



Design of an early alert system for PM_{2.5} through a stochastic method and machine learning models



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ABSTRACT

In Latin America, the levels of pollution have risen considerably in the last few years. 2019, for example, had one of the largest numbers of air quality alerts. These alerts signal an increase in respiratory diseases among the population. For this reason, this paper designs a preventive early alert system for air quality. This system compares three machine learning models and validates, through statistical and categorical parameters (9), that a stochastic model, combined with a convolution bidirectional recurrent neural network (1D-BDLM), has an accuracy of $\approx 93 \pm 4\%$ when forecasting the risk for each population group in all the monitoring stations. Likewise, it is also able to capture high pollution events without producing false alarms ($\approx 10 \pm 5\%$). This model is utilized to design an alert protocol (24 h in advance) before a pollution event occurs. The protocol distinguishes the level of alert and the type of population at risk, focusing on two objectives: pollution mitigation and risk reduction for the population. To reduce pollutant concentrations, this paper proposes limiting vehicle traffic in the most polluted city zones or, if necessary, throughout the entire area. In relation to stationary sources, this article proposes the implementation of monitoring measures in order to identify the most polluting factories and restrict their operation during a specific period of time. In regards to population risk, the protocol aims to reduce exposure time by recommending the avoidance of outdoor activities (in specific zones) and the use of protective gear, taking into consideration relevant differences between population groups.

1. Introduction

Air pollution has become a determining factor in the quality of life of highly populated and industrialized areas, as it has been associated with the emergence of respiratory diseases and an increase in public costs (Kelly et al., 2011; Maas and Gennfelt, 2016). High concentrations of particulate matter (PM), for instance, cause harmful effects on the respiratory system due to its composition and size (WHO, 2018). Hence, several countries have implemented early alert systems (EAS) for air quality, which can forecast PM concentrations. These systems have aided in the task of reducing harmful effects on human health and the government costs associated with them (airALERT, 2005; Wen et al.,

2009; Dominguez-Calle and Lozano-Báez, 2014). An important feature of the EAS is its air quality forecast focused on risk assessment, which allows an early detection of pollution, leading to a minimization of costs in public health and the coordination of meteorological and health agencies (Kumar et al., 2018).

Consequently, predictive models are the main component of the EAS: they are able to forecast pollutant concentrations in the short-term, strengthening the decision-making process during pollution events (Makowski, 2000; Longo et al., 2013; Casallas et al., 2020). Thus, in recent years, numerical models (e.g., WRF-CHEM, CAMS) (Byun and Schere, 2006; Kumar et al., 2016; González et al., 2018; Casallas et al., 2020), Machine Learning (ML) models (e.g., Artificial Neural Networks

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-ANN-, Support Vector Machines -SVM-) (Comrie, 1997; Shahraiyni and Sodoudi, 2016; Tao et al., 2019; Mogollón-Sotelo et al., 2020; Casallas et al., 2021a) and statistical approaches (Liao et al., 2021) have been used and have fostered great developments in PM predictions. Its use, in regards to air quality, generally focuses on the capability of the models to learn clear diurnal trends and their perturbations/peaks. These efforts can lead to better forecasting strategies that can be used to design, implement and evaluate air quality protocols and the model's performance (Zhang et al., 2012). Consequently, ML applications provide information on air quality through highly-precise forecasts (fine spatial and temporal resolution ≤ 24 h) that can contribute to risk management and to reduce air quality impacts on public health (Shahraiyni and Sodoudi, 2016).

Statistical analysis has been used to evaluate methodologies that increase the spatial distribution of air quality measurements. Tzanis et al. (2019) compared the Inverse Distance Weighting, three linear regression models, and the Linear Mixed Model, alongside a Feed Forward Neural Network (FFNN) model. The results highlight the effectiveness of the FFNN, as it is statistically superior when simulating the spatial variability of particulate matter. Regarding ANN, Huang and Kuo (2018) made a pioneering effort in the development of a deep Convolutional Neural Network (CNN) merged with Long Short-Term Memory (LSTM) (which they called APNet) to include air quality forecasting in smart cities, especially in terms of PM_{2.5} prediction. They compared seven ML models designed with historical data (precipitation, wind speed, and PM_{2.5}) using four statistical parameters. Their results indicate that the APNet has the highest forecasting accuracy. For this reason, a CNN-LSTM model is a good starting point to design an ANN as a tool for risk management in a tropical city.

Beijing was one of the first cities to use models to predict air pollution (since 2007), providing air quality forecasting information to more than 100 countries. This turned the city into a forerunner in the incorporation of forecasting simulations of the Copernicus Atmosphere Monitoring Service (CAMS) (Inness et al., 2019), using the topographic and meteorological conditions of each region (WAQI, 2007). In Latin America, Brasil made the first efforts in air quality prediction, through linear models and neural networks (Lira et al., 2007). The results indicated that the analyzed simulation tools have high accuracy and can be used by the local authorities, alongside the design of a risk management program regarding air quality, such as an EAS, to reduce the risk associated with air pollution (Lira et al., 2007). Chile has also made great efforts to forecast air quality in real-time in their main cities, including forecasts using physico-chemical models, with the aim of assisting the policy-making process, to avoid severe pollution events in their cities (Saide et al., 2015). Likewise, an analysis of air quality management in Chile found that the effectiveness of PM_{2.5} regulations have significantly decrease pollution and, thus, most cities have implemented an Air Quality Management Plan and applied regulations on mobile and residential sources, something that has produced positive impacts to air quality risk (Jorquera, 2021).

Colombia has also made efforts in this direction. The city of Medellín, for example, created an EAS for air quality using numerical models. Nonetheless, this alert does not consider the long-term toxic effects caused by a chronic exposure to PM or the increase in diseases associated with these pollutants (Martonen and Schroeter, 2003; Gómez Ortega et al., 2018; Baena-Salazar et al., 2019). In Bogotá, Franceschi et al. (2018) forecasted PM₁₀ and PM_{2.5} concentrations using an ANN, Principal Component Analysis, and k-means clustering. They managed to predict pollutant concentrations 24 h in advance, by using Multi-Layer Perceptron for the most polluted station of the city. The promising results of these studies prove that these models can be easily used for the issuance of precise early warnings with hourly forecasts in polluted areas to accurately reduce the risk.

These efforts join the increasing concern of the international community in relation to this issue, as demonstrated in the UNECE (2013)-amendment to the Gothenburg Protocol- (which entered into force in

2019): the first binding treaty with international obligations regarding levels of PM concentrations. Before this amendment, there were supranational provisions (binding to EU countries) in the same direction, such as the directive (2008/50/EC) (Commission directive, 2015), which aims at a general reduction in PM concentrations in urban areas, and directive (2016/2284) (Commission directive, 2016), which establishes commitments to a reduction in national emissions of, among other pollutants, PM_{2.5}. Likewise, the WHO (2015) and UNECE (2007) have reported on the importance, costs and benefits of reducing concentrations, showing progress in the implementation of not only effective, but also economically sustainable, measures.

This article seeks to design an EAS model based on risk, stochastic and ML models that predict PM_{2.5} behavior at least 24 h before an increase in concentrations. Its objective is to outline an EAS protocol, capable of being implemented in any region with an air quality monitoring network, using a general methodology that allows policy-makers to adapt it to their city, using local data (e.g., population groups, pollutant concentrations). To illustrate its possible application, the city of Bogotá, Colombia is utilized as a case study.

2. Method

2.1. Study area

Bogotá, Colombia (4.60971, −74.08175) is a city located in the tropics [where there is no framework of equations (as the geostrophic approximation) that can describe atmospheric dynamics (Holton, 2004), and local thermodynamic processes are important for the development of convective events (Casallas et al., 2021b)], in the eastern Andes Mountain range. Nevertheless, as mentioned, this design is intended to be used in any city that has an air quality monitoring network. Bogotá has 12 air quality monitoring stations, part of the Air Quality Monitoring Network of Bogotá (AQMNB), located throughout the city (Fig. 1): Guaymaral (S1) to the north, Usaquén (S2) northeast; Suba (S3) northwest; Las Ferias (S4) and Centro de Alto Rendimiento (CAR) (S5) downtown; Ministerio de Ambiente (MADS) (S6) to the east; Fontibón (S7) and Puente Aranda (S8) to the west; Kennedy (S9) and Carvajal (S10) southwest; Tunal (S11) to the south; and San Cristóbal (S12) southeast (SDA, 2020). The stations are divided into three categories: S4, S6, S7, S8, S10 are traffic-industrial stations; S1, S2, S3 are considered suburban; and S5, S9, S11, and S12 are urban background stations (Mogollón-Sotelo et al., 2020).

To determine the influence area of the stations, first, localities with only one station are represented by this sole station. However, if there are two stations within one locality, it is divided into Zonal Planning Units (ZPUs) and the closest ZPU to each station is selected. Lastly, if there are no stations in a locality, the ZPUs closest to a station are selected and integrated into its influence area.

2.2. Models

2.2.1. Deterministic models

This research evaluated 3 different models to forecast PM_{2.5}. Furthermore, the WRF-CHEM model Version 4.2 (Skamarock et al., 2019) was also evaluated, but due to large uncertainties (RMSE $\approx 38 \mu\text{gm}^{-3}$) produced by Bogotá's emission inventory (e.g., Kumar et al., 2016; Casallas et al., 2020; Ballesteros-González et al., 2020), it could not be fully validated for the EAS. Although the behavior of wind field, radiation, temperature, and precipitation are well represented, as identified by several authors (e.g., Kumar et al., 2016; Casallas et al., 2020; Guevara-Luna et al., 2020; Ballesteros-González et al., 2020), the pollutants have large uncertainties in their magnitudes. For this reason, it is important to make major efforts in order to develop a reliable emission inventory database for the city of Bogotá, which would allow the incorporation of this model to the EAS, bearing in mind that the

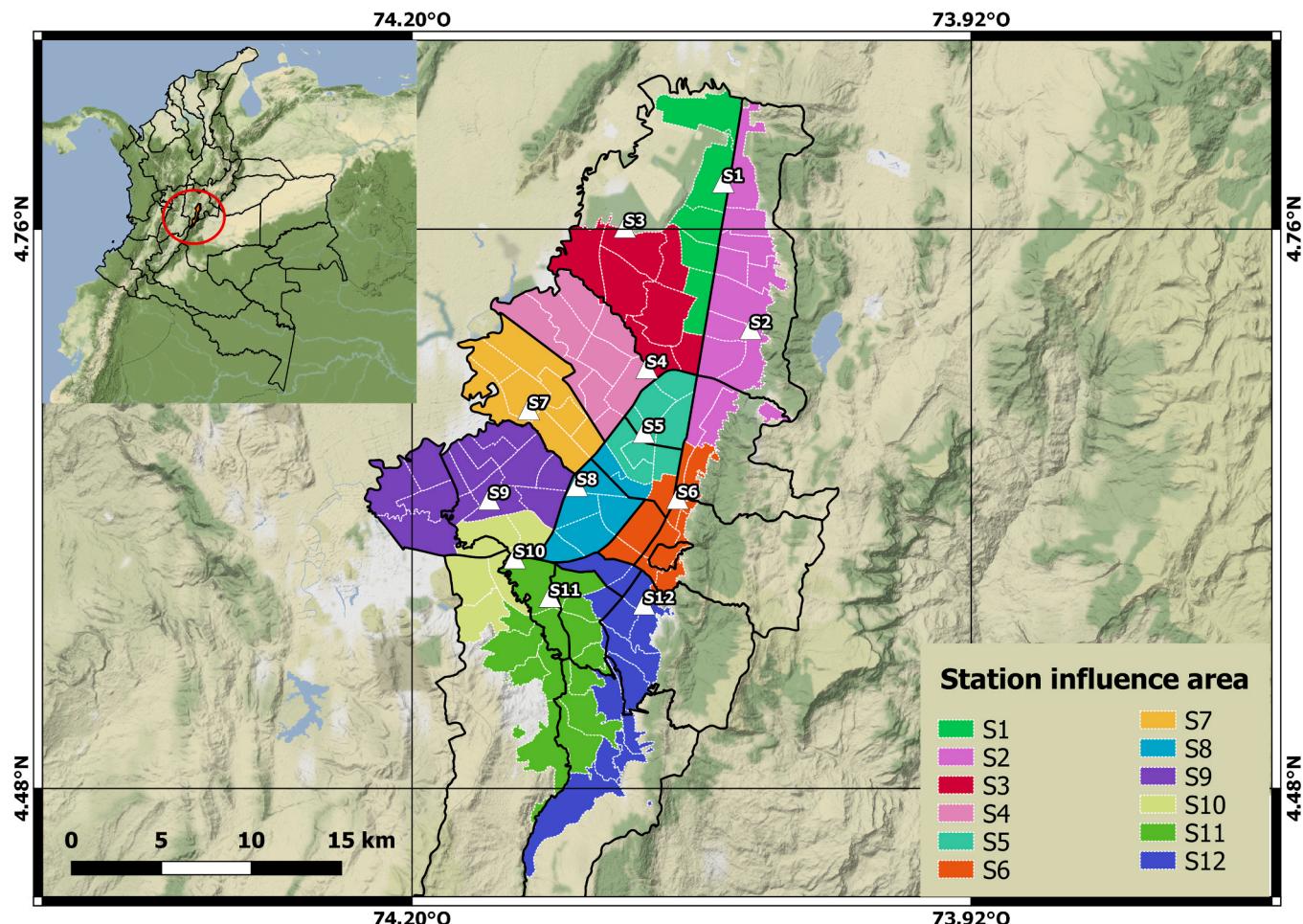


Fig. 1. Geographical location and influence area of the 12 stations (white triangles) of the AQMNB. The polygons indicate the division into localities (black borders) and the division into ZPUs (white borders) in the city of Bogotá.

WRF-CHEM model has proven to be useful in the comprehension of the fundamental behavior of contaminants and their sources, and in the evaluation of different air quality scenarios. For example, Sokhi et al. (2021) showed that understanding the behavior of pollutants (e.g., ozone), especially in low pollution conditions, is important because some contaminants can increase their concentrations in an undesired manner, something that must be accounted for when developing new policies.

Three different ML models were evaluated. The first model was the SVM model, created by Cortes and Vapnik (1995). This machine aims at orienting a hyperplane in a way that is the farthest possible from each data of the series, something that allows it to classify the data and make regressions with a classification function (Fletcher, 2009). For this reason, this tool has been used in air pollutant predictions (e.g., Lu and Wang, 2005; Hou et al., 2014; Mogollón-Sotelo et al., 2020), delivering satisfactory results in regards to describing PM_{2.5} behavior and magnitude. On the other hand, ANN were published for the first time by Ivakhnenko and Lapa (1965) and improved by Ivakhnenko et al. (1967). These networks are used to recognize images, to determine the precipitation of a day and to describe the behavior of a pollutant, among others (e.g., Hochreiter and Schmidhuber, 1997; Zhang et al., 2012; Shahraiyni and Sodoudi, 2016). As the accuracy of these techniques has been widely tested (e.g., Huang and Kuo, 2018; Franceschi et al., 2018; Tzanis et al., 2019) for air quality modeling, we evaluated their precision to simulate PM_{2.5} in a high-altitude tropical city and their capacity to work as an input tool for an EAS.

To build the training sets, air quality hourly data from 12 stations of

the AQMNB, with at least 70000 data points per station between 2015 and 2020, were used. In the cases where the data had missing values, they were imputed using the hourly mean of each station. Although not shown here, an imputation using linear regressions/dense neural networks, taking into account the closest station with available data, was performed for the station S10. However, the simulation results did not show considerable changes when following this procedure. Thus, the hourly mean imputation method was used, as it needs less computational resources. The X-vector (Input) and Y-vector (Output) are constructed equally for each model, the X-vector is designed with slices of 120 data points previous to the “present” time, and the Y-vector has 24 data points that represent 24 h in the “future”. This way, 120 data points (hours) from the “past” produce the simulation of 24 h in the “future” (See Fig. 2 and the Supplementary Material -hereafter SM- Table SM1). For the three models, a grid search method (e.g., Ndiaye et al., 2019) was performed to select the parameters that produce the best forecast (Table SM1). Additionally, an early stopping method is applied to the ANNs to prevent them from overfitting (e.g., Prechelt, 1998).

Here the SVM is built following the work of Mogollón-Sotelo et al. (2020). Nevertheless, it is important to acknowledge that this model has a limitation in comparison to the other two ML techniques: the forecast produces one value at a time, so the 24 h simulation has to use predicted values, something that increases the uncertainty with respect to the neural networks (for more details, see Mogollón-Sotelo et al., 2020). The LSTM network is based on (Casallas et al., 2021a), while the design of a 1-Dimension CNN merge with a bidirectional LSTM (hereafter 1D-BDLM) is based on Huang and Kuo (2018). However, the structure

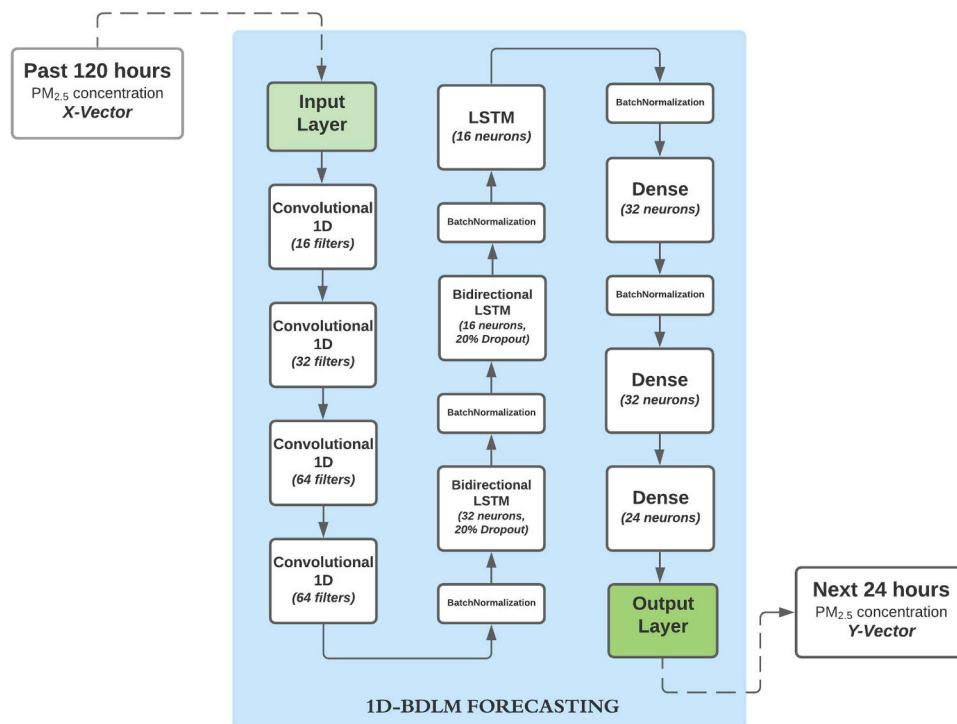


Fig. 2. 1D-BDLM neural network structure. Notice that every box has the number of neurons/filters in the layer and that the dropout percentage of a layer is also indicated.

and layers of the latter are modified to achieve the objective of forecasting 24 h as output (instead of one, as in Huang and Kao's case). The structure of the neural network models are described in Fig. 2 (1D-BDLM) and in Figure SM1 (LSTM), and the parameters of the three ML models are shown in Table SM1. The SVM was designed with SK-learn-0.24.1 (Pedregosa et al., 2011) and the ANNs were designed using Tensorflow-2.4.1 (Abadi et al., 2015) and Keras-2.4.3 (Chollet et al., 2015) libraries from Python-3.8.

2.2.2. Stochastic model

The Monte Carlo model (Eq. 1) includes the uncertainty present in every input data supplied by the AQMNB, through variables of a continuous distribution of PM_{2.5} concentrations. This allows the calculation of probabilistic risk for each population group of the selected stations. This was conducted to include the uncertainty of the input data and the effects of atypical data on the model's results and evaluation, something not included in the deterministic risk (Asante-Duah, 2017; McFarland and DeCarlo, 2020). In relation to most environmental problems, this differential and gender-based probabilistic approach is required to specify the spectrum of available information, which may contribute to the quality of the risk assessment task for each population group, and to simultaneously provide decision-makers with a robust analysis (Bu et al., 2019). To design this model, we identified the best data distribution adjustment for daily PM_{2.5} concentrations from January 1st, 2018 to December 31st, 2020, in each station of the AQMNB. Different probabilistic distributions are used (c.f. Table SM2) as the main input of the Monte Carlo model (Liu et al., 2020a).

$$E(\chi) \approx \frac{1}{N} \sum_{n=1}^N \chi_n \quad (1)$$

Eq. 1. Monte Carlo model. Where $E(\chi)$ is the expected value, χ is a random variable and N is the size of the sample.

2.3. Risk Assessment for PM_{2.5} in Bogotá

The city of Bogotá implemented a corrective air quality alert system

(Decreto 595 of, 2015), i.e., actions to mitigate population exposure, executed after a pollution event has occurred. For this reason, the protocol must be improved by designing an EAS that can be activated 24 h prior to the pollution event. To achieve this, the risk of acute exposure to PM_{2.5} is assessed, based on the negative effects on health (Xing et al., 2016). Thus, the method of risk assessment of the EPA (2020) was incorporated. This method is divided into three phases: 1. Identification and characterization of the danger; 2. Characterization of the risk; and 3. Risk management.

2.3.1. Identification and characterization of the danger

In this phase, the danger was identified based on the yearly maximum permitted level of PM_{2.5}, internationally suggested by the WHO, of 10 $\mu\text{gm}^{-3}\text{year}^{-1}$ (hereafter WHOYL) (WHO, 2018). We also identified the percentage of days that surpassed the WHO's daily limit of 25 $\mu\text{gm}^{-3}\text{day}^{-1}$ (hereafter WHODL) (WHO, 2018), and hourly composites are used to evaluate the hourly behavior of the pollutant and the risk associated with it. On the other hand, the Air Quality Index (AQI) is used, instead of Bogotá's Air Quality Index (BOAQI), as the former has been used internationally and, thus, can be utilized for any city. Once the risk is identified, PM exposure of the population can be assessed.

2.3.2. Characterization of the risk

The population of the studied zone (data from (DANE, 2018)) is classified into 5 subgroups: Infants (< 3 years), Children (3–11 years), Young people (12–29 years), Adults (30–65 years), and Older people (> 65 years). Furthermore, the last three groups are subdivided by gender. This selection of reference groups allows the EAS to mitigate the risk of developing diseases related to PM_{2.5} pollution in the entire population, through a differential approach (e.g., Wang et al., 2018; Lu et al., 2019; Gómez Peláez et al., 2020). To determine the risk for each population group, deterministic models coupled with a probabilistic model are used. These models, incorporated to the EAS, allow highly precise decision-making, in relation to risk management, in a preventive manner, instead of a corrective one (Liu et al., 2020b). Hence, this phase

quantitatively determines the probability of harmful effects occurring due to PM_{2.5} exposure for the entire population.

To quantitatively determine the population risk in relation to health, the methodology of Greene and Morris (2006), based on the EPA (2014), is used. With it, we can determine that non-carcinogenic population risk (R_p) (Eq. 2) depends on C (PM_{2.5} concentrations in $\mu\text{g m}^{-3}$) and UR , where UR becomes the percentage (c.f. Table SM3) of each population group of the studied zone. From Eqs. 1 and 2, we can derive Eq. 3, which implements the Monte Carlo model to stochastically predict population risk. With the determined model and distributions, 200000 random simulations are conducted to represent possible risk scenarios (Asante-Duah, 2017), obtaining the differential and gender-based risk, using a confidence interval of 95%.

$$R_p = C * UR \quad (2)$$

Eq. 2. Population Risk (R_p) (%)

$$R = \frac{1}{N} \left(\sum_{i=1}^N C_i * UR \right) \quad (3)$$

Eq. 3. Adaptation of the Monte Carlo equation to calculate population risk. Where C_i is the random variable of concentration for each of the i experiments and N is the number of experiments.

2.4. Statistical validation of the models

For the evaluation of the model, we used 182 days that are removed from the training set. These days were distributed in different AQI categories so that the model was capable of reproducing low, medium, and high air pollution scenarios. In addition, every month of the year has at least 10 days of representation (not continuous days, and taking weekend and week days to also account for weekly changes), in order to evaluate the different rainy seasons and also a variety of weather conditions (e.g., wind field, precipitation). To validate the model, we used the Root Mean Square Error (RMSE), the Mean Bias (MB), the R², the Index Of Agreement (IOA), the Factor of Two (FAC2), the Normalized Mean Bias (NMB) as statistical parameters (e.g., Willmott et al., 1985; Barnston, 1992; Boylan and Russell, 2006; Cobourn, 2010; Tzanis et al., 2019; Mogollón-Sotelo et al., 2020; Liao et al., 2021). As categorical statistics, the Hit rate (HIT), the False Alarm Rate (FAR) and the Proportion of Correctness (POC) were used (e.g., Chai et al., 2013; Sayeed et al., 2021). A further explanation of these parameters, including its equations, are found in Table SM4.

2.5. Risk management

Based on the examination of the monitoring information, the simulations and the risk calculations, the current District Protocol for the Response to Air Pollution Alerts in Bogotá (2015) and several international protocols (e.g., Liu et al., 2020b) are analyzed, in order to articulate and incorporate immediate responses and adequate management measures to minimize exposure and vulnerability. The technological tools articulated with preventive risk management may help state agencies to decrease PM concentrations and to avoid yellow or orange alert events. Likewise, measures related to actions and communication with the general public are incorporated, in order to improve their response and self-management concerning the risk of exposure to high concentrations of PM.

3. Results and discussion

3.1. Identification and characterization of the risk

To identify the risk in the studied zone, we performed three different evaluation criteria (Fig. 3). First, the PM_{2.5} hourly mean was calculated (Fig. 3a), showing that in the case of Bogotá there are two local

maximums in the day: the first one between 6 h and 8 h Colombian Local Time (CLT) and the second one between 18 h and 20 h CLT. These slots reflect the times when traffic sources are more present, taking into account that people are moving from and to work (Castillo-Camacho et al., 2020). The WHO does not have a limit for an hourly value. Indeed, when using the WHODL, at least 9 of the 12 stations surpass it for a few hours, something that must be addressed in air quality policies. In addition, a daily evaluation of PM_{2.5} concentrations shows that, between 2015 and 2020, all the stations surpassed the WHODL (blue bars in Fig. 3b) at least 10% of the days. In S8, S9, S10, S11, this limit is surpassed in \approx 20% of the days and, in S9/S10 the limit is crossed more than 40/70% of the days, respectively.

On the other hand, in 2020 all the stations had higher yearly mean concentrations (orange bars Fig. 3b) than the WHOYL. This situation happened even during the COVID-19 pandemic, where most of the pollutants decreased their concentrations due to the lack of mobility and a drop in industrial activities (Sokhi et al., 2021). Likewise, it is important to mention that, i) as seen in Fig. 3b, stations S8, S9, and S10, located in the southwestern area of the city, have concentrations 2 or 3 times higher than what the WHO provides. This is because this zone has the greatest number of industries and diesel-based public transport (e.g., Rojas, 2004; Castillo-Camacho et al., 2020) (see the method section for more details about the type of stations). ii) Colombia, especially Bogotá, suffers from Long Range Transport (LRT) such as biomass burning (wildfires) coming from the East and Southeast part of the country (e.g., Ballesteros-González et al., 2020; Mendez-Espinosa et al., 2020; Sokhi et al., 2021). These arguments lead to the conclusion that there is a risk to public health in the city in an hourly, daily, and yearly time resolution, especially in the southwestern polygon.

3.2. Exposure and risk assessment

To determine which tool has the highest precision when forecasting PM_{2.5}, the performance of the models (SVM, LSTM, and 1D-BDLM) is compared by simulating 182 days that are selected as described in Section 2.4. These days are evaluated by means of 9 statistical parameters for each station (Fig. 4 and details in Table SM2). Fig. 4 shows the comparison of three ML models using evaluation parameters, where the HIT, the FAR, and the POC are categorical parameters and their threshold is the WHODL. The parameters are calculated for the daily mean of each station and the mean station type (i.e., Industrial-Traffic Mean, Suburban Mean, and Urban-Background Mean), that is found using a virtual station: an hourly mean composite of the stations in the same category is calculated for the model's results and observations, and then the statistics are computed.

For all the parameters, except the HIT and the NMB, the 1D-BDLM has the best performance and the SVM the worst. The SVM has the lowest scores, mainly due to overestimations of PM_{2.5} concentrations. This is probably caused by their inability to grasp vastly fast changes (Mogollón-Sotelo et al., 2020) and the pollutant's behavior, as seen in the R² values. In spite of this, the precision of the SVM is better than the ones presented in previous studies of Bogotá (e.g., Zarate et al., 2007; Kumar et al., 2016; Casallas et al., 2020; Pulido et al., 2020; Ballesteros-González et al., 2020). The 1D-BDLM and the LSTM models have good performance when predicting PM_{2.5} and can be used as an input for the EAS system. Although, in the HIT parameter, the two networks have similar performances, for the other statistics, the 1D-BDLM has better results (except for NMB and MB where they are very close, but the LSTM is better, due to the consistency of the results throughout the stations), possibly due to the CNN's capability of identifying key features, and also because the bidirectional LSTM has the ability to learn more robustly and produce nowcasting's (e.g., Huang and Kuo, 2018; Sayeed et al., 2021). For this reason, this 1D-BDLM network is chosen to be further described and analyzed.

The 1D-BDLM model presents values higher than 0.6, 0.85, and 95% for the R², IOA, and FAC2, respectively. This indicates that the model is

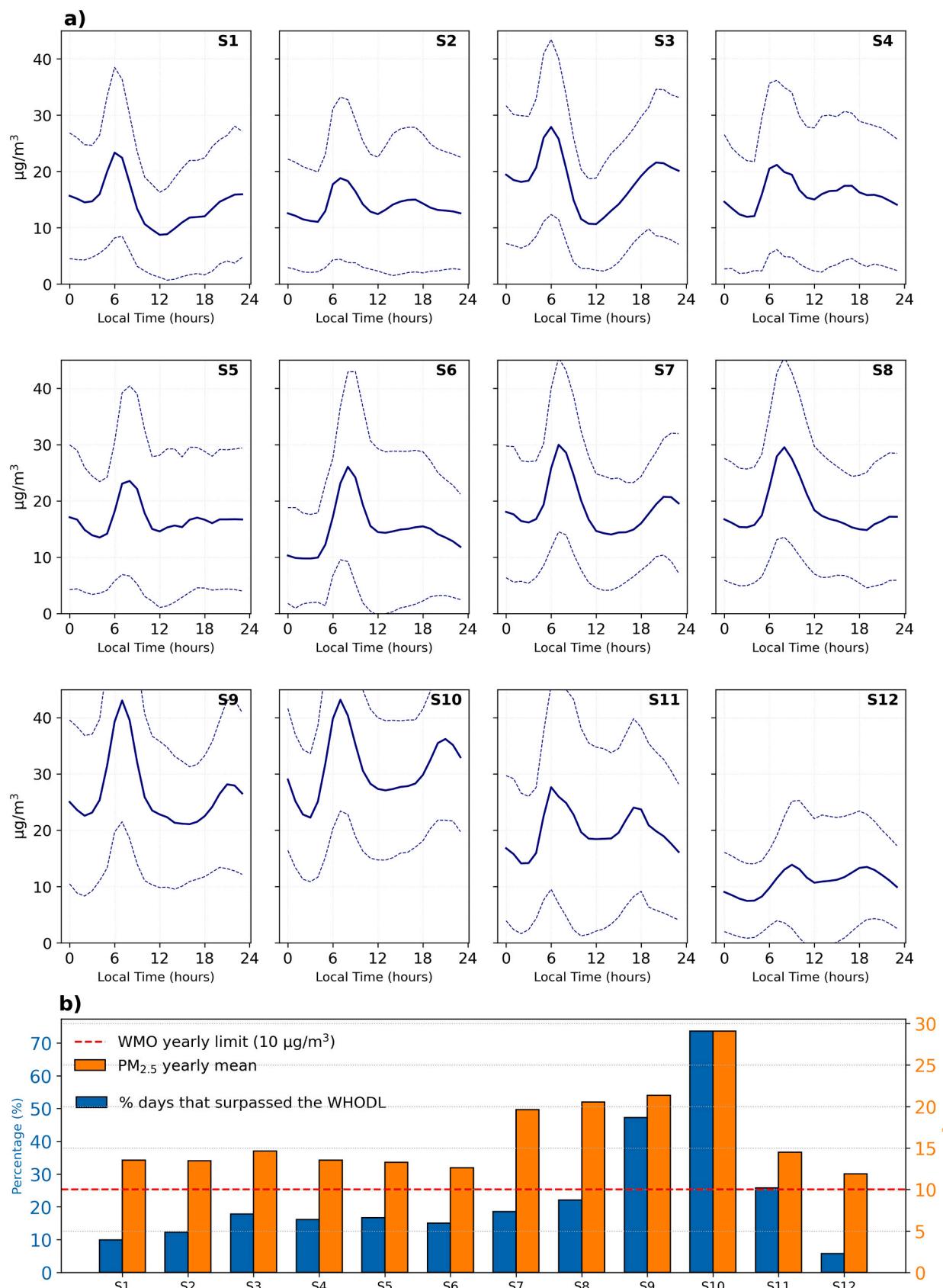


Fig. 3. a) PM_{2.5} hourly mean concentration for every station calculated for the period between 2015 and 2020. The dotted lines represent the standard deviation, to account for the data variability. b) The blue bars represent the percentage of days between 2015 and 2020 that surpassed the WHODL, per station. The orange bars show the PM_{2.5} yearly mean concentration of 2020 per station. Notice that the red dashed line is the WHOYL and has to be read alongside the orange bars.

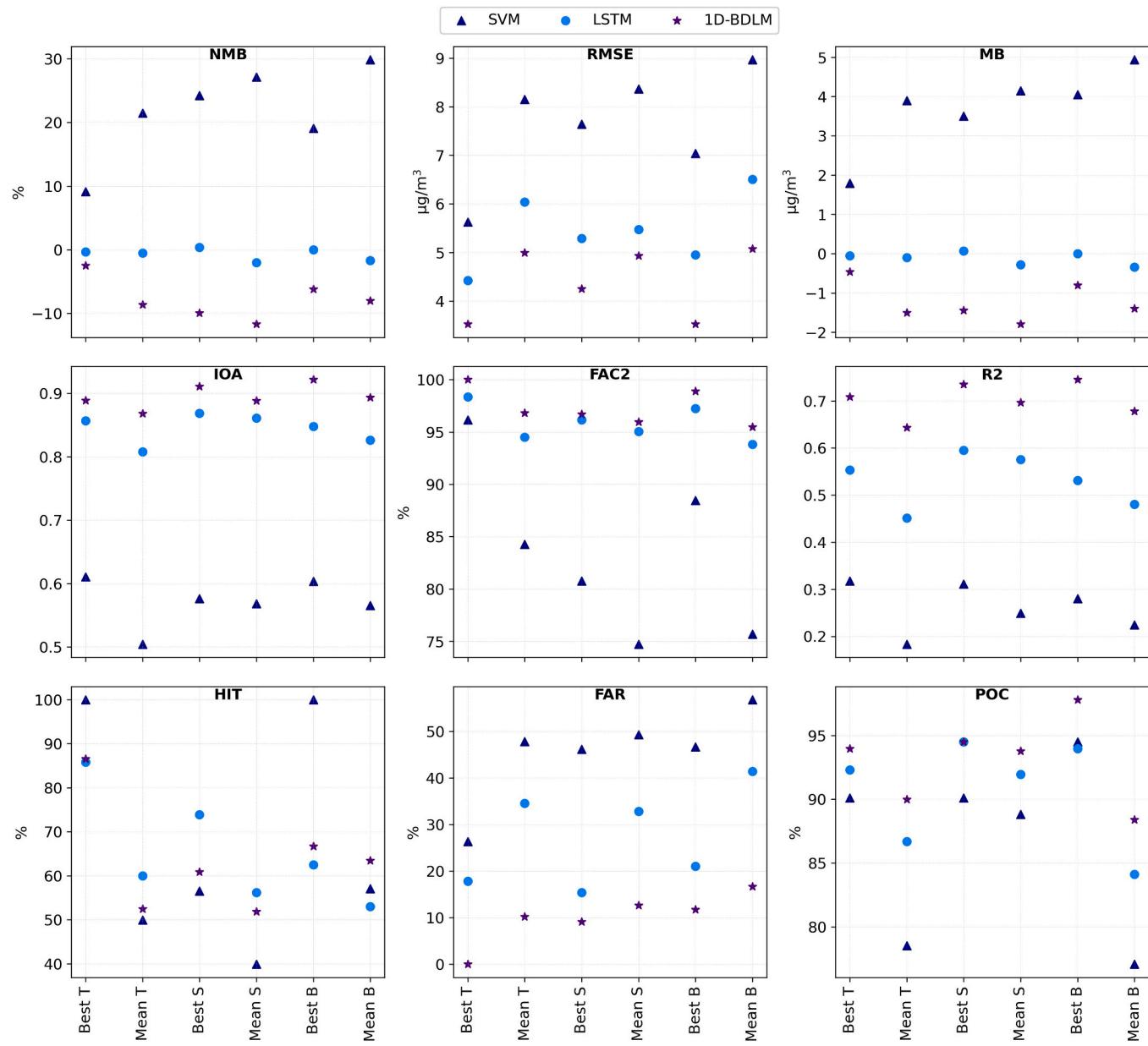


Fig. 4. Average of the 9 statistical parameters evaluated, calculated with the daily mean concentration, for the best -Traffic (T), Suburban (S), and Urban background (B)- station and for the virtual mean station per category. The models are represented by markers and each panel indicates a different evaluation parameter.

able to represent the behavior/tendencies of the pollutant in an efficient manner. Furthermore, the NMB ($\approx 7 \pm 4\%$), the RMSE ($\approx 4.5 \pm 1 \mu\text{gm}^{-3}$) and the MB ($\approx 1 \pm 0.7 \mu\text{gm}^{-3}$) show that the model is able to accurately simulate the magnitude of the pollutant, which demonstrates the high accuracy and low uncertainties associated with the model. Although the model is able to represent the magnitude and behavior of the pollutant, it is also important for an EAS that the 1D-BDLM can identify highly polluted events and not produce false alarms, something that is accounted for by the categorical statistics. The model identifies more than $\approx 63 \pm 8\%$ of the alarms produced in the 182 days evaluated, with a false alarm ratio smaller than $\approx 10 \pm 5\%$, and correctness of $\approx 92 \pm 3\%$, taking into consideration the WHODL as threshold. For these reasons, the network is validated (with high precision) to be used as input in the EAS.

To evaluate the spatial behavior of the 1D-BDLM in the studied area, an anomaly inspection was carried out for 30 days, following the methodology validated by [Mogollón-Sotelo et. al. \(2020\)](#). The results show a similar spatial distribution of the errors for the days examined

([Fig. 5](#)). Thus, a map of the most polluted day of the period (2019–03–28) is shown in [Fig. 5](#) as an example of the model's spatial performance. The highest anomalies (red) are in S8, S9 where the model sub-estimates the AQI values. These two stations are in the southwestern polygon where the concentration shows sudden and steeper changes in the morning, a feature that is not fully represented by any of the models and needs to be improved in future work, especially in stations where these changes and magnitudes are anomalous. Also, the S7, S6, S11 and S12 stations have low sub-estimation (yellow). In contrast, the northern, center zone (S1–S5) and S10 have the closest values to 0 (green and blue), which shows that the 1D-BDLM has a better precision when pollution does not have steeper (and high magnitude) changes in its concentration throughout the day, or when these changes normally occur in the stations. This, alongside the results of [Fig. 4](#), shows that the model has high spatial precision and is able to recreate the pollutant's behavior, magnitude, and alarms in each of the stations.

Once the precision of the 1D-BDLM is determined through the anomalies map, the range of population risk is calculated ([Eq. 2](#)) for each

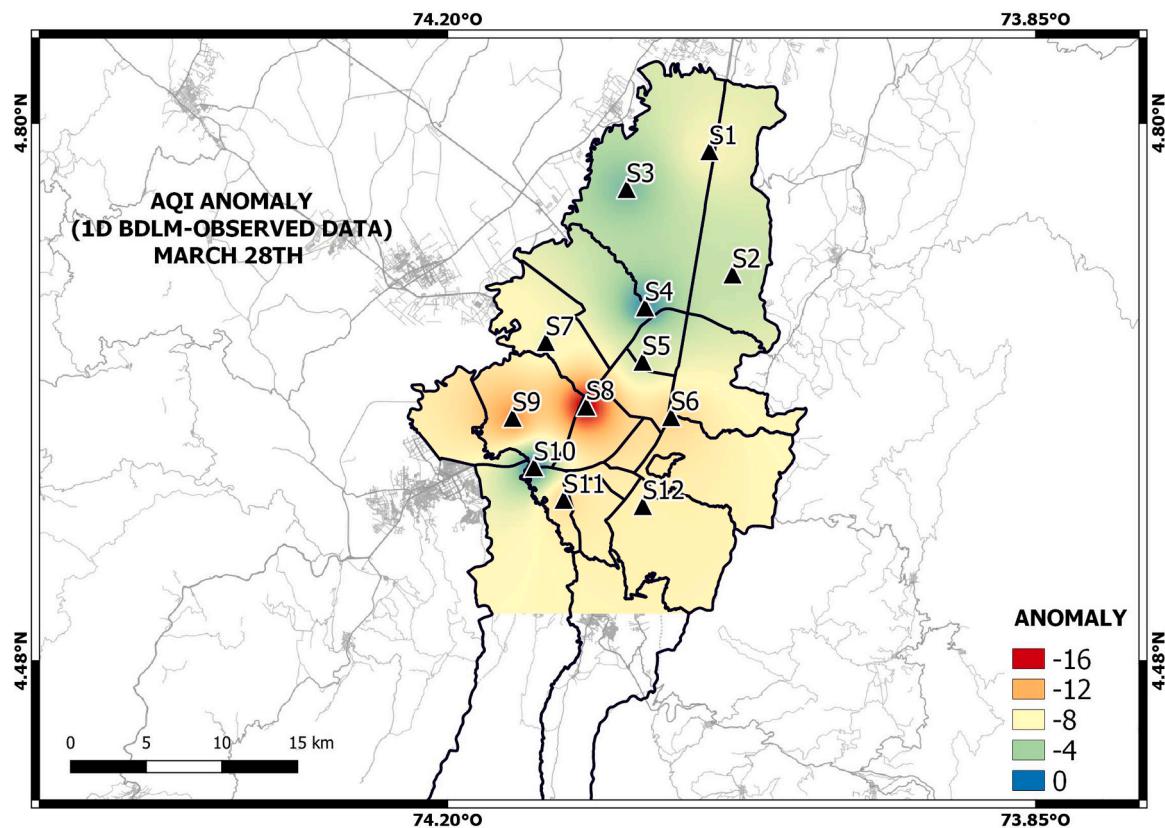


Fig. 5. AQI anomalies map between the 1D-BDLM and the observed data of the AQMNB on March 28th, 2019 in the city of Bogotá-Colombia.

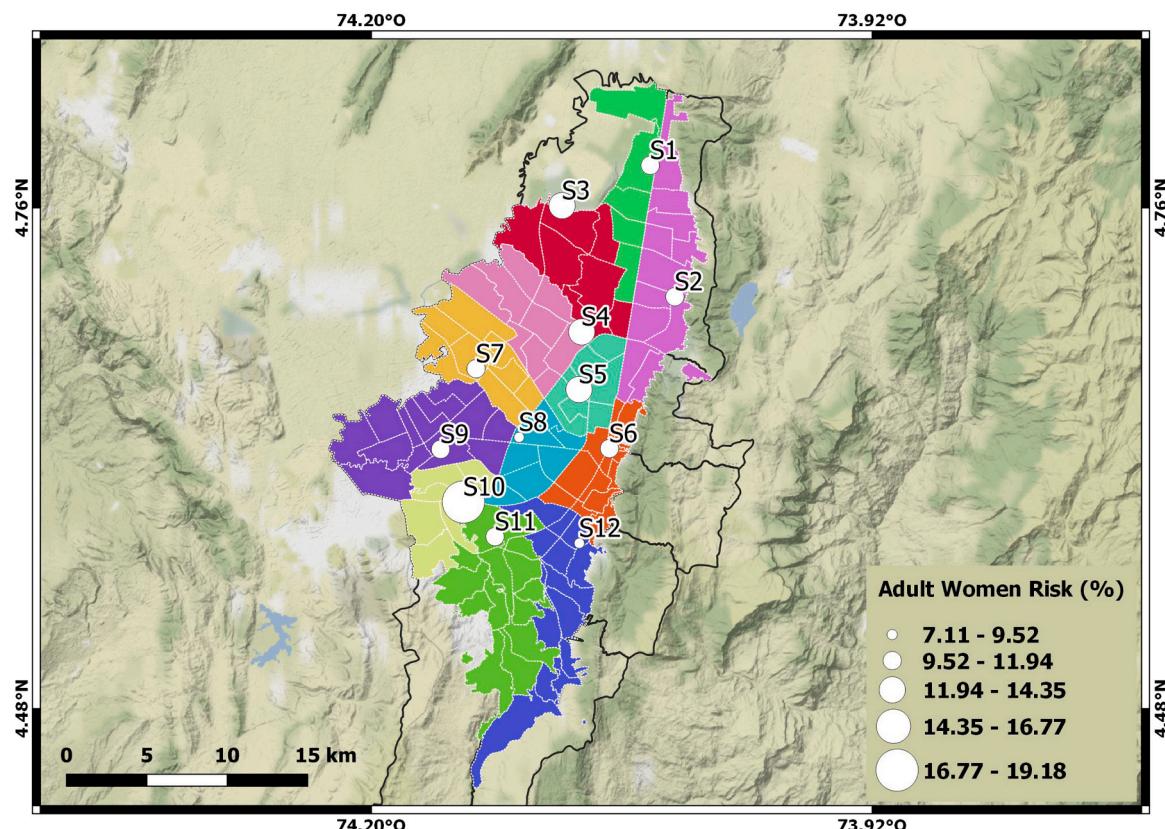


Fig. 6. Risk percentage for adult women on the most polluted day of 2019 (March 28th) in the city of Bogotá.

category of the AQI and each population group (c.f. Table SM5). Based on the 1D-BDLM, the risk is calculated (c.f. Table SM6 - 2019–03–28-), and the Monte Carlo method is performed to assess the randomness in model inputs (Eq. 3). This way, Monte Carlo accounts for uncertainties that are intrinsic to the data input, in order to obtain a probabilistic and more reliable result (McFarland and DeCarlo, 2020).

The output of these models can aid in the design of risk maps according to each population group and influence area. Although the risk values were found for the 182 days validated by the model, for the sake of simplicity, only the map of population risk for the most polluted day of the period (2019–03–28) and the population that suffers the greatest risk is shown (Fig. 6). In the southwestern zone of the city (S10), adult women present the highest risk ($19.18 \pm 1.5\%$ of the population) due to the PM_{2.5} concentration forecasts for this area. Nonetheless, in the other two stations within the same polygon (S8 and S9), PM concentrations also have special relevance (Fig. 3), but there are no considerable percentages of risk for adult women on this day. This suggests that, in order to determine the risk of a population group, it is important to evaluate each area of influence independently, taking into account that this risk does not only depend on the pollutant concentrations or the number of people from a specific population group living in the area. Hence, long-term strategies must not only be designed in relation to pollution mitigation but also concerning population distribution throughout the city. Consequently, this validates these models (especially the 1D-BDLM and the LSTM) to be used as an input tool in the EAS protocol.

3.3. Risk management concerning air quality

In relation to risk management concerning air quality, the city does not have an EAS that contemplates PM concentrations forecast and/or risk for each reference group. These flaws stem from the fact that the alert is issued based on real-time monitoring of pollutants, generating corrective protocols, rather than preventive ones. Thus, the risk of different vulnerable groups suffering harm is ignored in relation to air quality (Calderón-Garcidueñas et al., 2008; Brook et al., 2010).

The 1D-BDLM, with the input randomness of the Monte Carlo method, is a tool of predictive modeling that can be incorporated into the established procedures issued by public authorities in Bogotá pursuant to the District Protocol for the Response to Air Pollution Alerts (Decreto 595 of, 2015, for PM_{2.5}). In addition to the established protocol, the prediction 24 h before the occurrence of an event, and the inclusion of the risk factor for each level of alert and population group, generates a robust tool that can aid in the decision-making process and in the creation of adequate sectorized strategies to face the risk caused by the deterioration of air quality. Likewise, this paper suggests further monitoring during the 24 h prior to the simulated event. If the yellow alert persists, an official declaration of the alert is suggested, and the model can be used to determine the proper time to deactivate this alert and its measures.

The model identifies specific areas where an in-situ supervision is recommended, according to the intensity of the alert. The prediction can also establish recommendations to manage the risk and is capable of estimating the percentage of people at risk of developing respiratory diseases for each population group. This way, the incorporation of specific actions to protect human health, according to each vulnerable group, optimizes the task of risk management and reduces the impact on public health. Hence, to reduce the risk in possible alert events related to air quality, restrictive measures must be imposed concerning public and private transportation, which, due to vehicle age and/or the type of fuel used, can contribute to the increase of PM_{2.5} concentrations, leading to an increase in the alert level (e.g., Rojas, 2004). For stationary sources, in-situ monitoring in the influence area (i.e., zones in alert) allows the identification of emission hotspots. Furthermore, through a joint articulation with authorities, a temporal decrease in certain activities can be achieved, in order to control atmospheric concentrations of PM_{2.5}. This can be done in an optimal way, by means of possible restrictions (e.g.,

partial, hourly, by sectors, for specific processes in factories), as well as for vehicle traffic (e.g., hourly, depending on the type of fuel used, date of vehicle registration), in zones of possible alerts and not throughout the entire city.

In regards to public health, when a possible alert is declared, the active search for older adults in the influence area is recommended, according to the analysis of the spatial prediction. Also, a follow-up monitoring of the impact of the pollution event on human health for reference groups is suggested, in the cases where the event in fact occurs. In cases of a red alert issued by an intersectoral technical consensus, and taking into account the predictions in the behavior and toxicity of the pollutant, supplying N95 respirators may be deemed as necessary. Likewise, the evacuation and/or enforcement of transit restrictions in the influence areas is also suggested, as well as following health recommendations (Table 1) pursuant to the risk values for each AQI category (Table SM5), which follows the pollution thresholds established by the WHO (2018), and the percentage of population for each reference group defined in this research.

The implementation-validation of the protocol can be divided into two components, technical and social. Regarding the technical aspect, the results of this research can support governments in their decision-making strategies, by showing the importance of incorporating further monitoring to increase the efficiency of the current risk management protocol. The protocol could be validated through evaluation indicators that can determine the percentage of people/industries/mobile-sources that are following the protocol recommendations. It is also important to make real-time and widespread measurement campaigns in air quality hotspots that will aid in the task of tracking air quality in a more efficient and realistic way, to quantitatively identify pollution reduction due to the protocol measures.

Concerning the social aspect, the scientific community (including higher-education institutions and academic networks) and the general

Table 1

Recommendations for health notices in relation to risk probability for each AQI category.

Alert Level	Health recommendations for vulnerable population (i.e., infants, children and older adults)	Health recommendations for the general population
Yellow Alert	Reduce or reschedule strenuous outdoor activities if there are signs of asphyxia, coughing, sore throat, asthma, respiratory diseases.	Reduce physical outdoor activities, take breaks, and decrease the time of physical activity.
Orange Alert	Limit the practice of strenuous and prolonged outdoor activities and take more breaks when doing it. Keep doors and windows shut throughout the day to reduce interior personal exposure and engage in quiet indoor activities. Cover the air vents, and other similar holes through which air can flow, of your home with a wet cloth.	Limit outdoor time or completely reduce physical activities. Consider exercising at home to avoid outdoor exposure. Wash fruits and vegetables before consuming them. Clean utensils and surfaces with a wet cloth to remove any dust.
Red Alert or higher	Follow institutional measures when an evacuation order is issued. If not possible, avoid any physical activities and keep the doors and windows shut and cover air vents with a wet cloth. Stay home for 12 h after the alert has been issued and monitor outdoor atmospheric concentrations using public information websites. The use of N95 respirators is highly recommended, both indoors and outdoors.	Follow institutional measures when an evacuation order is issued. If not possible, reduce strenuous and prolonged physical outdoor activities to 15 min max. Stay home and monitor outdoor atmospheric concentrations using public information websites. The use of N95 respirators is highly recommended.

public can contribute with systems, surveys, research and measurement equipment with low-cost sensors and analysis tools. Likewise, the development of air governance criteria that include the affected community will allow concrete actions to be generated for the reduction of pollutants and self-management of risk from exposure to contaminated environments (Wan et al., 2020). In this way, we consider that it is possible to socialize and involve citizens in air quality monitoring, to empower them and educate them regarding the effects and characteristics of air pollution. This can be achieved by disseminating the results at events that include several actors involved in air governance such as the academia, governmental authorities and citizen groups.

4. Conclusions

In the city of Bogotá, PM_{2.5} is the most dangerous pollutant, due to its concentration exceeding daily and annual limits, alongside its hourly peaks (Fig. 3). 2019 had the highest number of alerts concerning air quality in the city, which suggests a negative impact on human health. This highlights the need of implementing a functioning preventive system. For this reason, this work focuses on the creation of a preventive EAS. In order to determine the best predictive models, three machine learning techniques (SVM, LSTM, and 1D-BDLM) are compared with the evaluation of 182 days by means of 9 statistical parameters. This evaluation led to the conclusion that the 1D-BDLM produces the most precise simulations and is able to predict the behavior, magnitude and air quality alarms in an effective manner, without producing false alarms.

The alert system, thus, incorporates a 1D-BDLM that accounts for data uncertainty through the Monte Carlo model and is capable of predicting the risk for each population group. Furthermore, a protocol is designed, using these models as the main input, which activates 24 h before a pollution event. The protocol distinguishes the level of alert (e.g., yellow, orange) and the type of population (e.g., vulnerable groups) at risk, with measures focusing on the mitigation of pollution and the reduction in population risk. To decrease concentrations, restrictions on vehicle traffic in specific zones of the city or, if necessary, in the entire city, are suggested. In relation to stationary sources, the implementation of monitoring measures is proposed, in order to identify the most polluting factories and to (partially or completely) restrict their operation during a specific period of time (e.g., in the peak of concentration levels). Concerning population risk, the protocol seeks to reduce the exposure time of population groups, by avoiding outdoor activities and through the use of protective gear (e.g., masks).

Based on what has been stated, we can conclude that the 1D-BDLM (the most precise model) integrated into the Monte Carlo model is capable of grasping the variability intrinsic to the nature of the data of each station. For example, S7 station has a high variability due to the low number of data and the fact that it does not behave as any statistical distribution. Nonetheless, the model has high accuracy, with an uncertainty of $\approx 7 \pm 4\%$ (Figs. 4–5) in relation to risk prediction, and can establish that the population groups most impacted are adult women (30–65 years) and younger men (12–29 years), due to the fact that these are the groups with the largest population in the city. It also suggests that vulnerable groups (older people, children, and infants) are not at the highest risk but are possibly the most prone to develop serious diseases caused by PM. In addition, it is clear that the protocol must have a preventive approach that starts with the mitigation of the contaminant and a decrease in the population risk, as this could lead to a reduction in the number of people that may suffer PM-related diseases and a reduction in the correlative costs. Accordingly, this alert system (the models and protocol) can be potentially used as a tool of air quality management in cities with PM-related risks.

For future work, it is important to make major efforts in the development of a reliable emission inventory database for the city of Bogotá, allowing the incorporation of the WRF-CHEM model to the EAS, which could aid in the creation of model ensembles, the evaluation of scenarios and the study of the fundamental behavior of the pollutants, something

essential in policy-making (Sokhi et al., 2021). It is also important to test more ANN structures to continue improving the results, especially in cases where steeper changes are presented, or when very anomalous pollutant behavior occurs. For example, the inclusion of a multi-input layer could, in principle, increase the precision of the model. Likewise, the coupling of WRF-CHEM model outputs with ANN can not only better account for meso/regional scale interactions of the atmosphere, but also assess the local behavior of the pollution captured by the networks. In addition, the inclusion of more methods (e.g., BenMAP, Air pollution Social Impact Using Regression -EASIUR-, Intervention Model for Air Pollution -InMAP-) that make the risk assessment calculation more robust are necessary, in order to include ensembles in both risk and air quality models to reduce the uncertainty of the results as much as possible and also to account for the economic impacts associated with PM_{2.5} concentrations.

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CRediT authorship contribution statement

Nathalia Celis and Alejandro Casallas: Conceptualization, Data Curation, Methodology, Software, Validation, Formal Analysis, Visualization, Writing - Original Draft. **Ellie Anne López-Barrera:** Conceptualization, Formal Analysis, Writing – Original Draft. **Hermes Martínez and Carlos A Peña Rincón:** Software, Validation. **Ricardo Arenas:** Formal Analysis, Writing – Original Draft. **Camilo Ferro:** Data Curation, Software, Validation, Formal Analysis.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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Appendix A. Supporting information

Supplementary data associated with this article can be found in the online version at doi:10.1016/j.envsci.2021.10.030.

References

- Abadi M. et al., 2015. TensorFlow: Large-scale machine learning on heterogeneous systems, 2015. vo.2.4.1. (Version 0.2.4.1). Tensorflow.
- airALERT, 2005. AirAlert information. (<http://www.airalert.info/>) (Accessed 19 June 2020).
- Asante-Duah, D.K., 2017. Public Health Risk Assessment for Human Exposure to Chemicals, second ed. Springer, Washington, DC.
- Baena-Salazar, D., Jiménez, J., Zapata, C., Ramírez-Cardona, Á., 2019. Red neuronal artificial aplicada para el pronóstico de eventos críticos de PM_{2.5} en el Valle de Aburrá. DYNA 86 (347–356). <https://doi.org/10.15446/dyna.v86n209.63228>.
- Ballesteros-González, K., Sullivan, A.P., Morales-Betancourt, R., 2020. Estimating the air quality and health impacts of biomass burning in northern South America using a chemical transport model Sci. Total Environ. 739, 139755 <https://doi.org/10.1016/j.scitotenv.2020.139755>.

- Barnston, A., 1992. Correspondence among the Correlation, RMSE and Heidke Forecast verification Measures; Refinement of the Heidke Score. *Weather Forecast.* 7, 699–709. [https://doi.org/10.1175/1520-0434\(1992\)007<0699:CATCRA>2.0.CO;2](https://doi.org/10.1175/1520-0434(1992)007<0699:CATCRA>2.0.CO;2).
- Boylan, J.W., Russell, A.G., 2006. PM and light extinction model performance metrics, goals, and criteria for three-dimensional air quality models. *Atmos. Environ.* 40, 4946–4959. <https://doi.org/10.1016/j.atmosenv.2005.09.087>.
- Brook, R.D., Rajagopalan, S., Pope, C.A., Brook, J.R., Bhatnagar, A., Diez-Roux, A.V., Holguin, F., Hong, Y., Luepker, R.V., Mittleman, M.A., Peters, A., Siscovich, D., Smith SC, Jr, Whitsel, L., Kaufman, J.D., American Heart Association Council on Epidemiology and Prevention, Council on the Kidney in Cardiovascular Disease, and Council on Nutrition, Physical Activity and, M., 2010. Particulate Matter Air Pollution and Cardiovascular Disease. *Circulation* 121, 2331–2378. <https://doi.org/10.1161/CIR.0.b013e3181dbece1>.
- Bu, Z., Mmereki, D., Wang, J., Dong, C., 2019. Exposure to commonly-used phthalates and the associated health risks in the indoor environment of urban China. *Sci. Total Environ.* 658, 843–853. <https://doi.org/10.1016/j.scitotenv.2018.12.260>.
- Byun, D., Schere, K.L., 2006. Review of the governing equations, computational algorithms, and other components of the Models_3 Community Multiscale Air Quality (CMAQ) modeling system. *Appl. Mech. Rev.* 59, 51–77. <https://doi.org/10.1115/1.2128636>.
- Calderón-Garcidueñas, L., Villarreal-Calderon, R., Valencia-Salazar, G., Henríquez-Roldán, C., Gutiérrez-Castrillón, P., Torres-Jardón, R., Osnaya-Brizuela, N., Romero, L., Torres-Jardón, R., Solt, A., Reed, W., 2008. Systemic Inflammation, Endothelial Dysfunction, and Activation in Clinically Healthy Children Exposed to Air Pollutants. *Inhal. Toxicol.* 20, 499–506. <https://doi.org/10.1080/08958370701864797>.
- Casallas, A., Celis, N., Ferro, C., López Barrera, E., Peña, C., Corredor, J., Ballen Segura, M., 2020. Validation of PM10 and PM2.5 early alert in Bogotá, Colombia, through the modeling software WRF-CHEM. *Environ. Sci. Pollut. Res* 27, 35930–35940. <https://doi.org/10.1007/s11356-019-06997-9>.
- Casallas, A., Ferro, C., Celis, N., Guevara-Luna, M., Mogollón-Sotelo, C., Guevara-Luna, F., Merchán, M., 2021a. Long short-term memory artificial neural network approach to forecast meteorology and PM_{2.5} local variables in Bogotá, Colombia. *Model. Earth Syst. Environ.* <https://doi.org/10.1007/s40808-021-01274-6>.
- Casallas, A., Hernandez-Deckers, D., Mora-Paez, H., 2021b. Understanding convective storms in a tropical, high-altitude location with in-situ meteorological observations and GPS-derived water vapor. *Atmósfera. Early Release.*
- Castillo-Camacho, M.P., Tunarrosa-Grisales, I.C., Chacón-Rivera, L.M., Guevara-Luna, M. A., Belalcázar-Cerón, L.C., 2020. Personal Exposure to PM2.5 in the Massive Transport System of Bogotá and Medellín, Colombia. *Asian J. Atmos. Environ.* 14, 210–224. <https://doi.org/10.5572/ajae.2020.14.3.210>.
- Chai, T., Kim, H.C., Lee, P., Tong, D., Pan, L., Tang, Y., Huang, J., McQueen, J., Tsidulko, M., Stajner, I., 2013. Evaluation of the United States National Air Quality Forecast Capability experimental real-time predictions in 2010 using Air Quality System ozone and NO 2 measurements. *Geosci. Model Dev.* 6, 1831–1850. <https://doi.org/10.5194/gmd-6-1831-2013>.
- Chollet, F., et al., 2015. Keras. GitHub. Retrieved from <https://github.com/fchollet/keras>. v0.2.4.3. (Version 0.2.4.3). Keras.
- Cobourn, W.G., 2010. An enhanced PM2.5 air quality forecast model based on nonlinear regression and back-trajectory concentrations. *Atmos. Environ.* 44, 3015–3023. <https://doi.org/10.1016/j.atmosenv.2010.05.009>.
- Commission Directive, 2015. Ambient air quality and cleaner air for Europe, European Parliament. Counc. Eur. Union. <http://extwprlegs1.fao.org/docs/pdf/eur80016.pdf>, accessed 3 July 2020.
- Commission Directive, 2016. The reduction of national emissions of certain atmospheric pollutants, amending Directive 2003/35/EC and repealing Directive 2001/81/EC. Eur. Parliam., Counc. Eur. Union. (https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=uriserv%3AOJ_L_2016_344_01.0001.001.ENG), accessed 3 July 2020.
- Comrie, A.C., 1997. Comparing Neural Networks and Regression Models for Ozone Forecasting. *J. Air Waste Manag. Assoc.* 47, 653–663. <https://doi.org/10.1080/10473289.1997.10463925>.
- Cortes, C., Vapnik, V., 1995. Support-vector networks. *Mach. Learn* 20, 273–297. <https://doi.org/10.1007/bf00994018>.
- Dominguez-Calle, E., Lozano-Báez, S., 2014. Estado del arte de los sistemas de alerta temprana en Colombia. *Rev. Acad. Colomb. Cienc.* 38, 321–332. <https://doi.org/10.18257/raccefn.132>.
- EPA, 2014. AQI - Air Quality Index. A Guide to Air Quality and Your Health. EPA-456/F.-14-002 (accessed 07 January 2020). https://www3.epa.gov/airnow/aqi_brochure_02_14.pdf.
- Decreto 595 of 2015, 2015. Adopting Bogotá's Environmental Early Warning System for its Air Component SATAB-air, EO, Office of the Mayor of Bogotá. (<https://www.alcaldiabogota.gov.co/sisjur/normas/Normal1.jsp?i=64242>) (accessed 12 January 2021).
- EPA, 2020. Probabilistic Risk Assessment to Inform Decision Making: Frequently Asked Questions (Washington (DC): Risk Assessment Forum, US Environmental Protection Agency). EPA/100/R-14/003. (<https://www.epa.gov/osa/probabilistic-risk-assessment-inform-decision-making-frequently-asked-questions>) (accessed 12 January 2021).
- Fletcher, T., 2009. Support vector machines explained. *Univ. Coll. Lond.* (https://clg.csd.uwo.ca/cs860/papers/SVM_Explained.pdf) (accessed 20 January 2020).
- Franceschi, F., Cobo, M., Figueiredo, M., 2018. Discovering relationships and forecasting PM10 and PM2.5 concentrations in Bogotá, Colombia, using Artificial Neural Networks, Principal Component Analysis, and k-means clustering. *Atmos. Pollut. Res.* 9, 912–922. <https://doi.org/10.1016/j.apr.2018.02.006>.
- Greene, N., Morris, V., 2006. Assessment of Public Health Risks Associated with Atmospheric Exposure to PM_{2.5}. 3. International Journal of Environmental Research and Public Health, Washington, DC, USA, pp. 86–97. <https://doi.org/10.3390/ijerph200603010>.
- Gómez Ortega, L.C., Muñoz Guerrero, M.N., Soto Alegría, L.F., 2018. Sistema de Alerta Temprana Ambiental y Efectos en Salud – SATAES. una Herram. Para. la Acción. (<https://www.ins.gov.co/buscador/IQEN/IQEN%20vol%2023%202018%20num%202.pdf>) (accessed 2 April 2020).
- Gómez Peláez, L.M., Santos, J.M., de Almeida Albuquerque, T.T., Reis, N.C., Andreão, W. L., de Fátima Andrade, M., 2020. Air quality status and trends over large cities in South America (<https://doi.org/10.1016/j.envsci.2020.09.009>).
- González, C.M., Ynoue, R.Y., Vara-Vela, A., Rojas, N.Y., Aristizábal, B.H., 2018. High-resolution air quality modeling in a medium-sized city in the tropical Andes: Assessment of local and global emissions in understanding ozone and PM10 dynamics. *Atmos. Pollut. Res.* 9, 934–948. <https://doi.org/10.1016/j.apr.2018.03.003>.
- Guevara-Luna, M.A., Casallas, A., Belalcázar Cerón, L., Clappier, A., 2020. Implementation and evaluation of WRF simulation over a city with complex terrain using Alos-Palsar 0.4 s topography. *Environ. Sci. Pollut. Res* 27, 37818–37838. <https://doi.org/10.1007/s11356-020-09824-8>.
- Hochreiter, S., Schmidhuber, J., 1997. Long Short-Term Memory. *Neural Comput.* 9, 1735–1780. <https://doi.org/10.1162/neco.1997.9.8.1735>.
- Hou, W., Li, Z., Zhang Yuhuan, Xu, H., Zhang Y., Li K., Li D., Wei, P., Ma, Y., 2014. Using support vector regression to predict PM10 and PM2.5. IOP Conference Series: Earth and Environmental Science. 17, 012268. <https://doi.org/10.1088/1755-1315/17/1/012268>.
- Holton, J.R., 2004. *An Introduction to Dynamic Meteorology*, fourth ed., Elsevier Academic Press., USA.
- Huang, C.J., Kuo, P.H., 2018. A deep CNN-LSM model for particulate matter (PM_{2.5}) forecasting in smart cities. *Sensors* 1, 2220. <https://doi.org/10.3390/s18072220>.
- Inness, A., Ades, M., Agustí-Panareda, A., Barré, J., Benedictow, A., Blechschmidt, A.M., Dominguez, J.J., Engelen, R., Eskes, H., Flemming, J., Huijnen, V., Jones, L., Kipling, Z., Massart, S., Parrington, M., Peuch, V.H., Razinger, M., Remy, S., Schulz, M., Suttie, M., 2019. The CAMS reanalysis of atmospheric composition. *Atmos. Chem. Phys.* 19 (6), 3515–3556. <https://doi.org/10.5194/acp-19-3515-2019>.
- Ivakhnenko, A.G., Lapa, V.G., 1965. *Cybernetic Predicting Devices*, first ed., CCM Information Corporation., New York.
- Ivakhnenko, A.G., Lapa, V.G., McDonough, R.N., 1967. *Cybernetics and forecasting techniques*, first ed., American Elsevier., New York.
- Jorqueria, H., 2021. Air quality management in Chile: Effectiveness of PM2.5 regulations. *Urban Clim.* 35, 100764. <https://doi.org/10.1016/j.ulclim.2020.100764>.
- Kelly, F.J., Fuller, G.W., Walton, H.A., Fussell, J.C., 2011. Monitoring air pollution: Use of early warning systems for public health. *Respirology* 17, 7–19. <https://doi.org/10.1111/j.1440-1843.2011.02065.x>.
- Kumar, A., Jiménez, R., Belalcázar, L.C., Rojas, N.Y., 2016. Application of WRF-CHEM model to simulate PM10 concentration over Bogotá. *Aerosol Air Qual. Res.* 16, 1206–1221. <https://doi.org/10.4209/aaqr.2015.05.0318>.
- Kumar, R., Peuch, V.H., Crawford, J.H., Brasseur, G., 2018. Five steps to improve air-quality forecasts. *Nature* 561, 27–29. <https://doi.org/10.1038/d41586-018-06150-5>.
- Liu, J., Zhang, A., Chen, Y., Zhou, X., Zhou, A., Cao, H., 2020a. Bioaccessibility, source impact and probabilistic health risk of the toxic metals in PM_{2.5} based on lung fluids test and Monte Carlo simulations. *J. Clean. Prod.* 283 (124667) <https://doi.org/10.1016/j.jclepro.2020.124667>.
- Liu, C., Chen, W., Hou, Y., Ma, L., 2020b. A new risk probability calculation method for urban ecological risk assessment. *Environ. Res. Lett.* 15, 024016. (<https://iopscience.iop.org/article/10.1088/1748-9326/ab6667/pdf>).
- Longo, K.M., Freitas, S.R.D., Pirre, M., et al., 2013. The chemistry CATT-BRAMS model (CCATT-BRAMS 4.5): a regional atmospheric model system for integrated air quality and weather forecasting and research. *Geosci. Model Dev. Discuss.* 6, 1173–1222. <https://doi.org/10.5194/gmd-6-1389-2013>.
- Lu, W.Z., Wang, W.J., 2005. Potential assessment of the “support vector machine” method in forecasting ambient air pollutant trends. *Chemosphere* 59, 693–701. <https://doi.org/10.1016/j.chemosphere.2004.10.032>.
- Lu, Y., Lin, S., Fatmi, Z., Malashock, D., Hussain, M.M., Siddique, A., Carpenter, D.O., Lin, Z., Khwaja, H.A., 2019. Assessing the association between fine particulate matter (PM_{2.5}) constituents and cardiovascular diseases in a mega-city of Pakistan. *Environ. Pollut.* 252B, 1412–1422. <https://doi.org/10.1016/j.envpol.2019.06.078>.
- Makowski, M., 2000. Modeling paradigms applied to the analysis of European air quality. *Eur. J. Oper. Res.* 122, 219–241. [https://doi.org/10.1016/S0378-4274\(02\)00411-3](https://doi.org/10.1016/S0378-4274(02)00411-3).
- Marion, T.B., Schroeter, J.D., 2003. Risk assessment dosimetry model for inhaled particulate matter: I. Human subjects. *Toxicol. Lett.* 138, 119–132. [https://doi.org/10.1016/S0378-4274\(02\)00411-3](https://doi.org/10.1016/S0378-4274(02)00411-3).
- Maas, R., Grennfelt, P., 2016. *Towards Cleaner Air. Scientific Assessment Report 2016: Summary for Policymakers. EMEP Steer. Body Work. Group Eff. Conv. Long. -Range Transbound. Air Pollut.*, Oslo.
- McFarland, J., DeCarlo, E.C., 2020. A Monte Carlo framework for probabilistic analysis and variance decomposition with distribution parameter uncertainty. *Reliab. Eng. Syst. Saf.* 197, 106807. <https://doi.org/10.1016/j.ress.2020.106807>.
- Mendez-Espinosa, J.F., Rojas, N.Y., Vargas, J., Pachón, J.E., Belalcazar, L.C., Ramírez, O., 2020. Air quality variations in Northern South America during the COVID-19 lockdown. *Sci. Total Environ.* 749, 141621. <https://doi.org/10.1016/j.scitotenv.2020.141621>.
- Mogollón-Sotelo, C., Casallas, A., Vidal, S., Celis, N., Ferro, C., Belalcazar, L.C., 2020. A support vector machine model to forecast ground-level PM_{2.5} in a highly

- populated city with a complex terrain. *Air Qual. Atmos. Health* 14, 399–409. <https://doi.org/10.1007/s11869-020-00945-0>.
- Ndiaye, E., Le, T., Fercoq, O., Salmon, J., Takeuchi, I., 2019. Safe Grid Search with Optimal Complexity. Proc. 36th Int. Conf. Mach. Learn., Proc. Mach. Learn. Res. 97, 4771–4780. In: (<http://proceedings.mlr.press/v97/ndiaye19a.html>).
- Liao, K., Huang, X., Dang, H., Ren, Y., Zuo, S., Duan, C., 2021. Statistical Approaches for Forecasting Primary Air Pollutants: A Review. *Atmosphere* 12, 686. <https://doi.org/10.3390/atmos12060686>.
- Lira, T.S., Barrozo, M.A., Assis, A.J., 2007. Air quality prediction in Uberlândia, Brazil, using linear models and neural networks. *Comput. Aided Chem. Eng.* 24, 51–56. [https://doi.org/10.1016/S1570-7946\(07\)80032-0](https://doi.org/10.1016/S1570-7946(07)80032-0).
- Pedregosa, F., et al., 2011. Scikit-learn: Machine learning in Python. *J. Mach. Learn. Res.* 12, 2825–2830 vo. 0.24.1. (Version o.0.24.1).
- Prechelt, L., 1998. Early Stopping - But When?. In: Orr G.B., Müller K.R. (eds) Neural Networks: Tricks of the Trade. Lecture Notes in Computer Science. 1524. https://doi.org/10.1007/3-540-49430-8_3.
- Pulido, J.C., Vasquez, J.A., Hernandez, L.A., 2020. Validación de los modelos de calidad del aire empleados por el SIMCAB. Final report. Bogotá, Colombia: Dept air, auditory and visual quality, District Secretary of Environment. Apr. Report No. 2020ER68620.
- Rojas, N., 2004. Revisión de las emisiones de material particulado por la combustión de Diesel y Biodiesel. *Rev. De. Ing.* 20. ISSN 0121-4993.
- Saide, P.E., Mena-Carrasco, M., Tolvett, S., Hernandez, P., Carmichael, G.R., 2015. Air quality forecasting for winter-time PM2.5 episodes occurring in multiple cities in central and southern Chile. *J. Geophys. Res.: Atmospheres* 121, 558–575. <https://doi.org/10.1002/2015JD023949>.
- Sayeed, A., Lops, Y., Choi, Y., Jung, J., Salman, A.K., 2021. Bias correcting and extending the PM forecast by CMAQ up to 7 days using deep convolutional neural networks. *Atmos. Environ.* 253, 118376. <https://doi.org/10.1016/j.atmosenv.2021.118376>.
- Shahraiyni, H.T., Sodoudi, S., 2016. Statistical modeling approaches for PM10 prediction in urban areas; A review of 21st century studies. *Atmosphere* 7, 15. <https://doi.org/10.3390/atmos7020015>.
- Skamarock, W., et al., 2019. A Description of the Advanced Research WRF Version 4. Tech. rep. NCAR Tech. Note NCAR/TN-556+STR. <https://doi.org/10.5065/1dfh-6p97>.
- Sokhi, R.S., Singh, V., Querol, X., Finardi, S., Targino, A.C., Andrade, M.F., Pavlovic, R., Garland, R.M., Massagué, J., Kong, S., Baklanov, A., Ren, L., Tarasova, O., Carmichael, G., Peuch, V.H., Anand, V., Arbillaga, G., Badali, K., Beig, G., Belalcazar, L.C., Bolignano, A., Brimblecombe, P., Camacho, P., Casallas, A., Charland, J.P., Choi, J., Chourdakis, E., Coll, I., Collins, M., Cyrys, J., da Silva, C.M., Di Giosa, A.D., Di Leo, A., Ferro, C., Gavidia-Calderon, M., Gayen, A., Ginzburg, A., Godefroy, F., Gonzalez, Y.A., Guevara-Luna, M., Haque, S.M., Havenga, H., Herod, D., Hörrak, U., Hussein, T., Ibarra, S., Jaimes, M., Kaasik, M., Khaiwal, R., Kim, J., Kousa, A., Kukkonen, J., Kulmala, M., Kuula, J., La Violette, N., Lanzani, G., Liu, X., MacDougall, S., Manseau, P.M., Marchegiani, G., McDonald, B., Mishra, S.V., Molina, L.T., Mooibroek, D., Mor, S., Moussiopoulos, N., Murena, F., Niemi, J.V., Noe, S., Nogueira, T., Norman, M., Pérez-Camano, J.L., Petajä, T., Pike, S., Rathod, A., Reid, K., Retama, A., Rivera, O., Rojas, N.Y., Rojas-Quincho, J.P., San José, R., Sánchez, O., Seguel, R.J., Sillanpää, S., Su, Y., Tapper, N., Terrazas, A., Timonen, H., Toscano, D., Tsegas, G., Velders, G.J.M., Vlachokostas, C., von Schneidemesser, E., VPM, R., Yadav, R., Zalakeviciute, R., Zavalá, M., 2021. A global observational analysis to understand changes in air quality during exceptionally low anthropogenic emission conditions. *Environ. Int.* 157, 106818.
- Tao, Q., Liu, F., Li, Y., Sidorov, D., 2019. Air Pollution Forecasting using a Deep Learning Model based on 1D Convnets and Bidirectional GRU. *IEEE Access* 7, 76690–76698. <https://doi.org/10.1109/access.2019.2921578>.
- Tzanis, C.G., Alimisis, A., Philippopoulos, K., Deligiorgi, D., 2019. Applying linear and nonlinear models for the estimation of particulate matter variability. *Environ. Pollut.* 246, 89–98. <https://doi.org/10.1016/j.envpol.2018.11.080>.
- UNECE, 2007. Report of the fourth and fifth meetings of the Expert Group on Particulate Matter (Report ECE/EB.AIR/WG.5/2007/18). UN Econ. Soc. Coun. (<https://www.unece.org/fileadmin/DAM/env/documents/2007/eb/wg5/WGSR40/ece.eb.air.wg.5.2007.18.e.pdf>) (accessed 9 september 2020).
- UNECE, 2013. Protocol to Abate Acidification, Eutrophication and Ground-level Ozone as amended on 4 May 2012 (Gothenburg Protocol). Treaties Other Int. (https://unece.org/DAM/env/documents/2013/air/eb/ECE.EB.AIR.114_ENG.pdf) (accessed 9 september 2020).
- WAQI, 2007. About the World Air Quality Index project. (<https://waqi.info/>). (accessed 10 April 2020).
- Wan, K., Shackley, S., Doherty, R.M., Shi, Z., Zhang, P., Golding, N., 2020. Science-policy interplay on air pollution governance in China. *Environ. Sci. Policy* 107, 150–157. <https://doi.org/10.1016/j.envsci.2020.03.003>.
- Wang, Q., Wang, J., He, M.Z., Kinney, P.L., Li, T., 2018. A county-level estimate of PM 2.5 related chronic mortality risk in China based on multi-model exposure data. *Environ. Int.* 110, 105–112. <https://doi.org/10.1016/j.envint.2017.10.015>.
- Wen, X.J., Balluz, L., Mokdad, A., 2009. Association between media alerts of air quality index and change of outdoor activity among adult asthma in six states. *Brfss. J. Com. Health* 34, 40–46. <https://doi.org/10.1007/s10900-008-9126-4>.
- WHO, 2015. Reducing Global Health Risks Through Mitigation of Short-Lived Climate Pollutants. Scoping Report for Policy-makers. (https://apps.who.int/iris/bitstream/handle/10665/189524/9789241565080_eng.pdf;jsessionid=1A08270BB7B2D3BC974EA81554DA2E0C?sequence=1). (accessed 01 March 2020).
- WHO, 2018. Ambien (outdoor) air pollution. ([https://www.who.int/news-room/fact-sheets/detail/ambient-\(outdoor\)-air-quality-and-health](https://www.who.int/news-room/fact-sheets/detail/ambient-(outdoor)-air-quality-and-health)) (accessed 24 December 2020).
- Willmott, C.J., Ackleson, S.G., Davis, R.E., Feddema, J.J., Klink, K.M., Legates, D.R., O'Donnell, J., Rowe, C.M., 1985. Statistics for the evaluation and comparison of models. *J. Geophys. Res.: Oceans* 90, 8995–9005. <https://doi.org/10.1029/JC090iC05p08995>.
- Xing, Y.F., Xu, Y.H., Shi, M.H., Lian, Y.X., 2016. The impact of PM_{2.5} on the human respiratory system. *Journal of thoracic disease*, 8 (E69–E74). <https://doi.org/10.3978/j.issn.2072-1439.2016.01.19>.
- Zarate, E., Belalcazar, L., Clappier, A., Manzi, V., van den Bergh, H., 2007. Air quality modelling over Bogotá, Colombia: Combined techniques to estimate and evaluate emissions inventories. *Atmos. Environ.* 41, 6302–6318. <https://doi.org/10.1016/j.atmosenv.2007.03.011>.
- Zhang, Y., Bocquet, M., Mallet, V., Seigneur, C., Baklanov, A., 2012. Real-time air quality forecasting, part I: history, techniques and current status. *Atmos. Environ.* 60, 632–655. <https://doi.org/10.1016/j.atmosenv.2012.06.031>.
- DANE, 2018. Proyecciones de Población Bogotá. (<https://www.dane.gov.co/index.php/estadisticas-por-tema/demografia-y-poblacion/proyecciones-de-poblacion/proyecciones-de-poblacion-bogota>) (accessed 13 february 2021).
- SDA, 2020. Reporte de estaciones. (<http://rmcab.ambientebogota.gov.co/Report/stat ionreport>) (accessed 02 february 2020).