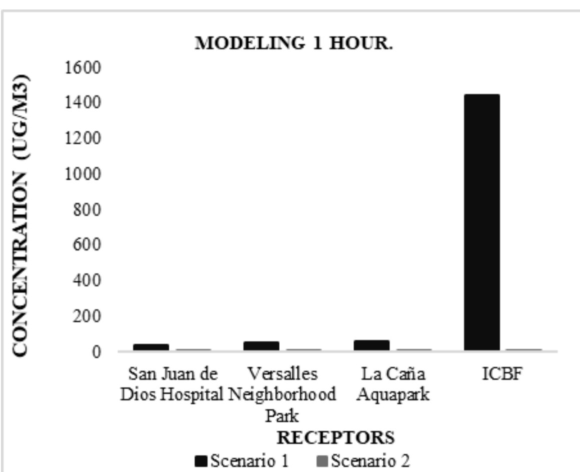

Figure 7. Modeling of SO_2 for 1 Hour.

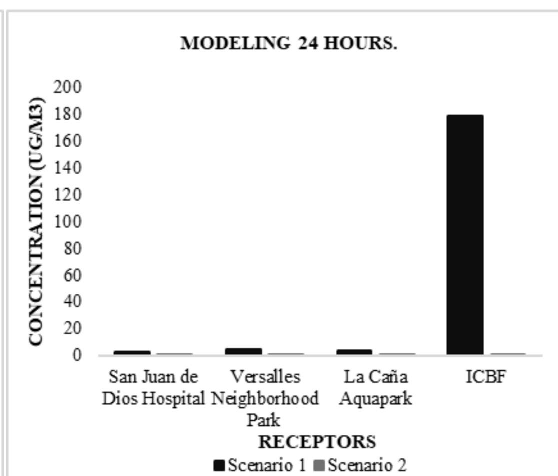

Figure 8. Modeling of SO_2 for 24 Hours.

Figures 9 and 10 show the percentage difference between the two scenarios according to the SO_2 modeling for 1 hour and 24 hours

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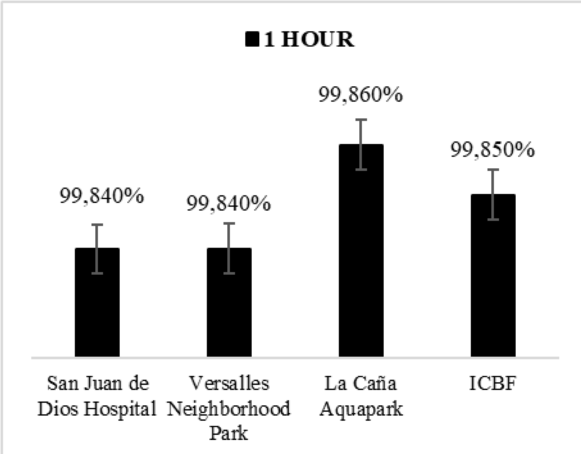

Figure 9. Percentage difference of SO_2 for 1 Hour.

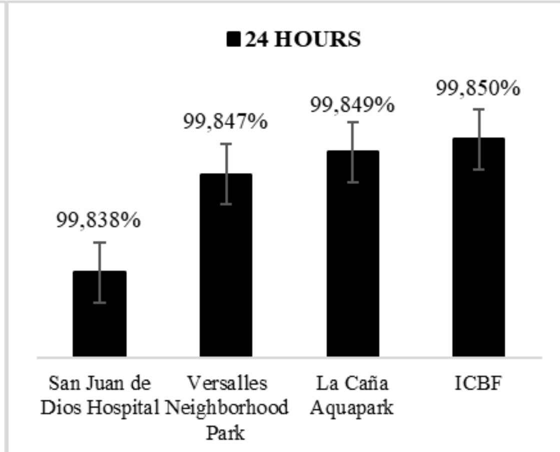

Figure 10. Percentage difference of SO_2 for 24 Hours.

Validation of the modeling results is essential for comparison with the data measured by the monitoring stations. In this case, due to the scope of the study, such validation was not carried out; however, the need to perform this analysis is emphasized.

Conclusions

In this work, the evaluation and modeling of SO_2 concentration was performed for two industries that use (Fuel Oil and Diesel) as boiler fuels. It was found that the fuel oil generates higher concentrations of SO_2, which are outside the maximum permissible values established by resolution 2254 of 2017. Therefore, a comparison was made through modeling with the change of fuel to natural gas for the two industries, where it was evidenced that this generates lower concentrations of SO_2, one of the options that positively impacts the environment. Therefore, it is recommended that this fuel change be made and thus contribute to improving urban air quality. The Aermod View software identifies the areas with the highest concentration of SO_2, not only in the receptors selected for this study but also in other points. For example, the residential area of Comuna 4 in the city has a concentration of 495.09 µg/m^3, which does not comply with resolution 2254 of 2017.

It is crucial that industries use liquid fuels with low sulfur content and implement programs to protect air quality, thus contributing to reducing atmospheric emission concentrations.
The validation of the modeling is crucial for the effective comparison with the data obtained by the monitoring stations; this study did not perform such validation due to the scope's limitations, which are of great importance to perform in future research.

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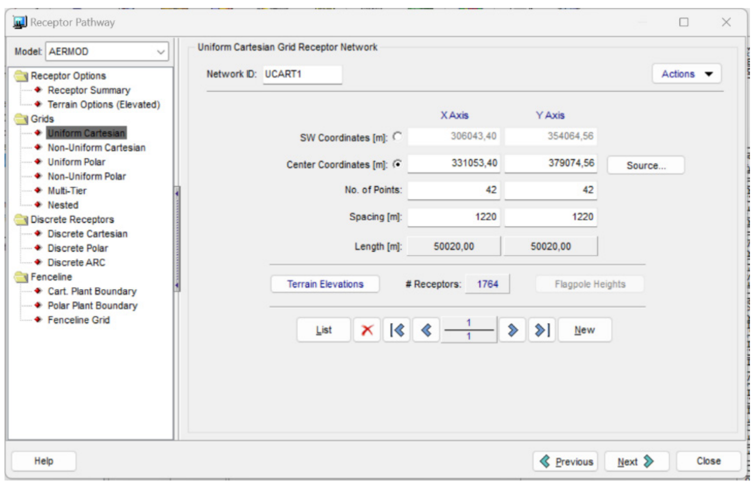
Annex 1.

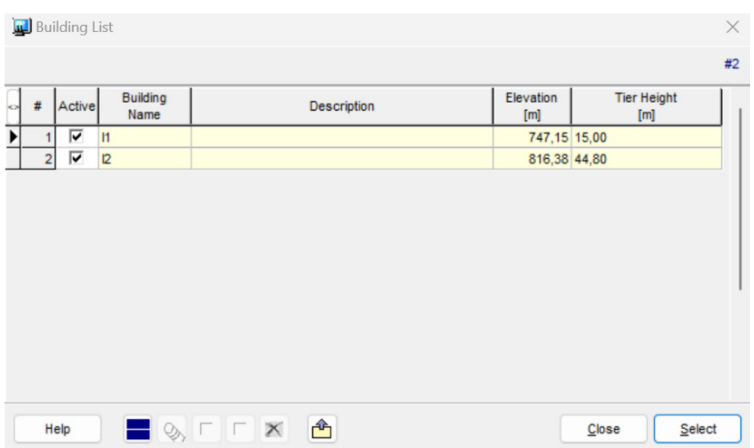
Guide to modeling using Aermod View software

As a first step, the coordinates of Santiago de Cali are X: 330866.7 Y: 380055.41 UTM 18 Zone, and the radius of the domain is 25.00 Km.

A grid of receptors was established as follows to estimate the field of concentrations.

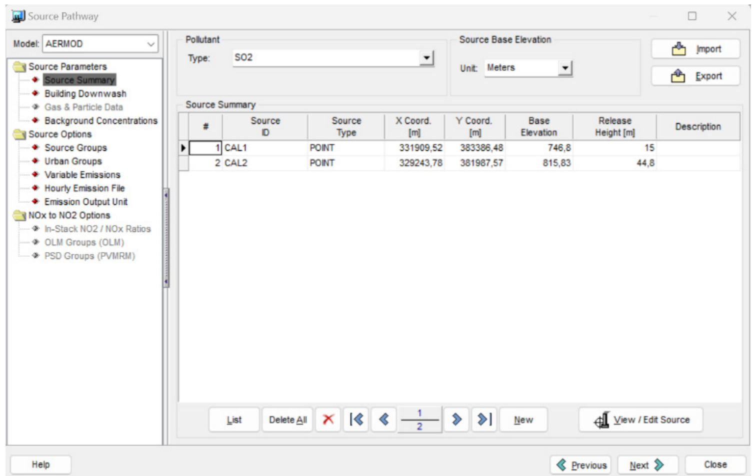


The coordinates of each of the industries were identified with their respective elevation and height.

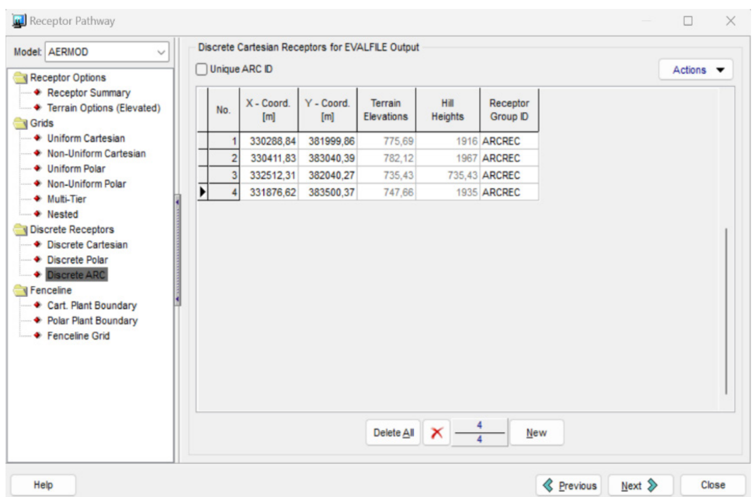


The criteria for pollutants to be modeled, in this case, SO_2, was established at 1 hour and 24 hours in urban areas. In addition, we proceed to add each of the emission sources, taking into account the parameters obtained through isokinetic sampling if the sources exist or if they are projected to be established in the design of chimneys and SO_2 emissions were made using the emission factors of the United States Environmental Protection Agency (AP-42).

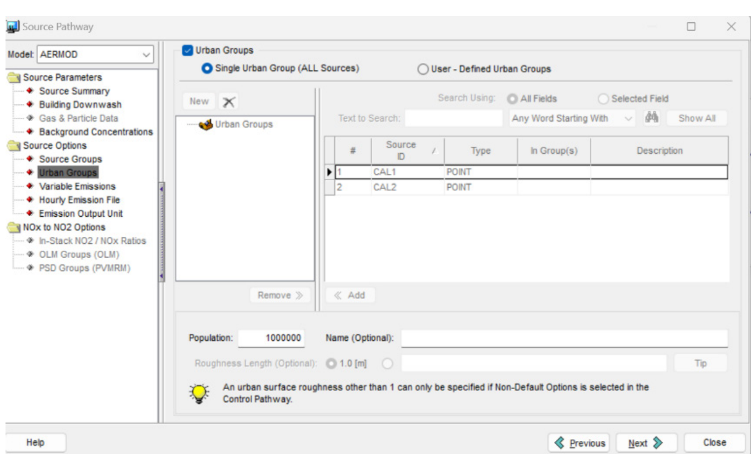
doi: 10.25100/iyc.v26i1.13337



The coordinates of each of the discrete receptors are added.



The sources are grouped as follows, considering a population of 1 000 000 inhabitants.



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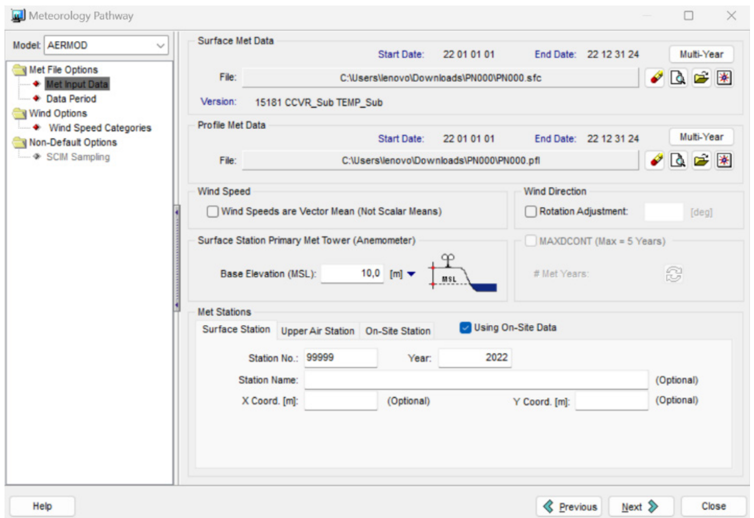
If it is successful, the software's BPIP is run, and the respective process is continued, which adds the meteorology of the year 2022, obtained from WRF from January 1 to December 31, and its topography, which in this case is GTOPO30/SRTM30. Finally, the model is run to obtain the modeling results.



Annex 2.

The following link goes to the meteorological data for the year 2022.https://drive.google.com/drive/folders/1OMiDfBc8SC72Gcs-Uxkf8GYTwnVqthEH?usp=sharing

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