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Evaluating Hourly Sulphur Dioxide and Ground Ozone Simulated with the Air Quality Model in Lima, Peru

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***Abstract*—**Sulphur dioxide (SO_2) and surface-ozone (O_3) concentrations are associated with diseases. The objective of this research is to evaluate the effectiveness of the air-quality Weather Research and Forecasting model coupled to Chemistry (WRF-Chem) model with a horizontal resolution of 5 km x 5 km. For this purpose, the measurements of the hourly SO_2 and O_3 concentrations available in three air quality monitoring stations in Lima, Peru were used for the purpose of validating the simulations of the SO_2 and O_3 concentrations obtained with the WRF-Chem model in February 2018. For the quantitative evaluation of the simulations of these gases, statistical techniques were implemented, such as the average of the simulations; the average of the measurements; the Mean Bias (MeB); the Mean Error (MeE); and the Root Mean Square Error (RMSE). The results of these statistical metrics indicated that the simulated SO_2 and O_3 values over-predicted the SO_2 and O_3 measurements. For the SO_2 concentration, the MeB values varied from 0.58 to 26.35 μg/m³; the MeE values varied from 8.75 to 26.5 μg/m³; the RMSE values varied from 13.3 to 31.79 μg/m³; while for O_3 concentrations the statistical values of the MeB varied from 37.52 to 56.29 μg/m³; the MeE values varied from 37.54 to 56.70 μg/m³; the RMSE values varied from 43.05 to 69.56 μg/m³.

***Keywords*—**Ground-ozone, Lima, Sulphur dioxide, WRF-Chem.

I. Introduction

EXPOSURE to high levels of air pollutants can cause a variety of adverse health outcomes. In research in Greece, [1] demonstrated that people who have been exposed to high SO_2 concentrations have a "carotid atherosclerotic burden". In research in South Korea, [2] found that an increase in ground-level ozone (O_3) exposure is associated with "dry-eye disease". Primary air pollutions, such as SO_2 in urban areas in a megacity such as Lima with 11 million inhabitants, is emitted mainly from vehicular, industrial emissions, and cooking anthropogenic activities [3]. For this reason, it is important to carry out simulations of these atmospheric pollutants in Lima, Peru, as estimates of these gases were made in other cities of the world [4]-[6]. The aim of this research is to evaluate the hourly sulphur dioxide concentrations and hourly ground-ozone simulated with photochemical-dynamic WRF-Chem model in February 2018 in Lima.

II. Methodology and Data

The hourly concentrations of sulphur dioxide (SO_2) and hourly ground-ozone concentrations (O_3) were simulated using the 4.0 Air Quality WRF-Chem model version [7]. This is a chemistry model coupled with a meteorological model named WRF (Weather Research Forecasting). The WRF-Chen model is simulated air pollution concentrations and meteorological variables. For the initial and boundary conditions of the WRF-Chem model, we utilized the NCP-FNL "Operational Model Global Tropospheric Analyses" [8] with 0.25° x 25° horizontal resolution. The simulations of SO_2 and O_3 with the WRF-Chem model were performed with a horizontal resolution of 5 km x 5 km, which is the same resolution set up by the authors of [9]. To evaluate the WRF-Chem outputs results of hourly SO_2 and hourly O_3 we chose three air quality monitoring stations due to availability of SO_2 and O_3 measurements concentrations in Lima. On the other hand, the hourly SO_2 and O_3 concentrations measurements were obtained from the Servicio Nacional de Meteorología e Hidrología del Perú (SENAMHI). The locations of the three measurements stations are shown in Fig. 1. These are the San Borja (SB), the Carabayllo (CR), and the Puente Piedra (PP) measurement stations. The evaluations of the WRF-Chem model performance were calculated using the statistical analysis: MeB, MeE, and RMSE defined in (1)-(3) [10]:

$$MeB = \frac{1}{N}\sum_{i=1}^{N}(P_{rei} - O_{bsi}) \quad (1)$$

$$MeE = \frac{1}{N}\sum_{i=1}^{N}|P_{rei} - O_{bsi}| \quad (2)$$

$$RMSE = \sqrt{\frac{1}{N}\sum_{i=1}^{N}(P_{rei} - O_{bsi})^2} \quad (3)$$

where the sub-index I means the pair between predicted (with the symbol P_{rei}) and observed (with the symbol O_{bsi}) for each air quality station and for each hourly variation in time.

III. Results and Discussion

SO_2 and O_3 concentrations were extracted from the WRF-Chem model outputs located in the volume cell (with horizontal resolution of 5 km x 5 km and vertical resolution of the first layer) of air quality stations or areas nearby the stations. Table

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I presents the statistical evaluations of the WRF-Chem model compared with the SO_2 and ground-O_3 measurements in the SB, CR and PP stations.

Fig. 1 Location of the three air quality measurement stations in Lima: the San Borja (SB), the Carabayllo (CR), and the Puente Piedra (PP) measurement stations

TABLE I
THE SO_2 AND GROUND-O_3 HOURLY EVALUATIONS PREDICTED WITH THE WRF-CHEM MODEL IN LIMA

Contaminants	SO_2	SO_2	SO_2	O_3	O_3	O_3
Air Quality Station	SB	CR	PP	SB	CR	PP
Observed	18.4	4.3	13.3	11.7	19.7	14.5
Predicted	19.6	31.4	30.5	48.6	60.1	57.3
MeB (µg/m³)	0.58	26.35	17.18	37.52	56.29	43.36
MeE (µg/m³)	8.75	26.50	23.81	37.54	56.70	44.57
RMSE (µg/m³)	13.30	31.79	29.05	43.05	69.56	63.95

SB = San Borja station, CR = Carabayllo station, PP = Puente Piedra station.

A. Sulphur Dioxide

At the SB station, the SO_2 observed concentration mean was 18.4 µg/m³, while the SO_2 predicted mean was 18.4 µg/m³. The SO_2 MeB was 0.58 µg/m³ which indicated a slight over-prediction of the simulated SO_2 concentration with respect to the measured SO concentration; the MeE was 8.75 µg/m³; and the RMSE was 13.30 µg/m³. At the CR station, the SO_2 observed concentration mean was 4.3 µg/m³, while the SO_2 predicted mean was 31.4 µg/m³. The SO_2 MeE was 26.35 µg/m³ which indicated large over-prediction of the simulated SO_2 concentration regarding the measured SO_2 concentration; the MeE was 26.50 µg/m³; and the RMSE was 31.79 µg/m³. At the PP station, the SO_2 observed concentration mean was 13.3 µg/m³, while the SO_2 predicted mean was 30.5 µg/m³. The SO_2 RMSE was 17.18 µg/m³ which indicated the model error in simulating the SO_2 concentration; the MeE was 23.81 µg/m³; and the RMSE was 29.05 µg/m³. The result of this research regarding SO_2 concentration coincides with the results of research in Lebanon conducted by [10] which found that the SO_2 MeB =17.8 µg/m³; and the RMSE = 31.3 µg/m³, just by comparing simulated and measured hourly concentrations. Fig. 2 shows that the SO_2 concentration in Metropolitan Lima has the highest values (around 30 µg/m³) compared to the northern areas (27 µg/m³ of SO_2), the western areas (21 µg/m³ of SO_2), and the southern areas of Metropolitan Lima (21 µg/m³ of SO_2).

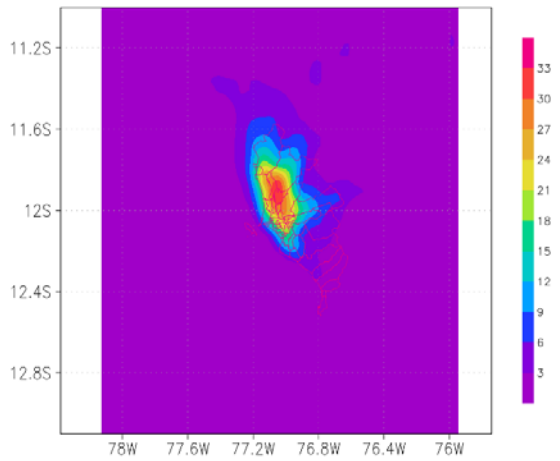

Fig. 2 Spatial variations of SO_2 concentration simulations (in µg/m³) over the Metropolitan Lima with the WRF-Chem model

B. Ground-Ozone

Regarding ground-O_3, the statistical analysis results showed that the model overpredicted at the SB, CR, and PP stations. The MeB, MeE, and RMSE over SB were 37.52 µg/m³, 37.54 µg/m³ and 43.05 µg/m³, respectively. Those over CR were MeB = 56.29 µg/m³, MeE = 56.70 µg/m³ and RMSE = 69.56 µg/m³, respectively. Those over PP were 43.36 µg/m³, 44.57 µg/m³ and 63.95 µg/m³, for MeB, MeE and RMSE respectively. On the other hand, over Beirut in the Easter Mediterranean, [11] showed RMSE = 38.6 µg/m³ and MeB = 25.7 µg/m³ for hourly ground-O_3 comparison. Fig. 3 shows that the highest ozone concentration (160 µg/m³) is located NNW (11.2 S, 70 W) of Metropolitan Lima.

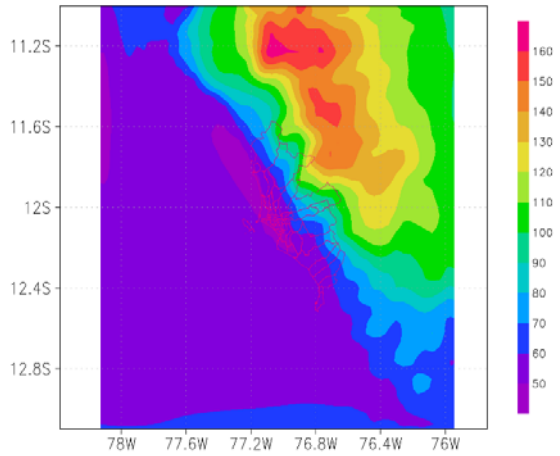

Fig. 3 Spatial variations of ground-ozone concentration simulations (in µg/m³) over Metropolitan Lima with the WRF-Chem model

Figs. 4-6 show the diurnal cycle of ground-ozone simulated using the WRF-Chem model on February 19, 2018 in the San Borja, Carabayllo, and Puente Piedra air quality stations in Lima, respectively, where the highest ozone value was noted around 13:00 local time in Lima (18 UTZ). Fig. 7 shows the vertical variations of ozone concentrations simulated with the WRF-Chem model with Lambert projections over the ozone peak (presented in Fig. 3) where the highest values of ozone

located in the middle of the troposphere can be observed. Fig. 8 shows that the highest value of ozone vertical variation (140 ug/m³) is located at level 10 of the WRF-Chem model.

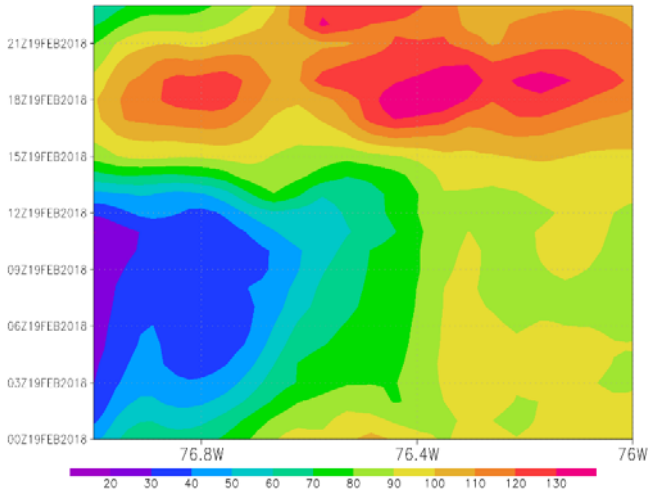

Fig. 4 Diurnal variations of ground-ozone concentration simulations (in µg/m³) over San Borja with the WRF-Chem model

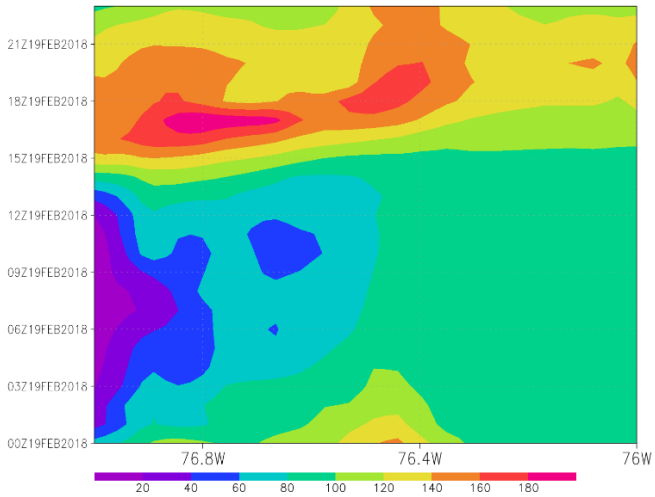

Fig. 5 Diurnal variations of ground-ozone concentration simulations (in µg/m³) over Carabayllo with the WRF-Chem model

C. Temperature and Relative Humidity Simulations with the WRF-Chem Model

Fig. 9 shows that the center of Metropolitan Lima and the coastal area have high temperature values (296 Kelvin) compared to southern Lima, northern Lima, and eastern Lima. Whereas Fig. 10 shows the spatial surface relative humidity (2 m above the surface) simulated with the WRF-Chem model in February 2018 where the relative humidity – HR in the central Lima area is drier (70-75% RH) compared to the Pacific Ocean (95% RH) and the northern Lima area (58% RH).

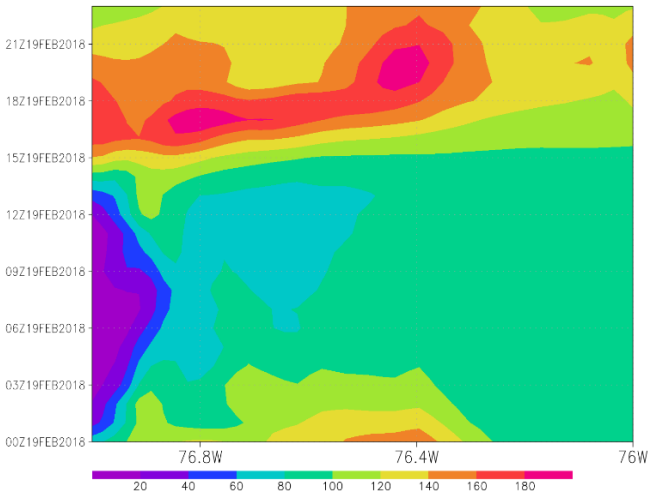

Fig. 6 Diurnal variations of ground-ozone concentration simulations (in µg/m³) over Puente Piedra with the WRF-Chem model

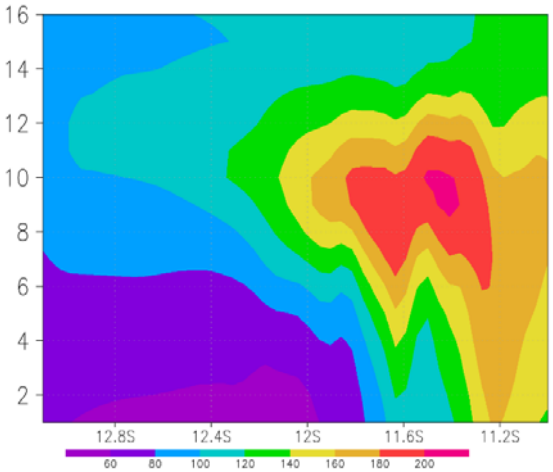

Fig. 7 Vertical variation of ozone was performed considering the fixed length (70° W) located in the highest ozone surface value zone of 160 ug/m³

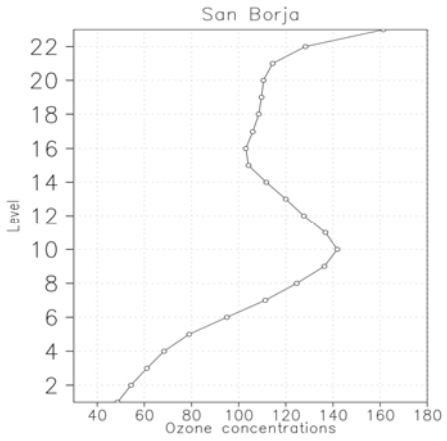

Fig. 8 Vertical variations of ozone concentration simulations (in µg/m³) over San Borja with the WRF-Chem model

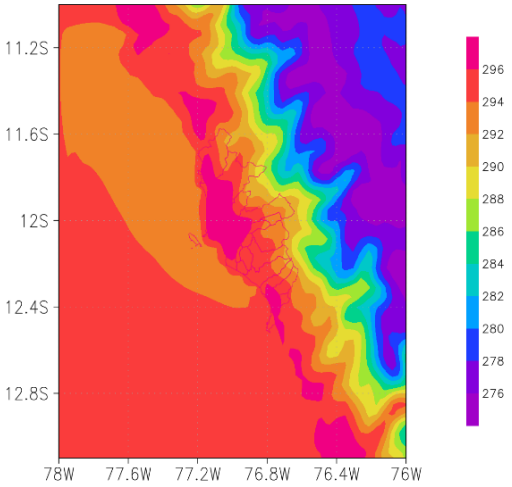

Fig. 9 Spatial variations of surface temperature simulations (K) over Metropolitan Lima with WRF-Chem model

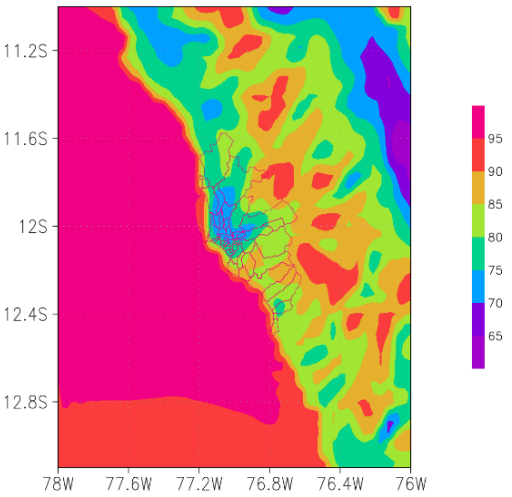

Fig. 10 Spatial variations of surface relative humidity (%) simulations over Metropolitan Lima with the WRF-Chem model

IV. Conclusion

This research shows the evaluation of sulphur dioxide (SO_2) and ground-ozone (O_3) simulations using the WRF-Chem model. For this reason, SO_2 and O_3 predicted were compared with the SO_2 and O_3 measurements using the statistical metric of MeB, MeE, and RMSE in Lima, Peru. The results of these statistical techniques noticed SO_2 were $0.58 \leq MeB \leq 26.35$ µg/m³, $8.75 \leq MeE \leq 26.5$ µg/m³, $13.3 \leq RMSE \leq 31.79$ µg/m³, while for O_3 were $37.52 \leq MeB \leq 56.29$ µg/m³, $37.54 \leq MeE \leq 56.70$ µg/m³, $43.05 \leq RMSE \leq 69.56$ µg/m³. The results of this research are consistent with the results of a research conducted in Lebanon by [11] published in an indexed journal. The future of this research project might be to carry out research to understand and reduce the overestimations in the estimates of the emission of SO_2 from the result of the simulations with the WRF-Chem model, in comparison with the measurements of SO_2.

References

[1] E. Oikonomou, G. Lazaros, and D. Tousilis, "The association of air pollutants exposure with subclinical inflammation and carotid atherosclerosis," International Journal of Cardiology, vol. 342, pp. 108–114, Nov. 2021, doi: 10.1016/j.ijcard.2021.07.056.

[2] Y. Kim, Y. H. Choi, M. K. Kim, H. J. Paik, and D. H. Kim, "Different adverse effects of air pollutants on dry eye disease: Ozone, PM2.5, and PM10," Environmental Pollution, vol. 265, Oct. 2020, doi: 10.1016/j.envpol.2020.115039.

[3] J. Ngarambe, S. J. Joen, C. H. Han, and G. Y. Yun, "Exploring the relationship between particulate matter, CO, SO_2, NO2, O_3 and urban heat island in Seoul, Korea," Journal of Hazardous Materials, vol. 403, Feb. 2021, doi: 10.1016/j.jhazmat.2020.123615.

[4] Z. He, P. Liu, X. Zhao, X. He, J. Liu, and Y. Mu, "Responses of surface O_3 and PM2.5 trends to changes of anthropogenic emissions in summer over Beijing during 2014–2019: A study based on multiple linear regression and WRF-Chem," Science of the Total Environment, vol. 807, Feb. 2022, doi: 10.1016/j.scitotenv.2021.150792.

[5] T. Sha, X. Ma, and J. Wang, "Improvement of inorganic aerosol component in PM2.5 by constraining aqueous-phase formation of sulfate in cloud with satellite retrievals: WRF-Chem simulations," Science of the Total Environment, vol. 804, Jan. 2022, doi: 10.1016/j.scitotenv.2021.150229.

[6] P. Wang, P. Wang, K. Chen, J. Du, and H. Zhang, "Ground-level ozone simulation using ensemble WRF/Chem predictions over the Southeast United States," Chemosphere, vol. 287, Jan. 2022, doi: 10.1016/j.chemosphere.2021.132428.

[7] G. A. Grell, S.E. Peckham, R. Schmitz, S. McKeen, G. Frost, W. C. Skamarock, and B. Eder, "Fully coupled 'online' chemistry within the WRF model," Atmospheric Environment, vol. 39, no. 37, pp. 6957–6975, 2005, doi: 10.1016/j.atmosenv.2005.04.027.

[8] NCEP, "National Centers for Environmental Prediction/National Weather Service/NOAA/U.S. Department of Commerce: NCEP FNL Operational Model Global Tropospheric Analyses, continuing from July 1999, Research Data Archive at the National Center for Atmospheric Research, Computational and Information Systems Laboratory, https://doi.org/10.5065/D6M043C6, 2000. Accessed 07 July 2021.

[9] O. R. Sánchez-Ccoyllo, C. G. Ordoñez-Aquino, Á G. Muñoz, A. Llacza, M. F. Andrade, Y. Liu, W. Reátegui-Romero, and G Brasseur. "Modeling Study of the Particulate Matter in Lima with the WRF-Chem Model: Case Study of April 2016," International Journal of Applied Engineering Research, vol. 13, no. 11, p. 10129, 2018, doi: 10.37622/ijaer/13.11.2018.10129-10141.

[10] M. T. Chuang, C. F. Wu, C. Y. Lin, W. C. Lin, C. C. K Chou, Lee, and S. S. K. Kong, "Simulating nitrate formation mechanisms during PM2.5 events in Taiwan and their implications for the controlling direction," Atmospheric Environment, vol. 269, Jan. 2022, doi: 10.1016/j.atmosenv.2021.118856.

[11] C. Abdallah, C. Afif, N. el Masri, F. Öztürk, M. Keleş, and K. Sartelet, "A first annual assessment of air quality modeling over Lebanon using WRF/Polyphemus," Atmospheric Pollution Research, vol. 9, no. 4. Elsevier B.V., pp. 643–654, Jul. 01, 2018. doi: 10.1016/j.apr.2018.01.003.