Study for the dispersion of particulate matter emissions from a steel industry using Gaussian Plume equation through computational modeling

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Abstract. Mathematical models allow evaluating air pollutants effects to the environment, being a relevant tool for planning and regulatory purposes. The present study aims to evaluate the air quality of Volta Redonda, Brazil, due to particulate matter emitted by stationary point sources of a large steel plant using meteorological data from three monitoring stations. A mathematical model was developed linking Matlab® and RStudio®, using the Gaussian dispersion equation and Google Maps to visualize the results. Observed data revealed southern, north-western and northern light prevailing winds that were used to simulate stable and unstable atmosphere conditions according Pasquill-Guifford classification. Results have exposed elevated concentrations of particulate matter in ambient air, reaching particularly Santa Cecilia neighbourhood. National air quality standards recently updated were partially met however numerous violations were indicated, considerably higher in Santa Cecilia station (47.98%), followed by Belmonte (6.69%) and Retiro (4.17%), indicating a forthcoming need for an update of the technologies and processes that emit particulate matter to improve the city air quality, preventing from environmental and human health effects.

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 also 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 (AERMOD) and CALPUFF, developed by the United States Environmental Protection Agency (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, the former continues to be extensively used, which can be explained by the unavailability or inaccessibility of input data required by AERMOD and other more sophisticated models [8].

In the present study, a Gaussian plume model was developed using Matlab® and 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 912,000 metric tons of steel in the third quarter of 2018, achieving approximately US $1.3 billion in profit in 2018 [10].

In order to obtain pollutant emission data, the steel plant’s atmospheric emissions inventory official report of 2011 was used [11]. The report includes all stationary and mobile sources emissions such as nitrogen oxides (NO and NO$_2$ as NOx); sulfur dioxide (SO$_2$) and particulate matter (total and PM$_{10}$), calculated based on emission factors proposed by EPA AP-42 [12]. The inventory has identified 23 zones/processes which emit air pollutants and 17 showed non-zero PM$_{10}$ emissions. Figure 1 shows the sources (points 1 to 23) and monitoring stations locations at the plant. Particulate matter emissions by process are presented in Table 1.

![Figure 1. Sources of air pollutants by process and monitoring stations surrounding the steel plant located in Volta Redonda, Brazil.](image-url)
Table 1. Inhalable particulate matter emissions reported by the steel plant in 2011.

| Zones/processes | Sinter plant | Blast furnace 2 | Thermoelectric CTE 02 | Coke oven battery 01 | Thermoelectric UG50Hz | Coke oven battery 04A, 04B and 05 | Continuous annealing | Steel casting |
|-----------------|--------------|-----------------|----------------------|---------------------|------------------------|----------------------------------|---------------------|-------------|
| Lat (º)         | -22.509      | -22.509         | -22.513              | -22.511             | -22.511                | -22.512                         | -22.514             | -22.516     |
| Long (º)        | -44.106      | -44.111         | -44.105              | -44.112             | -44.105                | -44.116                         | -44.121             | -44.124     |
| PM$_{10}$ (g/s) | 64.95        | 4.61            | 8.41                 | 13.12               | 5.79                   | 31.260                          | 2.09                | 0.13        |

| Zones/processes | Zinc plating | Cold rolling | Lime plant | Basic oxygen furnace | Hot rolling | Acid regeneration Plant | Coke handling | Blast furnace 03 | Coal yard |
|-----------------|--------------|--------------|------------|----------------------|-------------|------------------------|---------------|------------------|-----------|
| Lat (º)         | -22.518      | -22.519      | -22.524    | -22.514              | -22.517     | -22.521                | -22.509       | -22.510          |           |
| Long (º)        | -44.122      | -44.120      | -44.132    | -44.110              | -44.115     | -44.125                | -44.116       | -44.106          | -44.113   |
| PM$_{10}$ (g/s) | 0.52         | 1.64         | 4.59       | 15.13                | 1.51        | 0.020                  | 6.37          | 10.96            | 6.19      |

2.2. Meteorological data
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.

2.3. Dispersion model: structure and configuration
The program was developed in Matlab® and divided into five sections: variable definitions, model configuration, cases selection, equation resolution and post-processing. First section describes possible input values that will be chosen by the user in configuration module. Case selection defines the routines required to generate wind direction distribution, atmosphere stability pattern and output type. Post-processing section allows visualizing the results in Matlab or exporting them to a .mat file (Matlab data files) or .txt (text file). A statistical R package called R.matlab was used for reading .mat files, 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 Gaussian model is derived from the advection-diffusion equation, reduced to a differential form with analytical solution. The concentration ($C$) at a point in space ($x, y, z$) considering a point source with continuous emission and effective height, $He$, is given by the following Equation 1.

$$C(x,y,z,He) = \frac{Q}{2\pi \upsilon \sigma_y \sigma_z} \cdot \frac{\pi}{4} \cdot \left( \frac{\upsilon}{\sigma_y} \right)^2 \left[ e^{-\left( \frac{(z-He)^2}{2\sigma_y^2} \right)} + e^{-\left( \frac{(z+He)^2}{2\sigma_z^2} \right)} \right]$$

(1)

Where $C$ is the pollutant concentration (g m$^{-3}$), $Q$ is the emission rate from the source (g s$^{-1}$), $He$ is the effective height, $\upsilon$ is the mean horizontal wind speed at He (m s$^{-1}$), $\sigma_y$ and $\sigma_z$ are the horizontal and vertical dispersion coefficients respectively, $x$ is the downwind distance from source to receptor (m) and $y$ is lateral distance from source to receptor (m) and $z$ is the vertical direction (m).

The model was configured according 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. Four effective
heights (10, 25, 50 and 100 meters) were settled and a trial was performed for each of Pasquill-Guifford stability class (A/B, C, D and E/F).

The model has some limitations. It does not take into account wind variability, atmospheric turbulence, chemical transformation, wet deposition or inhomogeneous terrain [5,6]. Due to unavailability of emission point data such as gas exit velocity and source geometrical height, plume rising calculations were not included in the model. All emissions were presumed simultaneous and released at the same effective height He and total emission rate (stacks and fugitive) of each zone/process were concentrated to a spatially representative point inside its boundaries.

3. Results and discussion

3.1. Wind and stability analysis

Wind roses were generated using openair R package and have shown dissimilar wind pattern 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 [13]. 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. Considering all seasons showed very similar wind speeds, for comparison purposes, it was assumed stability classes A/B during the daytime and stable classes E/F during the night period.

![Figure 2. Wind roses of Santa Cecilia, Belmonte and Retiro station by season.](image-url)
3.2. Modelling results

It is possible to observe in Figure 3 and Figure 4 that prevailing north-western winds lead to high PM$_{10}$ concentrations in Santa Cecilia zone, reaching 584.6 μg m$^{-3}$, in case of 50 m effective height and stable conditions. Belmonte and Retiro, under same configuration, reached 50.5 μg m$^{-3}$ and 18.5 μg m$^{-3}$ of PM$_{10}$ concentration, respectively.

![Figure 3. PM$_{10}$ dispersion plumes under NW winds of 2.5 ms$^{-1}$ and unstable conditions.](image1)

![Figure 4. PM$_{10}$ dispersion plumes under NW winds of 2.5 ms$^{-1}$ and stable conditions.](image2)

For E-SE winds, conserving 2.5 ms$^{-1}$ and stable atmosphere, reducing to 10 m of effective height, a peak was also recorded at Santa Cecilia station, reaching 18823.5 μg m$^{-3}$, and at Belmonte and Retiro, 970.8 μg m$^{-3}$ and 439.8 μg m$^{-3}$. Using 50 m as He, concentrations of 62.7 μg m$^{-3}$ (Santa Cecilia), 821.1 μg m$^{-3}$ (Belmonte) and 399.2 μg m$^{-3}$ (Retiro) were found.

Figure 5 and Figure 6 show hourly mean and 24-hour running average (24-h RA) for a 90-days trial period at Retiro location, considering 50 m as effective height and 2.5 ms$^{-1}$ as wind speed, for unstable and stable atmosphere conditions. Horizontal lines represent national standards for PM$_{10}$ according to the Conselho Nacional de Meio Ambiente (CONAMA) Resolution 491/2018, which establishes maximum values currently in force 120 μg m$^{-3}$ (PI-1) and final standard (PF) as 50 μg m$^{-3}$ [14], which is expected to be achieved in the next years, same as presently recommended by the World Health Organization [1].

![Figure 5. Hourly mean and 24-hour running average simulated concentrations of PM$_{10}$ under unstable atmosphere for Retiro station.](image3)
Figure 6. Hourly mean and 24-hour running average simulated concentrations of PM$_{10}$ under stable atmosphere for Retiro station.

Retiro presented slightly favourable conditions for PM$_{10}$ dispersion under eastern flow and unstable atmosphere, however, for a stable atmosphere, hourly mean values exceeding four times PI-1 were verified. For 24-hour running average values, several exceeds of PF were also presented under stable conditions, however, there was no violation of PI-1 standard. Table 2 presents PI-1 and PF standards exceeds for hourly mean and 24-hour running average.

Table 2. National standards exceeds for a 90-day period simulation using $He = 10m$.

| Station    | Wind Direction (°) | PG stability class | Hourly Mean $>$ PI-1 | 24h RA $>$ PI-1 | Hourly Mean $>$ PF | 24h RA $>$ PF |
|------------|--------------------|--------------------|----------------------|-----------------|-------------------|---------------|
| Belmonte   | 135                | B                  | 0.0%                 | 0.0%            | 0.0%              | 0.0%          |
|            | 315                | E                  | 0.2%                 | 0.0%            | 3.2%              | 0.0%          |
|            |                    | B                  | 0.0%                 | 0.0%            | 0.0%              | 0.0%          |
|            |                    | E                  | 15.8%                | 5.0%            | 19.2%             | 69.7%         |
| Retiro     | 315                | B                  | 0.0%                 | 0.0%            | 0.0%              | 0.0%          |
|            | 90                 | E                  | 0.0%                 | 0.0%            | 2.3%              | 0.0%          |
|            |                    | B                  | 0.0%                 | 0.0%            | 0.0%              | 0.0%          |
|            |                    | E                  | 12.3%                | 0.3%            | 15.2%             | 43.5%         |
| Santa      | 135                | B                  | 21.2%                | 4.4%            | 26.5%             | 76.5%         |
| Cecilia    | 90                 | E                  | 14.6%                | 82.6%           | 16.2%             | 95.7%         |
|            |                    | B                  | 58.3%                | 100.0%          | 68.2%             | 100.0%        |
|            |                    | E                  | 45.0%                | 100.0%          | 47.8%             | 100.0%        |

Considering all estimated concentrations, Santa Cecilia revealed the highest number of ambient air standards exceeds, reaching the totality for 10 m of effective height emission and 48% for 50 m, while Belmonte showed 6.7% of violations under stable conditions, using NO and SE winds. The lowest number of exceeds occurred in Retiro, presenting 4.2% of the total estimated values, related to E winds, 10 m and 50 m and PG classes E.
4. Conclusion
Wind rose analysis showed that prevailing wind directions, taking account on season variability, was from NW, N, E and SE, which are mainly responsible for the pollutants dispersion in the study domain.

The developed model showed a trend of high concentrations of particulate matter to the south of the steel complex and indicated a strong contribution of sintering and coke processes in Santa Cecilia air quality. SE winds appeared to facilitate the pollutants dispersion, indicating that the most extreme concentrations simulated for further wind directions are less probable, nevertheless might over acceptable values. There were a substantial number of PI-1 and PF standards violations, noticeably higher in Santa Cecilia zone (48%), followed by Belmonte (6.7%) and Retiro (4.2%). The results showed, therefore, a need to update the processes performed at the steel plant that emit particulate matter, in order to meet the national air quality standards currently in force and to improve Volta Redonda air quality.

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