COMPARISON OF MARITIME TRANSPORT INFLUENCE OF SO2 LEVELS IN ALGECIRAS AND ALCORNOCALES PARK (SPAIN)

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ABSTRACT

The main aim of this work was to measure the influence of the volume of shipping over the Sulphur dioxide (SO2) concentration in the air pollution in two monitoring stations located at Algeciras city and Alcornocales Park developing the same analysis in these two locations.

The target is to demonstrate the assumption that Algeciras is more affected by SO2 than Alcornocales Park which is 30 km far away from Algeciras Port. A multiple regression approach has been applied using wind data: wind direction (degrees) and wind speed (km/h) recorded in two weather stations, together with the volume of the gross tonnage per hour (GT/h) of vessels in the Bay of Algeciras to estimate SO2 concentration values in the two stations Algeciras and Alcornocales. The database contains records of hourly samples of these variables during the year 2019. Different artificial neural networks (ANNs) models were compared and the results showed that SO2 in Algeciras station could be better explained than the same pollutant in Alcornocales station. On the other hand, ANNs produced better results than linear models which means that nonlinear models fit best the data. A cross- validation procedure has been applied in order to assure the generalization capabilities of the tested models. The results showed that in Algeciras a more reliable estimation could be done reaching a correlation estimation between the model and the target (real) values of SO2. This fact highlights the major influence of maritime transport in the Bay of Algeciras

1. INTRODUCTION

The importance of cities outdoors in pandemic times has increased substantially since people are doing their lives in streets, parks, and common zones.

It is now, more than ever, when the air surrounding cities becomes essential to develop secure sports activities and their day to day life. This is what motivates this study, in order to gain knowledge about how ports can affect towns. Algeciras city is highly populated with a total of 123,000 inhabitants in 2020, and the Bay of Algeciras is a big exchange site of winds, which makes it interesting analysing this area in concordance with a pollution scenery. For this reason, this study is developed in this location due to its connection with chemical and steelmaking industries, Gibraltar airport, and Algeciras Port, one of the most important ports of goods in Europe, which is a hub of economic activity. Maritime traffic has experienced a massive increase in Europe, and in the whole Globe. The low offer of public transport in the bay makes this zone full of constant private traffic which decreases the air quality. All the transportation sources contribute to a complex pollution scenario, although we focus on Algeciras Port. As one of the main ports in Spain and Europe, the relevance of maritime traffic evinces not only goods movement but also air pollution.

Therefore, the appearance of particulate matter is higher in port zones (González et al., 2011, Viana et al., 2014) often motivated by the ineffective maintenance of vessel engines that makes them unnecessarily consume and waste more fuel (Moreno-Gutiérrez et al., 2015). High rates of the total ships' emissions can be dispersed to 400 km inland (González et al., 2011). Worldwide estimations suggest that vessels are responsible for 15% of NOx and 8% of SO2 emissions all around the Globe, involving 20- 28% of the total emitted gases in the transport sector (Corbett et al., 2007). Besides, other estimations calculated that vessels produce 3% of the total human greenhouse gases, double of aviation (IMO). Not only do navigating ships discharge fumes to the atmosphere but also docked vessels, which can be considerably reduced by switching to lower-sulphur fuel in the ECAs (Emission Control Areas) (Wan et al., 2019). Some pieces of research estimated that 172,000 vessels consumed during voyages about 47 million metric tons of heavy fuel oil and emitted about 2.4 million metric tons of SO2 (Wang et al., 2007). The database provided by Algeciras Port Authority showed that about 29,000 vessels berthed during the year 2019 in the Bay and, while berthing only the auxiliary engine (AE) is functioning to generate electricity onboard what produces lower emissions than cruising (Durán-Grados et al., 2020). Lee et al., (2020) estimated other emissions from several types of ships (general cargo, cruise, container, and tankers vessels) facing the docking process.

Calculations in SOx emissions in the Strait of Gibraltar went from 8.20 ton/km2/year in 2007 (Moreno-Gutiérrez et al., 2015) to 11.60 ton/km2/year in 2017 (Nunes et al., 2020). As a curious fact, Durán- Grados et al., (2020) estimated how Ro-Pax passenger-ships affected the atmosphere in the Strait of Gibraltar during the 90 days of COVID-19 pandemic lockdown while all vessels were berthed in the port of Algeciras taking into account the auxiliary engine and, they obtained a reduction of 12% of emissions. Several studies present an overview of air quality in Europe and port cities (Guerreiro, et al., 2014; Wagner 2019).

Others, the relationship between transport-related air pollutant concentrations to integrate new models for sustainable mobility of vehicles (Catalano, et al., 2016) and the usage of different methods to predict peaks of pollution in critical meteorological situations, particularly in the Bay of Algeciras (Muñoz et al., 2014). Due to huge vessels with engines run on heavy fuel oil (2,700 times higher than road fuel), the shipping emissions are tackled in many manuscripts (Corbett et al., 2007; Liu, et al., 2014; Nunes, et al., 2019; Puig, et al., 2020; Bilgili, et al., 2021; Moreno-Gutiérrez and Durán-Grados (2021)).

Nunes, et al., (2019) evaluated four important ports in Portugal in terms of environmental, social, and economic criteria to evaluate the implementation of policies for in-port emissions. Other authors have studied four types of marine fuels on the environment and human health and concluded that IMO 2020 Sulphur Cap are not at a desirable level yet (Bilgili, et al., 2021). Sanchez et al., (2020) detailed methods to reduce traffic emissions and to implement policy interventions in cities.

In terms of meteorological events that affect pollution, winds seem to be important. Meteorology contribution to pollution events together with forecasting models are faced by Muñoz et al., (2014); Gonzalez-Enrique et al., (2019b); Vellalassery et al., (2021).

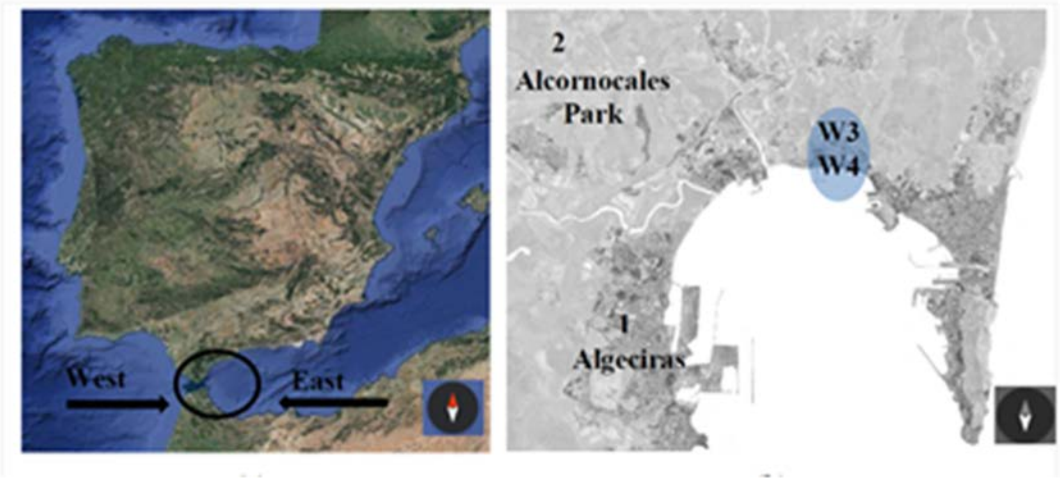
Estimations related to urban areas are tackled in Hu et al., (2021) and in Johnson et al., 2020). The evolution of the interaction between ports and cities is shown in Hesse (2013) adapted from Hoyle (1988). Sustainable cities are related to green transport but Wagner (2019) revealed also multiple factors such as economics, planning development, civil engineering, geography, and of course, transportation.

In this work, the best estimation model of SO2 concentrations in Algeciras and Alcornocales Park is achieved using historical data resolving an input-output fitting problem with feedforward artificial neural network (ANNs). Linear regression models are applied and compared as a benchmark. The rest of this manuscript is organised as follows.

Sect. 2 describes the study case, the database and the methodology. Sect. 3 presents the experimental procedure and the different tested approaches. Sect. 4 discusses the obtained results, and finally, Sect. 5 states the main conclusions.

2. MATERIALS AND METHODS

The Bay of Algeciras is located in the south of Spain, Figure 1(a), and the port of Algeciras is shown in Figure 1(b). The strategic position of the port due to its specific orographic location and the two main directions of wind, East winds (Levante) and West winds (Poniente), affect this area. Figure 1(b) highlights the monitoring stations over the Bay, described in Table 1. Weather stations were denoted using Wn (W3- 4) and listed Algeciras and Alcornocales Park correspond to pollutant monitoring stations



(a) **(b)**

Figure 1 – (a) Bay of Algeciras location and its frequent winds; (b) Monitoring stations (air pollution 1- 2, and meteorological W3- 4)

This study area was chosen due to the importance of maritime transport in this bay. As well, road traffic that moves the goods from this point to the rest of Spain has increased substantially during the last ten years in Algeciras. The two monitoring stations tested, Algeciras and Alcornocales Park are located in Figure 1(a). Alcornocales Park was chosen because it is a remote unspoilt green area where, theoretically, pollution does affect less.

The hypothesis is that Algeciras city is more affected by maritime transport than Alcornocales station. Therefore, a prediction model in Algeciras should be better explained than another in Alcornocales station, due to the effect of maritime transport.

Looking at Figure 1(b), the localization of the Bay of Algeciras is clear and also the different monitoring stations spread over the region. The two dominant winds in the bay are shown in Figure 1(a), Levante (East) and Poniente (West). These peculiar ways in which the wind blows are due to the funnel factor of the bay contained by the Rock of Gibraltar and due to the connection between the Atlantic Ocean and the Mediterranean Sea.

Code	Monitoring/weather station	Latitude	Longitude
1	Algeciras (EPSA)	36º8’11.7” N	5º27’11.44” W
2	Alcornocales	36º13’35” N	5º31’11.44” W
W3	Cepsa (60 m high)	36º11’37.66” N	5º24’1.24” W
W4	Cepsa (15 m high)	36º10’54.7” N	5º25’43.42” W

Table 1 – Location of the meteorological and SO2 monitoring stations

2.1. Materials

Andalusian Government and Algeciras Bay Port Authority (APBA) have provided to the University of Cádiz the recorded values of SO2 concentration, wind, and GT (Gross tonnage) of vessels. The database was recorded hourly for SO2 concentration and wind speed and direction. Then, a new data imputation procedure was performed to complete the missing values. Here, missing data values have been included using a data imputation algorithm considering the measured values in other monitoring stations close to each station, following a proceeding previously used in other works by authors (Turias et al., (2006), Turias et al., (2008), Martín et al., (2008), Moscoso-López et al., (2016), González-Enrique et al., (2019a), Ruiz-Aguilar et al., (2020)). Figure 2(a)(b) shows SO2 concentration time-series and Figure 3(a) shows the wind rose representation of W3 station (Cepsa at 60 m high) and Figure 3(b) the wind rose of W4 station (Cepsa at 15 m high).

The vessel database provided by APBA contains a register for each vessel in the Bay in 2019 (with corresponding timestamps of arrival and departure). The database was transformed into a GT/h (Gross-tons per hour) computing the number of vessels in an hour and the total of Tons of those registered ships. Therefore, each hour a certain number of vessel-tons are located into the Bay, and theoretically affecting the air pollution.

The pollutant data are collected in two monitoring stations in Algeciras and Alcornocales Park, and the weather data are collected in two meteorological stations located in Cepsa refinery at 60 m high (W3) and 15 m high (W4) (see Figure 1b). The SO2 concentration (μg/m3) is recorded in Algeciras city and Alcornocales Park to verify the initial hypotheses (that Algeciras is more affected by SO2 than Alcornocales Park). The weather variables used in this research are the two components of the wind; wind speed (km/h) and wind direction (degrees).

Code	Variables	Measurement	Station
Output1	SO_2	$\mu g/m^3$	Algeciras (EPSA)
Output2	SO_2	$\mu g/m^3$	Alcornocales
Input1	Vessels	GT/h	-
Input2	WS (Wind speed)	Km/h	Cepsa (60 m)
Input3	WS (Wind speed)	Km/h	Cepsa (15 m)
Input4	WD (Wind direction)	Degrees	Cepsa (60 m)
Input5	WD (Wind direction)	Degrees	Cepsa (15 m)

Table 2 – Variables of the study

2.2. Methods

Artificial Neural Networks (ANNs) have been tested in this work together with the use of vessel and wind information in order to predict SO2 concentrations. In this sense, this system could be seen as a virtual sensor SO2 concentrations as a function of maritime transport and wind variables. ANNs require no prior assumptions about the model in terms of mathematical relationships or data distribution. Feedforward ANNs based on a backpropagation learning rule has been used (Rumelhart et al., (1986)). The output was the hourly SO2 concentrations, and the inputs were the gross tons of vessels summed each hour in the Bay of Algeciras, and the wind speed and wind direction in a certain timestamp.

Furthermore, different models were built, some of them using only the pollutant information and the rest considering exogenous variables (vessel and wind information).

The purpose of this modelling approach is to establish a quantitative relationship between a group of predictor variables, X, and a response Y (in this case, the SO2 concentration to be predicted). ANNs have found many applications on air pollution (Jorquera et al., (1998); Nunnari at al., (1998); Gardner et al., (1999); Balaguer, et al., (2002); Perez et al., (2001); Perez et al., (2002); Viotti et al., (2002); Kukkonen et al., (2003); Turias et al., (2003); Turias et al., (2006); Turias et al., (2008); Martín et al., (2008); González-Enrique et al., (2019a)).

For feedforward ANNs, a pattern is formed by inputs together with the pollutant concentration to be forecasted, named real or desired output. There is no way to determine the optimum although Hornik et al., (1989) show the capabilities of backpropagation feedforward networks. An experimental procedure has been used to determine the best ANN configuration.

A standard Multiple Linear Regression (MLR) model has been used as a benchmark in this study.

3. EXPERIMENTAL PROCEDURE

A procedure of resampling simulation was designed to select the model with the best generalization capabilities. First of all, data were selected to create and train the network.

Then its performance was evaluated using mean square error and regression analysis. A feedforward artificial neural network with sigmoid hidden neurons and linear output neurons can fit multi-dimensional mapping problems arbitrarily well, given consistent data and enough neurons in its hidden layer. Authors have successfully used similar procedures in other problems (Ruiz-Aguilar et al., (2014); Moscoso-López et al., (2016); Gonzalez-Enrique et al., (2019b); Ruiz-Aguilar et al., (2020)). Besides, in this problem, the best ANN model using 1000 replications was chosen. ANNs were trained with the Levenberg-Marquardt backpropagation algorithm. Finally, the obtained results were statistically analysed and compared in order to select the model with the best generalisation capabilities.

ANN models with different hidden units were compared to determine the effect of the addition of non-linear processing capabilities on model performance. The resampling procedure was found to reduce test set prediction error and to mitigate the effects of overfitting.

The strategy split randomly the database into three portions (training 70%, validation 15%, and test 15% sets) and the performance results were collected only for the test set in order to estimate the generalization error of each model using unseen data as .

Approach	Input variables	Wind direction
1	Vessels	Levante (East Wind)
2	Vessels	Poniente (West Wind)
3	Vessels, WS, WD	Levante (East Wind)
4	Vessels, WS, WD	Poniente (West Wind)

Table 3 – List of the tested approaches in the experimental procedure

The approaches 1 and 2 are represented in Equation (1):

$$\hat{SO}_2(t) = f(vessels(t)) \qquad (1)$$

The approaches 3 and 4 are represented in Equation (2):

$$\hat{SO}_2(t) = f(vessels(t), wind\ direction(t), wind\ speed(t)) \qquad (2)$$

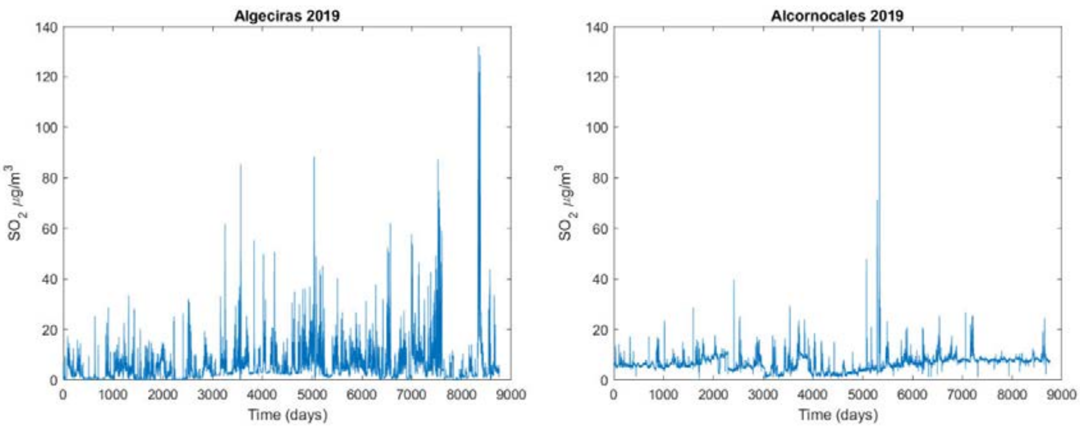
where vessels(t) are the hourly sum of the gross freight in tonnes of all the vessels in the Bay.

The output in each approach is the concentration of SO2 recorded in every station (Algeciras or Alcornocales Park). The models have been subdivided into three submodels: the first one for wind patterns of "Levante" (East wind), the second one for wind patterns of "Poniente" (West wind), and the last one for the rest of the examples in the database. Figure 3(a)(b) shows the winds of roses where these two main wind scenarios can be seen

4. RESULTS AND DISCUSSION

The Bay of Algeciras supports a mean of tons of vessels of one million tons per day as we can see in Figure 4. Moreover, Figure 2(a) shows the large variability of SO2 concentrations in Algeciras and higher concentration values. In contrast, Figure 2(b) indicates a low variability in Alcornocales Park and lower data.
The simulations were run in MATLAB environment. A complete experiment using shallow.

ANNs was developed to prove the efficiency and reliability of SO2 concentration estimation in two monitoring stations in the Bay of Algeciras (Spain) as a function of the total gross tons each hour. Levenberg-Marquardt was used as optimization algorithm and early stopping to avoid overfitting.



(a) **(b)**

Figure 2 – Hourly SO2 data from stations in 2019 (a) Algeciras; (b) Alcornocales Park

Figure 2 shows a considerable number of concentration peaks of SO2 pollutant in Algeciras than in Alcornocales Park monitoring station, also these values in Algeciras station fluctuate considerably more and in Alcornocales Park the values are significantly more stable. Table 4 shows their means and standard deviation.

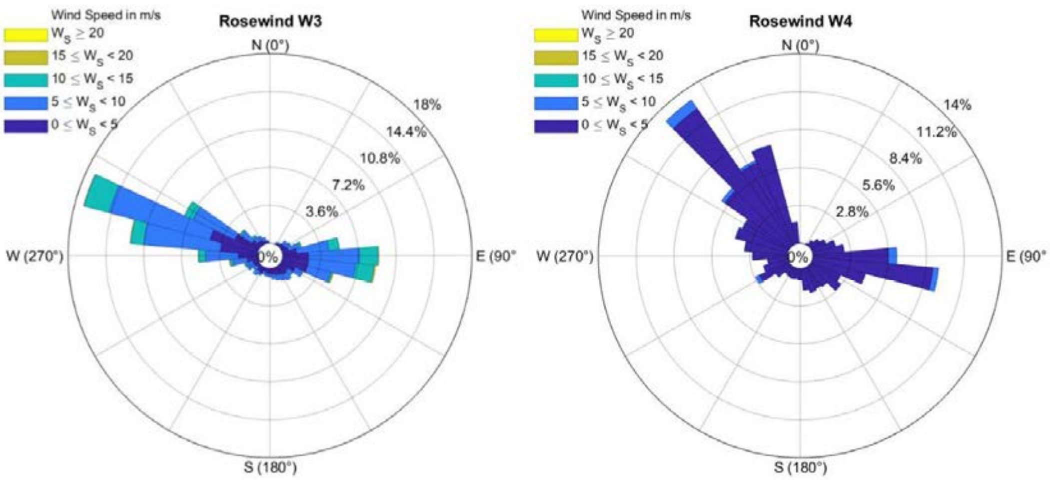
Station	Mean Value	Standard deviation
Algeciras	5.8168	8.5573
Alcornocales Park	6.7610	3.6223

Table 4 – Descriptive statistics of SO_2 monitoring stations

Characteristic winds in the Bay of Algeciras are drawn in the wind roses in Figure 3(a)(b). Both clearly show pure East winds 90º (Levante) and pure West winds 270º (Poniente), although in the Bay the West encompasses an angular range of 270º ± 30º approximately.

Most of the winds are normally lower than 54 km/h (15 m/s) and only a few episodes a year are higher than 70 km/h (20 m/s).

Figure 4, shows the 2019 vessel database provided by APBA. This data contains a register for each vessel in the Bay in 2019 (with corresponding timestamps of arrival and departure). In order to check if this data leverage SO2 concentrations, the database was transformed into a GT/h (Gross-tons per hour) calculating the number of vessels in an hour and the total of tons of those registered ships. Thus, a certain number of vessel-tons are located into the Bay each hour. In Figure 4(b), a data histogram is shown. The most frequent data is about 1E+06 GT/h. This amount of vessels produces emissions that can affect a certain area of influence



(a) (b)

Figure 3 – Wind roses year 2019 (a) station W3 at 60 m high; (b) station W4 at 15 m high

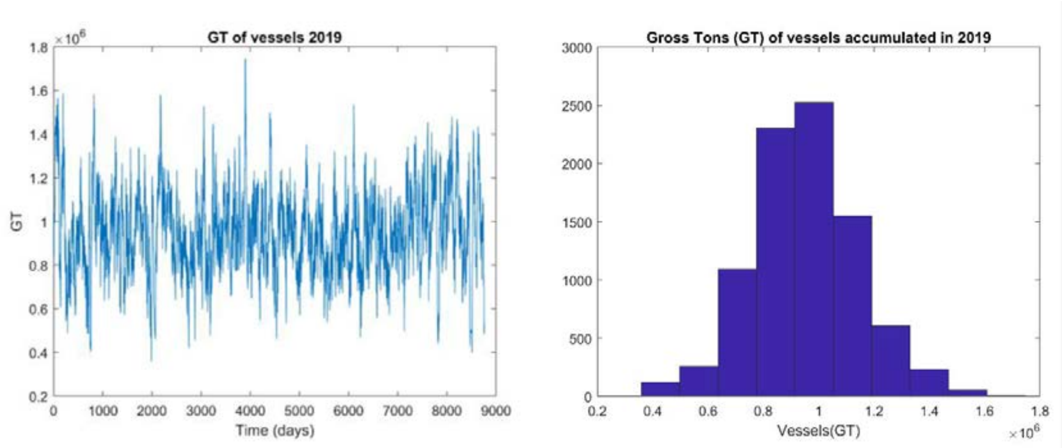


Figure 4 – Hourly vessel data 2019 in Gross Tons recorded in the port of Algeciras

In Tables 5-6 the results of linear regression models are exhibited for every approach. The highest regression coefficient (r = 0.4499) using the linear model is obtained in Algeciras for approach 4 (vessels + West wind) compared to r = 0.2432 in Alcornocales, which indicates a better explanation of the linear model in Algeciras. Analysing Table 6, approaches 1 and 2, it is observed that if we consider only the vessels as input, the model seems to show more leverage in Alcornocales in the case of East wind conditions. In the case of Algeciras, the linear model produces better results when Poniente conditions are registered. This fact could be explained due to in these specific conditions the SO2 concentration values show lower values in Algeciras and they are easier to model linearly.

Approaches 3 and 4 get better results than approaches 1 and 2, which means that input variables affect more strongly if interactions are considered.

Tables 7-8 show the results of ANN models. It is worth mentioning that ANN models fit better the database than MLR models. This fact is explained due to nonlinear behavior of the pollutant dispersion around the study area. One more time, the best results were found when approaches 3 and 4 were used. In the case of Alcornocales, better estimation results were obtained in Levante conditions, and the case of Algeciras, the best estimation model was found in Poniente conditions. The highest result is obtained in Algeciras with 20 hidden neurons (r = 0.7810) compared to the highest coefficient (r = 0.6356) in Alcornocales for approach 4 and only 1 hidden neuron.

Globally, the results show a poor linear relation amongst variables which means that, in comparison to ANNs models in Tables 7-8 with better regression coefficients, the inputs do not follow linear relations. ANNs models work better in general when exist non-linear behaviors and this fact is observed in the obtained results.

Besides, better results were obtained when wind variables are also used. Furthermore, a differentiation between Poniente models and Levante models improves the obtained results as we can see in Tables 5-8.

Weather station W3	Approach	r (MLR model)
Alcornocales	1	0.0853
	2	0.1727
	3	**0.2432**
	4	0.0854

Table 5 – Highest comparison results in Alcornocales Park station using RML

Weather station W4	Approach	r (MLR model)
Algeciras	1	0.1229
	2	0.0583
	3	0.2596
	4	**0.4499**

Table 6 – Highest comparison r results in Algeciras station using RML

Weather station W3	Approach	Neurons (ANNs model)				
		1	**5**	**10**	**20**	**50**
Alcornocales	1	0.3693	**0.3951**	0.3781	0.3744	0.3594
	2	0.4183	0.4264	0.4457	**0.4549**	0.4472
	3	**0.6356**	0.5665	0.6062	0.5608	0.5878
	4	0.4835	0.4968	**0.5552**	0.4646	0.5420

Table 7 – Highest comparison r results in Alcornocales Park station using ANNs

Weather station W4	Approach	Neurons (ANNs model)				
		1	**5**	**10**	**20**	**50**
Algeciras	1	0.4272	0.4559	0.4301	0.4607	**0.5012**
	2	0.3179	0.3167	0.3021	0.4122	**0.4259**
	3	**0.5740**	0.5567	0.5508	0.5623	0.4978
	4	0.7287	0.7586	0.6965	**0.7810**	0.7055

Table 8 – Highest comparison r results in Algeciras station using ANNs

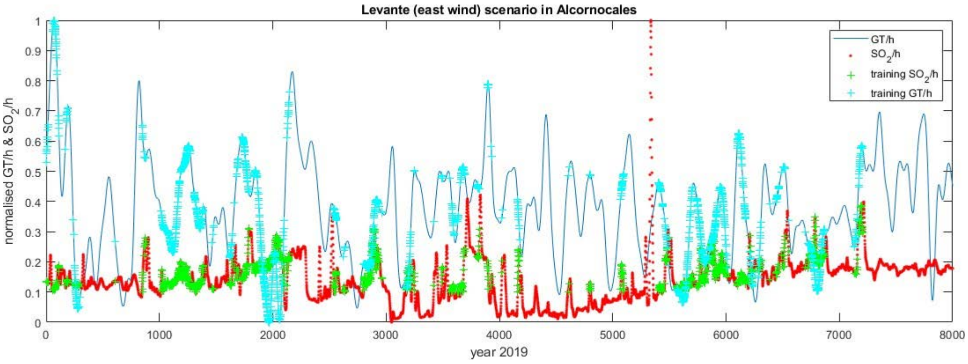


Figure 5 – Levante scenario in Alcornocales Park in the year 2019

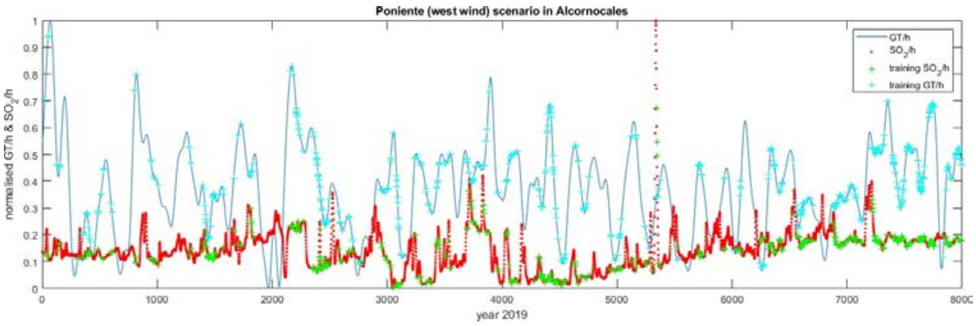


Figure 6 – Poniente scenario in Alcornocales Park in the year 2019

Figures 5-8 show the different variables used and also show the training examples in order to analyse how in each case, different conditions appear. Figures 5-8 show data after applying normalisation. The training examples of SO_2 are shown in green evidencing

Poniente and Levante events in both monitoring stations, Algeciras and Alcornocales Park. Ingeneral, West winds (Poniente) produce lower SO_2 situations and the reverse occurs with East winds (Levante). In both stations, West winds (Poniente) events models produce a better fitting in training data for SO_2 (green crosses) than in East wind due to the fluctuating nature of the SO_2 time-series in Levante conditions. Generally, in Poniente conditions, SO_2 data are more stable.

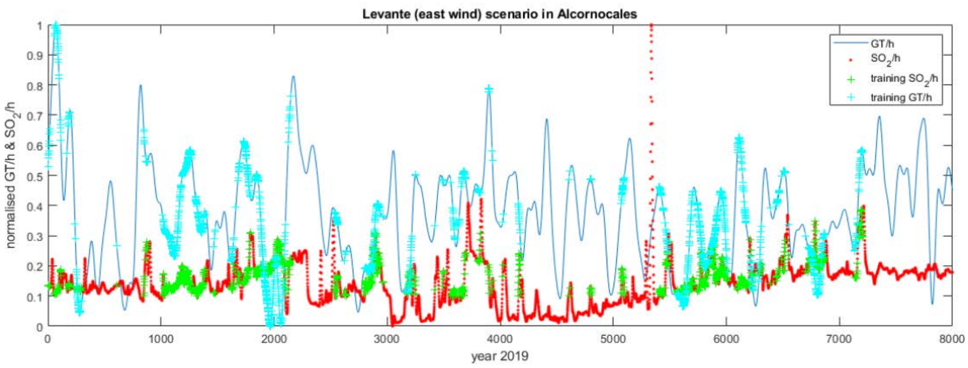


Figure 7 – Levante scenario in Algeciras city in the year 2019 (W4)

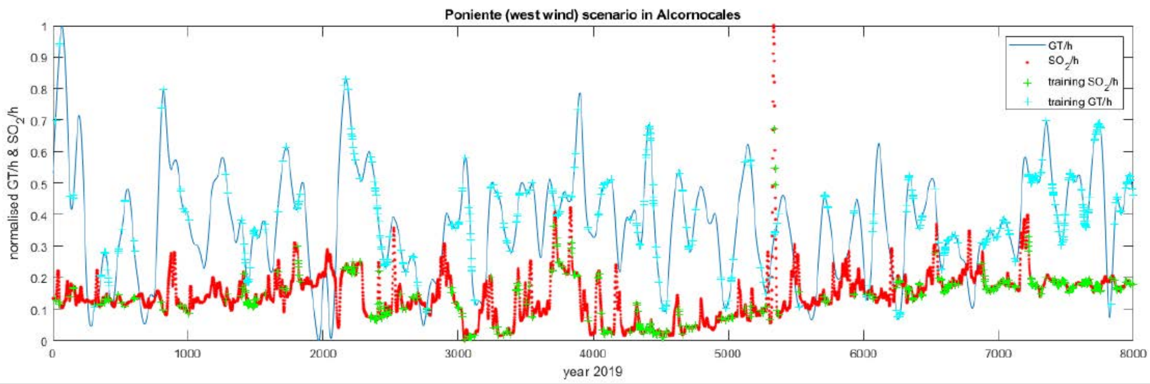


Figure 8 – Poniente scenario in Algeciras city in the year 2019 (W4)

5. CONCLUSIONS

The SO2 database is better suited to non-linear models as we can see from the results in Tables 5-8. ANNs models show better results than linear models, going from 0.7810 with 20 hidden neurons to 0.4499 in linear models in Algeciras. Although East winds are supposed to fit better the data in Algeciras, the results show that West winds produce a better fitting training data for SO2 due to the stability of SO2 data in Poniente conditions.

Once the study is developed, several conclusions can be extracted:

ANNs models deeply improve results of MLR revealing a strong non-linear behavior.
The usage of separated models for the two dominant winds (Poniente events and Levante events) also enhances the results of an individual model.

Future researches will focus on the usage of non-supervised clustering algorithms such as Kohonen’s self-organising (SOMs) maps to produce patterns to which separate models can be applied and also deep learning approaches.

The analysis presents promising results to be used afterward in SO2 forecasting models .
together with historical data of the time-series of SO2. In this research, the SO2 data were only used as outputs. Therefore, using a wind separation stage (Levante and Poniente), a robust estimation was developed and the obtained results have allowed us to confirm that this approach can serve as a support decision tool to citizens and/or institutions.

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