A RSTUDIO-based modeling program for dispersion of particulate matter emissions using Gaussian plume equation

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Abstract. Mathematical models allow evaluating the air pollutants effects to the environment under several conditions, being a relevant and a low-cost tool for planning and regulatory purposes. Recent studies have shown the effects of particulate matter on environment and human health, especially cardiovascular and respiratory diseases. This study aims to evaluate the air quality of Volta Redonda, Brazil, due to particulate matter emitted by stationary point sources of a steel industry using meteorological data from three monitoring stations. A mathematical model was developed RStudio®, using the Gaussian dispersion equation and Google Maps API to visualize the results. Davidson-Bryant plume rise equation was included. Observed data revealed southeastern, southeastern, northern and eastern light prevailing winds that were used to simulate particulate matter concentrations for 24-hour periods, under stable and unstable conditions according Pasquill-Guifford classification. The results show that the stations exceed the daily standards determined by the legislation in different scenarios, with Santa Cecília station, being the one that violated these standards the most, reaching an average daily value of 3673.04 µg m⁻³, with an hourly peak of 7712.76 µgm⁻³, for the scenario of prevailing northwest winds and wind speed of 1 m s⁻¹. Other stations also violated the standards, with the Retiro station showing better results for the north and northwest wind directions.

1. Introduction
Air pollution is one of the biggest environmental concerns in recent decades, due to industrial growth, high volume of traffic fossil-fuel vehicles and a significant increase of respiratory, cardiovascular, and neurological diseases attributed to the inhalation of these pollutants [1], causing approximately three million premature deaths per year [2].

Besides human health, the intensification of air pollutants in atmosphere and consequential deposition on soil and water bodies may cause acidification, affecting photosynthesis capacity, reducing agricultural productivity, changing natural nutrient balance [3] and being responsible for phenomena such as photochemical smog, stratospheric ozone depletion and global warming. [4].

Mathematical models are currently used to estimate potential impacts on air quality [5]. Dispersion modelling allows to assess the local atmospheric circulation and its influence on pollutants concentration and to verify if legal air quality standards are attained [6].

Gaussian plume model is the most widely used model for point source emissions and it is based on the transport and diffusion of the air pollutant particle, using empirical parameters (sigmas) as function of atmospheric stability [7]. Gaussian plume models such as industrial source complex (ISC), AERMIC Model of AERMOD software, and CALPUFF, developed by the United States
Environmental Protection Agency (US EPA) and the Atmospheric Dispersion Modeling System-Urban (ADMS-Urban) developed by Cambridge Environmental Research Consultants (CERC) are frequently used for regulatory purposes and environmental licensing processes. Thus, although the ISC model has been replaced by AERMOD software, the former continues to be extensively used, which can be explained by the unavailability or inaccessibility of input data required by AERMOD software and other more sophisticated models [8].

In the present study, a Gaussian plume model was developed using RStudio® platforms to perform air pollution dispersion studies. The model was used to simulate the dispersion of inhalable particulate matter (PM$_{10}$) emissions from a steel production plant located in Volta Redonda, Brazil, and an R package based on Google Maps API was managed to visualize the results.

2. Materials and methods

2.1. Emission data

This study was carried out in Volta Redonda city, located in Rio de Janeiro State, Brazil. The city is approximately 130 km far from the state capital and it is surrounded by mountains and valleys. The city has a mesothermal climate with an average annual precipitation of 1300 mm and relative humidity around 75% [9]. The main economic activity is the steel industry, sheltering the largest plant in Latin America, whose production reached 912000 metric tons of steel in the third quarter of 2018, achieving approximately US $ 1.3 billion in profit in 2018 [10].

As input emission data, steel plant’s point emissions inventory of 2017 [11], which includes 35 chimneys and measured data as nitrogen oxides (NO and NO$_2$ as NOx); sulfur oxides (SOx) and inhalable PM$_{10}$ from seven different processes within the plant. Figure 1 shows the sources and monitoring stations locations surrounding the plant. The average emissions from point sources by productive area are shown in Table 1.

![Figure 1. Sources by process and monitoring stations surrounding the steel plant located in Volta Redonda, Brazil.](image-url)
Table 1. Averages from point emissions reported by the steel plant in 2017.

| Zones/Processes         | Stacks (units) | Geometric height (m) | Stack diameter (m) | Gas temperature (°C) | Gas exit speed (m/s) | PM$_{10}$ (g/s) | NO$_x$ (g/s) | SO$_x$ (g/s) |
|-------------------------|----------------|----------------------|--------------------|----------------------|---------------------|----------------|-------------|-------------|
| Sinter plant            | 5              | 47.0                 | 4.1                | 28.4                 | 4.4                 | 7.6            | 11.2        | 19.9        |
| Basic oxygen furnace    | 5              | 22.4                 | 2.3                | 12.7                 | 3.4                 | 0.8            | 0.0         | 0.0         |
| Blast furnace           | 10             | 24.8                 | 2.6                | 17.5                 | 4.1                 | 1.3            | 0.0         | 0.0         |
| Coke oven plant         | 5              | 84.4                 | 4.4                | 35.1                 | 2.3                 | 1.4            | 2.1         | 8.4         |
| Lime plant              | 6              | 35.9                 | 1.2                | 13.8                 | 3.0                 | 0.3            | 1.6         | 0.0         |
| Thermoelectric power    | 3              | 45.3                 | 2.6                | 41.1                 | 6.8                 | 2.2            | 9.8         | 16.5        |
| Lamination              | 1              | 33.2                 | 3.3                | 170.9                | 1.7                 | 1.1            | 7.6         | 3.6         |

Meteorological data comprising wind temperature and relative humidity from January 2007 to December 2016 were collected from three meteorological stations placed near the complex. Due to unavailability data from Volta Redonda, other meteorological variables such as solar radiation, accumulated precipitation in 24 h and cloud cover were obtained from the National Institute of Meteorology (INMET) conventional and automatic meteorological stations, both located in the nearby city of Resende, Brazil.

2.2. Dispersion model: structure and configuration

The program was developed in RStudio® and divided into three components: variable definitions and model configuration, equation resolution and post-processing. First script describes possible input values and allows the user to set the model configuration. The second defines routines of wind direction distribution, atmosphere stability pattern and output data, and in sequence, provide concentration values using the Gaussian plume model; post-processing scripts use the Openair R package for plotting and providing general statistics of observed data and RgoogleMaps package to get background maps through Google Static Map API.

The model was configured according to wind speed and direction obtained from monitoring stations, using the inverse standard normal probability distribution to generate a prevailing wind field for each season/station; coefficients $\sigma_y$ and $\sigma_z$ were defined using McElroy-Pooler urban fit; effective emission heights were obtained by Davidson-Bryant plume rise formula to each stack. All emissions were presumed simultaneous; the model does not consider wind variability, atmospheric turbulence, chemical transformation, wet deposition, inhomogeneous terrain, and fugitive emissions [5,6].

3. Results and discussion

3.1. Wind and stability analysis

Wind roses were generated using the Openair R package and have shown dissimilar wind patterns in each station, both in the seasonal variability and in the prevailing wind directions. Average wind speed, however, shown prevailing light winds, ranging between 1.0 ms$^{-1}$ and 2.5 ms$^{-1}$. Wind directions ranged from northern (N) to north-western (NW) in summer and autumn and eastern (E) to south-eastern (SE) during winter and spring. SE winds occurred for 10% of all seasons, indicating the influence of cold fronts passages, and north-quadrant winds is believed to occur by the presence of mountain ranges positioned north of the steel complex, as observed by Guimaraes [12].

Figure 2 shows wind roses for each monitoring station. The average daily variation of stability classes, according to the Pasquill-Guifford classification [5] was made using average wind speed and climatological data from Resende station.
3.2. Modeling results

It can be seen from Figure 3 that northwest predominant winds of 1.0 ms\(^{-1}\) and a moderately stable atmosphere triggered high concentrations near to Santa Cecília station, Brazil, where the average daily concentration reached the value of 3673 μg m\(^{-3}\).

**Figure 2.** Wind roses of Santa Cecilia, Belmonte and Retiro station by season.

**Figure 3.** PM\(_{10}\) dispersion plumes under NW winds of 2.5 ms\(^{-1}\) and unstable conditions.

**Figure 4.** PM\(_{10}\) dispersion plumes under NW winds of 2.5 ms\(^{-1}\) and stable conditions.
Retiro and Belmonte stations, under these same conditions, met the national air quality standards. For East winds, conserving 1.0 ms⁻¹ and stable atmosphere, highest concentration values were found at Belmonte and Retiro stations with average values of, respectively, 324.15 μg m⁻³ and 850.89 μg m⁻³. Santa Cecília station, under the same configuration, met the air quality limits, indicating a high influence of the direction of prevailing winds on PM₁₀ concentrations.

Figure 5 shows that, for prevailing winds from Northwest of 2.5 ms⁻¹, Santa Cecília station exceeded the limit PI-1 (120 μg m⁻³) [13], currently the national air quality standard, and consequently, the intermediate (PI-2) and final (PF) values, which are both lower than PI-1. The exceed occurred for both stability conditions, however, under more stability as shown in Figure 6, simulated values were shown to be lower with the daily average of 149.58 μg m⁻³, approaching to PI-1, while unstable conditions reached 1480.63 μg m⁻³.

Table 2 shows the highest rates of exceedance of the national air quality standard PI-1 of 120 μg m⁻³. Santa Cecília station presented the first and second highest rates, for Northwest and North directions of similar wind speed conditions (1.0 ms⁻¹) and stability. Belmonte had the third highest rate for the prevailing East winds. Table 2 also demonstrates the direct influence wind directions over Santa Cecília station, performing lower concentrations of pollutants for the S-SE winds while Retiro and Belmonte stations, Brazil, showed better air quality over N-NO prevailing winds conditions.
Table 2. Exceed rate of the national standard PI-1 of 24-hour running average.

| Wind direction (°) | Station      | Wind speed (ms⁻¹) | PG stability class | 24h RA / PI-1 | 24 RA (µg / m³) |
|-------------------|--------------|-------------------|--------------------|---------------|----------------|
| 315               | Sta. Cecília| 1.0               | A/B                | 30.61         | 3673.04        |
|                   | Belmont     | 1.0               | A/B                | 0.62          | 74.89          |
|                   | Retiro      | 2.5               | E/F                | 0.36          | 43.35          |
| 0                 | Sta. Cecília| 1.0               | A/B                | 20.65         | 2477.47        |
|                   | Belmont     | 1.0               | E/F                | 2.20          | 264.78         |
|                   | Retiro      | 1.0               | A/B                | 0.13          | 16.23          |
| 90                | Sta. Cecília| 1.0               | A/B                | 0.98          | 117.11         |
|                   | Belmont     | 1.0               | E/F                | 10.17         | 1220.50        |
|                   | Retiro      | 1.0               | A/B                | 2.70          | 324.15         |
| 135               | Sta. Cecília| 2.5               | A/B                | 0.00          | 0.06           |
|                   | Belmont     | 1.0               | A/B                | 5.79          | 695.74         |
|                   | Retiro      | 1.0               | A/B                | 7.11          | 853.63         |

4. Conclusion

The results analysis pointed to a high influence of prevailing wind directions on the concentrations of particulate matter, most related to permanent and transient pressure systems that appear over the area throughout the year. Santa Cecília station revealed high concentration results for the N-NO wind directions, while Retiro and Belmonte stations showed higher concentrations for S-SE winds. The south of the complex near Santa Cecília exposed the highest concentration results, mainly for the NO winds of 1.0 ms⁻¹, under which the highest average concentration was reached. Air quality standards have been exceeded in several conditions, with high overtaking rates, indicating the need to improve air quality control, to meet national and local standards and provide environmental health and protection.

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