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SIRANE modeling of oxides nitrogen (NO_x) and ozone (O_3) in the area of Agadir city, southwestern Morocco.

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Abstract

This work aimed to model the dispersion of the traffic emissions for the first time in the area of Agadir city (Morocco). The estimate of road emission (from vehicle counts) was performed with Circul'air software version 4.0 which is based on the European methodology Copert 4. While the dispersion modelling was performed using SIRANE model, an important tool which adopts the classic NO_x photochemical process. The input data are pollutant emissions, background concentrations, meteorological parameters and building configuration data from QGIS software as well as a list of other factors such as latitude, albedo, etc.

Finally, the quality of the output results was validated by comparing observed measurements and modelled data.

Keywords: *Circul'air, SIRANE model, dispersion, modelling, Agadir, Morocco*

1.Introduction

The World Health Organization (WHO) and the International Agency for Research on Cancer (IARC) has identified outdoor air pollution as a main cancer agent on a global scale [1]. A large part of it may be ascribed to the emissions from automobile traffic, which impacts the air quality in cities by increasing the pollution levels [2,3]. In many countries, ambient air quality is monitored by a network of fixed stations. Such a network is not dense in Morocco, with only 29 stations installed in 15 cities of the Kingdom [4]. The importance of the air pollution problem is nonetheless recognized, a recent study [5] has estimated the cost of environmental degradation for Moroccan society at about 1 billion US $, or 1.05% of GDP in 2014. Moreover, even in countries where such a regulatory network exists, the limited number of stations makes the correct description of the general population exposure almost impossible, which represents the critical relationship between ambient air pollution levels and the induced human health effects [6,7]. In particular, they provide a general description of the pollution levels in cities and over the territories, but they fail to identify the local effects, such as the air pollutants freshly emitted by local sources [8,9], or the trapping of pollutants in urban canyons. An alternative to the physical measurements of air pollutants is the use modeling tools. These tools allow the understanding of the phenomena, the extrapolation of existing measurements to places not equipped with instruments, and most importantly the evaluation of operational solutions to control the emissions and the impacts, such as changes in the urban pattern, in the composition of the fuel, of the land use parameters, in the establishment of alternative, intermodal or cleaner transportation systems. … Among of these models, Operational Street Pollution Model OSPM [10], AERMOD [11], CALINE4 [12], ADMS-Urban [13] and SIRANE [14] are often used. The models can treat simultaneously both the atmospheric dynamics, i.e. the transport of pollutants away from their emission sources, and the complex reactive chemical and photochemical processes, though all the reactions are not systemically included, in particular at the local scale.

The urban community of Agadir, located at 30°56'N, 9°13'W, is the largest city of southern Morocco, counting over 420,000 inhabitants [15]. Agadir is a dynamic metropolitan area, with a rapidly expanding population, in parallel with its fast economic growth, driven by many industrial zones and industrial units, such as food-processing, agriculture, concrete, cement plants, steel mills, fertilizer plants, chemical factories, and rubber processing plants, in and around the city, which release significant amounts of gaseous pollutants into the atmosphere. The increase in population and economic activity, including tourism, leads to an increase in the number of vehicles in the city. Traffic congestion is omnipresent during peak hours and week-ends. The vehicle fleet remains relatively old despite strong renewal efforts, with a large number of vehicles imported from Europe, therefore in accordance with European standards on the environment. Additionally, over the past ten years, the characteristics of petroleum products have tended towards those of the European Union. Still, environmental issues such as air and noise pollution are of prime importance for the Agadir population, and are addressed by the local authorities, who are investigating the possibility of creating a public transportation system with a high quality of service. A prerequisite to this creation is the detailed characterization of the present situation and the evaluation of possible scenarios and routes for the buses. In previous works [16-18], we have investigated experimentally the pollutant (NO_x, carbonyls, BTX) levels in the area. We have shown that the specific topographical and meteorological conditions of the area, with the city bordered on the West by the Atlantic Ocean and on the East by the Atlas mountain range, as well as the wind mainly in the west-northwest direction, can create a temperature inversion leading to an accumulation of pollutants in the lower layer of the atmosphere [16-18]. We have also previously demonstrated that the photostationary state (PSS) normally leading to equilibrium between NO, NO_2 and O_3 concentrations through the Leighton cycle [19], is not reached in roadside environments [17], mainly because of the different timescales between the chemical reactions and physical (dilution and mixing) phenomena.

NO, which accounts for ~ 85% of the NO_x emitted by cars [20, 21], is quickly converted into NO_2 which subsequently undergoes complex chemical processes [22, 23]. But the PSS is disrupted by possible additional chemical reactions, for instance with VOCs, and also by incomplete mixing of the exhaust plumes with the surrounding air [24]. This implies that roadside measurements by monitoring stations, if any, will not be able to correctly capture both mobile emission concentrations and background concentrations. This will also limit the direct interpretation of the output of modeling tools, because they rely on the PSS for the NO_x chemistry. But these modeling tools can still be used with profit to estimate the emissions and their global impact at the city scale, particularly through the identification of pollution hot spots. In the present study, we have constructed the first inventory of the pollutants emitted by the traffic in the urban community of Agadir city, and applied the SIRANE model [14], with the limitations stated above, to investigate the NO_x distribution over the area. The SIRANE model has been selected for the ease of creating input files, the unlimited number of sources and receptor points in the input and output grids, the speed of calculation thanks to parallel computing techniques, and the demonstrated performances. The output of the SIRANE model was compared with measurements performed throughout the city between January and June 2014.

2. Modeling methodology

The SIRANE model developed by the Air Impact and Risk laboratory of the Ecole Centrale de Lyon [14,25] was used to simulate the NO_x atmospheric dispersion. As regards the reactivity, the SIRANE model only considers basic NO_x chemistry, according to the Leighton cycle linking the NO, NO_2 and O_3 concentrations [19]. The model computes the concentrations of NO, NO_2 and O_3 from the emissions of NO_x, evaluated using the Circul'air software of ASPA (2005) [26], described below. This methodology makes two important assumptions: (i) the pollutants emitted by the traffic are inert substances at the local scale, and (ii) the photostationary equilibrium is reached, which we have shown earlier not to be completely true at proximity of the traffic sources [17]. The input data necessary for the SIRANE modeling tool are the topographical information on the road network and the surrounding buildings, the meteorological data, the total NO_x traffic emissions and the background concentrations measured at different receptor points. All these parameters are described in more details below.

2.1. Meteorological data

The climate is semi-arid to arid, influenced by the proximity of the Atlas mountain range and of the Atlantic Ocean coast. The average annual rainfall is about 260 mm. The annual average maximum and minimum temperatures are 27 °C (August) and 11 °C (January) respectively, with a relative humidity ranging between 32% and 85%. The wind is mostly in the west-northwest direction, with a wind speed ranging from 0.1 to 3.6 m/s.

The hourly meteorological data for the period under investigation (wind speed and direction, temperature, relative humidity, cloud cover, precipitations) were recovered from the Infoclimat association website (http://www.infoclimat.fr/). The measurements, taken at the meteorological station located at Agadir airport, about 20 km away from the centre of the city, are considered also representative of the city weather conditions.

2.2. Road network

The road network file is created using the open source QGIS program suite (www.qgis.org). The file contains information on the position and the geometry of the roads, in particular their width W, and the positions and parameters of the buildings, in particular their height H. This allows determining the topographical type of the roads, that is whether they are in open terrain (W/H > 3) or in a street canyon (W/H ≤ 3). The global road network

of the city is shown on Fig 1. Only the major roads (blue lines) are taken into account in this work, for a total of 208 km. All roads are considered as open streets type, and most of them have a zero slope. Each road is divided into several sections, according to the number of lanes, the maximum authorized speed and the absence of traffic lights, stops or intersections. A total of 534 road sections was found. The lengths of these sections range from 10 m to 2.7 km. In each of these sections, the traffic, and therefore the emissions, is considered homogeneous. For calculation purposes, these 534 sections are further divided by QGIS into 2737 smaller linear segments. The length of each segment was calculated directly under QGIS. The capacity of the road is estimated by Circul’Air from the number of lanes, speed limit, and slope. Preliminary calculations were performed to ensure that the rest of the road network did not play a significant role in the output result. Therefore, they are considered tertiary sources with negligible importance according to the tests carried out in this way.

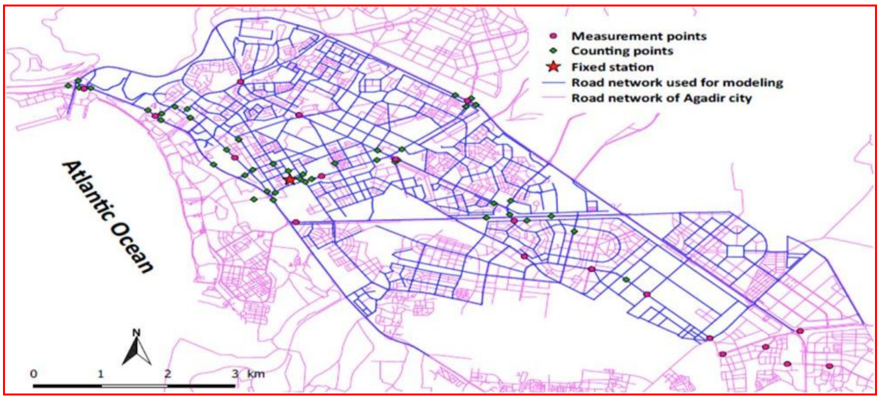

Figure 1. Map of the area under study, with the localization of the traffic counting stations, the NO_x background monitoring station and the NO_x measurement points.

2.3. Estimation of NO_x traffic emissions

The traffic emissions were calculated using Circul'air. The software version, Circul'air 3.0, is based on the European methodology for calculating the emissions from road transport COPERT IV version 10 [27]. Circul'air calculates for each road segment the annual road traffic emissions of greenhouse gases (CO_2, N_2O, and CH_4) and air pollutants CO, NO_x (NO_2 and NO), PM_{10}, $PM_{2.5}$. Circul’air also computes the fuel and oil consumption. The required input data are mainly the annual average daily traffic (AADT), the percentage by type of vehicle (% of trucks, % of buses, % of cars), the temporal profiles of the traffic, the meteorological data (average monthly minimum daily temperatures and average monthly maximum daily temperatures, monthly average relative humidity), the capacity of the road, the rolling automobile park, the length of each axis, the slope and the percentage of cold start vehicles.

2.3.1. Vehicle fleet

In the absence of information on the composition of the Moroccan vehicle fleet, we assumed that it could be represented by the French rolling park fleet of the year 2010, as was done during a previous study [28] with Moroccan specificities. Briefly, this fleet is 15% gasoline, 85% Diesel, 81% private cars, 1% trucks, 3% buses, 14% motorcycles, with vehicles with a mean age of 10-15 years. The number of buses and the number of daily trips were communicated by the transport services at the city. For Moroccan fuel quality, since 2008, their specificities tend towards those of European fuels.

2.3.2. Traffic counts and temporal (day, week, month) profiles

The evaluation of the annual traffic on each road and for each type of vehicle passes by the collection and the exploitation of the data of counting all vehicles and the part of trucks in this value [29, 30]. Temporary traffic counting campaigns were conducted by the Agadir urban community (AUC) on the main roads of the city during two weeks in December 2013. The locations of the traffic counters were decided by AUC for operational purposes. They are indicated by green markers on Figure 1. The permanent counting station operates in “all vehicle mode” without distinguishing between car and trucks. Two complementary methodologies for traffic data surveys were mainly implemented during the survey campaign: Automatic counts in current section and directional counts at intersections. In the case of the most complex intersections (more than 4 branches and with significant traffic volumes) the directional counting by Mineralogical Plates has been adopted allowing to carry out additional interesting analyzes. Six intersections were counted by number plate readings (from 7:30 to 8:30 am and 17:00 to 18:00 segregated in 15-minute periods) and thus 38 intersections were processed by manual directional counts.

A total of 86 pneumatic counters were placed at 44 sites to count traffic in both directions; two meters were placed on one-way streets. The counters operate in "all vehicles" mode and thus provide the series of traffic volumes per hour for seven consecutive days. These measurements allow determining for each counting point the daily total number of vehicle and the daily profile. It has been found that the hourly profiles of each counting station are similar. The typical profile is presented on Figure 2. We therefore make the (strong) assumption that at all timescales (week, months) the temporal profiles at all counting stations are similar. The detailed analysis of the traffic patterns will be published separately. This assumption allows determining at each traffic counting station the Annual Average Daily Traffic (AADT), by comparison with the AADT measured on RN1.

2.3.3. Temporal profiles

The temporal profiles used for calculating road emissions are traffic estimates based on the month, day and hour of 2014. From temporal profiles (monthly profile, daily profile, hourly profile), the road traffic for each axis and each type of vehicle is calculated for each hour, each day and each month of the year. The road count data correspond to the Annual Average Daily Traffic (AADT) as well as the percentage of trucks (% HT) associated with each road sections. For all counting sites, the automatic counts carried out on roads allows to know the AADT with similar hourly profiles: the peaks are reached as early as 7:30 to stabilize at hourly volumes of 1500 and 2500 vehicles up to 17.00 with light falls around 9.00, between 12.00-13.00 and 15.30-16.30 (Local Time).

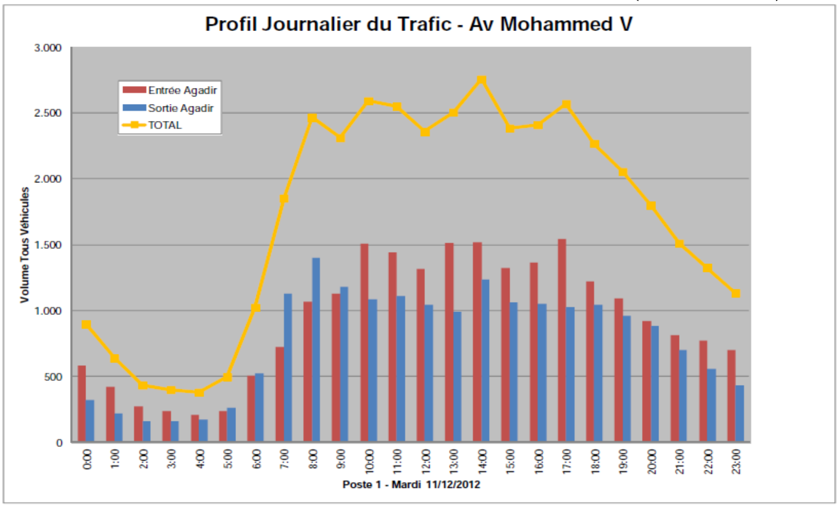

Figure 2 : The daily profile of the flows recorded on Tuesday 11 December 2013 at Mohammed V Avenue.

2.3.3. Output of Circul'air: congestion status, traffic speed, and annual emissions

From the parameters of the road (number of lanes, slope, speed limit) and the number of light vehicles and trucks, Circul'air allows to compute, with a time step of one hour, the congestion status and average traffic speed on each section of the road network [31]. The hourly traffic is then distributed by means of a detailed characterization of the vehicle fleet. Air emissions are thus estimated on each road or each road section and for each type of vehicle. Finally, these hourly emissions are summed to provide, for each pollutant, the annual emission (kg/km/year) per road section, which constitutes the input data for the SIRANE model.

3. Measurement of NO_x and O_3 concentrations

NO_x and O_3 concentrations were measured with online gas analyzers, to provide the background concentrations necessary to run the SIRANE model, and also to provide experimental determinations that can be compared to the output of the SIRANE model. Ozone was measured with an Environnement SA model 41M, based on UV absorption at 253.7 nm, with a detection limit of 0.4 ppb. NO_x (NO and NO_2) were measured with an Environnement SA model 31M, based on chemiluminescence, with a detection limit of 0.35 ppb. Two background sites were selected. The first one is located at the reference station of the city, the second site is located on the campus of the Faculty of Science of the Ibn Zohr University, and it was already demonstrated that this site is not influenced by the traffic or any other source of nitrogen oxides [17]. Roadside measurements were performed between January and June 2014. The sampling points were placed at a height of 4 m above the ground, 10 to 100 m away from the roadside [32].

3.1. Measured background concentrations of O_3 and NO_x

As an example, Figure 3a and 3b shows the time evolution of the O_3 and NO_x concentrations in March and May 2014 at the background sites, located on the Campus of the Faculty of Sciences of the University Ibn Zohr of Agadir. NO level is continuously around 10 $\mu g.m^{-3}$, with a few data points spiking above 20 $\mu g.m^{-3}$. NO_2 level is generally between 20 and 30 $\mu g.m^{-3}$, occasionally up to 40 $\mu g.m^{-3}$. Ozone shows more frequent and larger variations, between 5 and 40 $\mu g.m^{-3}$.

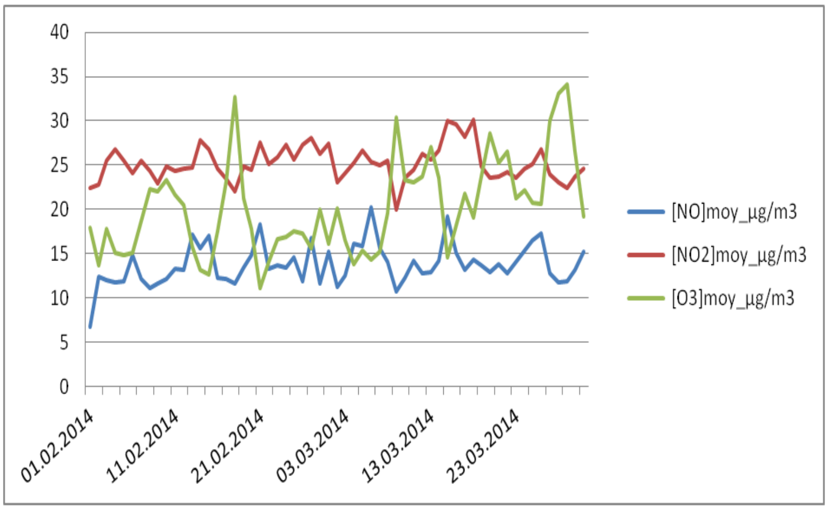

Figure 3a. Background ozone and NO_x concentrations measured at the reference station of Agadir city.

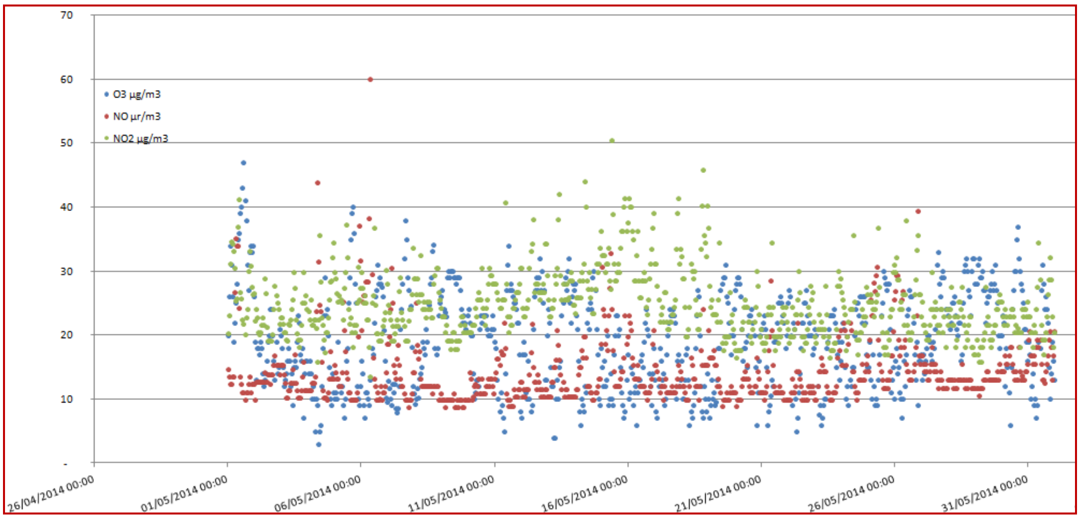

Figure 3b. Background ozone and NO_x concentrations measured at the Faculty of Sciences of the Ibn Zohr University.

3.2. Measured roadside concentrations of O_3 and NO_x

An example of the daily concentration evolution of NO_x (ppb) measured from 8:00 to 18:00 during 4 days in December 2014 at four selected sites is reported on the Figure 4. The three curves corresponding to roadside measurements follow the same behavior, characterized by two peaks corresponding to the morning and evening rush hours. The three curves still differ in their baseline concentration, from ~80 ppb at P2 to ~160 ppb at P1, and in the intensity of the peak concentration, reaching 200 ppb at P2 and P3 and up to 320 ppb at P1. This is consistent with the traffic at the three measurement locations, more important at P1 than at the two other places. By comparison, the background site also reported on the same graph shows a much lower NO_x concentration of about 40 ppb, not influenced by rush hour traffic.

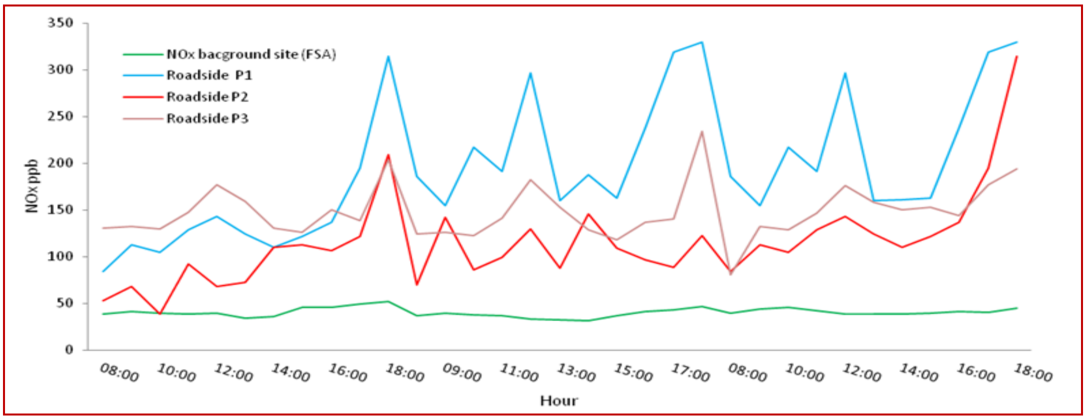

Figure 4. Example of hourly concentrations of NO_x (ppb) in background site (FSA) and three roadside locations.

4. Results and Discussions

4.1. Output of Circul'Air model

From these input parameters, the total annual traffic emissions of NO_x are computed by the Circul'Air model. Assuming that at the tailpipes, the NO_x are constituted by 85% of NO_2 and 15% of NO, the resulting maps are shown on Figure 5a and 5b.

Figure 5a. Annual emissions of NO calculated by Circul'Air.

Figure 5b. Annual emissions of NO_2 calculated by Circul'Air.

4.2. NO_2, NO and O_3 modelled dispersion

The output of Circul'Air is injected into the SIRANE model to take into account the dispersion of pollutants and the reactivity of NO_x through the Leighton cycle, considering also the measured background, large scale concentrations of NO_x and ozone. This allows reconstructing maps of selected parameters on the concentrations of these species. As an example, the resulting maps of the average concentrations of NO_2, NO and O_3, calculated for the period from January to June 2014 for which background concentrations measurements were available, are shown on Figure 6a, 6b, 6c respectively.

Figure 6a. Simulated NO_2 average concentrations obtained between January 1th and June 30th 2014.

Figure 6b. Simulated NO average concentrations obtained between January 1th and June 30th 2014.

Figure 6c. Simulated O_3 average concentrations obtained between January 1th and June 30th 2014.

The analysis of these maps shows that the NO_x concentrations are elevated only close to the roads, with maximal concentrations around 45 to 50 µg/m3 in average for both NO and NO_2. At the same time, the ozone concentration close to the roads is about one half of the background concentration. The effect of traffic is however very limited, and the NO_x concentrations in the surrounding residential areas are on average around 30 µg/m^3 for NO_2 and 10 µg/m^3 for NO, which are similar to the measured values presented on Figure 3a and 3b. The modeled concentrations of NO_x and O_3 are therefore globally lower than the WHO recommendations. Only at the roadsides that these recommendations are exceeded.

4.3. Comparison of predicted NO_2 concentrations with measured ones

To further validate the methodology and results of this work, we examine here in detail the output of the modeling tools, through the comparison between the modeled NO_2 concentrations and the measured NO_2 concentrations in six different sites within the Agadir urban community [32,17]. The overall performances of the SIRANE model have already been evaluated for field studies using such a comparison between modeled and measured concentrations. However, in the present work, we have made several strong assumptions regarding the vehicle fleet, its emissions, the daily traffic profile, the exclusion of the secondary network of roads within the city, and most importantly, the measurement of background and roadside concentrations and the counting of vehicles were not performed simultaneously. It is therefore important to verify whether these assumptions do not impact the validity of the procedure. For this comparison, we use several classical statistical indicators [33-36]. These include the mean absolute percentage error (MAPE), the fractional bias (FB), the normalized mean square error (NMSE),

the fraction of prediction within a factor of two of observations (FAC2), and the geometric variance (VG). The meaning and the mathematical definition of these parameters can be found in [35,37]. We also used the standard acceptance criteria recommended for urban areas [35]: MAPE values below 30%, FAC2 values above 0.3, FB below 0.67 and $(NMSE)^{1/2}$ below 2.4.

Table 1, summarizes the different average, minimum and maximum values of the four performance indices, calculated using the NO_2 hourly concentration values, for each day where experimental measurements were available.

Site	Date	MAPE (%)		FB		$(NMSE)^{1/2}$	FAC2	
		mean	max	mean	max	mean	mean	min
	06/6/14							
1	11/6/14							
	18/6/14						0.42	0.26
	6/1/14							
2	11/6/14	36%					0,77	0.45
	10/6/14							
	1/3/14	31,5					0.47	0.31
3	25/1/14						0.39	0.24
	8/3/14						0.69	0.40
	3/2/14	22	51	0.22		0.07	0.93	
9	6/2/14	25	49	0.23		0.67	1.08	
	8/2/14	11	23	0.11		0.09	0.94	
	14/4/14						0.76	0.11
	4/2/14	17	46	0.16		0.04	1.03	
10	9/3/14	39					1.21	0.18
	15/4/14	27					0.43	0.19
11	5/2/14	28	67	0.24		0.10	1.18	
	7/2/14	25	52	0.23		0.08	1.09	

For our case, we obtained an average MAPE mean of 26.2% and MAPE max of 48% which validates on average the forecasting model since the MAPE is lower than 30%. Unlike the FB, the FAC2 is a robust and appropriate indicator for assessing the performance of the air quality model since it is not overly influenced by outliers. FB can be negative (underestimated) or positive (overestimated). The values of FAC2 < 0.5 indicate that it is important to consider the canyon approach and not "open or partially open terrain". Indeed, among the considered measurement points, the sites 3 and 10 tend towards canyon avenues, while the other sites are mostly semi-open bordered sites where the canyon effect depends on the position of the measuring point by compared to neighboring buildings.

The model results underestimate (when FB > 0) or overestimate measures (when FB < 0). The few differences between the predicted and the measured values may be due to the homogeneity of the meteorological conditions, whereas in reality they vary over time under the effect of buildings. In this work, the simulation was carried out under open environment conditions (W/H > 3) and most of the measurements were performed in a partially open

manner where wind recirculation is no longer homogeneous and where, in the SIRANE model, the stability is based on the approach of [38], which most other dispersion systems use specifically in rural areas. In urban areas, this atmospheric stability is based on the approaches [39]. If the measurements are very close to the axes of the roads, the difference between measurements and predictions is very wide. This can be explained by the chemistry of the Chapman cycle (R1, R2 and R3) and by the photostationary equilibrium defect "PSS" at the edges of the channels. From the analysis of the ozone map generated by SIRANE model, it can be noted that its values are very low compared to the minimum values, which can be explained by the chemical processes: the reaction (O_3 + NO) is important, the effect of OH and RO_2 are also minimal and the VOC rate is therefore relatively low in the environment. The chemical transformation of NO_2 includes two mechanisms, photochemical reactions and exchange processes with ambient air. The chemical transformation module in SIRANE tends to decrease the predicted NO_2 concentrations in the open zone, in the canyons zone it uses background ozone concentrations to form NO_2, generating higher concentrations reducing the gap between measured and modelled concentrations. In conclusion, the SIRANE model underestimates the NO_2 concentrations observed in an open or partially open area. While it overestimates the concentrations near the open area channels although it has a Gaussian algorithm for modelling dispersion outside urban canyons. According to [40], neglecting the contribution of other sources of pollution in urban areas can lead to lower concentrations of about 30%. For our study we obtained a MAPE of 26.2%, which validates the forecast model. According to [37] the MAPE needs to be inferior to 30% for model validation and which returned a MAPE of 21.15%, for sites in city-center. The underestimation may be due to the emission rates that do not take in to account daily traffic variation or meteorological inputs.Comparison with background values, the model error was minor between the dispersion modelling and the background values of the fixed automatic station as indicated on the figure 7.

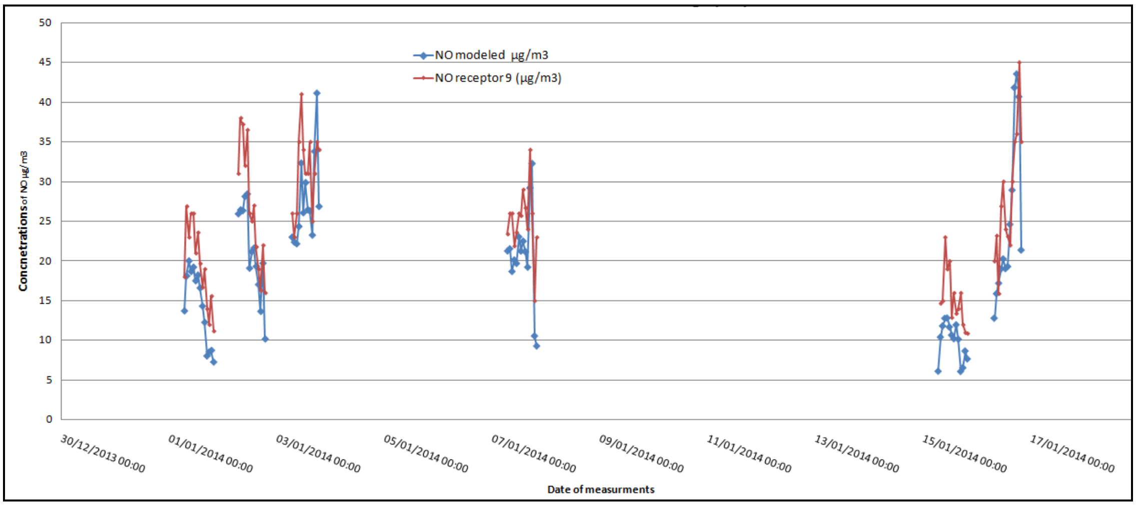

Figure 7. Comparison between background values and modelled values.

5. Conclusion

The paper focused on the SIRANE model as an operational model of urban dispersion and also as the first attempt realized for Agadir (Morocco). The aim of this work is to evaluate and study the dispersion of NO_x and O_3 using the SIRANE model. It consists of two main steps: traffic estimation and dispersion modelling. Traffic estimation was done by on-site traffic fleet counting and the European methodology COPERT for emission factors.

The SIRANE model has proved effective when applied to traffic pollution as it is monitored in busy urban area, for example, the application of ADMS-Urban to pollution in London.

The simulated data were correlated to the measured values using on-line analyzers located at a distance of approximately 10 m from the roads of six sites during the study period. Efforts are needed to improve the traffic conditions within the city, to encourage public transport, to develop the lanes (increasing the number of lanes); the BHLS line remains an important solution.

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