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Insights to WRF-Chem Sensitivity in a Coastal Region of Morocco: Chemical Mechanisms, Nesting Options, and Physical Parametrization

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Abstract: The performance of the Weather Research and Forecasting model coupled with chemistry (WRF-Chem) relies on the accuracy of the input data and its parameterization schemes. This study investigated the sensitivity of WRF-Chem version 4.4.2 to domain configuration, chemical mechanisms, and physics parameterizations. The model was used to predict air quality criteria pollutants (PM10, O3, CO, NO2, and SO2) and meteorological variables (wind speed (WS) and temperature (T)) for the first time over the Moroccan domain, in Agadir City. This region is located on the southwestern coast of Morocco and has a complex topography and land use configuration. We ran various simulations to test the sensitivity of the selected variables' predictions. These simulations explored different options for chemical mechanisms (MOZART, RACM, and GOCART), nesting configurations (three nested domains with a 1:4 nesting ratio and four nested domains with a 1:3 nesting ratio), and planetary boundary layer (PBL) parameterizations (YSU, MYJ, MYNN2, and QNSE). Modeled values of air quality and meteorological variables were then compared with surface observations using various statistical metrics. The results show that ozone O3 and NO2 are less sensitive to changes in domain configuration or chemical mechanisms, suggesting that ambient concentrations of these pollutants are more influenced by local factors. In particular, variations in NO2 are closely linked to local emission patterns. However, CO shows greater sensitivity to changes in nesting options, which is attributed to the dependence of CO modeling on accurate capture of local emission sources and atmospheric mixing. Similarly, concentrations of PM10, SO2 and CO are highly dependent on how physical and chemical processes are represented in the domain configurations and chemical mechanisms. On the other hand, O3 estimates are very sensitive to physical parameterization, which can affect meteorological parameters such as temperature. This underlines the significant influence of temperature and sunlight on ozone levels. For sensitivity analysis, the results indicate that the best optimal configuration varies depending on the variable, utilizing both qualitative (spatial variations) and quantitative (statistical metrics) approaches. Furthermore, for physics parameterizations, the chosen PBL for predicting WS and T is YSU. Concerning chemical mechanisms, GOCART emerges as the best scheme for predicting PM10, SO2, and CO, while MOZART is optimal for O3 and

NO2. Regarding nesting options, the most efficient choice is to utilize three nested domains with a 1:4 ratio, optimizing modeling time. These indicate significant improvements in air quality prediction over the region, however, there are still improvements to be made, especially in PM10, which has the lowest accuracy of the model and could be the objective of further research in this study area.

1 Introduction

Air pollution is a pervasive and complex environmental problem that demands careful attention on a global scale. It is a complex interplay between anthropogenic activity and natural processes that is altering the composition of the atmosphere on earth (World Health Organization, 2006). The consequences of air pollution figure large as human continue its trajectory of industrialization, urbanization, and energy consumption, which need an extensive investigation supported by solid research (Ciencewicki & Jaspers, 2007). Due to the rising levels of air pollution, billions of people are at danger for health problems (Sicard et al., 2021). Among air pollutants, the following have the most concerning effects on public health: ground-level ozone (O_3), nitrogen dioxide (NO_2), Sulphur dioxide (SO_2) and particulate matter ($PM_{10}/PM_{2.5}$) (Bălă et al., 2021; Regional, 2003), which are all related to health diseases such asthma, chronic obstructive pulmonary disease, and cardiovascular problem (Arghavani et al., 2019; Ciencewicki & Jaspers, 2007; Luo et al., 2020). In addition to causing visual harm, air pollution may also retard plant development and decrease its ability to resist certain pathogenic agents. For example, ozone may reduce agricultural production of cereals (Arghavani et al., 2019; Manisalidis et al., 2020). For these reasons it is important to study and forecast the concentrations of those pollutants in order to reduce their effects on human health, climate change, and atmospheric visibility (Lecoeur & Seigneur, 2013).

Anthropogenic air pollution emissions significantly impact the concentration and variety of chemical components found in the atmosphere. However, these emissions are just one piece of the puzzle when it comes to air quality. Weather conditions also play a significant role; Studies have shown that atmospheric stability, which is influenced by large-scale weather patterns (synoptic systems) and factors like wind speed, humidity, and temperature, can significantly impact air quality (Alapaty et al., 2012; Bounakhla et al., 2023). Particulate matter, a major air pollutant, is formed through chemical reactions, highlighting the crucial role of these reactions in air quality (Park, 2021a, 2021b; Taşpınar, 2015). Additionally, elements including terrain, land use, and others affect how pollutants spread throughout the environment. Numerical models are useful tools for predicting air pollution and comprehending involved physical and chemical processes (Sha et al., 2019). These tools, particularly meteorological models, play a vital role in our understanding of how meteorological conditions influence air quality (Liu et al., 2022). The appropriate simulation of meteorological variables and chemical species depends on an accurate understanding of local meteorological processes, topography and pollutant emissions (Misenis & Zhang, 2010a). Since air pollutants undergo complex chemical reactions in the atmosphere, air quality models combine meteorological forecasts with atmospheric chemistry modelling tools to predict pollution levels (Menut et al., 2021).

Currently, there are two different approaches for analyzing air quality: (i) a qualitative approach based on the study of factors affecting air quality from industrial activities, society, etc., taking into account a variety of factors like growing populations, waste incineration, coal combustion, and vehicle exhaust emissions, (ii) a quantitative approach based on pollutant transportation and diffusion mechanisms (Li et al., 2021; Liu et al., 2022). As an example of quantitative analysis, there are statistical models and deterministic models. Statistical method is about using the historical data to predict the future behavior of various air quality parameters (Qiu et al., 2022). This approach has been used extensively for air pollution prediction. For instance, studies have assessed patterns of PM_{10} levels and ozone using standard statistical methods like multiple linear regression (MLR) (e.g., Iraoui et al., 2023; Mohammed & Abualqumboz, 2018; Mohd Napi et al., 2020; Nazif et al., 2016; Siegfried et al., 2005; Yorkor & Leton, 2017) as well as artificial intelligence (AI) approaches such as support vector machines (SVMs), neural networks (ANNs), and deep learning (DL) (Abdul-Wahab & Al-Alawi, 2002; Adnane et al., 2020; Bozkurt, 2014; Chen et al., 2013; Luna et al., 2014; Park, 2021b; Taşpınar, 2015; Tebal & Pinang, 2011; W. Wang et al., 2003).While some studies suggest artificial intelligence methods can achieve higher accuracy, conventional statistical techniques offer valuable insights. Statistical models may not explicitly identify influential variables, treating the system as a "black box». Additionally, their accuracy relies heavily on the quality and amount of historical data (Mohan et al., 2011).

Unlike statistical models, deterministic models rely on established principles from chemistry, meteorology, and fluid dynamics. They utilize mathematical equations that explain how pollutants are transported, changed, and deposited in the atmosphere and establish the cause-and-effect relationship between the model's inputs (initial conditions) and its outputs (predictions). Deterministic models fall into two categories: sequential (also called coupled offline) models and integrated (online) models. Unlike sequential methods that treat meteorology and chemistry separately, online models like WRF-Chem simulate both processes simultaneously. This allows for a more comprehensive understanding, as online models can account for how meteorology patterns influence the formation, transport, and removal of pollutants. In WRF-Chem, both chemical and meteorological calculations share the same time step and utilize identical horizontal and vertical grids, facilitating this two-way interaction (Grell et al., 2005).

In recent years, WRF-Chem has become a popular tool for researchers worldwide. Studies have used it to simulate both weather and air quality by employing various options for chemical reactions, aerosols, and light-driven processes. Studies around the world have been using different configurations within the model, including various options for chemistry, aerosols, and how sunlight interacts with chemicals (photolysis). However, there are only a few studies focused on evaluating WRF-Chem specifically in Morocco, as well as the wider African context, where air quality modeling becomes increasingly challenging (Ajdour et al., 2020). Table 1 and

Table **2** provide a summary of recent WRF-Chem studies from various locations worldwide. These studies highlight limitations in simulating certain air quality parameters, particularly PM10 and PM2.5. This shortcoming likely stems from uncertainties in input data and the lack of local emission inventories(Schindlbacher et al., 2021). To address discrepancies between modeled and observed pollutant concentrations, studies highlight the need to investigate the influence of input data sources and model configurations as a means to enhance model performance. In this vein, a great deal of research has focused on evaluating how WRF-Chem performance changes with different chemical mechanisms, nesting ratios, and physical parameterizations. These studies play a crucial role in understanding how these adjustments affect the model's accuracy. Analyzing these sensitivities helps to determine the optimal configuration for WRF-Chem in various situations. For instance, Khan et al. (Khan & Kumar, 2019) focused on how the initial and boundary conditions for chemical species affect predictions using the MOZART-4 mechanism. Shimada et al (Shimada et al., 2011) compared various PBL schemes within the WRF-ARW model to see which best replicates wind speeds over Japan. Yu et al. (Yu et al., 2022) evaluated different parameterization options for the planetary boundary layer (PBL), microphysics (MP), and shortwave/longwave radiation (SW-LW) to find the WRF model setup most accurate for wind fields under stable weather conditions in North China. Finally, Cifuentes et al. (Cifuentes et al., 2021) analyzed how factors like lateral chemical boundary conditions (LCBC), domain configurations, nesting options, and chemical mechanisms impact the model's ability to predict CO, O_3, PM_{10} and $PM_{2.5}$.

While previous studies have helped understand air quality modeling, there's a gap in knowledge regarding the best chemical mechanism scheme across different regions. These schemes can vary significantly in their effectiveness depending on location. This study aims to address this gap by identifying a mechanism that accurately reflects air quality conditions specific to Morocco and North Africa, a region lacking such studies. For these reasons, this study uses the WRF-Chem model for the first time to simulate meteorological fields and air quality specifically over Agadir, Morocco. We aim to identify the best model configuration by testing different chemical mechanisms, nesting ratios, and physics parameterizations. This optimal setup will then be used for future air quality simulations in Agadir and potentially adapted for other Moroccan cities. This research not only advances air quality modeling in Agadir by employing a more comprehensive model (WRF-Chem) compared to previous studies (e.g., (Ajdour et al., 2020; Ajdour, 2022), using WRF-CHIMERE), but also establishes a foundation for future research in this field.

The methodology employed to assess the WRF-Chem system's performance and the sensitivity analyses conducted in this study involve several stages, which are elaborated upon in the following sections. First, we describe the study area (Morocco, centered on Agadir City) and the model configuration used (domain size, nesting options, etc.). We also explain the data used and the physics options chosen for the simulations. Next, we present the results of sensitivity tests focusing on how different chemical mechanisms and nesting scenario impact pollutant concentrations. This will help us understand how these settings influence the model's overall accuracy. Finally, we summarize the key findings of this investigation and highlight the most impactful settings on model performance.

Table 1 Summary of WRF-Chem Studies Reviewed, Highlighting Geographic Focus and Key Findings.

Study	Model/study area	Study overview
(Kant et al., 2021)	WRF-Chem/India	• In this study, the WRF-Chem numerical model was used to analyze the effects of aerosols on cloud microphysical properties during winter in India, February 2016. The model's performance was assessed for rainfall, aerosol optical depth (AOD), temperature, and wind, showing consistent RMSE, MSE, and MB values in simulations DEF (which deactivated wet filtering and cloud chemistry but activated both aerosol effects) and INDEF (considering indirect aerosol impacts). However, the LCINDEF simulation, which included all INDEF factors with a 50% reduction in anthropogenic emissions, exhibited significant errors.
(Singh et al., 2021)	WRF-chem/India	• This study analyzes an extreme dust episode in India using WRF-Chem, focusing on atmospheric dust dynamics and its impacts on ecosystems and human health. Model evaluation, through categorical validation, indicates a strong correspondence between reanalysis and observational datasets and WRF-Chem's dust load

		simulations, showing a 0% false alarm rate, a detection likelihood between 78% and 92%, and an accuracy range of 79% to 90%.
(Sicard et al., 2021)	WRF-Chem/ Asian region	• The study evaluates the WRF-Chem model's effectiveness in simulating atmospheric physics and chemistry over Asia. It found that the model accurately approximates spatial distributions of O3, especially in summer, but significantly underestimates NO2 concentrations.
(P. Wang et al., 2020)	WRF-Chem/ Sichuan Basin (China)	• In this study, the WRF-Chem model was utilized to simulate PM2.5 and O3 in the Sichuan Basin of China during January and July 2015. The results indicated that PM2.5 levels were accurately modeled for all cities in both months, with mean fractional bias of 0.6 and mean normalized bias of 0.7. Ozone simulation showed good agreement with observational data in July, but concentrations were generally overestimated in January, primarily due to uncertainties in emissions and photochemical processes affecting winter O3 levels.

Table 2 continued

Study	Model/study area	Study overview
(Saidou Chaibou et al., 2019)	WRF-Chem/ North Africa	• This study analyzes dust extinction and vertical profiles in North Africa using data from CALIPSO and AERONET, combined with WRF-chem simulations from the summer of 2006. Its aim is to enhance understanding of atmospheric dust behavior and its regional impacts. The results indicate that all modeling schemes effectively captured the spatial coherence of total dust emissions. However, differences in threshold friction velocity and soil moisture adjustments led AFWA and UoC schemes to diverge from GOCART regarding extent, magnitude, and patterns, while still showing comparable regional distribution. GOCART displayed good consistency with AFWA and UoC schemes, evidenced by correlation coefficients of 0.5 and 0.8, respectively, despite emitting larger dust flows at times.

2 Data and Methods

2.1 Description of case study

Agadir, is a prominent city located along the southwestern coast of Morocco (see Fig. 1), recently, it is becoming an area of increasing scientific interest due to its unique geographic and climatic conditions that impact local air quality(Ajdour et al., 2020; Chirmata et al., 2017). As the capital of the Agadir-Ida Outanane Province and a bustling hub for tourism and agriculture (Bouchriti et al., 2023), Agadir experiences a range of air quality issues that reflect both its economic activities and natural settings. The city's positioning by the Atlantic Ocean and at the foothills of the Atlas Mountains offers distinctive meteorological patterns that can influence pollutant dispersion and accumulation (UNECA and UNECE, 2014). After Agadir's reconstruction from the 1960 earthquake, the city boomed with urbanization and industry. While these advancements have boosted the local economy, they have also led to increased emissions of air pollutants, compounded by pesticide application and fertilizer dust. Additionally, the city's major seaport adds to the issue by introducing marine and shipping emissions, further worsening the urban air pollution situation. While other Moroccan cities have received more attention regarding air quality, Agadir remains understudied. This lack of existing information concerning air quality dynamics in Agadir motivated this study, which investigates the sensitivity of the WRF-Chem model for this specific region.

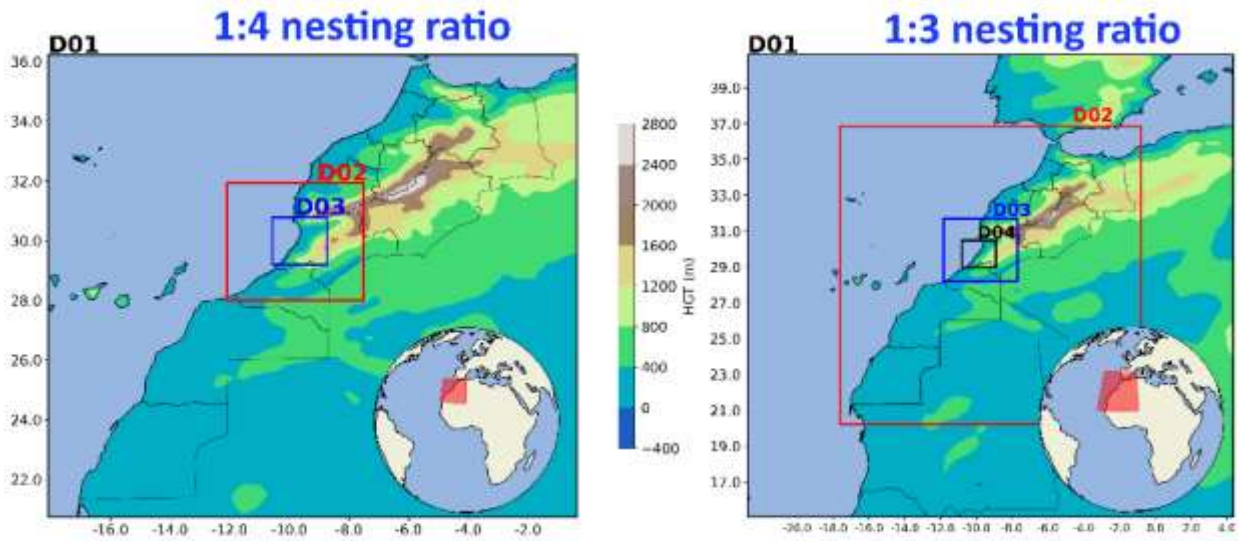

Fig. 1. Study area and domain configuration for nesting ratios of 1:4 (left panel) and 1:3(right panel).

2.2 WRF-chem model and setup

WRF-Chem (Weather Research and Forecasting model with Chemistry) is an advanced numerical tool designed to integrate atmospheric chemistry with meteorology. The model has been developed collaboratively by NOAA, DOE/PNNL, NCAR, and other research institutes (https://www2.acd.ucar.edu/wrf-chem). It simulates the interaction between chemical and meteorological processes to predict air quality outcomes under varying atmospheric conditions. The model captures both anthropogenic emissions and biogenic sources, allowing for detailed investigations into the formation, dispersion, and deposition of pollutants (Grell et al., 2005).

In this study, WRF-Chem was utilized to simulate local air quality and atmospheric chemistry. The setup for lateral chemical boundary conditions (LCBC) was based on output provided every 6 hours, from the Community Atmosphere Model with Chemistry (CAM-Chem), which supplied comprehensive global atmospheric composition information essential for initializing and constraining the regional chemical environment. Meteorological boundary conditions were derived from the National Centers for Environmental Prediction (NCEP) Global Forecast System (GFS) data, with a spatial resolution of 0.5°×0.5° and forecast lead time of 3 hours.

We configured our simulation domain using the Mercator projection to include multiple nested domains, which allowed for increasingly refined spatial resolutions. As illustrated in Fig. 1, two configurations were employed: the first configuration comprised three nested domains with a 1:4 nesting ratio, where D01 (the coarsest domain) had a resolution of 16 km, D02 had a resolution of 4 km, and D03 had a resolution of 1 km. The second configuration consisted of four nested domains using a 1:3 nesting ratio, with a resolution of 27 km for D01, 9 km for D02, 3 km for D03, and 1 km for D04.

For 1:3 nesting ratio, the largest domain (D01) encompassed the southern region of Spain, northern Mauritania, eastern Algeria, and extended eastwards into the Atlantic Ocean. The second domain (D02) specifically covered the entirety of Moroccan territory. The inner domains (D03 and D04) were specifically designated to focus on the study area around Agadir city. A one-way nesting technique was employed for this domain configuration. In this approach, the outermost domain (D01) provided meteorological data and boundary conditions that influenced the simulations within the smaller nested domains. There was no feedback from the smaller domains influencing the larger one. Table 3 summarizes the different model configurations used in this study.

Table 3 Setup and Sensitivity Testing of the WRF-Chem Model (version 4.4.2) used in this study.

Model configurations	**Options used and sensitivity analysis**
Domain	Agadir, Morocco
Domain resolution	3 nested domains (16km,4km,1km)
	4 nested domains (27km,9km,3km,1km)
Vertical levels	31 vertical layers
Simulation time	7 days (02–08 May)
Spin-up time	24 h
IC/BC (chemistry)	MOZART global model
IC/BC (meteorology)	NCEP (resolution: 0.5°×0.5°, 3h interval)
Biogenic emission inventory	MEGAN
Anthropogenic emission inventory	EDGAR
microphysics	Morrison double moment
Longwave radiation	RRTMG (Rapid Radiative Transfer Model)
Shortwave radiation	RRTMG (Rapid Radiative Transfer Model)
Surface layer	MM5 similarity based on Monin–Obukhov scheme
Land-surface physics	Noah-MP (multi-physics) land surface model
Planetary boundary layer	Yonsei University scheme
	Mellor-Yamada-Janjic
	Quasi-Normal Scale Elimination
	Mellor-Yamada-Nakanishi-Niino Level 2.5
Chemistry options	Regional Atmospheric Chemistry Mechanism (RACM)/ chem_opt=201
	Model for Ozone and related chemical Tracers (MOZART) / chem_opt=43
	Global Oceans Chemistry Aerosol Radiation and Transport (Gocart) / chem_opt=301

Regarding emissions data, our study utilized a combination of datasets to precisely represent various emission sources. And Due to the absence of a local emission inventory for Agadir, we employed the Emission Database for Global Atmospheric Research (EDGAR), which offers a global inventory of anthropogenic emissions at a 1° × 1° horizontal resolution for the year 2010. The EDGAR emissions were spatially interpolated to the nested WRF-Chem domains using the prep_chem_sources utility, which conserves total mass while redistributing emissions according to the model grid resolution (16 km, 4 km, and 1 km over Agadir). The fine-resolution inner domain allows emissions to be redistributed according to local land-use patterns, road density, and urban extent implicitly represented in the WRF geographical datasets. This robust framework enabled a detailed representation of anthropogenic emissions across our simulation domains. Fig. 2 and Fig. 3 illustrate the spatial distribution of these anthropogenic emissions from EDGAR across domains D01 and D02 in case of nesting ratio 1:4, respectively. Biogenic emissions were computed online using The Model of Emissions of Gases and Aerosols from Nature (MEGAN) based on environmental conditions and vegetation types. High-resolution emissions from biomass burning were incorporated from the Fire Inventory from NCAR (FINNv1.5). Model for Ozone and Related Chemical Tracers (MOZART-4) was used to provide initial and lateral boundary conditions (IC/BC) for chemical species in WRF-Chem.

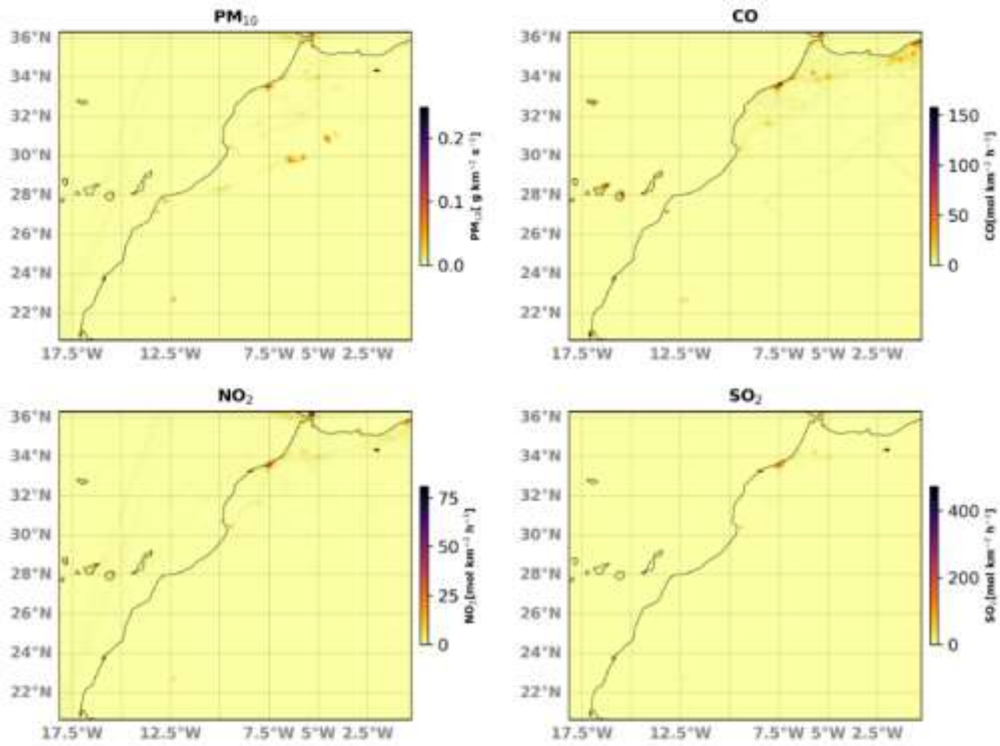

Fig. 2. Spatial pattern of Anthropogenic emission from EDGAR over D01.

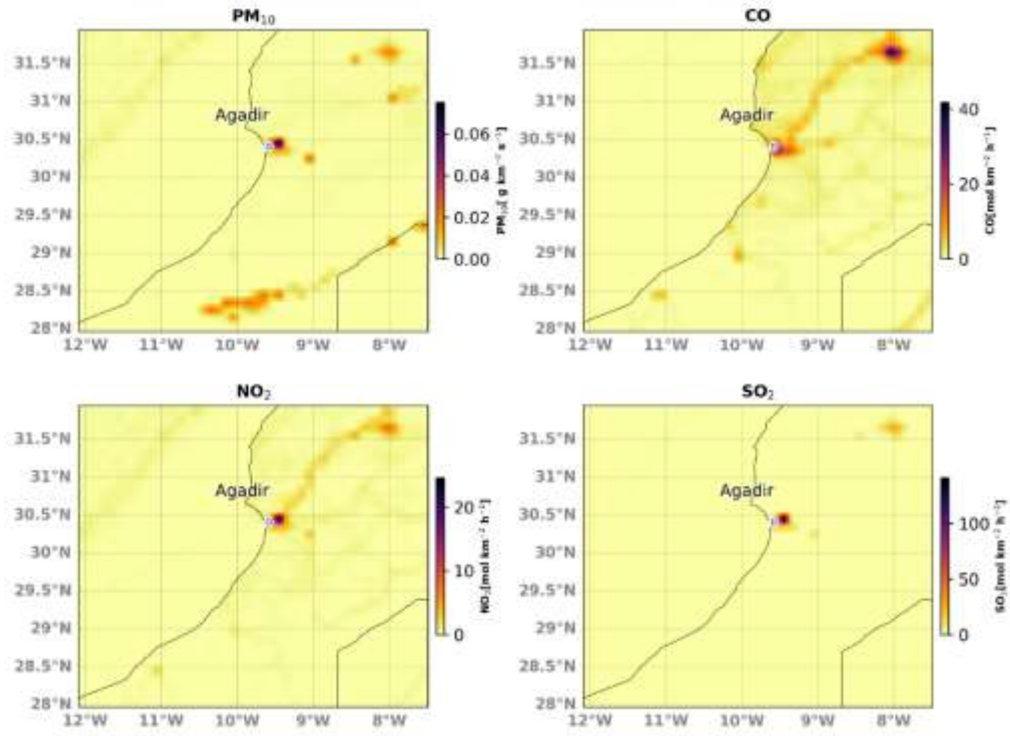

Fig. 3. Spatial pattern of Anthropogenic emission from EDGAR over D02.

2.3 Sensitivity runs

To identify the optimal configuration for WRF-Chem version 4.4.2 in predicting air quality (Carbon Monoxide (CO), Nitrogen Dioxide (NO_2), Ozone (O_3), Fine Suspended Particles (PM_{10}), and Sulphur Dioxide (SO_2)) and meteorological variables (wind speed (WS), temperature (T)) over the study area, an investigation into the model's sensitivity to domain configuration, chemical mechanisms, and physics parameterizations was undertaken. This involved systematic exploration through a series of controlled simulations. Each factor was varied to isolate its influence on the accuracy of model outputs. The selection procedures for these tests are detailed in Fig. 4. Domain configuration sensitivity was investigated using various nesting strategies, ranging from broader regional scales to more focused local scales. Specifically, simulations were conducted with both three nested domains (1:4 nesting ratio; (3D)) and four nested domains (1:3 nesting ratio; (4D)), as previously described.

Three chemical mechanisms were evaluated for their suitability in WRF-Chem simulations: The first mechanism, the Regional Atmospheric Chemistry Mechanism (RACM), includes over 240 chemical species and 840 reactions, offering a comprehensive representation of atmospheric chemistry (Ha, 2022).it was chosen as a revised version of the RADM2(Regional Acid Deposition version 2) mechanism to provide more detailed organic chemistry for regional atmospheric pollution modeling. The Model for Ozone and Related chemical Tracers (MOZART) was also assessed. This mechanism features around 150 species and over 300 reactions, providing a more focused approach (Emmons et al., 2010) and is consistent with the chemistry used in the global model that provides the chemical boundary conditions for our simulations. Finally, the Global Oceans Chemistry Aerosol Radiation and Transport (GOCART) mechanism was included in the evaluation. GOCART specializes in modeling complex aerosol interactions, complementing the capabilities of RACM and MOZART (Mian Chin & Lin, 2000) . The GOCART module simulates major tropospheric aerosol components, including sulfate, dust, black and organic carbon, and sea salt, and includes algorithms for dust and sea salt emissions, dry deposition, and gravitational settling. These mechanisms offer a detailed description of atmospheric chemistry across various atmospheric layers and scales, ranging from regional to global.

In terms of physics schemes, four planetary boundary layer (PBL) parameterization schemes were employed to assess their impact on model simulations. The Yonsei University Scheme (YSU) was implemented due to its non-local closure approach, known to be effective for vertical transport in convective conditions (Hu et al., 2013). The Mellor-Yamada-Janjic (MYJ) scheme was chosen for its detailed representation of turbulence kinetic energy under both stable and unstable atmospheric conditions (Hu et al., 2010). The Quasi-Normal Scale Elimination (QNSE) scheme was included for its ability to simulate stable boundary layers by incorporating scale-dependent dynamical processes (Sukoriansky et al., 2006). Lastly, the Mellor-Yamada-Nakanishi-Niino Level 2.5 (MYNN2) scheme was utilized for its comprehensive treatment of boundary layer turbulence and cloud-top cooling effects (Kitamura, 2010). This comprehensive sensitivity analysis, encompassing various physics schemes and chemical mechanisms (as illustrated in Fig. 4), aimed to refine the WRF-Chem model for improved predictive performance and reliability in air quality management and research within the target region. More details on the physical parameterizations used can be found at http://www2.mmm.ucar.edu/wrf/users/phys_references.html.

2.4 Datasets for model evaluation

Over the year 2010, daily average concentrations of air quality pollutants and meteorological parameters were collected from a fixed monitoring station situated at a school within Agadir's city center (urban area). This data acquisition was facilitated by the Department of Environment, Wilaya of Agadir, Morocco. The pollutants monitored included CO, NO_2, O_3, PM_{10}, and SO_2. Meteorological data encompassed T, and WS. While limited data availability restricted the analysis to this timeframe (using older data due to the lack of more recent information), this study still provides valuable insights into air quality trends and their impacts within Agadir. The established methodologies can be applied to future datasets upon their availability, ensuring the ongoing relevance and applicability of this research.

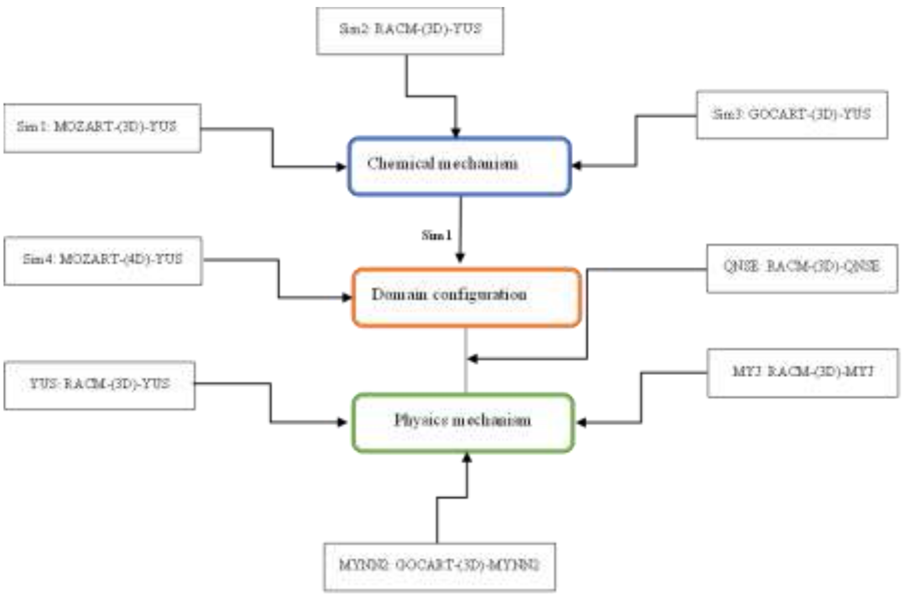

Fig. 4. Flowchart of the research workflow, outlining the specific steps followed in this study to analyze the sensitivity of the WRF-Chem model.

Acronyms: RACM: Regional Atmospheric Chemistry Mechanism; **MOZART**: Model for OZone And Related chemical Tracers; **GOCART**: Global Oceans Chemistry Aerosol Radiation and Transport; **3D**: Three nested domains with a 1:4 nesting ratio; **4D**: Four nested domains with 1:3 nesting ratio; **YUS**: Yonsei University Scheme; **MYJ**: Mellor-Yamada-Janjic; **QNSE**: Quasi-Normal Scale Elimination; **MYNN2**: Mellor-Yamada-Nakanishi-Niino Level 2.5.

2.5 Model evaluation

The performance of the model was evaluated by comparing the simulated values of air quality parameters (PM_{10}, O_3, NO_2, CO, SO_2) and meteorological parameters (T, WS) with in-situ measurements. Various performance metrics were employed, including Pearson's correlation coefficient (r), mean bias (MB), normalized mean bias (NMB), root mean squared error (RMSE), mean absolute gross error (MAGE), and agreement index (IOA). These metrics were calculated as follows:

$$r = \frac{\sum_i^n [(O_i - \bar{O})(P_i - \bar{P})]}{\sqrt{\sum_i^n (O_i - \bar{O})^2 * \sum_i^n (P_i - \bar{P})^2}} \tag{1}$$

- Where r ranges between -1 and 1, with $r = 0$ indicating no correlation, and the correlation increases as the coefficient approaches -1 or 1.

$$MB = MAGE = \frac{1}{n}\sum_{i=1}^{n}(P_i - O_i) \tag{2}$$

- Positive value of MB indicates an overestimation of the simulated data while the negative value implies underestimation. A MB value of zero suggests that model predictions are perfectly unbiased relative to observations.

$$NMB = \frac{\sum_{i=1}^{n}(P_i - O_i)}{\sum_{i=1}^{n} O_i} \tag{3}$$

- A positive NMB indicates that predicted variables are higher than observed ones, while a negative NMB indicates under-prediction. A value of zero implies no bias indicating ideal model performance.

$$MAGE = \frac{1}{n}\sum_{i=1}^{n}|P_i - O_i| \tag{4}$$

- Low value of $MAGE$ indicates greater similarity between observed and simulated values.

$$RMSE = \sqrt{\frac{\sum_{i=1}^{n}(P_i - O_i)^2}{n}} \tag{5}$$

- a lower value of $RMSE$ indicates a good agreement between simulated and observed data.

$$IOA = 1 - \frac{\sum_{i=1}^{n}(P_i - O_i)^2}{\sum_{i}^{n}(|P_i - \bar{O}| + |O_i - \bar{O}|)^2} \tag{6}$$

- The *IOA* provides a value between 0 and 1, where 1 indicates perfect agreement between model predictions and observed data. A higher *IOA* value indicates a better predictive performance, taking into account both the magnitude and the direction of deviations between the model and observations.

Where:

P_i and O_i represent the predicted and the observed variables respectively,

$\bar{P}$ and $\bar{O}$ are the mean values of the predicted and the observed values respectively,

n is the total number of observation data used.

3 RESULTS AND DISCUSSION

This section presents the results of simulations for air quality (PM_{10}, O_3, CO, and NO_2) and meteorological variables (WS and T). Sensitivity tests were performed using varying chemical mechanisms, nesting ratios, and physical parameterizations to identify the most effective configurations for WRF-Chem in the study area. These configurations can be recommended for future research. Python was used to analyze the model outputs and calculate performance metrics. The results of this study are compared with a previous WRF-CHIMERE simulation realized in the same area and for the same period of time (Ajdour et al., 2020; Ajdour, 2022) using both qualitative (spatial variations) and quantitative (statistical metrics) approaches.

Prior to a detailed examination of model sensitivity, an evaluation of the spatial distributions of pollutants is undertaken. Fig. 5 and Fig. 6 depict the average pollutant concentrations simulated across two domains (D01 and D02) for a 1:4 nesting ratio. These figures serve as foundational elements, providing a baseline for the sensitivity analysis by establishing the initial pollutant dispersion patterns within the two domains. Visualizations of this nature are essential for understanding the initial conditions and environmental setting, which influence the model's subsequent sensitivity evaluation to various parameters.

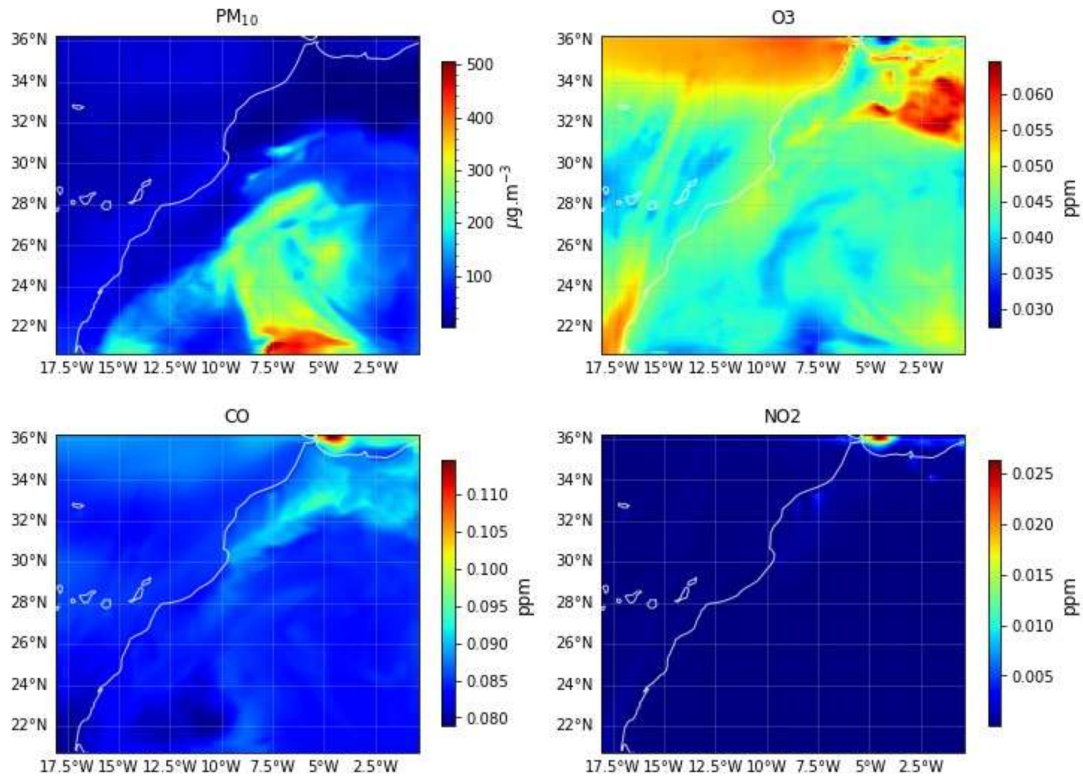

Fig. 5. Average concentration maps for various pollutants across the study domain on May 2, 2010 (D01)

The study area has been ascribed having a high PM_{10} concentration due to various sources of pollution, such as industrial activities, waste incineration, and traffic-related emissions. In 2010, the main sources of pollution were the cement plant, which was still operational at the time and the traffic(Leghrib et al., 2018). In addition to the sources already mentioned, this region is affected by the phenomenon of the rise of sand of Saharan origin. Let us recall that the region is located in the south of Morocco, which makes it influenced by a dynamic southern flow that brings dust storms, these storms in turn brought with them high levels of concentrations of PM_{10}. The figures distinctly show that pollutant concentrations are denser near the Sahara, underscoring the impact of geographical and environmental factors on air quality.

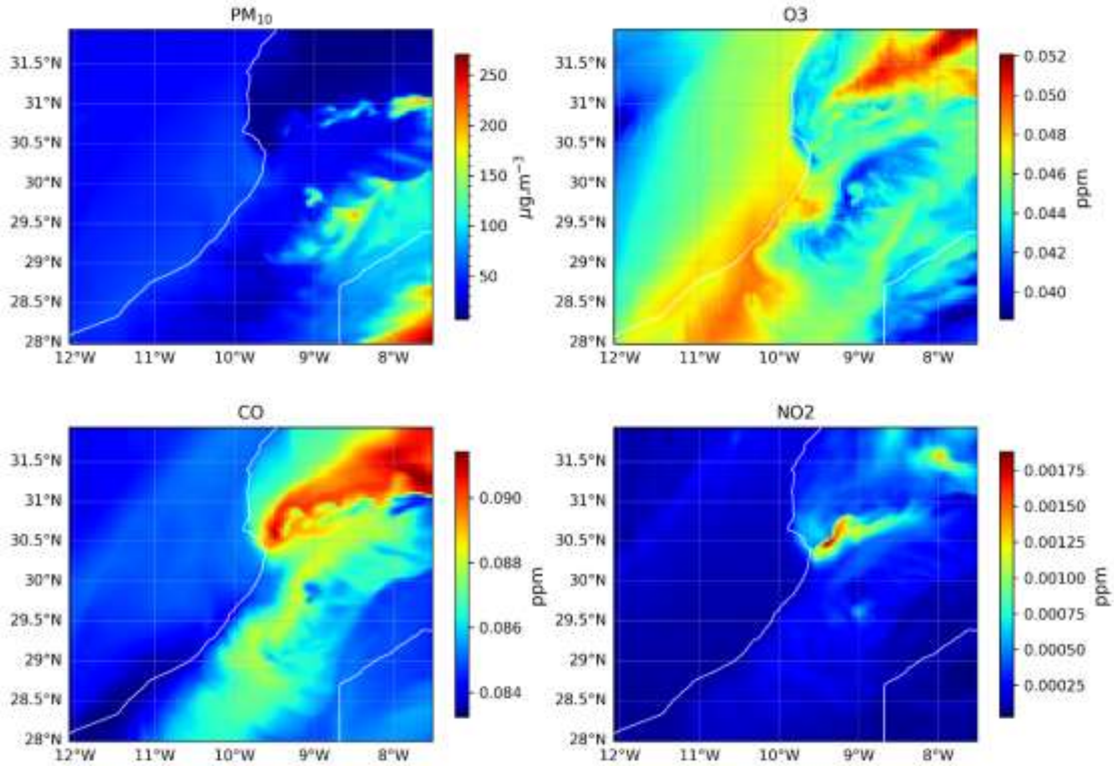

Fig. 6. Average concentration maps for various pollutants across the study domain on May 2, 2010 (D02)

3.1 Model evaluation

3.1.1 Model evaluation of meteorological variables

Table ***4*** provides insight into the performance metrics of the model compared with WRF-CHIMERE for the same study case, with a particular focus on meteorological variables such as wind speed and temperature. Analysis of Table 4 reveals strong Pearson correlation coefficients (ranging from 0.84 to 0.90) for all forecasted temperatures. This indicates a good correlation between observed and simulated temperature values. All models exhibited satisfactory results, with RMSE values ranging from 2.5 to 3.0 °C. Furthermore, the temperature Mean Bias (MB) ranged from 2.12 to 2.77 °C, suggesting a tendency for the model to overestimate temperature in most cases. Similarly, wind speed MB values (ranging from 0.92 to 1.32 m/s) indicate consistent overestimation. However, correlation coefficients for wind speed remained satisfactory (between 0.68 and 0.78), and RMSE values (ranging from 0.95 to 1.53 m/s) were considered acceptable compared to the previous study using WRF-CHIMERE (Ajdour et al., 2020; Ajdour, 2022). It was noted that both WRF-Chem and WRF-CHIMERE historically struggled with wind speed and direction (Yu et al., 2022). To address this, this study aimed to improve the physical parameterization, minimizing the bias between observed and simulated wind speed due to its critical role in pollutant dispersion.

The simulation results indicate that the predictions of wind speed and temperature are satisfactory. This study represents an enhancement in modeling specifically for wind speed compared to a previous study using WRF-CHIMERE for the same case study. This improvement is clearly demonstrated in Fig. 7 which presents the time series plot of WS and T over the simulation period. These advancements are crucial for more accurately forecasting pollutant distribution, which is significantly influenced by meteorological conditions (Q. Wang & Li, 2022).

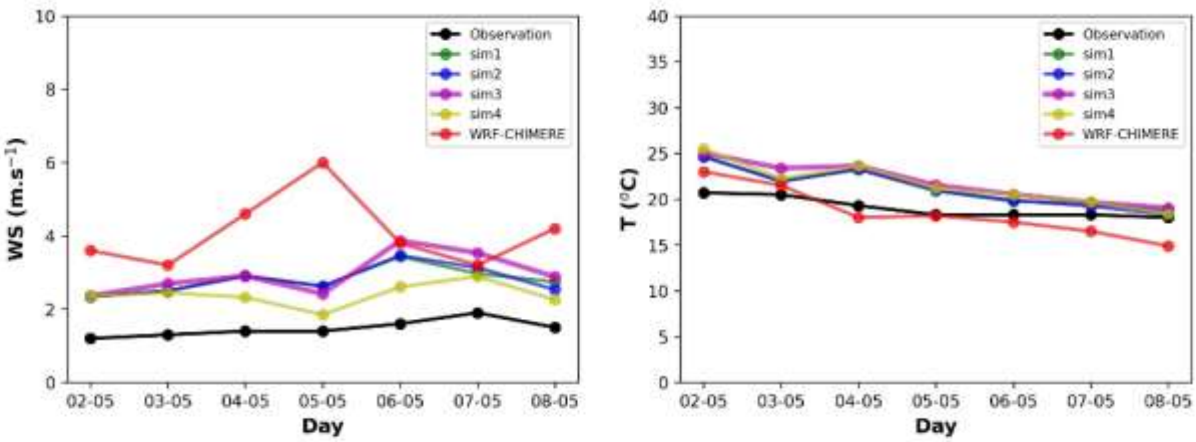

Fig. 7. Time series of daily ground-level wind speed (WS) and temperature (T) during the simulation period from May 02 to May 08.

Table 4 Summary of performance statistics for the sensitivity analyses

Options	Variable	MB	MAGE	RMSE	NMB	NME	IOA	r
MOZART-(3D)-YUS	T(°C)	2.2	2.2	2.53	11.55	11.55	0.57	0.86
	WS	1.32	1.32	1.34	89.49	89.49	0.23	0.68
	O_3	-1.12	2.14	3.26	-2.04	3.9	0.93	0.92
	CO	2.02	6.65	8.06	10.09	33.25	0.26	-0.13
	NO_2	-15.79	15.79	15.83	-76.75	76.75	0.11	0.38
	PM_{10}	-47.39	47.39	50.23	-72.75	72.75	0.29	-0.13
	SO_2	0.39	1.64	1.98	3.97	16.92	0.37	0.05
RACM-(3D)-YUS	T(°C)	2.12	2.12	2.5	11.11	11.11	0.58	0.84
	WS	1.32	1.32	1.34	89.4	89.4	0.24	0.73
	O_3	8.63	8.63	9.59	15.69	15.69	0.69	0.83
	CO	5.99	7.89	9.46	29.97	39.44	0.46	0.31
	NO_2	-15.37	15.37	15.41	-74.72	74.72	0.11	0.21
	PM_{10}	-39.81	39.81	42.95	-61.12	61.12	0.32	-0.21
	SO_2	1.08	1.29	1.63	11.11	13.24	0.45	-0.01
GOCART-(3D)-YUS	T(°C)	2.53	2.53	2.93	13.28	13.28	0.53	0.84
	WS	0.92	0.92	0.95	62.54	62.54	0.33	0.63
	O_3	-7.95	7.95	8.95	-14.46	14.46	0.64	0.86
	CO	0.42	6.29	7.57	2.08	31.46	0.23	0.1
	NO_2	-15.2	15.2	15.21	-73.9	73.9	0.11	0.91
	PM_{10}	-28.38	28.38	33.85	-43.57	43.57	0.41	0.03
	SO_2	1.53	1.86	2.03	15.72	19.11	0.55	0.52
MOZART-(4D)-YUS	T(°C)	2.77	2.77	3.03	14.56	14.56	0.52	0.9
	WS	1.48	1.48	1.53	100.65	100.65	0.23	0.79
	O_3	-5.7	6.24	7.43	-10.37	11.34	0.75	0.76
	CO	1.97	7.52	8.84	9.87	37.62	0.18	-0.36
	NO_2	-15.9	15.9	15.98	-77.31	77.31	0.1	-0.02
	PM_{10}	-50.03	50.03	52.11	-76.81	76.81	0.28	0.02
	SO_2	-0.96	1.6	1.9	-9.91	16.47	0.49	0.23

WRF-CHIMERE	T(°C)	-0.54	1.49	1.75	-2.85	7.8	0.77	0.94
	WS	2.61	2.61	2.79	177.67	177.67	0.08	-0.22
	O_3	21.29	21.29	21.7	38.7	38.7	0.42	0.81
	CO	102.29	102.29	102.53	511.43	511.43	0.1	0.38
	NO_2	-18.5	18.5	18.53	-89.93	89.93	0.09	-0.22
	PM_{10}	-55.79	55.79	57.33	-85.64	85.64	0.26	-0.09
	SO_2	-7.17	7.17	7.34	-73.82	73.82	0.17	-0.31

3.1.2 Model evaluation of air quality variables

Table ***4*** summarizes the statistical metrics from various simulations of air quality variables, offering detailed insights into model performance across pollutants. Notably, O_3 simulations demonstrated strong Pearson correlation coefficients, ranging from 0.76 to 0.92, indicating good agreement between observed and modeled values. In the case of NO_2, the correlation coefficients varied, with generally medium values (0.21 to 0.36), except for the Sim3 (GOCART-(3D)-YUS) which exhibited a strong correlation of 0.91. However, the model had a low value of r in the case of PM_{10} and SO_2 that suggest a less accuracy in these simulations. In terms of MB, O_3 concentrations were typically underestimated by the models, with one exception (Sim2: RACM-(3D)-YUS) where overestimation occurred. Conversely, both PM_{10} and NO_2 were consistently underestimated across all simulations. CO and SO_2 exhibited contrasting behavior with overestimations in their concentrations. This diverges from WRF-CHIMERE results, which tended to overestimate O_3 and underestimate SO_2. Low RMSE values were obtained for O_3, CO, and SO_2, indicating good model performance for these variables. The best RMSE values were recorded at 3.26 µg/m³ for O_3, 8.06 µg/m³ for CO, and 1.63 µg/m³ for SO_2. In contrast, PM_{10} and NO_2 simulations showed higher RMSE values (42.95 µg/m³ for PM_{10} and 15.98 µg/m³ for NO_2). A comparison with WRF-CHIMERE performance metrics emphasizes the improvements achieved in this study:

- O_3 exhibited substantial improvement with RMSE of 3.26 µg/m^3 compared to 21.7 µg/m^3 for WRF-CHIMERE. Similarly, MB improved from 21.29 µg/m^3 to -1.12 µg/m^3, and the correlation coefficient increased from 0.81 to 0.92. A significant reduction in Normalized Mean Error (NME) was also observed, from 38.7 to 3.9.
- CO accuracy also improved. The RMSE was reduced to 7.0 µg/m^3 from 102.53 µg/m^3, and the MB improved from 102.29 µg/m^3 to 0.42 µg/m^3.the correlation coefficient is the same for both studies (0.36 in this study versus 0.36 in WRF-CHIMERE).
- Improvements were observed for NO_2 as well. The RMSE decreased from 18.53 µg/m3 to 15.21 µg/m^3, and the MB improved from -18.5 µg/m^3 to -15.2 µg/m3. The correlation coefficient showed a marked increase (0.91 versus -0.22). Additionally, the NME was reduced from 89.93 to 73.9.
- PM_{10} also showed improvement, with a reduced RMSE of 33.86 µg/m^3 compared to 57.33 µg/m^3 for WRF-CHIMERE. The MB improved from -55.79 µg/m3 to -28.38 µg/ m^3, although the correlation coefficient remained weak (-0.21 versus 0.09). The NME also decreased from 85.64 to 43.57.
- Finally, SO_2 experienced a significant drop in RMSE (from 7.34 µg/m^3 to 1.63 µg/m^3) and MB (from -7.17 µg/m^3 to 0.39 µg/m^3). The correlation coefficient improved from -0.31 to 0.52. The NME showed a marked improvement, reaching 13.24 µg/m^3 compared to 73.82 µg/m^3 for WRF-CHIMERE.

These results highlight advancements in air quality predictions across the region, particularly for O_3, CO, and SO_2, exceeding the benchmarks established by WRF-CHIMERE.

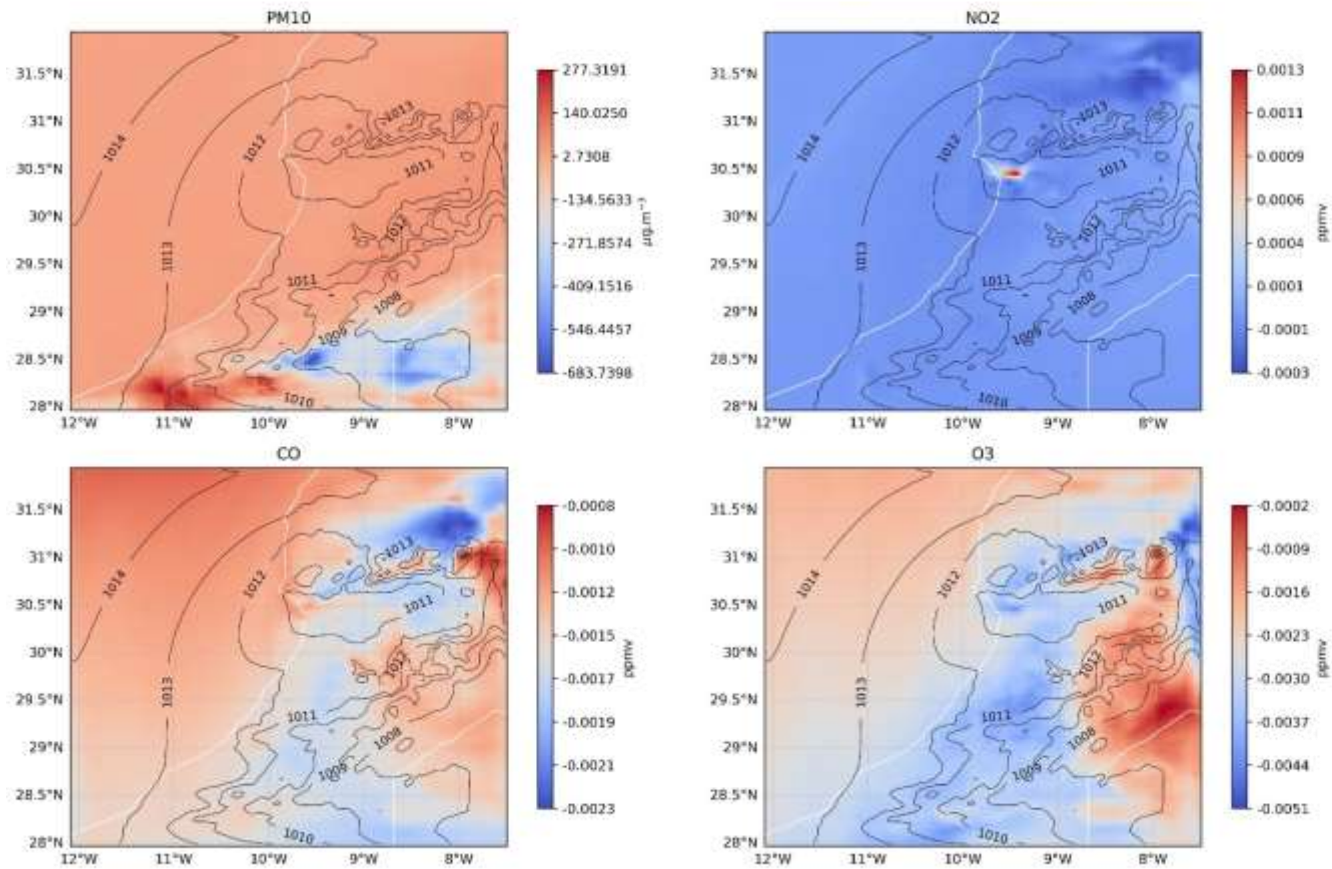

Fig. 8. Mean difference of PM_{10}, NO_2, CO and O_3 concentrations between MOZART and GOCART.

3.2 Chemical mechanisms comparison

Fig. 8 illustrates the mean differences in PM_{10}, O_3, CO, and NO_2 concentrations between the MOZART and GOCART chemical mechanisms. This figure provides a comprehensive perspective on how each mechanism influences the simulation of various air pollutants. Positive differences indicate areas where MOZART predicts higher concentrations compared to GOCART. Conversely, negative differences highlight regions where GOCART predicts higher concentrations. PM_{10} concentrations are found to be sensitive to changes in chemical mechanisms. Throughout most of the domain, MOZART predicts higher PM_{10} concentrations compared to GOCART. This can be attributed to MOZART's more detailed treatment of non-methane volatile organic compound (NMVOC) emissions (Emmons et al., 2010) and their conversion into secondary organic aerosols (SOA)(Clappier et al., 2021), which are key components of PM_{10}. An exception is observed in the southeastern Saharan region, where the opposite trend is seen. In the case of O_3, a predominance of negative differences is observed, indicating that GOCART generally produces higher ozone concentrations than MOZART. This is likely due to GOCART's specific treatment of aerosol interactions, which may scavenge ozone precursors differently(Kong et al., 2015). Similarly, all areas exhibit negative differences for CO compared to GOCART, suggesting lower concentrations predicted by MOZART. Finally, the differences in NO2 concentrations mirror those seen in O_3 due to their close chemical interdependencies in urban photochemistry. Consequently, negative NO_2 differences are observed across most of the study area. An exception is found around the Agadir city, where MOZART predicts higher NO_2 concentrations due to its comprehensive treatment of NO_2 emissions and lifetimes(Y. Wang et al., 2021). To facilitate comparisons between different chemical mechanisms, results from this study can be compared with the previous study in Fig. 9. This figure displays a time series plot of air quality variable concentrations simulated by various chemical models (Sim1, Sim2, and Sim3). Additionally, Fig. 10, Fig. 11, and Fig. 12, which illustrate plots of principal statistical metrics alongside specific statistical criteria, can be used to select the most suitable chemical mechanism. An analysis of Fig. 10 reveals that for sim1 (MOZART), the Pearson coefficient achieves the desired goal (>= 0.75%) for O_3 and temperature, and exceeds the threshold (>= 0.50%) for wind speed (WS). However, it falls below the established criteria for the other variables. Similarly, the Index of Agreement (IOA) for ozone and temperature is close to 1, and the Normalized Mean Error (NME) is less than or equal to 25%, indicating good accuracy for this model in predicting ozone concentrations within the study area. For sim2 (RACM), an improvement in the correlation coefficient (r) is observed for all variables except SO_2 and O_3, where r has decreased (refer to Fig. 11). In the case of sim3 (GOCART), a significant improvement in r is observed for NO_2 and SO_2, with similar improvements in IOA (refer to Fig. 12).

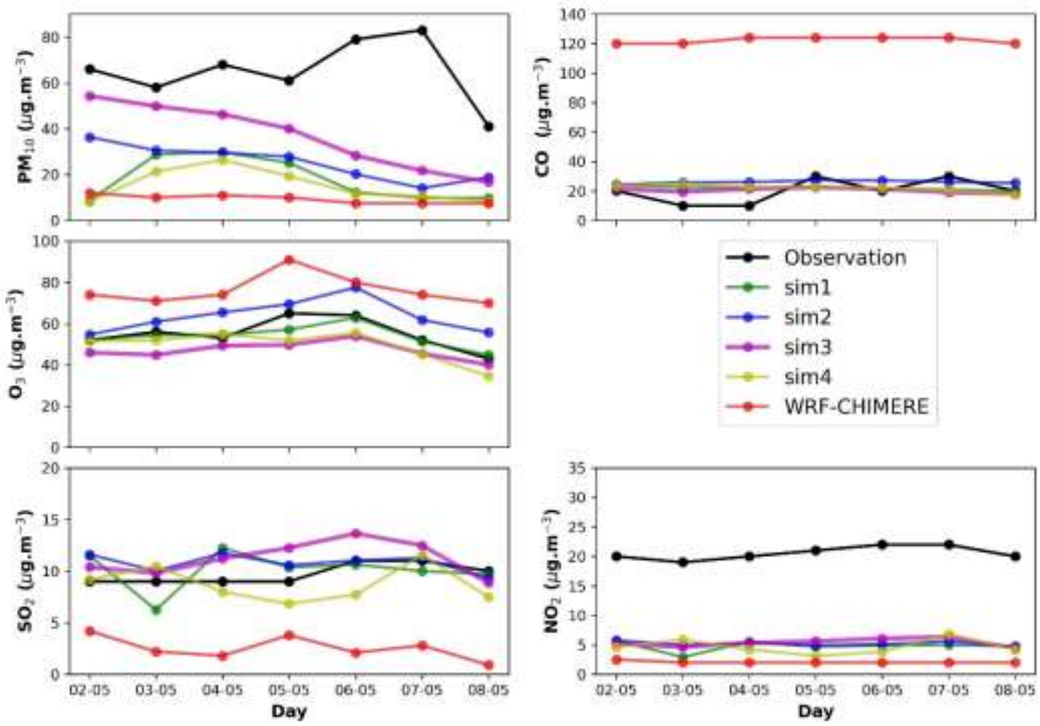

Fig. 9. Time series plot of daily concentrations of air quality variables (PM_{10}, O_3, SO_2, NO_2 and CO) during the simulation period from May 02 to May 08

Based on these results and the time series shown in Fig. 9 we can conclude that the best chemical mechanism for predicting PM_{10}, SO_2, and CO is GOCART, while the best mechanism for O_3 and NO_2 is MOZART.

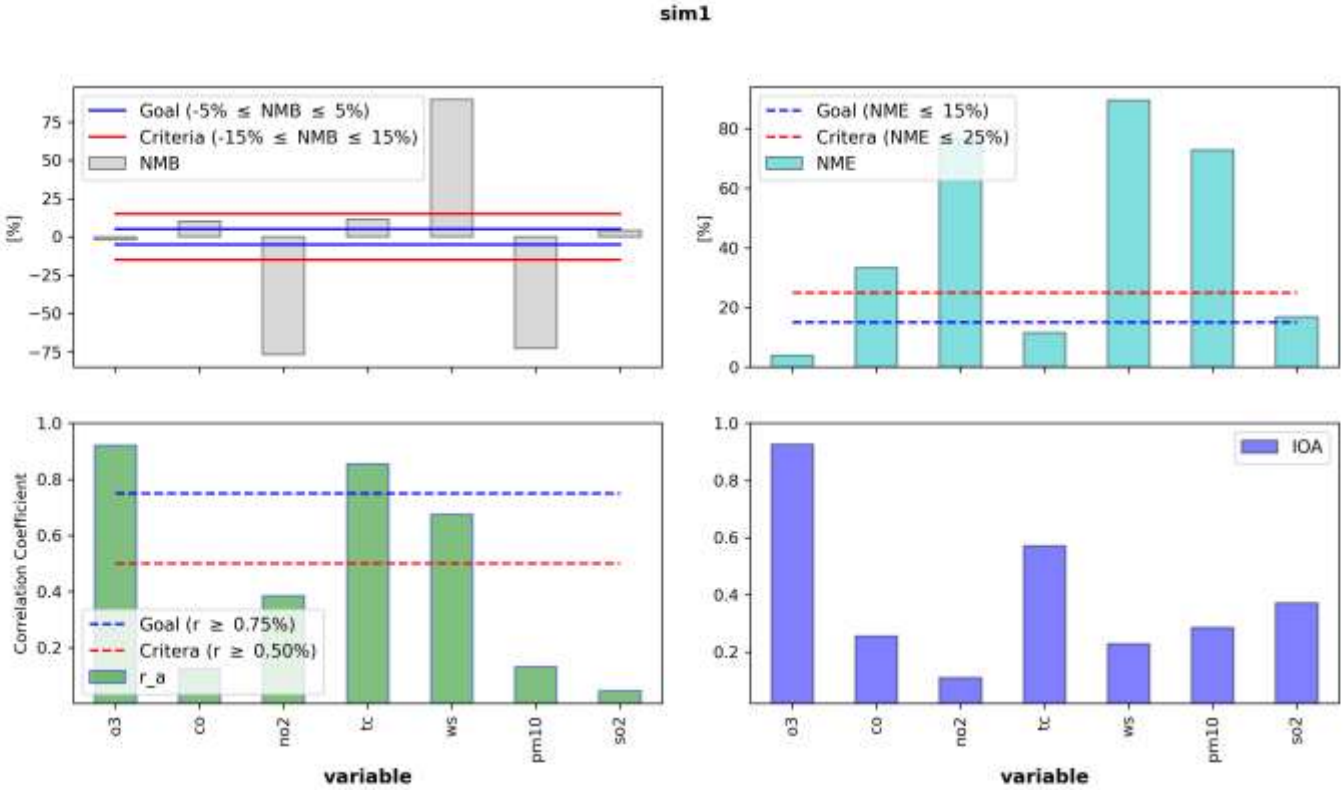

Fig. 10. Statistical plot for the first chemical mechanism, MOZART (simulation 1).

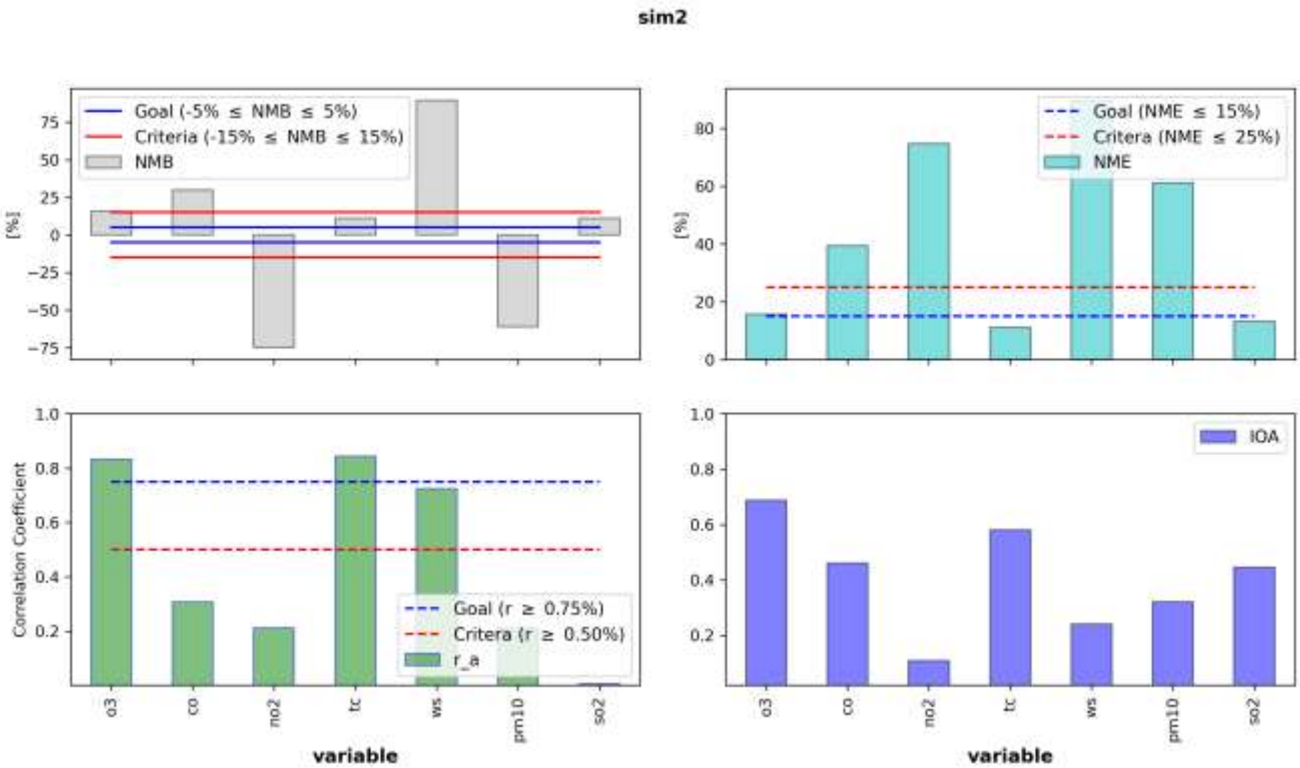

Fig. 11. Statistical plot for the second chemical mechanism, RACM (simulation 2).

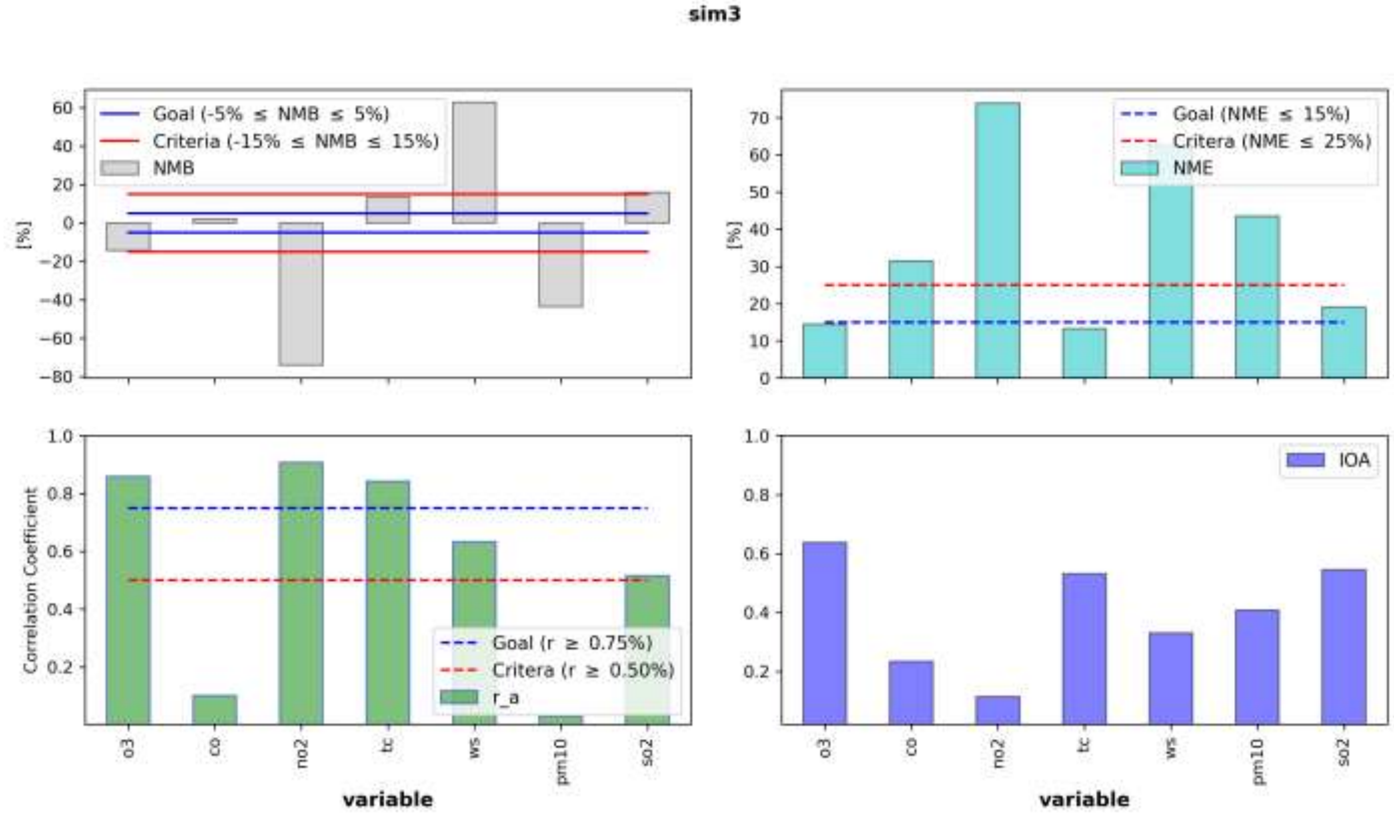

Fig. 12. Statistical plot for the third chemical mechanism, GOCART (simulation 3).

3.3 Nesting ratio comparison

This section investigates the impact of varying the nesting ratio on modeled meteorological (wind speed, temperature) and air quality (PM_{10}, CO, NO_2, O_3) variables. Two nesting configurations were employed: one with a 1:4 nesting ratio, where the nested domain has a resolution four times finer than its parent domain, and another with a 1:3 nesting ratio, where the nested domain has a resolution three times finer than its parent domain.

3.3.1 Impact of nesting ratio on meteorological variables

Fig. 13 presents the mean difference in wind speed and temperature between simulations with 3 and 4 nested domains. For wind speed, positive values dominate, indicating higher values in the 3-nested domain simulation (Sim1) compared to the 4-nested domain simulation (Sim4). These discrepancies are most pronounced in high-elevation regions. Conversely, the opposite trend is observed for temperature, except in the Sahara region where Sim1 exhibits higher values with increasing differences towards the domain boundaries.

An evaluation of Fig. 10 and Fig. 14 reveals that the 4-nested domain simulation (Sim4) achieves higher Pearson correlation coefficient for both temperature and wind speed, exceeding the target threshold ($r \geq 0.75\%$). However, Sim4 also exhibits a higher Normalized Mean Error (NME) for wind speed, which exceeds the established criteria (NME $\leq$ 25%). Faced with difficulties in determining the optimal nesting ratio for enhancing model performance for temperature and wind speed. As shown, Fig. 7 displays the time series of ground-level wind speed and temperature for Sim1 and Sim4. Based on this comparison, Sim1 appears to produce better results for wind speed, with values closer to observations. However, for temperature, Sim4 occasionally exhibits better performance on specific days, while on others, both models perform similarly.

Taking these results into account, along with the computational cost, which is roughly three times higher for Sim4 compared to Sim1, a 3-nested domain configuration with a 1:4 nesting ratio is suggested as a more effective approach for predicting ground-level temperature and wind speed (Cifuentes et al., 2021).

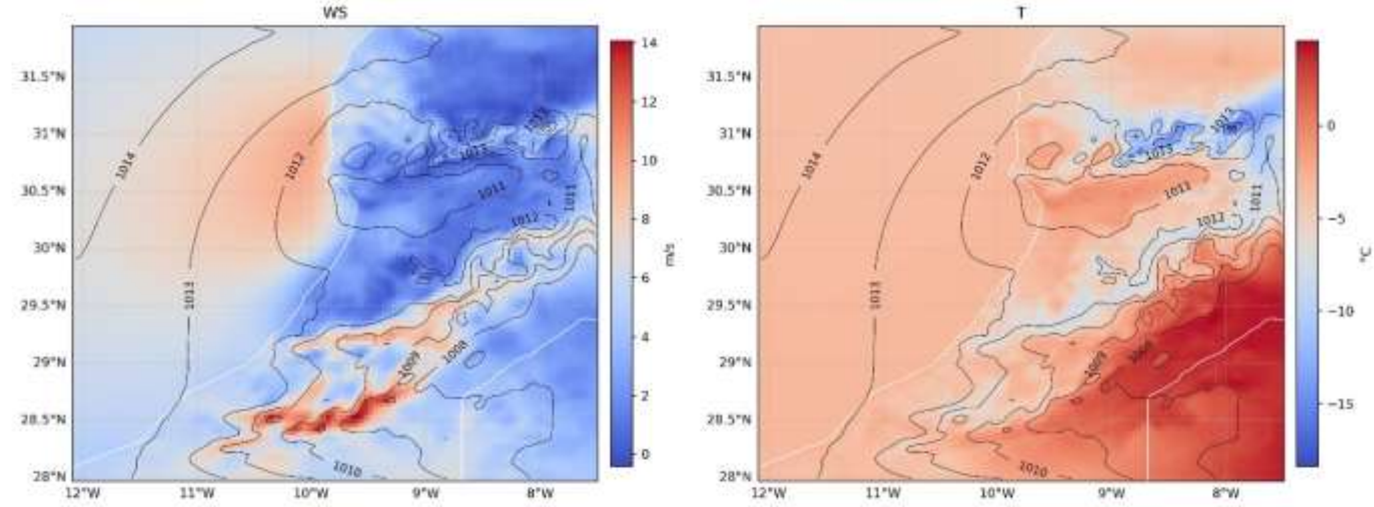

Fig. 13. Mean difference of ground level WS (left panel) and T (right panel) between 3 nested domains (1:4 nesting ratio) and 4 nested domains (1:3 nesting ratio).

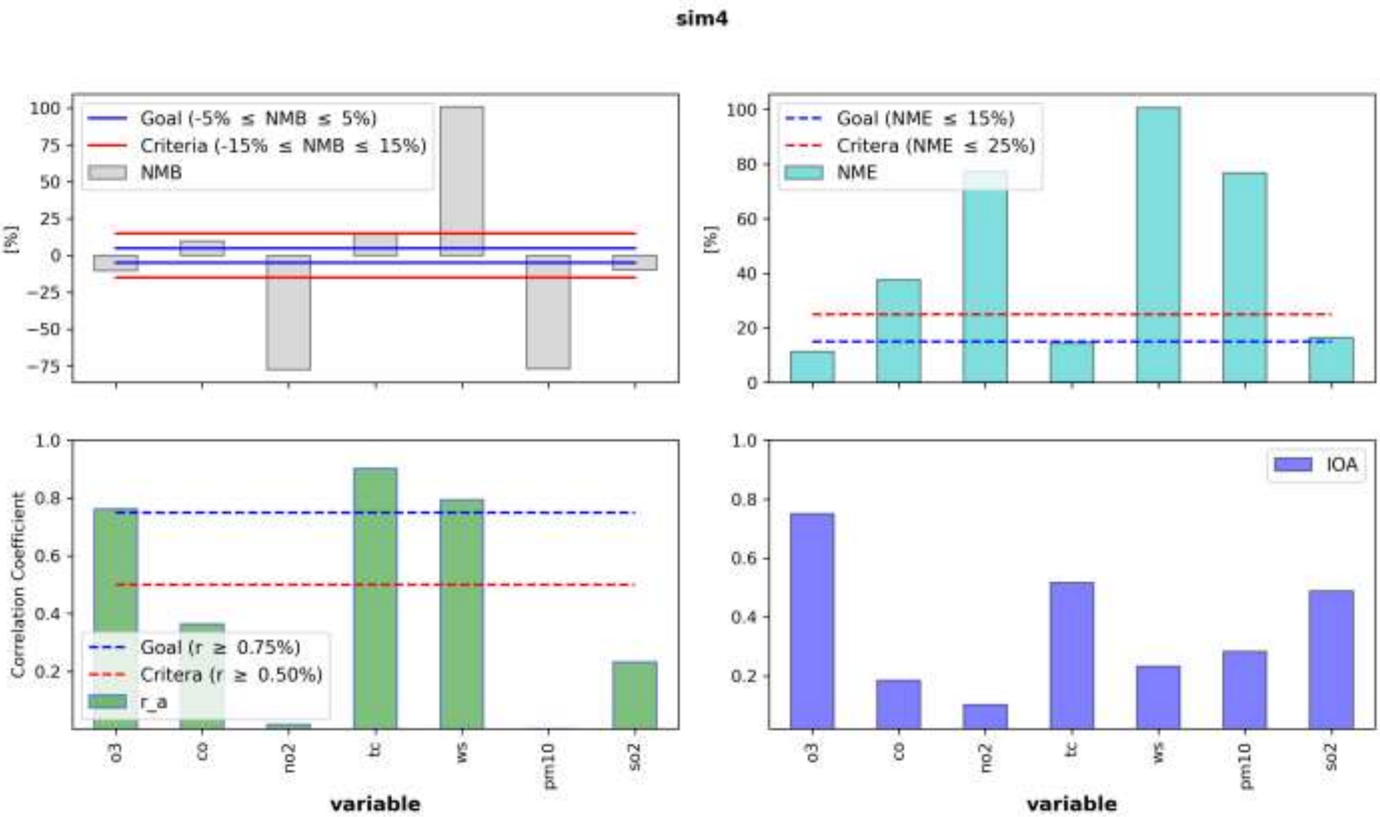

Fig. 14. Statistical plot for the 4 nested domains (1:3 nesting ratio).

3.3.2 Impact of nesting ratio on air quality variables

Fig. 15 presents the mean difference of PM_{10}, NO_2, CO and O_3 concentrations between simulations with 3 and 4 nested domains. This figure demonstrates a predominance of positive values for PM_{10}, which indicates that predicted concentrations using the 3-nested domain configuration are higher than those predicted using 4 nested domain configurations. Conversely, higher concentrations of NO_2, O_3, and CO are observed with the 4 nested domain configurations. An analysis of Fig. 14 reveals that the 4 nested domain configuration increases the Pearson correlation coefficient (r) for CO from 0.1 to 0.3, while it decreases the value of r for O_3 from 0.9 to 0.79. Similarly, for PM_{10} and NO_2, the 4-nested domain configuration significantly decreases their concentrations. As depicted in Fig. 9, it can be concluded that the performance for O_3 and PM_{10} accuracy is negatively affected when using the 4-nested domains. For CO and NO_2, both configurations exhibit similar performance.

As previously mentioned, the 4 nested domain option incurs computational time issues. Therefore, for predicting air quality in this region, a 3-nested domain configuration with a 1:4 ratio is suggested. This approach offers an efficiency time gain(Cifuentes et al., 2021; Misenis & Zhang, 2010b).

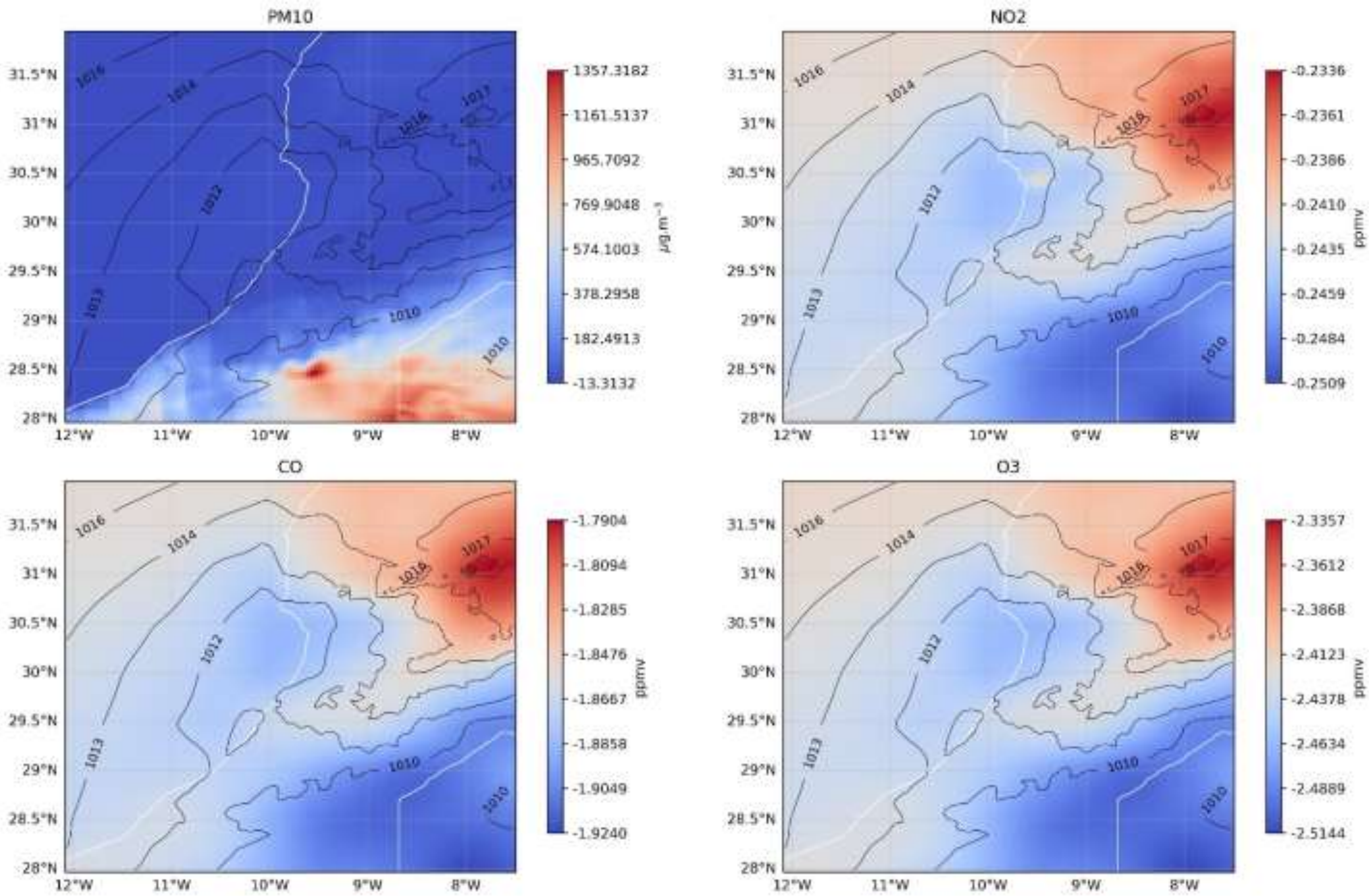

Fig. 15. Mean difference of PM_{10}, NO_2, CO and O_3 concentrations between 3 nested domains (1:4 nesting ratio) and 4 nested domains (1:3 nesting ratio).

3.4 *Effect of Resolution*

Fig. 16 illustrates the impact of resolution on ozone concentration. The figure reveals a clear trend: finer resolutions provide more detail in the predicted variable. This suggests that the grid resolution of a model significantly affects its ability to capture and resolve atmospheric processes at finer scales (Tao et al., 2020). Consequently, simulations with higher resolutions, exemplified by the 4-nested domain setup, generally offer more detailed and accurate representations of local phenomena, particularly important for air quality and meteorological variables. However, this increased detail comes at the cost of higher computational demands. Considering these trade-offs, the selection between the 3 and 4 nested domain configurations necessitates a balance between the requirement for and available computational resources. The 3 nested domain configuration with a 1:4 ratio offers efficiency advantages, making it a more suitable option for studies with significant time and resource constraints (Misenis & Zhang, 2010a).

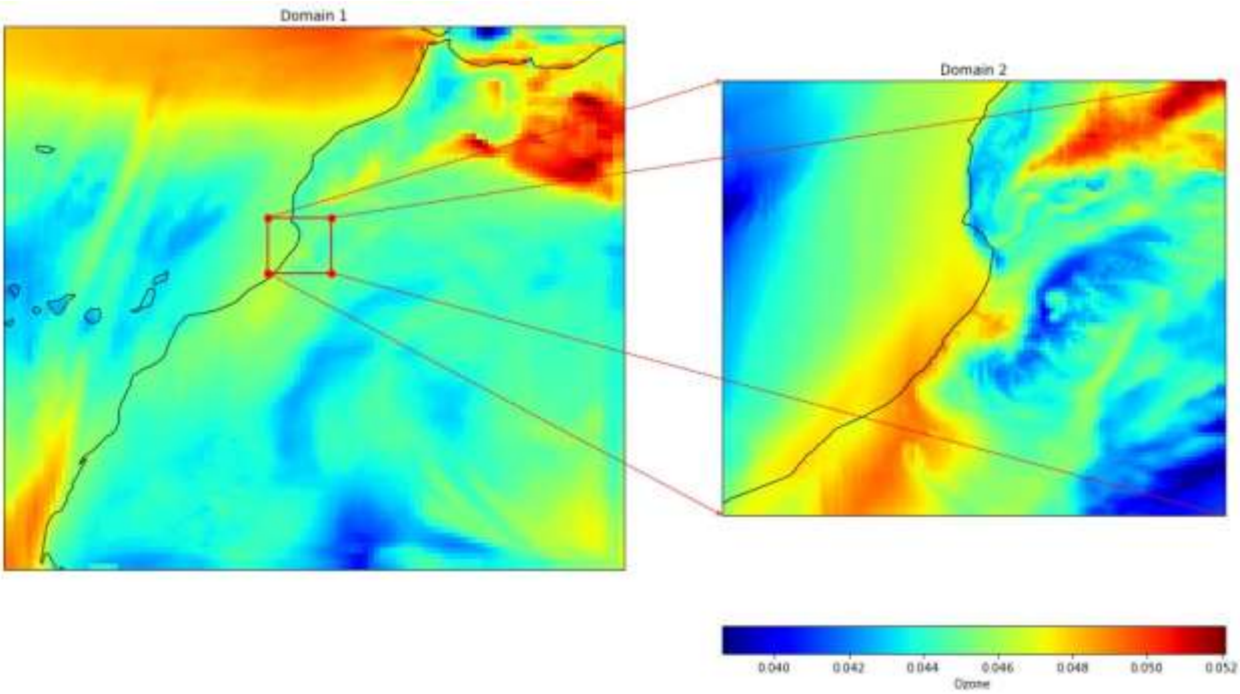

Fig. 16. Plot illustrating the effects of resolution changes between the first domain (D01) and the third one (D03).

3.5 *Impacts of PBL parameterizations on meteorological variable*

The selection of a Planetary Boundary Layer (PBL) parameterization scheme significantly impacts the simulation of meteorological parameters. Fig. 17 presents a comparison between different PBL schemes, including YSU, MYJ, MYNN2, and QNSE. An analysis of wind speed (WS) and temperature (T), reveals that the YSU scheme is the best for predicting ground-level WS. Likewise, for temperature, the YSU scheme demonstrates the most effective performance, followed closely by MYJ. These findings underscore the importance of employing an appropriate PBL parameterization to enhance the accuracy of meteorological forecasts (Banks & Baldasano, 2016; Rizza et al., 2020), particularly for variables such as WS and T, which directly influence various applications (Misenis & Zhang, 2010a).

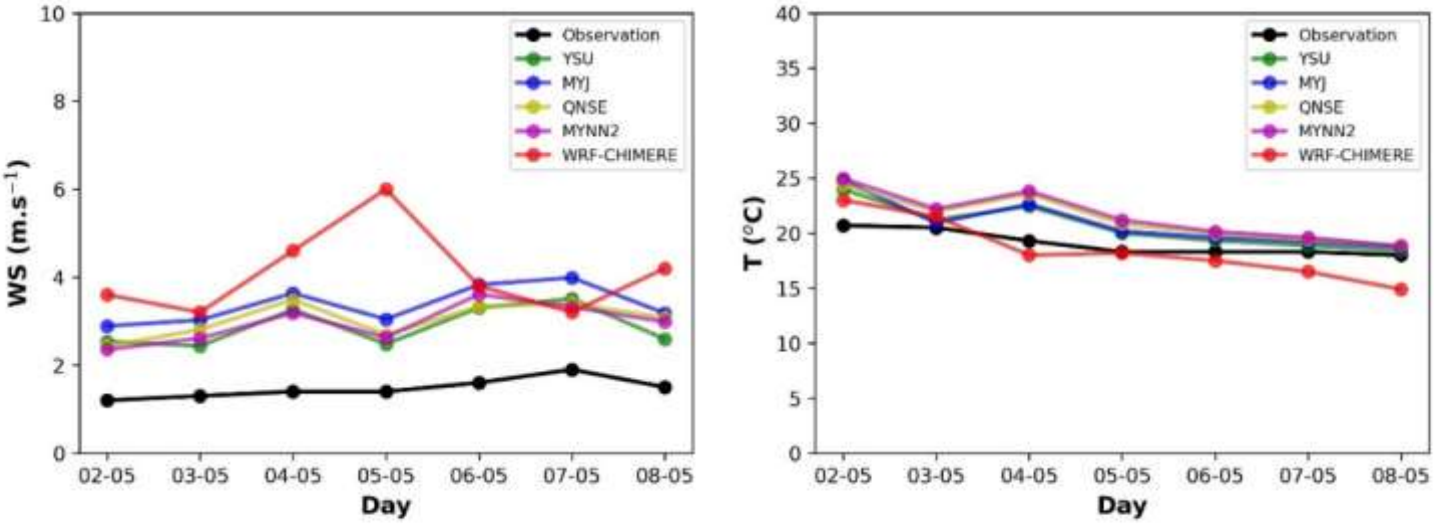

Fig. 17. Time series plot of daily ground-level wind speed (left panel) and temperature (right panel) during the simulation period from May 02 to May 08, showing the impact of different PBL parametrizations (YSU, MYJ, MYNN2, and QNSE).

4 Conclusion

This study successfully implemented the WRF-Chem model within the Moroccan domain for the first time. The model was used to simulate both meteorological variables (WS and T) and air quality variables (PM_{10}, O_3, CO, NO_2, and SO_2). The sensitivity of the model to changes in configuration was also evaluated. This included testing different nesting options (three nested domains with a 1:4 nesting ratio and four nested domains with a 1:3 nesting ratio), examining the effects of three chemical mechanisms (MOZART, RACM, and GOCART), and evaluating four PBL schemes (YSU, MYJ, MYNN2, and QNSE) to determine the optimal configuration.

Simulated meteorological and chemical variables were compared with observations and with a previous study over Agadir City that utilized WRF-CHIMERE. Statistical metrics were calculated for the same period for comparison. Overall, the results show that this study improved air quality prediction within the study area compared to WRF-CHIMERE.

Sensitivity analysis revealed good biases and correlations consistent with other studies. The performance of the model was found to be case-dependent, with optimal configurations varying based on the study's focus. For studies focused on ozone and nitrogen dioxide, MOZART was identified as the best chemical mechanism, GOCART produced the best results for PM_{10}, SO_2, and CO. The three nested domains configurations with a 1:4 nesting ratio emerged as the optimal choice, offering a 15% reduction in computational time compared to the 1:3 nesting ratio. Additionally, the YSU scheme was determined to be the optimal PBL scheme for enhancing the model's performance in producing WS and T.

Despite the improvements observed, the performance of the model, particularly for PM_{10}, NO_2, and wind speed (WS), remains lower than desired. WS is a crucial factor influencing pollutant transport and air-quality distribution, especially in coastal regions like Agadir where sea- and land-breeze phenomena strongly impact local meteorology. The study is also constrained by the limited observational data, relying on a single monitoring station from 2010, and by the lack of high-resolution local emission inventories, which may contribute to underestimation of urban-scale pollutants. Furthermore, while the MOZART, RACM, and GOCART schemes capture key chemical and aerosol processes, simplifications in secondary aerosol formation and heterogeneous reactions limit the accuracy of PM predictions. Despite these limitations, the results provide a benchmark for future studies and highlight the importance of improving local emission datasets, expanding observational networks, and refining model configurations to better represent air-quality processes in Morocco.

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Author Contributions: Karima Iraoui **:** Conceptualization, Methodology, Validation, Writing-Original draft, software. Charifi Hicham, Moustabchir Rachid, Abdelfettah Benchrif, Ahmed Chirmata: Conceptualization, Methodology, Validation, Writing - review & editing.

REFERENCES

Abdul-Wahab, S. A., & Al-Alawi, S. M. (2002). Assessment and prediction of tropospheric ozone concentration levels using artificial neural networks. *Environmental Modelling and Software*, *17*(3), 219–228. https://doi.org/10.1016/S1364-8152(01)00077-9

Adnane, A., Leghrib, R., & Chaoufi, J. (2020). The Use of a Recurrent Neural Network for Forecasting Ozone Concentrations in the City of Agadir (Morocco). *Journal of Atomic, Molecular, Condensed Matter & Nano Physics*, *7*(3), 197–206. https://doi.org/10.26713/jamcnp.v7i3.1545

Ajdour, A., Leghrib, R., Chaoufi, J., Fetmaoui, H., Bousseta, M., & Chirmata, A. (2020). Assessment of Particulate Matter (PM\(_{10}\)) using Chemistry Transport Modeling in Agadir City, Morocco. *Journal of Atomic, Molecular, Condensed Matter and Nano Physics*, *7*(3), 231–240. https://doi.org/10.26713/jamcnp.v7i3.1547

Ajdour, A. (2022). Surveillance et modelisation de la pollution atmospherique urbaine au Maroc: Cas des villes d'Agadir et Casablanca. *PhD Thesis*. Faculty of Science. Ibn Zohr University.

Alapaty, K., Mathur, R., Pleim, J., Hogrefe, C., Rao, S. T., Ramaswamy, V., Galmarini, S., Schaap, M., Makar, P., Vautard, R., Baklanov, A., Kallos, G., Vogel, B., & Sokhi, R. (2012). New Directions: Understanding interactions of air quality and climate change at regional scales. *Atmospheric Environment*, *49*, 419–421. https://doi.org/10.1016/j.atmosenv.2011.12.016

Arghavani, S., Malakooti, H., & Bidokhti, A. A. (2019). Numerical evaluation of urban green space scenarios effects on gaseous air pollutants in Tehran Metropolis based on WRF-Chem model. *Atmospheric Environment*, *214*(June), 116832. https://doi.org/10.1016/j.atmosenv.2019.116832

Bălă, G. P., Râjnoveanu, R. M., Tudorache, E., Motișan, R., & Oancea, C. (2021). Air pollution exposure—the (in)visible risk factor for respiratory diseases. In *Environmental Science and Pollution Research* (Vol. 28, Issue 16). https://doi.org/10.1007/s11356-021-13208-x

Banks, R. F., & Baldasano, J. M. (2016). Impact of WRF model PBL schemes on air quality simulations over Catalonia, Spain. *The Science of the Total Environment*, *572*, 98–113. https://doi.org/10.1016/j.scitotenv.2016.07.167

Bouchriti, Y., Korrida, A., Ait Haddou, M., Achbani, A., Sine, H., Rida, J., Sine, H., Amiha, R., & Kabbachi, B. (2023). Assessment of health impact of the surface ozone on a population residing at Agadir city (Morocco) using the AirQ+ model. *E3S Web of Conferences*, *364*, 0–5. https://doi.org/10.1051/e3sconf/202336402003

Bounakhla, Y., Benchrif, A., Costabile, F., Tahri, M., Gourch, B. El, Kafssaoui, E., Hassan, E., Zahry, F., & Bounakhla, M. (2023). *Overview of PM10, PM2.5 and BC and Their Dependent Relationships with Meteorological Variables in an Urban Area in Northwestern Morocco*.

Bozkurt, Z. (2014). *prediction of daily maximum PM10 concentration in Düzce , Tukey application pf artifcial neural networks and regression modekls in the prediction of daily maximum PM10 concentratiion in DÜZCE , TURKEY. January-2014*.

Chen, Y., Shi, R., Shu, S., & Gao, W. (2013). Ensemble and enhanced PM 10 concentration forecast model based on stepwise regression and wavelet analysis. *Atmospheric Environment*, *74*, 346–359. https://doi.org/10.1016/j.atmosenv.2013.04.002

Chirmata, A., Leghrib, R., & Ichou, I. A. (2017). Implementation of the Air Quality Monitoring Network at Agadir City in Morocco. *Journal of Environmental Protection*, *08*(04), 540–567. https://doi.org/10.4236/JEP.2017.84037

Ciencewicki, J., & Jaspers, I. (2007). Air pollution and respiratory viral infection. *Inhalation Toxicology*, *19*(14), 1135–1146. https://doi.org/10.1080/08958370701665434

Cifuentes, F., González, C. M., & Aristizábal, B. H. (2021). Insights to WRF-Chem sensitivity in a zone of complex terrain in the tropical Andes: Effect of boundary conditions, chemical mechanisms, nesting, and domain configuration. *Atmospheric Pollution Research*, *12*(6). https://doi.org/10.1016/j.apr.2021.101093

Clappier, A., Belis, C. A., Pernigotti, D., Thunis, P., Clappier, A., Belis, C. A., Pernigotti, D., Thunis, P., Clappier, A., Belis, C. A., Pernigotti, D., & Thunis, P. (2021). *Source apportionment and sensitivity analysis : two methodologies with two different purposes To cite this version : HAL Id : hal-03254557 Source apportionment and sensitivity analysis : two methodologies with two different purposes*.

Emmons, L. K., Walters, S., Hess, P. G., Lamarque, J. F., Pfister, G. G., Fillmore, D., Granier, C., Guenther, A., Kinnison, D., Laepple, T., Orlando, J., Tie, X., Tyndall, G., Wiedinmyer, C., Baughcum, S. L., & Kloster, S. (2010). Description and evaluation of the Model for Ozone and Related chemical Tracers, version 4 (MOZART-4). *Geoscientific Model Development*, *3*(1), 43–67. https://doi.org/10.5194/gmd-3-43-2010

Grell, G. A., Peckham, S. E., Schmitz, R., McKeen, S. A., Frost, G., Skamarock, W. C., & Eder, B. (2005). Fully coupled "online" chemistry within the WRF model. *Atmospheric Environment*, *39*(37), 6957–6975. https://doi.org/10.1016/j.atmosenv.2005.04.027

Ha, S. (2022). Implementation of aerosol data assimilation in WRFDA (v4.0.3) for WRF-Chem (v3.9.1) using the RACM/MADE-VBS scheme. *Geoscientific Model Development*, *15*(4), 1769–1788. https://doi.org/10.5194/gmd-15-1769-2022

Hu, X. M., Klein, P. M., & Xue, M. (2013). Evaluation of the updated YSU planetary boundary layer scheme within WRF for wind resource and air quality assessments. *Journal of Geophysical Research Atmospheres*, *118*(18), 10,490-10,505. https://doi.org/10.1002/jgrd.50823

Hu, X. M., Nielsen-Gammon, J. W., & Zhang, F. (2010). Evaluation of three planetary boundary layer schemes in the WRF model. *Journal of Applied Meteorology and Climatology*, *49*(9), 1831–1844. https://doi.org/10.1175/2010JAMC2432.1

Iraoui, K., Moustabchir, R., Charifi, H., Ouattab, M., & Chirmata, A. (2023). Ozone concentrations Predicting in Agadir city (Morocco) using the Multiple Linear Regression (Forward Regression Analysis). *2023 3rd International Conference on Innovative Research in Applied Science, Engineering and Technology, IRASET 2023*, 1–4. https://doi.org/10.1109/IRASET57153.2023.10152974

Kant, S., Panda, J., Rao, P., Sarangi, C., & Ghude, S. D. (2021). Study of aerosol-cloud-precipitation-meteorology interaction during a distinct weather event over the Indian region using WRF-Chem. *Atmospheric Research*, *247*(July 2020), 105144. https://doi.org/10.1016/j.atmosres.2020.105144

Khan, A. W., & Kumar, P. (2019). Impact of chemical initial and lateral boundary conditions on air quality prediction. *Advances in*

Space Research, *64*(6), 1331–1342. https://doi.org/10.1016/j.asr.2019.06.028

Kitamura, Y. (2010). Modifications to the mellor-Yamada-Nakanishi-Niino (MYNN) model for the stable stratification case. *Journal of the Meteorological Society of Japan*, *88*(5), 857–864. https://doi.org/10.2151/jmsj.2010-506

Kong, X., Forkel, R., Sokhi, R. S., Suppan, P., Baklanov, A., Gauss, M., Brunner, D., Barò, R., Balzarini, A., Chemel, C., Curci, G., Jiménez-Guerrero, P., Hirtl, M., Honzak, L., Im, U., Pérez, J. L., Pirovano, G., San Jose, R., Schlünzen, K. H., … Galmarini, S. (2015). Analysis of meteorology-chemistry interactions during air pollution episodes using online coupled models within AQMEII phase-2. *Atmospheric Environment*, *115*, 527–540. https://doi.org/10.1016/j.atmosenv.2014.09.020

Lecoeur, E., & Seigneur, C. (2013). Dynamic evaluation of a multi-year model simulation of particulate matter concentrations over Europe. *Atmospheric Chemistry and Physics*, *13*(8), 4319–4337. https://doi.org/10.5194/acp-13-4319-2013

Leghrib, R., Ajdour, A., Chirmata, A., Chaoufi, J., Kaaya, A., Fatmaoui, H., Ichou, I. A., Menut, L., & Mailler, S. (2018). Particulate matter monitoring in Souss Massa Region. *SMETox Journal*, *1*(04), 128–136.

Li, X., Hussain, S. A., Sobri, S., & Md Said, M. S. (2021). Overviewing the air quality models on air pollution in Sichuan Basin, China. *Chemosphere*, *271*, 129502. https://doi.org/10.1016/j.chemosphere.2020.129502

Liu, Y., Wang, P., Li, Y., Wen, L., & Deng, X. (2022). Air quality prediction models based on meteorological factors and real-time data of industrial waste gas. *Scientific Reports*, *12*(1), 1–15. https://doi.org/10.1038/s41598-022-13579-2

Luna, A. S., Paredes, M. L. L., de Oliveira, G. C. G., & Corrêa, S. M. (2014). Prediction of ozone concentration in tropospheric levels using artificial neural networks and support vector machine at Rio de Janeiro, Brazil. *Atmospheric Environment*, *98*, 98–104. https://doi.org/10.1016/j.atmosenv.2014.08.060

Luo, C., Wang, W., Sheng, L., Zhou, Y., Hu, Z., Qu, W., Li, X., & Hai, S. (2020). Influence of polluted dust on chlorophyll-a concentration and particulate organic carbon in the subarctic North Pacific Ocean based on satellite observation and the WRF-Chem simulation. *Atmospheric Research*, *236*(August 2019), 104812. https://doi.org/10.1016/j.atmosres.2019.104812

Manisalidis, I., Stavropoulou, E., Stavropoulos, A., & Bezirtzoglou, E. (2020). Environmental and Health Impacts of Air Pollution: A Review. *Frontiers in Public Health*, *8*(February), 1–13. https://doi.org/10.3389/fpubh.2020.00014

Menut, L., Bessagnet, B., Khvorostiyanov, D., Monge, J., Valari, M., & Vautard, R. (2021). *To cite this version : de la troposphère*.

Mian Chin, R. b. R., & Lin, S.-J. (2000). *Atmospheric sulfur cycle* (p. 17). Journal of geophysical research.

Misenis, C., & Zhang, Y. (2010a). An examination of sensitivity of WRF/Chem predictions to physical parameterizations, horizontal grid spacing, and nesting options. *Atmospheric Research*, *97*(3), 315–334. https://doi.org/10.1016/j.atmosres.2010.04.005

Misenis, C., & Zhang, Y. (2010b). An examination of sensitivity of WRF/Chem predictions to physical parameterizations, horizontal grid spacing, and nesting options. *Atmospheric Research*, *97*(3), 315–334. https://doi.org/https://doi.org/10.1016/j.atmosres.2010.04.005

Mohammed, A. N. N. I., & Abualqumboz, A. M. M. S. (2018). Multivariate analysis of monsoon seasonal variation and prediction of particulate matter episode using regression and hybrid models. *International Journal of Environmental Science and Technology*, *0123456789*. https://doi.org/10.1007/s13762-018-1905-6

Mohan, M., Kandya, A., & Yadav, M. (2011). An evaluation and comparison of the various statistical and deterministic techniques for forecasting the concentration of criteria air pollutants. *International Journal of Environment and Pollution*, *44*(1–4), 96–105. https://doi.org/10.1504/IJEP.2011.038407

Mohd Napi, N. N. L., Noor Mohamed, M. S., Abdullah, S., Mansor, A. A., Ahmed, A. N., & Ismail, M. (2020). Multiple Linear Regression (MLR) and Principal Component Regression (PCR) for ozone (O3) concentrations prediction. *IOP Conference Series: Earth and Environmental Science*, *616*(1). https://doi.org/10.1088/1755-1315/616/1/012004

Nazif, A., Mohammed, N. I., Malakahmad, A., & Abualqumboz, M. S. (2016). Application of Step Wise Regression Analysis in Predicting Future Particulate Matter Concentration Episode. *Water, Air, and Soil Pollution*, *227*(4). https://doi.org/10.1007/s11270-016-2823-1

Park, J. (2021a). *A Particulate Matter Concentration Prediction Model Based on Long Short-Term Memory and an Artificial Neural Network*.

Park, J. and seonju chang. (2021b). *A Particulate Matter Concentration Prediction Model Based on Long Short-Term Memory and an Artificial Neural Network _ Enhanced Reader.pdf* (p. 15). https://doi.org/https://doi.org/10.3390/ijerph18136801

Qiu, M., Zigler, C., & Selin, N. E. (2022). Statistical and machine learning methods for evaluating trends in air quality under changing meteorological conditions. *Atmospheric Chemistry and Physics*, *22*(16), 10551–10566. https://doi.org/10.5194/acp-22-10551-2022

Regional, W. H. O. (2003). *Health Aspects of Air Pollution with Particulate Matter , Ozone and Nitrogen Dioxide*. *January*.

Rizza, U., Mancinelli, E., Canepa, E., Piazzola, J., Missamou, T., Yohia, C., Morichetti, M., Virgili, S., Passerini, G., & Miglietta, M. M. (2020). WRF sensitivity analysis in wind and temperature fields simulation for the northern sahara and the mediterranean Basin. *Atmosphere*, *11*(3). https://doi.org/10.3390/atmos11030259

Saidou Chaibou, A. A., Ma, X., Kumar, K. R., Jia, H., Tang, Y., & Sha, T. (2019). Evaluation of dust extinction and vertical profiles simulated by WRF-Chem with CALIPSO and AERONET over North Africa. *Journal of Atmospheric and Solar-Terrestrial Physics*, *199*(2019), 105213. https://doi.org/10.1016/j.jastp.2020.105213

Schindlbacher, S., Matthews, B., & Ullrich, B. (2021). *Uncertainties and recalculations of emission inventories submitted under CLRTAP*. 1–26. https://www.ceip.at/fileadmin/inhalte/ceip/00_pdf_other/2021/uncertainties_and_recalculations_of_emission_inventories_submitted_under_clrtap.pdf

Sha, T., Ma, X., Jia, H., Tian, R., Chang, Y., Cao, F., & Zhang, Y. (2019). Aerosol chemical component: Simulations with WRF-Chem and comparison with observations in Nanjing. *Atmospheric Environment*, *218*, 116982. https://doi.org/10.1016/j.atmosenv.2019.116982

Shimada, S., Ohsawa, T., Chikaoka, S., & Kozai, K. (2011). Accuracy of the wind speed profile in the lower PBL as simulated by the WRF model. *Scientific Online Letters on the Atmosphere*, *7*(1), 109–112. https://doi.org/10.2151/sola.2011-028

Sicard, P., Crippa, P., De Marco, A., Castruccio, S., Giani, P., Cuesta, J., Paoletti, E., Feng, Z., & Anav, A. (2021). High spatial resolution WRF-Chem model over Asia: Physics and chemistry evaluation. *Atmospheric Environment*, *244*(October 2020), 118004. https://doi.org/10.1016/j.atmosenv.2020.118004

Siegfried, H., Pfeiler, B., & Stadlober, E. (2005). *Analysis and Prediction of Particulate Matter PM10 for the Winter Season in Graz 1 1 Introduction*. *34*(4), 307–326.

Singh, C., Singh, S. K., Chauhan, P., & Budakoti, S. (2021). Simulation of an extreme dust episode using WRF-CHEM based on optimal ensemble approach. *Atmospheric Research*, *249*(July 2020), 105296. https://doi.org/10.1016/j.atmosres.2020.105296

Sukoriansky, S., Galperin, B., & Perov, V. (2006). A quasi-normal scale elimination model of turbulence and its application to stably stratified flows. *Nonlinear Processes in Geophysics*, *13*(1), 9–22. https://doi.org/10.5194/npg-13-9-2006

Tao, H., Xing, J., Zhou, H., Pleim, J., Ran, L., Chang, X., Wang, S., Chen, F., Zheng, H., & Li, J. (2020). Impacts of improved modeling resolution on the simulation of meteorology, air quality, and human exposure to PM2.5, O3 in Beijing, China. *Journal of Cleaner Production*, *243*, 118574. https://doi.org/https://doi.org/10.1016/j.jclepro.2019.118574

Taşpınar, F. (2015). Improving artificial neural network model predictions of daily average PM10 concentrations by applying principle component analysis and implementing seasonal models. *Journal of the Air and Waste Management Association*, *65*(7), 800–809. https://doi.org/10.1080/10962247.2015.1019652

Tebal, N., & Pinang, P. (2011). *Comparison Between Multiple Linear Regression And Feed forward Back propagation Neural Network Models For Predicting PM 10 Concentration Level Based On Gaseous And Meteorological Parameters Ahmad Zia Ul-Saufie (Corresponding author) Clean Air Research G. 1*(4), 42–49.

UNECA and UNECE. (2014). Morocco Environmental Performance Reviews. In *The United Nations*. http://www.unilibrary.org/transportation-and-public-safety/the-united-nations-motorcycle-helmet-study_c92c1aa7-en

Wang, P., Qiao, X., & Zhang, H. (2020). Modeling PM2.5 and O3 with aerosol feedbacks using WRF/Chem over the Sichuan Basin, southwestern China. *Chemosphere*, *254*, 126735. https://doi.org/10.1016/j.chemosphere.2020.126735

Wang, Q., & Li, X. (2022). Correlation Analysis between Meteorological Factors and Pollutants Based on Copula Theory. *Journal of Physics: Conference Series*, *2168*(1). https://doi.org/10.1088/1742-6596/2168/1/012028

Wang, W., Lu, W., Wang, X., & Leung, A. Y. T. (2003). Prediction of maximum daily ozone level using combined neural network and statistical characteristics. *Environment International*, *29*(5), 555–562. https://doi.org/10.1016/S0160-4120(03)00013-8

Wang, Y., Yuan, Q., Li, T., Zhu, L., & Zhang, L. (2021). Estimating daily full-coverage near surface O3, CO, and NO2 concentrations at a high spatial resolution over China based on S5P-TROPOMI and GEOS-FP. *ISPRS Journal of Photogrammetry and Remote Sensing*, *175*, 311–325. https://doi.org/10.1016/j.isprsjprs.2021.03.018

World Health Organization. (2006). *Health risks of particulate matter from long-range transboundary air pollution*. http://www.euro.who.int/pubrequest.

Yorkor, B., & Leton, T. (2017).Prediction and modeling of seasonal concentrations of air pollutants in semi urban region employing artificial neural . *July*-2017.

Yu, E., Bai, R., Chen, X., & Shao, L. (2022). Impact of physical parameterizations on wind simulation with WRF V3.9.1.1 under stable conditions at planetary boundary layer gray-zone resolution: a case study over the coastal regions of North China. *Geoscientific Model Development*, *15*(21), 8111–8134. https://doi.org/10.5194/gmd-15-8111-2022