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Use of atmospheric modeling system to identify possible sources of pollution

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ABSTRACT
The increase in industrialization makes critical episodes of air quality degradation more and more common. In Pernambuco, similar cases can be observed in the vicinity of the Suape Industrial Port Complex, where this study found that, between 2017 and 2021, O_3 was the pollutant that most exceeded the final standard established in national legislation (100 µg/m³). Therefore, this work aimed to identify the possible emission sources during critical pollution episodes. For this purpose, backward trajectories associated with cluster analysis were calculated using the Hysplit atmospheric model. The simulations showed that 89% of the trajectories that exceeded the final standard originated in the ocean, indicating the possibility that the NO_x emitted by ships traveling on the coast is converted into O_3 still in the sea and taken inland by the wind. The other 11% came from areas where port and industrial activities are carried out, indicating the possibility that ozone also has VOCs emitted by petrochemicals as precursors. These results demonstrate that modeling systems can be used satisfactorily in monitoring air quality, contributing to support decision-making by public authorities.

Keywords: Ozone. Hysplit. Cluster Analysis.

1. INTRODUCTION

The Industrial Revolution brought about significant changes in the production of goods, resources, and the provision of services. Consequently, more significant environmental impacts were observed, as the growth of the industrial sector, while crucial for the economy, also significantly contributes to the emission of atmospheric pollutants (LAN et al., 2023). In addition to direct emissions from anthropogenic activities, increased urbanization poses risks of natural vegetation loss, leading to substantial air quality deterioration (PRAKASAM; ARAVINTH; NAGARAJAN, 2022).

The speed of industrialization growth has resulted in even more pronounced emissions, mainly when multiple industries concentrate in the same area. These industrial clusters form industrial parks or complexes, ranging from diverse sectors to companies with similar activities, such as chemical and petrochemical industries. The ventures' potential environmental and human health impacts warrant increased attention to monitoring, control, and safety in their vicinity (YANG; CHEN, 2022). However, each city has a unique industrial organization, causing pollutant concentrations to vary according to local characteristics (SUN et al., 2020).

In Pernambuco, the Governor Eraldo Gueiros Industrial Port Complex, better known as the Suape Industrial Port Complex (CIPS), houses numerous industries from various sectors and the Port of Suape. Prominent activities in CIPS include the Abreu e Lima Refinery, Petrochemical Suape, and the Port of Suape. This factor is significant because petrochemical industries are potential sources of various contaminants, such as volatile organic compounds (VOCs), particulate matter (PM), carbon monoxide and dioxide (CO and CO_2), sulfur oxides (SO_x), and nitrogen oxides (NO_x) (LIN et al., 2021). On the other hand, ports emit contaminants from anchored or transiting ships and activities within the port, such as loading and unloading, truck use, cranes, and trailers. Another relevant factor influencing pollutant emissions is the type of vessel, including cargo and tanker ships. Key pollutants associated with port activities include $PM_{2.5}$, PM_{10}, SO_x, NO_x, and ozone (O_3) (LEDOUX et al., 2018; MUELLER; WESTERBY; NIEUWENHUIJSEN, 2023; SIM; PARK; BAE, 2022).

As a secondary pollutant formed through photochemical reactions, O_3 is not directly emitted from the abovementioned sources. However, its formation is associated with primary precursor pollutants, such as NO_x and VOCs, local meteorological conditions, and air transport,

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among other factors. These factors, aside from determining O_3 production, are crucial in its loss, transformation, and spatial distribution (WANG et al., 2022a). When meteorological conditions are favorable, and there is an adequate quantity of primary pollutants, photochemical reactions are likely to generate tropospheric ozone (SONG et al., 2018). Furthermore, the O_3 formation process can be sensitive or limited by VOCs or NO_x. When it is sensitive to one of these pollutants, its production is influenced, leading to higher environmental concentrations. Conversely, when either of these pollutants limits it, its formation depends on the presence of that specific pollutant. Therefore, reducing the production of the primary pollutant also reduces ozone levels (SONG et al., 2021; QU et al., 2023).

Although this pollutant plays a crucial role in the stratosphere by filtering ultraviolet radiation and protecting planet life, its tropospheric formation can be devastating.
Studies indicate that exposure to tropospheric ozone may be associated with various adverse effects on human health (CHIQUETTO et al., 2019; GOMES et al., 2019; ROVIRA; DOMINGO; SCHUHMACHER, 2020; WANG et al., 2022b), besides provoking social and economic impacts, related to agricultural productivity. Such occurrence is due to the presence of O_3, which can lead to losses and reduction of crop growth, resulting in decreased harvests, which threatens food security (DONG; WANG, 2023; QI et al., 2023).

Given the presented issue, it is evident that monitoring O_3 behavior is necessary to reduce the impacts caused by this pollutant. Monitoring to predict, control, and mitigate events that may compromise air quality is a matter of public and environmental health. Therefore, public management must take the lead in decision-making. In Brazil, the legislation defining standards for atmospheric pollutant emissions is Resolution Conama No. 491 (CONAMA, 2018), followed in Pernambuco state.

However, there is a considerable need for more air quality monitoring stations in the country (REQUIA; ROIG; SCHWARTZ, 2021), necessitating the search for alternative methodologies to assist decision-making. One option to achieve this goal is through modeling systems, which have been globally employed over the decades through various applications, yielding positive results. This model exemplifies the studies conducted by Casciaro, Cavaiola, and Mazzino (2022), Silveira, Ferreira, and Miranda (2023), and Wu et al. (2023). One of the atmospheric models with a high degree of application is the Hybrid Single-Particle Lagrangian Integrated Trajectory (Hysplit) model, which enables the analysis of pollutant behavior from the emission source, identification of possible pollution sources affecting a given location, and characterization of air trajectory behavior through cluster analysis. Hysplit analyses can be conducted for both natural events (IRAJI et al., 2021; GHOSH et al., 2023) and pollution events associated with anthropogenic activities (CHEN et al., 2013; FRANZIN et al., 2020; BOLAÑO-TRUYOL et al., 2022). Furthermore, it is an open and freely accessible model, facilitating access and application.

2. OBJECTIVES

This study analyzed data from five monitoring stations located in CIPS, in the Metropolitan Region of Recife, from 2017 to 2021. When exceeding the legal limit, the atmospheric model Hysplit was used to identify potential polluting sources.

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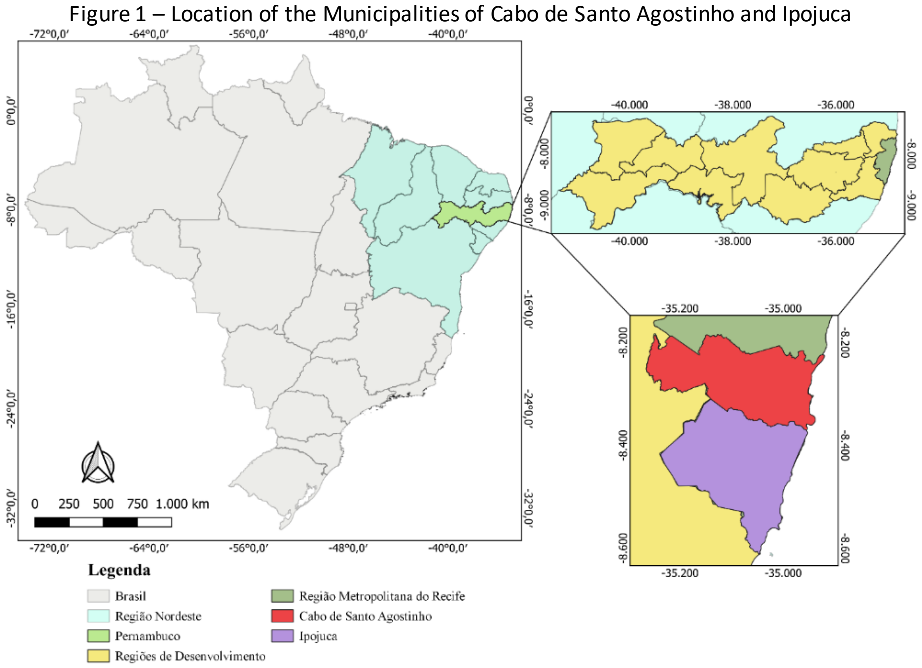
3. METHODOLOGY

3.1 Study Area

In June 2023, Pernambuco had six automatic monitoring stations, with five in active operation and one inactive. However, the most recent of these, the Suape Station, commenced activities in 2022 and needed data wasn’t available at the time of this research. Therefore, only the other five stations – CPRH, Cupe, Gaibu, IFPE, and Ipojuca – were analyzed from 2017 with the first available data until 2021, the last year with disclosed information. All stations have data for the five observed years except for Gaibu Station, which was deactivated in the first half of 2020, and Cupe, whose operations started in the second half of the same year.

These mentioned stations are located in the Metropolitan Region of Recife (RMR), and out of the five studied stations, two are in the municipality of Cabo de Santo Agostinho, and three are in the municipality of Ipojuca (Figure 1). The municipality of Cabo de Santo Agostinho has a territorial area of 445.386 km², an urbanized area of 43.47 km², and an estimated population of 210,796 inhabitants in 2021. The municipality of Ipojuca, with an estimated population of 99,101 inhabitants in 2021, has a territorial area of 521.801 km² and an urbanized area of 29.39 km². Both are part of the Recife Population Arrangement which, according to the Brazilian Institute of Geography and Statistics (IBGE), occurs when municipalities are highly integrated and effectively constitute a single city for urban hierarchy. Furthermore, both are in the Atlantic Forest biome and belong to the Coastal-Marine System (IBGE, 2023a; 2023b).

Figure 1 – Location of the Municipalities of Cabo de Santo Agostinho and Ipojuca



Source: The Authors (2023).

The cities of Cabo de Santo Agostinho and Ipojuca share similar economic activities, with their primary activities being the tourism potential of their beaches, industrial activities within the Suape Industrial Port Complex (CIPS), and sugarcane production from various mills

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and distilleries (CARDOSO; SILVA; LIMA, 2021; MORETTI; COX, 2016). Local employment opportunities stimulate the migration of workers from other cities and states (CARDOSO; SILVA; LIMA, 2021), and the tourism potential attracts people from around the world, contributing to increased urbanization (SIQUEIRA et al., 2021). The rise in urbanization and the numerous economic activities are potential sources of pollution and significant factors in environmental degradation.

Established in 1979, the CIPS is currently managed by the state-owned Industrial Complex Port Governor Eraldo Gueiros, which is linked to the Economic Development Secretariat of Pernambuco (CARDOSO; SILVA; LIMA, 2021). It is located approximately 40 kilometers south of Recife. It covers areas in Cabo de Santo Agostinho and Ipojuca (OLIVEIRA et al., 2021), which used to be occupied by mills involved in sugarcane production (MORETTI; COX, 2016).

All air quality monitoring stations are situated near CIPS, which includes the Port of Suape and 84 companies with various operations, such as food, chemical, pharmaceutical, liquid and gaseous bulk industries, and petrochemicals, including Petroquímica Suape and the Abreu e Lima Refinery (RNEST) (SUAPE, 2023). Petrobras maintains the air quality monitoring network as a requirement for obtaining the Environmental Operating License for RNEST from the state's environmental control and monitoring agency, the State Agency for the Environment (CPRH, 2023). The network monitors CO, MP_{10}, NO_2, O_3 and SO_2 pollutants. This study used as an evaluation criterion the final emission standard (FS) established in Resolution No. 491 of the National Council of the Environment (CONAMA, 2018) to determine if the values harmful to health and the environment exceeded the limit (Table 1). This resolution specifies that for CO and O_3, the maximum daily rolling averages calculated every 8 hours should be observed; for MP_{10} and SO_2, the daily averages should be used; and for NO_2, hourly averages should be employed.

Table 1 – National air quality standards. IS – Intermediate Standard; FS – Final Standard

Pollutant	Reference period	IS-1	IS-2	IS-3	FS
CO (ppm)	8 hours	---	---	---	9
MP_{10} (µg/m³)	24 hours	120	100	75	50
NO_2 (µg/m³)	1 hour	260	240	220	200
O_3 (µg/m³)	8 hours	140	130	120	100
SO_2 (µg/m³)	24 hours	125	50	30	20

Source: Adapted from Conama (2018).

However, although the CO and O_3 criteria consider only the maximum daily rolling average, this study chose to analyze all rolling averages to determine how many times the limit concentration was exceeded. Considering all exceedances at all five analyzed stations, the study found that O_3 was the pollutant that exceeded the Conama limit most frequently (Table 2), with all exceedances occurring at the Cupe Station – the station with the shortest operational time among those studied. Based on this finding and the significantly lower number of exceedances for the other pollutants, was decided to analyze the behavior of O_3 in the monitoring network, as well as variations in concentrations during legal limit violations and the primary air trajectories in these situations.

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Table 2 – Number of exceedances by pollutant from 2017 to 2021

	CO	PM_{10}	NO_2	O_3	SO_2
CPRH	6	4	---	---	4
Cupe	---	5	---	214	8
Gaibu	---	110	---	---	---
IFPE	---	11	1	---	4
Ipojuca	---	2	---	---	43
Total	**6**	**132**	**1**	**214**	**59**

Source: The Authors (2023).

3.2 Backward Trajectory Simulations and Cluster Analysis

The use of mathematical models to study air quality characteristics is a widely used method that allows for observing trajectory patterns, particle transmission, and diffusion. This system provides a better understanding of air pollution episodes, ranging from dust storms (IRAJI et al., 2021) to radioactive elements (GUTIÉRREZ-ÁLVAREZ et al., 2019).

To analyze the behavior of the central air trajectories during O_3 exceedances, the Hysplit (Hybrid Single-Particle Lagrangian Integrated Trajectory) mathematical atmospheric model was employed. This model utilizes a hybrid Lagrangian and Eulerian approach to calculate air pollutant trajectory, dispersion, and concentration simulations (STEIN et al., 2015). The version used was the unregistered 5.2.1 version for computers, provided by the Real-time Environmental Applications and Display System (READY) of the Air Resources Laboratory (ARL) at the National Oceanic and Atmospheric Administration (NOAA). The model allows for both forward and backward trajectory calculations. The forward trajectory identifies the behavior of air parcels from a simulated source point. In contrast, the backward trajectory determines the path from the detected point of the air parcel's origin and links it to emitting sources that may be at a considerable distance (FRANZIN et al., 2020).

Another functionality Hysplit offers and is used in this research is the cluster analysis, a data analysis technique that aims to create relevant subgroups of elements with similar characteristics while differing from others (HAIR JR. et al., 2010). One of the techniques used in this method and applied in Hysplit (KASPAROGLU; INCECIK; TOPCU, 2018) is the k-means method, which iteratively groups elements until the elements in each group possess the specified characteristics, resulting in the final number of clusters (GUTIÉRREZ-ÁLVAREZ et al., 2019). However, although this method suggests the number of clusters, the model allows the user to choose the number of groups for analysis, thereby relating them to specific atmospheric circulations in the region. The global meteorological database GDAS (Global Data Assimilation System) was used for trajectory calculations and cluster analysis. This database has a spatial resolution of 1.0° and contains information available since 2005 through weekly files (DRAXLER et al., 2022; KHAIRULLAH; EFFENDY; MAKMUR, 2017). For trajectory model execution, this study chose backward trajectory type, the Cupe Station as the receptor point with a latitude of -8.3996° and a longitude of -35.0398°, a 1-hour analysis time, and an altitude above ground level of 10 meters. For the cluster analysis, five clusters were selected, ensuring that they exhibited

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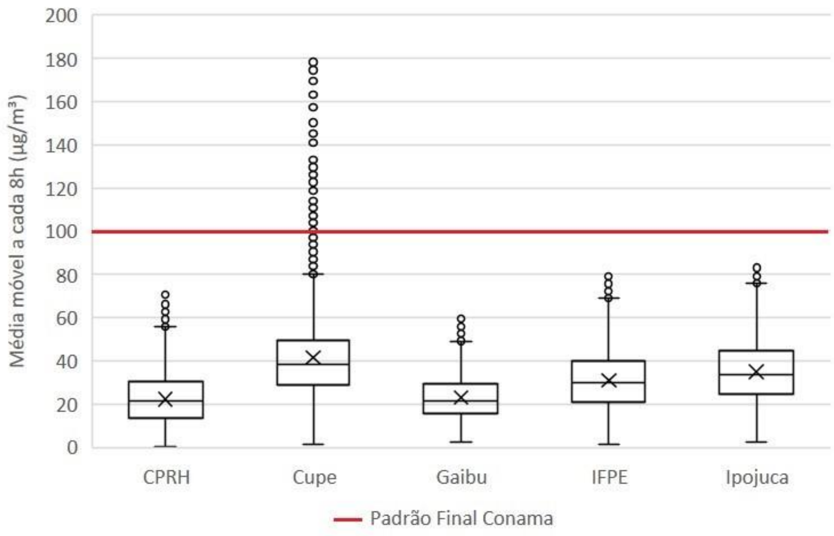
different behaviors and fairly consistent numbers of trajectories. This choice allowed for a better distribution of trajectories. This criterion is similar to that used by Gutiérrez-Álvarez et al. (2019).

4. RESULTS AND DISCUSSION

In coastal cities worldwide, particularly those with industrial and port activities, O_3 can be the primary air pollutant affecting air quality. This occurrence may be attributed to rapid economic and industrial development and local meteorological conditions, which can make ozone formation sensitive to NO_x or VOC depending on the time of the year (CHEN et al., 2023) and the activities conducted.

By applying the representativeness criterion and calculating the number of times each pollutant exceeded the final standards Conama (2018) set in the analyzed air quality monitoring stations, it was evident that O_3 was the pollutant with the highest number of cases that exceeded these limits (Table 2). The behavior of this pollutant across all studied stations was analyzed using a boxplot (Figure 2).

Figure 2 – Boxplot of hourly O_3 mobile mean concentrations from 2017 to 2021 by Monitoring Station. The red line represents the limit value established by Conama.



Source: The Authors (2023).

Upon examining the boxplot, it is noticeable that, for all stations, O_3 demonstrates similar behavior concerning symmetry. The same holds for dispersion, except for the Gaibu Station, which has a minor difference between the values of the first and third quartiles (13.34 µg/m³). Concerning medians, the CPRH and Gaibu Stations have similar values, around 20 µg/m³; the IFPE and Ipojuca Stations, on the other hand, approach 30 and 34 µg/m³, respectively, while the Cupe Station has an approximate value of 38 µg/m³, being the station with the highest median.

Regarding outliers, they can be observed at all stations, with 5, 24, 4, 4, and 3 at the CPRH, Cupe, Gaibu, IFPE, and Ipojuca Stations, respectively. Upon analyzing them, the study found that Gaibu was the only one not to present concentrations above 60 µg/m³. CPRH was

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the second with the lowest concentrations, with a maximum value of approximately 70 µg/m³. In contrast, the IFPE and Ipojuca stations had values closer to the final standard, with roughly 79 and 83 µg/m³ concentrations, respectively. Cupe was the station with the highest number of outliers, the only one to exceed the average concentration of 100 µg/m³, the limit established as the FS for O_3 by the legislation.

Furthermore, although it has the most minor data (10,386 hourly averages), as its activities began only in the second half of 2020, the Cupe Station has the most extensive range of mobile average means, with an approximate value of 79 µg/m³. The means of the 8-hour average concentrations were 22.3 µg/m³, 41.5 µg/m³, 23 µg/m³, 31.1 µg/m³, and 35.1 µg/m³ for the CPRH, Cupe, Gaibu, IFPE, and Ipojuca Stations, respectively. Through the outliers, the study observed that the maximum average concentrations were 70.6 µg/m³, 179.8 µg/m³, 59.4 µg/m³, 79.1 µg/m³, and 83 µg/m³. By the lower limits, the minimums were 0.3 µg/m³, 1.4 µg/m³, 2.4 µg/m³, 1.2 µg/m³, 2.4 µg/m³, for the CPRH, Cupe, Gaibu, IFPE, and Ipojuca Stations, respectively.

In other regions of Brazil, these values may vary, presenting similar or different concentrations. In a study conducted in the industrial district of Maracanaú, in the metropolitan region of Fortaleza, Ceará, with approximately 2,000 industries from various sectors, it was observed that, during the analyzed period, the average concentration of O_3 for 8-hour periods was 38.5 µg/m³, while the maximum and minimum were 48.8 µg/m³ and 27.9 µg/m³, respectively (LIMA et al., 2020). The average concentration in Maracanaú is similar to that observed at the Cupe and Ipojuca Stations, with a difference of approximately 3 µg/m³ more and less, respectively. The maximum concentration recorded is about 11 µg/m³ less than the one observed at the Gaibu Station, the closest value found. In contrast, the minimum concentration is significantly different from all, with a minimal difference of 25.5 µg/m³.

In São Gonçalo do Amarante, which hosts part of the Pecém Industrial Complex, also part of the metropolitan region of Fortaleza, Ceará, and the average concentration was 79.2 µg/m³, with a maximum of 122.8 µg/m³ and a minimum of 55.2 µg/m³. This complex houses steel mills, power plants, refineries, and various other industries, forming the Pecém Industrial Port Complex and the Pecém Port Complex (FERREIRA JÚNIOR et al., 2020). All the concentrations observed by these authors differ from those recorded in the stations analyzed in the present study. The minor difference for the average concentration was approximately 38 µg/m³, and for the maximum, approximately 57 µg/m³, both at the Cupe Station. As for the minimum concentration, the slightest difference was about 53 µg/m³ at the Gaibu and Ipojuca Stations.

In the city of Santos, in the state of São Paulo, episodes of pollution from vehicle traffic and port activities were analyzed, with average concentrations of 45.17 µg/m³, a maximum of 138.00 µg/m³, and a minimum of 2.00 µg/m³ observed (GUEDES et al., 2021). The average concentration observed in Santos is similar to that at the Cupe Station, with approximately 4 µg/m³ more. The maximum concentration differs from that recorded in all stations, having a value closer to that of the Cupe Station, with approximately 42 µg/m³ less. The minimum concentration has an approximate value that aligns with all the stations, especially Gaibu and Ipojuca.

The Air Quality Report for the State of São Paulo in 2021 presents episodes of high ozone concentrations in the second half of August and throughout September in the

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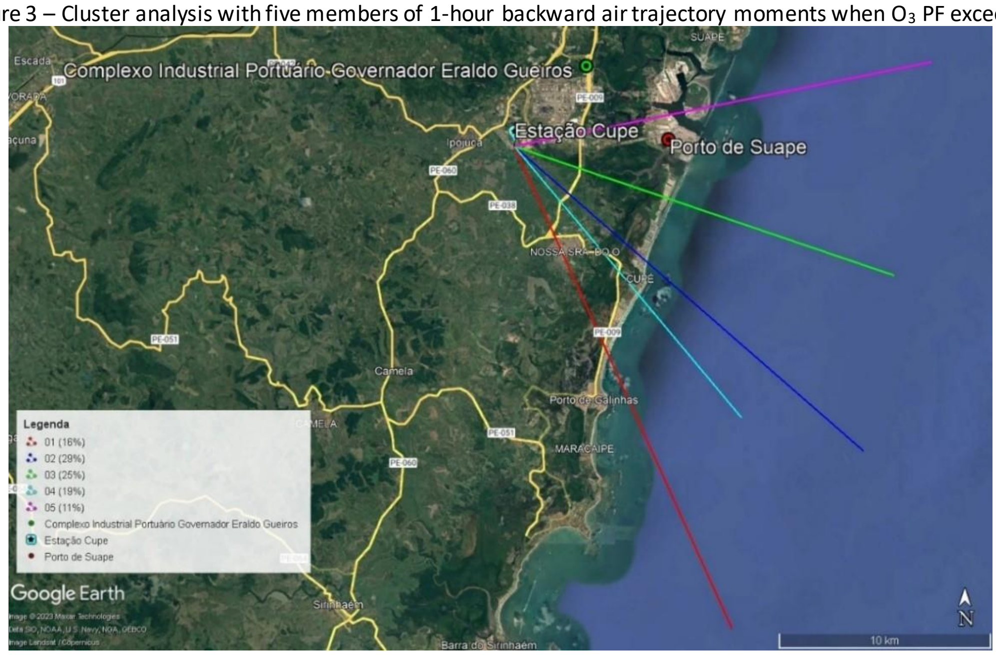
Metropolitan Region (RMSP) and the state’s interior and coastal areas, with maximum daily concentrations in 8-hour averages. For the RMSP, the lowest concentration observed was 30 µg/m³ on September 17, 2021, at the Nossa Senhora do Ó and Pinheiros Stations, while the highest was 187 µg/m³ on September 4, 2021, at the Cidade Universitária-USP-Ipen Station. For the interior and coastal areas, the lowest concentration was 16 µg/m³ on August 28, 2021, at the Cubatão-Vale do Mogi Station, and the highest was 168 µg/m³ on September 29, 2021, at the Americana Station (CETESB, 2022). The minimum concentrations observed by Cetesb differ by about 28 µg/m³ (RMSP) and 14 µg/m³ (interior and coastal) from those observed at the Gaibu and Ipojuca Stations. The maximum concentrations differ by approximately 7 µg/m³ (RMSP) and 12 µg/m³ (interior and coastal) from those observed at the Cupe Station.

To identify the origin of air parcels over the Cupe station during the exceedance of the FS, backward trajectory simulations with a 1-hour lead-time for these hours were employed. Subsequently, these trajectories were collectively analyzed using cluster analysis to identify their main paths (Figure 3). This research observed that most trajectories (clusters 01 to 04, 89%) originate from urban areas and the ocean. In contrast, the smallest group (cluster 05, 11%) passes through the CIPS, across the sea, Port of Suape, and areas near some industries, such as Petroquímica Suape and RNEST.

Figure 3 – Cluster analysis with five members of 1-hour backward air trajectory moments when O_3 PF exceeded



Source: Adapted from Google Earth and Hysplit (2023).

This result may be directly influenced by the ships that traverse the area destined to or departing from the Port of Suape since maritime diesel engines can emit significant amounts of NO_x (DENG et al., 2021), which can lead to the secondary pollutant O_3 through photochemical reactions. Additionally, petrochemical industries are potential sources of nitrogen oxides and VOC, contributing to the generation of tropospheric ozone (LU et al., 2023). Due to the low concentration of NO_2 measured by the monitoring stations, especially at the Cupe Station (Figure 4), it is possible that the ozone formed near the CIPS area (cluster 05), particularly in the

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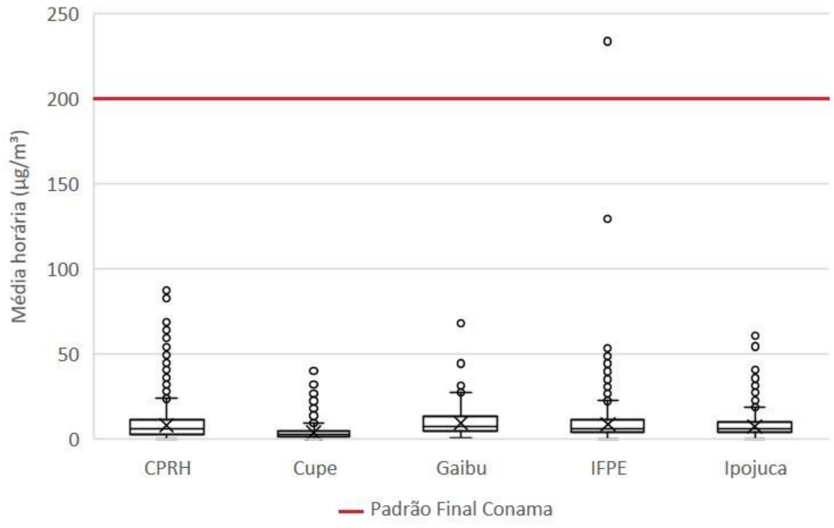
vicinity of petrochemical plants, is sensitive to VOC. Those originating from urban areas and the ocean (clusters 01 to 04), may be sensitive to NO_x, as the conversion of solar radiation is fast. This factor allows the transformation to occur near the emission source, in the ocean, and for O_3 to be transported by the wind to the mainland. Thus, the low values of NO_2 concentrations that the present study observed may be attributed the conversion process far from the monitoring network and transformations sensitive to VOC.

These results are consistent with other studies, which observed that the NO_x level increases when many ships traverse and that the emitted pollutants may remain in the route, affecting the O_3 formation (SIM et al., 2022). Therefore, in areas with high ship concentrations, ozone transformation may be firmly controlled by NO_x, being produced in the ocean and transported to the mainland according to wind patterns (WANG et al., 2019), as both pollutants have a high capacity for long-distance transport (WANG et al., 2023), causing critical episodes of pollution. About industrial complexes, the type of industry established in the area is a determining factor in the emitted pollutant type, with potentially significant concentrations of compounds such as VOCs (CHOI et al., 2023), which, unlike NO_x, have a low capacity for long-distance transport and, therefore, contribute to the formation of ozone near the emission source (WANG et al., 2023). The transformation of O_3 from sensitivity to VOC is a common characteristic in most industrialized cities (WANG et al., 2022a). One of these industries, present in the study area, is the petrochemical industry, whose refining process may be one of the primary sources of VOCs with a high potential for ozone formation (SHI et al., 2022).

Figure 4 – Boxplot of hourly average NO_2 concentrations from 2017 to 2021 by Monitoring Station. The red line represents the limit value established by Conama.



Source: The Authors (2023).

Regarding the values of ozone excess concentrations analyzed through boxplot (Figure 5), this research observed that although the fifth cluster has the lowest number of grouped trajectories (11%, 24 trajectories), it has the second largest data range (20.9 µg/m³). It presents significant variation in average concentrations, with an upper limit of 133.2 µg/m³ and a lower limit of 100.1 µg/m³, and is nearly symmetric. The trajectory direction of this cluster suggests

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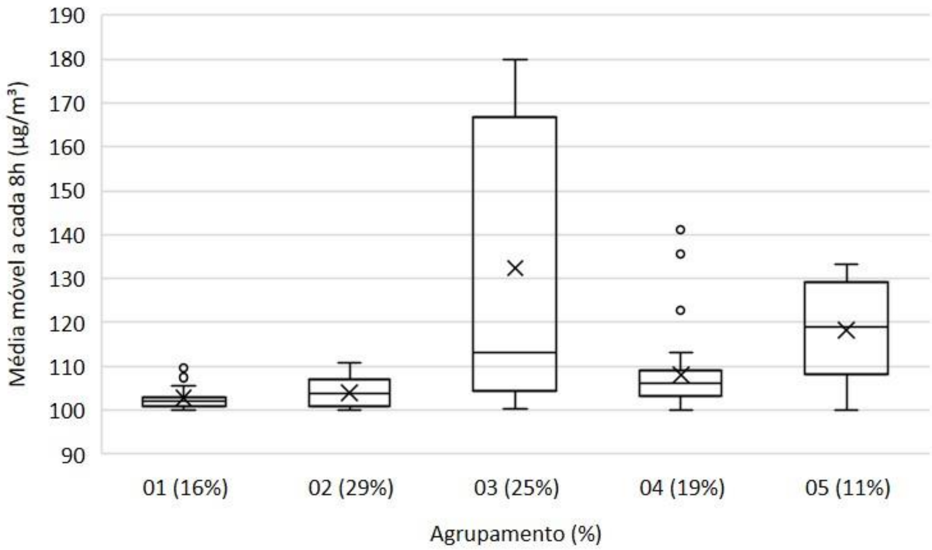
that 11% of the exceedance cases of the FS originate from conversions of primary pollutants emitted through maritime activities—whether from operations at the port or vessels—and industrial activities—mainly from the petrochemical industries located in the CIPS. The third cluster, on the other hand, is the second largest in number of trajectories (25%, 53 trajectories). It has a wider data range (62.5 µg/m³), is positively skewed, with a median (113.1 µg/m³) close to the first quartile (104.3 µg/m³). The same cluster has an upper concentration limit of 179.8 µg/m³ and a lower limit of 100.24 µg/m³.

The trajectory direction of this cluster indicates that out of the 214 times the FS was exceeded, 53 times are potentially due to the ocean, mainly in areas closer to the port, suggesting that the primary pollutants that lead to O_3 are related to vessels arriving or departing from the Port of Suape.

Figure 5 – Boxplot of O_3 mean concentrations above the final standard, separated by a cluster



Source: The Authors (2023).

Although the second cluster has a low range (6.03 µg/m³), it has the highest number of trajectories (29%, 62 trajectories), with a median of 103.87 µg/m³, an upper limit of 110.93 µg/m³, and a lower limit of 100.88 µg/m³. The other clusters have low ranges, and the first and fourth have two (107.5 µg/m³ and 109.2 µg/m³) and three (122.7 µg/m³, 135.5 µg/m³, and 141 µg/m³) outliers, respectively. Like Cluster 03, Clusters 01, 02, and 04 originate from the ocean, suggesting the potential contribution of primary pollutant NO_x from maritime emissions as the main precursor in ozone pollution episodes. The averages of the 8-hour mobile average concentrations for the exceedance cases were 102.75 µg/m³, 104.03 µg/m³, 132.42 µg/m³, 108.08 µg/m³, and 118.18 µg/m³ for Clusters 01, 02, 03, 04, and 05, respectively.

Although the monitoring stations are close to each other and monitor the same facilities, the impacts on the network occur differently. On a large scale, different regional emission and weather scenarios will likely hinder the creation of suitable and effective measures at the municipal level (DING et al., 2023), highlighting the need to apply measures considering each location's reality.

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5 CONCLUSION

With the increasing levels of urbanization and industrialization, critical air quality degradation has become more common. Similar cases can be observed in Pernambuco, near the Industrial Port Complex of Suape, the only place in the state with an air quality monitoring network. Network monitoring showed that between 2017 and 2021, O_3 was the pollutant that exceeded the final national standard (100 µg/m³) the most. Through cluster analysis executed by the Hysplit atmospheric trajectory and dispersion model, it was observed that most air trajectories (clusters 01 to 04, 89%) at the times of exceedance originate from the ocean, indicating that these contaminants may result from emissions from ship traffic. The smallest group (cluster 05, 11%) comes from areas where both port and industrial activities are conducted, making it possible for these contaminants to originate from the port and petrochemical industries, such as the Abreu e Lima Refinery and Petroquímica Suape.

Ships destined for the Port of Suape may emit NO_x during the voyage, which, through photochemical reactions, could be converted into ozone in the ocean and transported by the wind to the mainland. Other port activities, such as anchoring and product transportation, could also contribute to air pollution episodes. Regarding industrial activities, O_3 likely has VOC as the primary pollutant commonly emitted in petrochemical industries.

These results demonstrate that ozone is one of the pollutants related to the most critical episodes of pollution, whose transformation depends not only on the availability of primary pollutants but also on suitable weather conditions. Therefore, to implement satisfactory measures, it is necessary to consider the reality of each location. One way to achieve this goal is through atmospheric pollution modeling systems, which can serve as decision support tools, aiding real-time monitoring and forecasting. Moreover, they allow the analysis of past events to identify possible sources of pollution so that mitigating and preventive measures can be adopted.

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