Proceedings of the 6th World Congress on Civil, Structural, and Environmental Engineering (CSEE'21)
~~Lisbon, Portugal~~ Virtual Conference – June 21 – 23, 2021
Paper No. ICEPTP 105
DOI: 10.11159/iceptp21.lx.105

Evaluating Predicting Aerosol PM_{10} Concentrations with the WRF-Chem Model, in Lima, in February 2018

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Abstract **–** Particulate matter with aerodynamic diameters equal to or less than 10 µm (PM_{10}) concentration in the Metropolitan Area of Lima – Callao (MALC) frequently exceeds the daily Peruvian National Ambient Air Quality Standard for PM_{10} (100 µg/m^3) and the daily World Health Organization Guideline (50 µg/m^3). The aim of this study was to simulate the hourly PM_{10} concentration and evaluate the model performance. The prediction of PM_{10} concentration was done using the "Weather Research and Forecasting Model Coupled with Chemistry" (WRF-Chem) air pollution modeling system. Therefore, in this study, WRF-Chem (version 4.0) was applied to simulate PM_{10} concentrations from January 30, 2018 to February 28, 2018. The first 2 days were used as spin-up in order to minimize the influence of the initial conditions with a 5-km-by-5-km grid over MALC. This PM_{10} concentrations prediction was validated against ground-based observations. For validating the aerosol PM_{10} simulations, hourly PM_{10} in-situ measurements from two traffic air quality monitoring stations named Ate and Puente Piedra in the MALC were used. The results showed that the prediction of PM_{10} mass concentration at the (Ate and Puente Piedra) traffic air quality monitoring stations reasonably captures the observed PM_{10} temporal. However, PM_{10} concentrations estimated were under-estimated by the WRF-Chem model.

Keywords**:** Atmospheric modeling, air quality, chemistry, air pollution

1. Introduction

Efficient air pollution simulations are necessary because they could help policymakers to develop air quality regulation and decide on emission reduction [1]. In this study, a coupled on-line modeling system, the Weather Research and Forecasting model coupled with chemistry (WRF-Chem) [2] was used to simulate the hourly PM_{10} mass concentration. WRF-Chem is a regional air pollution model [2]. The WRF-Chem model is a completely coupled online meteorology-chemistry in which the same diffusion, advection, and convection schemes were used for the PM_{10} mass concentration prediction [3]. The WRF–Chem dynamically manages different processes such as photolysis, transport, gas-phase chemical mechanism, plume rise, aerosol chemistry, wet and dry deposition, anthropogenic, aerosol radiation, and biogenic emission, etc. [2]. Detailed descriptions of the WRF-Chem model can be found on the website (https://ruc.noaa.gov/wrf/wrf-chem/). The WRF-Chem model performance was evaluated by many researchers in the world, for example [4, 5, 6]. However, there are only few studies about numerical estimation of air quality in the MALC for example [4]. This study aims to predict the hourly PM_{10} concentration and evaluate the WRF-Chem model performance in the MALC in February 2018.

2. Methods

2.1. Study Area

In this study, we have chosen two traffic air quality monitoring stations named Ate (A) (76° 55' 7" W, 12° 1'34" S) and Puente Piedra (P) (77° 4' 26.88" W, 11° 51'47.7" S) (Fig. 1) in order to evaluate predicting PM_{10} concentration in the MALC. Heavy vehicular traffic, population, and industries are concentrated in the Lima districts of Ate and Puente Piedra. They are places where PM_{10} concentrations air pollution problems are severe. The hourly near-surface PM_{10} concentration observation

for Ate's and Puente Piedra's air quality monitoring stations was obtained from the National Service of Meteorology and Hydrology of Peru (https://web2.senamhi.gob.pe/?p=calidad-de-aire).

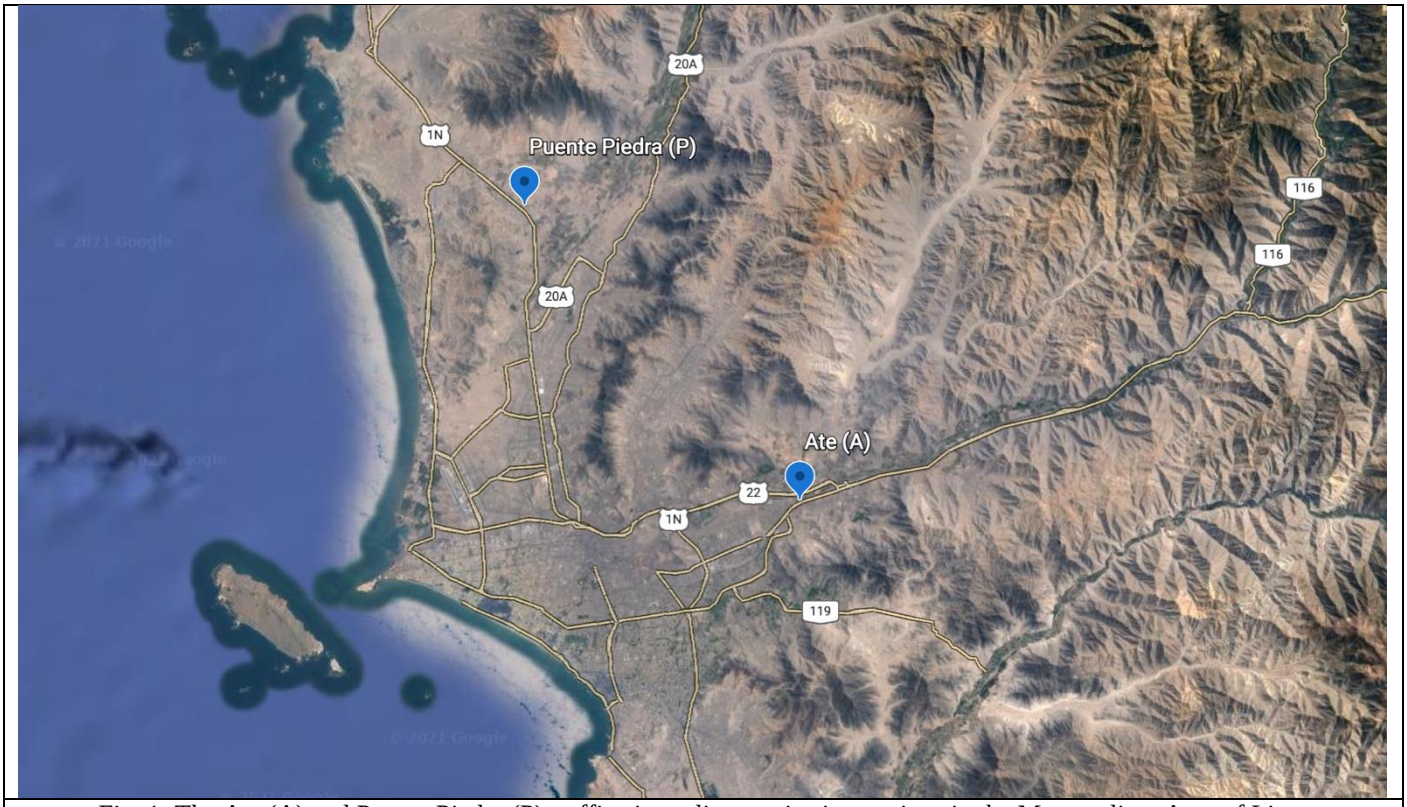

Fig. 1: The Ate (A) and Puente Piedra (P) traffic air quality monitoring stations in the Metropolitan Area of Lima

2.2. WRF-Chem Modeling Setup

The WRF-Chem (version 4.0) used to simulate PM_{10} mass concentrations in the MALC. In this study, the gas-phase chemical reactions were calculated using the RADM2 (Regional Acid Deposition Model, version 2) chemical mechanism. It is a reduced gas-phase photoxidation mechanism [5]. Included in the "RADM2 are: i) three classes of alkanes; ii) aromatic chemistry; iii) two alkenes classes; iv) ketones and dicarbonysls are distinct classes; v) isoprene is an explicit species; and peroxy radical reactions" [6]. The aerosol chemical reactions were calculated using the MADE-SORGAM (Modal Aerosol Dynamics Model for Europe-Secondary Organic Aerosol Model) model. It is a modal scheme that expresses three log-normal distribute modes to predict particle size distribution: i) the Aitken mode (< 0.1 μm diameter); ii) the accumulation mode (0.1-2 μm diameter); and, iii) the coarse mode (2-10 μm diameter) [5].

The Operational Global Analysis "National Centers for Environmental Prediction" (NCEP) – Final Analysis (FNL) with spatial resolution of 0.25-degree-by-0.25-degree grids every six hours (00, 06, 12 and 18 UTC) was used for the initial and physical conditions for WRF simulations (https://rda.ucar.edu/datasets/ds084.1/). The geo-physical parameters such as orography was taken from ASTER GDEM (Advanced Spaceborne Thermal Emission and Reflection Radiometer, Global Digital Elevation Model), and land use was taken from USGS (U.S. Geological Survey) datasets. The anthropogenic emissions of air contamination in a 5 km horizontal resolution grid domain [4] were based on the emission vehicular model [7]. This model considers that air atmospheric emission only comes from on-road vehicles [7]. Finally, WRF-chem model output was gotten on hourly PM_{10} concentrations.

3. Results and Discussion

WRF-Chem results at the lowest model layer for the Ate and Puente Piedra traffic air quality monitoring stations with with in-situ PM_{10} data were extracted, and, for these stations, statistical metrics to provide a measure model's error were calculated. Statistical parameters were implemented to evaluate the effectiveness of PM_{10} mass concentrations predictions. predictions. That parameters used were Mean Bias (MB), Mean Normalized Bias (MNB), Mean Gross Error (MGE), Mean Mean Normalized Gross Error (MNGE), and Root Mean Square Error (RMSE) as metric indicators to evaluate the WRF-Chem model performance. These indices are described as shown in Eqs. (1)- (5) [8]:

$$MB = \frac{1}{N}\sum_{i=1}^{N}(M_i - O_i) \quad (1)$$

$$MNB = \frac{\sum_{i=1}^{N}(M_i - O_i)}{\sum_{i=1}^{N} O_i} \quad (2)$$

$$MGE = \frac{1}{N}\sum_{i=1}^{N}|M_i - O_i| \quad (3)$$

$$MNGE = \frac{\sum_{i=1}^{N}|M_i - O_i|}{\sum_{i=1}^{N} O_i} \quad (4)$$

$$RMSE = \left[\frac{1}{N}\sum_{i=1}^{N}(M_i - O_i)^2\right]^{1/2} \quad (5)$$

Where N is the total number of data pairs; M_i is the predicted PM_{10} concentrations, and O_i is the observed PM_{10} concentrations. The results of these metric indices for PM_{10} mass concentrations are presented (Table 1). The MB (-67.1 $\mu g/m^3$) and MNB (-62.2%) for Ate and the MB (-63.3 $\mu g/m^3$) and MNB (-57.5%) for Puente Piedra were negative indicating that the PM_{10} total mass was under-predicted by the WRF-Chem model. The MGE (61.7 $\mu g/m^3$), MNGE (62.4 %,), and RMSE (84.9 $\mu g/m^3$) for Ate and the MGE (64.2 $\mu g/m^3$), MNGE (55.6 %,), and RMSE (77.6 $\mu g/m^3$) for Puente Piedra indicate that the WRF-Chem model performed badly. The PM_{10} concentrations estimated (40.5 ± 33.8) for Ate and (46.4 ± 27.4) for Puente Piedra were under-estimated by the WRF-Chem model, because average and standard deviation of PM_{10} observed were 107.9 ± 61.1 for Ate and 110.2 ± 47.4 for Puente Piedra respectively. The PM_{10} predicted reasonably captured the temporal variation of the PM_{10} observed (figure not shown).

Table 1: WRF-Chem model evaluation for PM_{10} mass concentrations at the Ate and Puente Piedra traffic air quality monitoring stations in Lima

Statistical measure	Ate traffic air quality monitoring station	Puente Piedra traffic air quality monitoring station
PM_{10} observed	107.9 ± 61.1	110.2 ± 47.4
PM_{10} predicted	40.5 ± 33.8	46.4 ± 27.4
MB ($\mu g/m^3$)	-67.1	-63.3
MNB (%)	-62.2	-57.5
MGE ($\mu g/m^3$)	61.7	64.2
MNGE (%)	62.4	55.6
RMSE ($\mu g/m^3$)	84.9	77.6

Fig. 2 shows the PM_{10} concentration simulated in the MALC, which is average for the month of February 2018. An of maximum PM_{10} concentration predicted by the model is noted in northern Lima, whose values vary from 55 to 60 However, there is a small area with a maximum value of PM_{10} (greater than 60 $\mu g/m^3$) located at the intersection of three districts as mentioned here: (i) east of the Puente Piedra district; (ii) west of the Carabayllo district; and (iii) north of the Comas district (Fig. 2). In downtown MALC, the simulated PM_{10} concentration ranges from 20 to 35 $\mu g/m^3$. Meanwhile, in the eastern MALC, the PM_{10} concentration predicted varies from 25 to 55 $\mu g/m^3$ (Fig. 2).

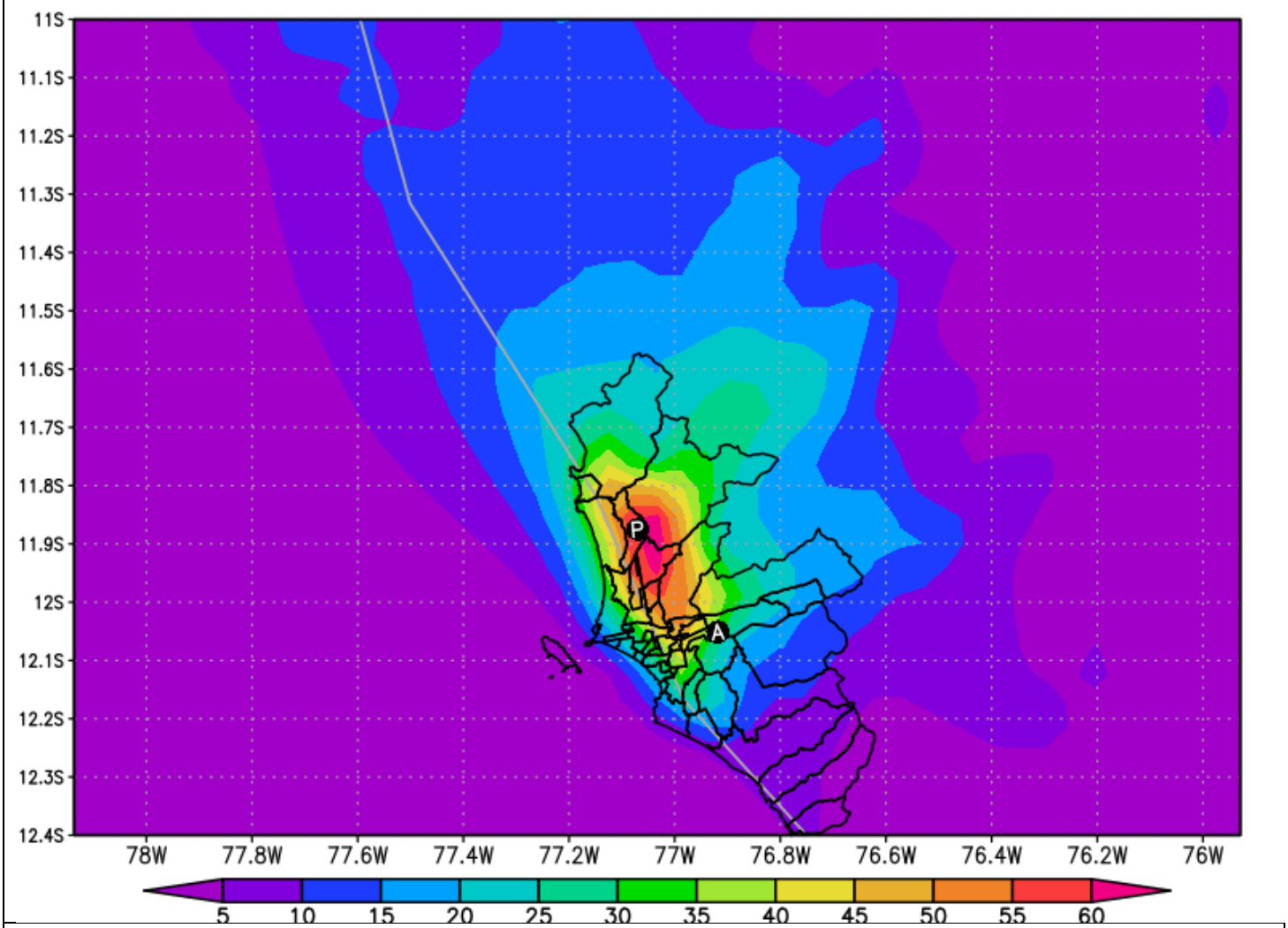

Fig. 2: Spatial variation of PM_{10} concentrations simulated with WRF-Chem model for February 2018 over the Metropolitan Area of Lima. The letters P and A indicate the Puente Piedra and Ate air quality monitoring stations respectively

4. Conclusion

In this study, numerical simulations were performed in the MALC in February 2018 using the WRF-Chem (version 4.0) 4.0) model to simulate the hourly PM_{10} concentration and evaluate the model performance. First, the model performance on on PM_{10} concentrations was calculated using in-situ observations at two traffic air quality monitoring stations named Ate Ate and Puente Piedra. In general, WRF-Chem model output reasonably captured the temporal variations of PM_{10} concentrations. However, the PM_{10} concentrations predicted were under-simulated by the model.

Acknowledgements

This research was supported under the CONCYTEC/FONDECYT contract 424-2019-FONDECYT with the Universidad Nacional Tecnológica de Lima Sur.

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