

Green AI

A Study About Paris' Air Pollutants

Élèves :

Nour AFFES Lucas BLANCHET Hugo BONNELL Ryan HAMADEH Yasmine MAARBANI

Enseignants:
Nathan ELBAZ
Ali MOKH

9 décembre 2024





Table des matières

1	ntroduction	:
	.1 Presenting the pollutants 1.1.1 PM10 : Particular Matter 1.1.2 NO : Nitric Oxide 1.1.3 NO2 : Nitrogen Dioxide 1.1.4 NOX : Nitrogen Oxides 1.1.5 O3 : Ozone	
2	Temporal Analysis	(
3	Policy Impact	(
4	Inter-Pollutant Relationships 1.1 Chemical Interactions and Relationships 4.1.1 Chemical Reactions of PM10 4.1.2 Chemical Reactions of NO 4.1.3 Chemical Reactions of NO2 4.1.4 Chemical Reactions of NOX 4.1.5 Chemical Reactions of O3 (Ozone) 1.2 Takeaways about air chemistry	
5	Comparative Studies	;
6	Event-based Analysis	
7	Forecasting 7.1 Forecasting Pollutant Concentrations for the next 6 months	
8	Conclusion	10



1 Introduction

Air pollution is a pressing environmental issue that affects the health and well-being of millions of people worldwide. In urban areas, such as Paris, the impact of pollutants like particulate matter (PM10), nitrogen oxides (NO, NO2, NOX), and ozone (O3) is especially critical due to the high population density and traffic congestion. Understanding the trends, sources, and behavior of these pollutants is essential for formulating effective policies and strategies to improve air quality and mitigate the risks posed by air pollution.

This study, conducted as part of the "Green AI" course, focuses on the temporal and chemical dynamics of air pollutants in Paris, specifically using data from the air quality monitoring station located in the 18th arrondissement. The dataset, which spans from 2018 to the present, provides valuable insights into the concentrations of key pollutants in the city. By examining this data, we aim to identify trends, patterns, and correlations that can inform better public health and environmental policies.

The study is structured around several key areas of analysis. First, we explore the temporal trends of pollutants to determine whether their concentrations have been increasing or decreasing over the years, and investigate seasonal patterns and daily cycles that influence air quality. We also examine the potential impact of specific policies and events on pollutant levels, such as the implementation of low-emission zones or the reduction in activity during the COVID-19 lockdowns.

Another important aspect of the study is the exploration of inter-pollutant relationships, where we analyze the chemical and atmospheric interactions between pollutants like NO2 and O3, or NO and NOX. These interactions can provide deeper insights into the causes of pollution and help identify critical thresholds at which one pollutant's increase significantly influences the concentration of others.

To further enrich our analysis, we conduct comparative studies by benchmarking Paris's air quality against other major cities around the world, providing a contextual understanding of how the city fares in terms of pollution levels. Additionally, we explore event-based analyses to assess the impact of specific occurrences, such as public holidays, protests, or transportation strikes, on pollutant levels.

Finally, in line with modern advancements in data science, we apply machine learning techniques to develop predictive models that can forecast pollutant levels based on historical data. This approach will provide a better understanding of future pollution patterns and help inform decision-making.

By combining data-driven insights with a comprehensive understanding of pollution dynamics, this study aims to contribute to the broader conversation about air quality in urban environments and its effects on public health and the environment.



1.1 Presenting the pollutants

1.1.1 PM10 : Particular Matter

Overview:

- Sources: Combustion (vehicles, industries), construction dust, agricultural activities, and natural sources like pollen or sea spray.
- **Behaviour**: Particles remain airborne and can travel long distances. They act as surfaces for chemical reactions involving gaseous pollutants.
- **Health impact**: Penetrates the respiratory system, causing cardiovascular and respiratory diseases.

What is it?

PM10 refers to particulate matter with a diameter of 10 micrometers or less. These fine particles are primarily produced from combustion processes (e.g., vehicles and industrial activities), construction dust, agricultural activities, and natural sources such as pollen and sea spray. Due to their small size, PM10 particles can remain suspended in the air for extended periods, potentially traveling over long distances. They act as surfaces for chemical reactions involving gaseous pollutants, including nitrogen oxides and volatile organic compounds. PM10 is a significant concern for human health, as it can penetrate deep into the respiratory system, leading to cardiovascular and respiratory diseases, particularly in vulnerable populations such as children and the elderly.

1.1.2 NO: Nitric Oxide

Overview:

- Sources: Emitted directly from combustion processes in vehicles and power plants.
- **Behaviour**: A reactive gas that plays a key role in forming NO2 and other nitrogen oxides.
- Health impact: Precursor to NO2 and ozone (O3) formation.

What is it?

Nitric oxide (NO) is a colorless and odorless gas primarily emitted from combustion processes, including vehicle engines, power plants, and industrial facilities. It plays a crucial role in atmospheric chemistry, particularly in the formation of nitrogen dioxide (NO2) and ozone (O3). NO is highly reactive and can quickly react with other compounds, making it a key precursor in the production of secondary pollutants. In urban areas, NO



levels are closely associated with traffic emissions, and its concentration tends to be higher in the colder months when heating and combustion activities peak. Though it is not directly harmful in low concentrations, its role in the formation of smog and acid rain underscores its importance in air quality studies.

1.1.3 NO2: Nitrogen Dioxide

Overview:

- Sources: Oxidation of NO in the atmosphere; direct emissions from diesel engines and industrial activities.
- **Behaviour**: A toxic gas contributing to smog formation and secondary particulate matter.
- **Health impact**: Contributes to acid rain and ozone production.

What is it?

Nitrogen dioxide (NO2) is a reddish-brown gas that forms primarily through the oxidation of nitric oxide (NO) in the atmosphere. Major sources of NO2 include diesel engines, industrial processes, and power plants. This toxic gas is a key component of urban air pollution, contributing to the formation of ground-level ozone and photochemical smog. NO2 is also a precursor to acid rain, which can have harmful effects on ecosystems and infrastructure. Additionally, NO2 contributes to the formation of secondary particulate matter, worsening air quality. Long-term exposure to elevated NO2 levels is linked to respiratory diseases, particularly in children and individuals with pre-existing lung conditions.

1.1.4 NOX: Nitrogen Oxides

Overview:

- Sources: Collective term for NO and NO2. Mainly produced from combustion.
- Behaviour: Highly reactive, leading to the formation of ozone and nitrates.
- **Health impact**: Major contributor to photochemical smog and secondary aerosol formation.

What is it?

NOX refers to the collective group of nitrogen oxides, primarily NO and NO2, which are produced during combustion processes such as those from vehicles, power plants, and



industrial activities. These gases are highly reactive and play a central role in atmospheric chemistry, particularly in the formation of ozone and secondary particulate matter. NOX is a major contributor to photochemical smog, a key component of urban air pollution, and its presence in the atmosphere leads to the formation of nitric acid and nitrates. NOX emissions are also associated with several environmental issues, including acid rain, which harms aquatic ecosystems and soil quality. Due to its significant role in air pollution, controlling NOX emissions is essential for improving urban air quality and mitigating its harmful effects on human health.

1.1.5 O3 : Ozone

Overview:

- Sources: Not emitted directly. Formed by photochemical reactions involving NOX and volatile organic compounds (VOCs) in the presence of sunlight.
- Behaviour: A secondary pollutant that peaks during sunny days.
- **Health impact**: Toxic to plants, humans, and animals. A greenhouse gas in the troposphere.

What is it?

Ozone (O3) is a secondary pollutant that forms in the atmosphere through photochemical reactions involving nitrogen oxides (NOX) and volatile organic compounds (VOCs) under the influence of sunlight. Unlike stratospheric ozone, which forms the ozone layer and protects life from harmful ultraviolet radiation, ground-level ozone is harmful to human health and the environment. Ozone exposure can cause respiratory problems, aggravate asthma, and lead to premature death in individuals with cardiovascular conditions. It is also toxic to plants, reducing crop yields and forest productivity. Ozone levels typically peak during sunny days and are closely linked to the concentration of precursor pollutants like NOX and VOCs, making it a significant focus for air quality monitoring and regulatory efforts.



- 2 Temporal Analysis
- 3 Policy Impact
- 4 Inter-Pollutant Relationships
- 4.1 Chemical Interactions and Relationships

4.1.1 Chemical Reactions of PM10

PM10 particles themselves do not directly participate in chemical reactions in the atmosphere, but they play a crucial role in facilitating reactions between gaseous pollutants. Due to their large surface area, PM10 particles can adsorb and react with gases like sulfur dioxide (SO2), nitrogen oxides (NOX), and volatile organic compounds (VOCs). This results in the formation of secondary pollutants, including sulfate and nitrate particles. For instance, nitrogen oxides can react with ammonia to form ammonium nitrate (NH4NO3), a major component of fine particulate matter. Moreover, PM10 particles can serve as carriers for harmful metals, such as lead and mercury, which have significant environmental and health impacts.

4.1.2 Chemical Reactions of NO

Nitric oxide (NO) is a highly reactive molecule that plays a central role in atmospheric chemistry. NO is primarily produced through combustion, where nitrogen in the air reacts with oxygen at high temperatures. Once released into the atmosphere, NO can quickly react with ozone (O3) to form nitrogen dioxide (NO2), a process that is often referred to as **NO titration.** This reaction reduces the local concentration of ozone:

$$NO + O_3 \Rightarrow NO_2 + O_2$$

NO can also react with other compounds, such as VOCs, in the presence of sunlight to form secondary pollutants like ground-level ozone. In addition, NO plays a key role in the formation of acid rain, as it can react with water vapor to produce nitric acid (HNO3), which is then deposited into the environment through precipitation.

4.1.3 Chemical Reactions of NO2

Nitrogen dioxide (NO2) is a product of the oxidation of NO, and it plays a pivotal role in the formation of ground-level ozone, particularly in urban environments. NO2 absorbs sunlight and undergoes photolysis, breaking down into NO and an oxygen atom (O). This free oxygen atom can then combine with molecular oxygen (O2) to form ozone (O3):

$$NO_2 + hv_{(sunlight)} \Rightarrow NO + O$$



$$O + O_2 \Rightarrow O_3$$

In addition to ozone formation, NO2 is also involved in the creation of particulate matter. NO2 reacts with hydroxyl radicals (OH) and water vapor to form nitric acid (HNO3), which can combine with ammonia (NH3) in the atmosphere to form ammonium nitrate, a major component of secondary aerosol pollution.

4.1.4 Chemical Reactions of NOX

NOX, which refers to the combined presence of nitric oxide (NO) and nitrogen dioxide (NO2), is a major driver of both ozone and particulate matter formation. In the presence of sunlight, NOX reacts with volatile organic compounds (VOCs) to produce ozone through a series of complex photochemical reactions. This process is especially prominent in urban environments with high levels of traffic and industrial emissions. The general mechanism for ozone formation involves the following steps:

- 1. NO2 is photolyzed by sunlight to produce NO and atomic oxygen (O), which then reacts with molecular oxygen (O2) to form ozone (O3).
- 2. NO combines with ozone in the atmosphere to form NO2, continuing the cycle and contributing to higher concentrations of both NO2 and ozone. Furthermore, NOX also plays a key role in the formation of particulate matter, particularly secondary organic aerosols (SOAs). These aerosols form through the oxidation of VOCs in the presence of NOX, leading to the creation of fine particles that contribute to smog and reduced air quality.

4.1.5 Chemical Reactions of O3 (Ozone)

Ozone (O3) is a secondary pollutant, meaning it is not directly emitted but rather forms through complex photochemical reactions involving nitrogen oxides (NOX) and volatile organic compounds (VOCs) under the influence of sunlight. Ozone plays a dual role in the atmosphere, with beneficial effects in the stratosphere and harmful effects at ground level. In the troposphere, ozone is a powerful oxidant, capable of reacting with numerous organic and inorganic compounds. This reactivity makes it a major player in air pollution.

The formation of ozone begins with the photolysis of nitrogen dioxide (NO2), producing NO and an oxygen atom (O). The oxygen atom then reacts with O2 to form ozone:

$$NO_2 + hv_{(sunlight)} \Rightarrow NO + O$$

 $O + O_2 \Rightarrow O_3$

Ozone can also be depleted in the atmosphere by reactions with nitrogen oxides (NO) in a process known as ozone titration (mentionned earlier) :



$$NO + O_3 \Rightarrow NO_2 + O_2$$

This reaction reduces ozone concentrations, particularly in urban areas with high NO emissions. Additionally, ozone is highly reactive with organic compounds, and its presence in the lower atmosphere can contribute to the formation of secondary particulate matter, such as fine particulate matter (PM2.5), which can have significant health impacts.

4.2 Takeaways about air chemistry

The chemical interactions between PM10, NO, NO2, NOX, and O3 reveal a complex web of processes that influence air quality and environmental health. NO and NO2 are central to the formation of both ozone and particulate matter, with their interactions driving the production of ground-level ozone, which exacerbates smog and contributes to adverse health outcomes. Furthermore, particulate matter like PM10 can act as a carrier for other pollutants and facilitate chemical reactions, while ozone itself plays a crucial role in both pollutant formation and degradation. Understanding these chemical reactions is essential for developing effective strategies to mitigate air pollution and improve urban air quality.

- 5 Comparative Studies
- 6 Event-based Analysis
- 7 Forecasting

7.1 Forecasting Pollutant Concentrations for the next 6 months

In this section of the study, we aim to forecast the concentrations of key air pollutants (PM10, NO2, NO, NOX, and O3) for the next six months using the ARIMA model. The ARIMA (AutoRegressive Integrated Moving Average) model is well-suited for time series forecasting due to its ability to capture temporal dependencies and trends in sequential data. For this analysis, we applied ARIMA with optimized hyperparameters to the historical hourly pollutant data.

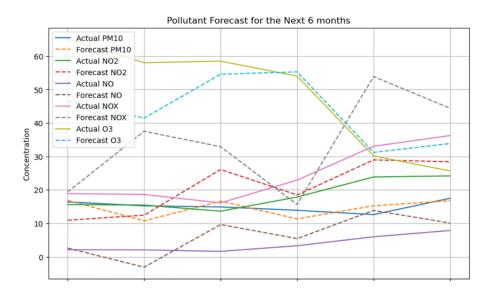
The code implemented for this forecasting task first defines a function, which uses the ARIMA model to forecast pollutant concentrations. The model parameters were set as (50, 1, 10) (Found by tweaking them), where:

- 50 is the number of lag observations included in the model (AR term),
- 1 represents the differencing order (I term) to make the data stationary, and



• 10 is the number of lag observations in the moving average model (MA term).

Using this function, we forecast the concentrations of five pollutants: PM10, NO2, NO, NOX, and O3 for the next six months, as shown in the plot below.



7.2 Plotting the Forecast

The resulting forecasted values (dashed lines) are overlaid with the actual historical values (solid lines) for each pollutant, with the date on the x-axis and pollutant concentration on the y-axis. The forecast is conducted on the test dataset, which includes actual pollutant concentrations up to the current period.

The forecasted trends suggest how each pollutant may evolve in the next 6 months, providing valuable insights into the potential future air quality scenario in Paris. For example, pollutants like NOX and O3 exhibit fluctuations that could help in formulating effective air quality management strategies.

7.3 Model Evaluation: MAE and RMSE

To assess the accuracy of the forecast, we calculated the Mean Absolute Error (MAE) and Root Mean Squared Error (RMSE) for each pollutant. These metrics provide a quantitative measure of the model's prediction error. The results of the evaluation are as follows:

MAE PM10: 2.10, RMSE PM10: 2.49
MAE NO2: 5.02, RMSE NO2: 6.20
MAE NO: 4.32, RMSE NO: 5.21



• MAE NOX: 12.07, RMSE NOX: 14.10

• MAE O3: 8.24, RMSE O3: 10.81

These values reflect a reasonable forecast performance, with lower errors for pollutants like PM10 compared to others like NOX and O3. The higher errors in NOX and O3 could be due to their greater variability, which is more difficult to model accurately with the chosen ARIMA configuration. These errors indicate areas where the model could potentially be refined by adjusting parameters or using more advanced forecasting techniques.

8 Conclusion