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Analytical Decision Supports System for Urban Air Quality Management in Tehran: Meteorological and Photochemical models

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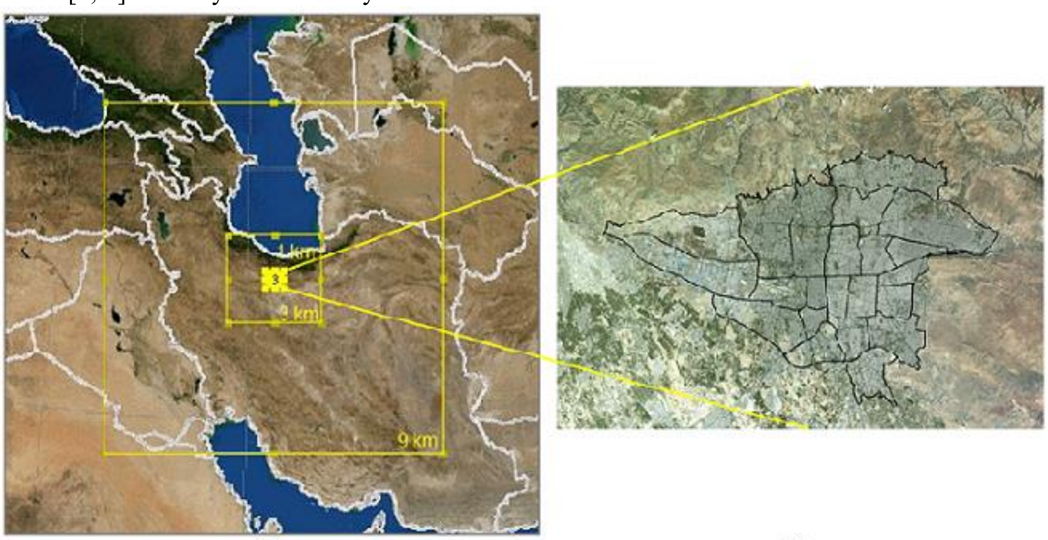
ABSTRACT
A new analytical air pollution modeling system is introduced in this paper to estimate concentrations of primary and secondary air pollutants and using it for further studies in order to improve the knowledge of pollutants emission and dispersion over Tehran, and developing a decision support system. For this purpose, WRF/CAMx modeling system was used to simulate the gas-phase pollutants concentrations including primary and secondary pollutants, over Tehran during a wintertime episode, which is characterized by very high concentrations of pollutants. Pollutants were triggered by meteorological conditions leading to a forced holiday imposed on citywide operations to protect the health of citizens. Based on calculated Values of NMB error, WRF performs acceptable in predicting temperature and wind speed. Generally, time series plots show that WRF performs acceptable in mild selected episode. Also, the daily trends of pollutant concentrations are greatly affected by changes in local meteorological conditions such as planetary boundary layer (PBL) height, temperature, wind, and relative humidity over the Tehran area. An underestimation in prediction of all pollutants concentrations episode at Poonak and Aghdasyeh sites show due to the insufficient emission data at the site position used for the simulation were seen. Results showed that WRF/CAMx modeling system proved to be a useful tool for analyzing urban environmental problems, investigating the impact of air quality control policies, and predicting critical conditions. However, there were weaknesses in input data and modeling system calibration that should be improved before using the system for further studies.

Key words: Air Quality Management; Air Quality Modeling; WRF; CAMx.

List of Abbreviations
WRF: Weather Research and Forecasting.
CAMx: Comprehensive Air Quality Model with extensions.
NMB: Normalized Mean Bias.
PBL: Planetary Boundary Layer.
CO: Carbon Monoxide.
NOx: Nitrogen Oxides.
PM: Particulate Matter.
HC: Hydrocarbon.
SO_2: Sulfur Dioxide.
CH_4: Methane.
AQCC: Tehran's Air Quality Control Company.
NCEP: National Centers for Environmental Prediction.
FNL: Final Analyses.
VOC: Volatile Organic Carbon.
FE: Fractional Error.

INTRODUCTION
Atmospheric pollutants which are of climate change, have dangerous impacts on human health and environment [1]. Developing countries usually experience severely high concentrations of air pollutants because of the rapid increase in industrialization, population, urbanization, and transportation without prompt emission controls. Tehran is the capital city of Iran, with an estimated area of 780km², and a population of 8.5 million. This city is Home to nearly half of the country's industrial firms, more than 10% of the country's population, and

more than three million vehicles. Tehran city is choked by air pollution, with more than one third of the year characterized by unhealthy air pollution conditions [2]. Pollutant emissions are caused by a variety of vehicular, commercial, and industrial sources in Tehran. Mobile sources are responsible for the majority of nitrogen oxides (NOx), carbon monoxide (CO), particulate matter (PM), hydrocarbon (HC) emissions. Also, stationary sources are account for the majority of sulfur dioxide (SO_2) emissions [3, 4]. Its geographic coordinates are 35°7′N and 51°4′E [5, 6]. As showed in Fig. 1b, Tehran has complex terrain conditions, which intensifies the city's air pollution problem [3, 7].Tehran sits on a sloping plateau at the foot of high-altitude mountain range Alborz, downstream of the prevailing winds. It is limited on three sides by hills. Therefore, the bowl form of the city adds to pollution entrapment, hampering the valley's ventilation. In winter time, due to the temperature inversions, stagnant polluted air remains close to the surface, increasing the pollutant concentrations to high levels. During the day, the wind blows from the city to the mountains and reverses direction during the night. In addition to the effect of the northern mountains, the western area of Tehran is affected by a dominant wind that blows from west to east and has a crucial role in spreading air pollution over the city. To estimate pollutants levels in Tehran, a few studies have been carried out that apply such air quality models [8, 9]. A study conducted by Tehran's Air Quality Control Co. (AQCC) shows that more than 70% of the air pollutants are generated by a mobile sources [10]. Shahbazi [11] showed the performance of WRF/CAMx modeling in estimation of primary and secondary gas phase pollutants. A significant impact of the initial and boundary concentrations on the accuracy of the model and level of pollutant concentrations over the city, was detected. Also, the effect of Odd-Even day traffic restriction policy on Tehran air quality was investigated using WRF/CAMx modeling system [11]. The results illustrated a satisfactory performance for both models in predicting meteorological parameters and pollutants concentrations. It was seen that the effectiveness of such scheme is highly related to the meteorological conditions, the type of the pollutant and the location under study. In similar studies, WRF/CAMx couple was used to in the eastern United States to simulate the relative contribution of and regional sources of surface ozone. Any reduction in emissions led to increase in ozone photochemical lifetime. The main purpose of this study was to introduce a useful tool using the Comprehensive Air Quality Model with Extensions (CAMx) model coupled with meteorological data obtained through the Weather Research and Forecasting model (WRF), for Tehran air pollution studies and developing an analytical modeling system in order to be used in decision making and improving the knowledge of pollutants behavior over Tehran.



(a) (b)

Fig. 1: (a) Tehran modeling domain, and (b) topography, which is surrounded by the Alborz Mountains on the north and east side.

MATERIALS AND METHODS

Photochemical modeling domain selection

In this study, The Comprehensive Air Quality Model with extensions (CAMx model, v6.0), [12]was used to model gas-phase pollutants over the Tehran modeling domain for the calendar year 2012, during a wintertime episode from November 30th to December 6th, 2012. In the study episode, because of the very high concentration of pollutants triggered by meteorological conditions, a forced holiday was imposed on citywide operations to protect the health of citizens. CAMx is an Eulerian photochemical model used for simulation of emissions, dispersion, chemical reactions, and removal of pollutants in the troposphere over a wide spatial range from urban up to continental scales. It has been thoroughly validated and has been extensively used worldwide for environmental impact assessment and state policy analyses [13- 19]. Therefore, CAMx model was used to compute pollutant concentrations over Tehran modeling domain. The first day of simulation was ignored to avoid the impact of initial conditions on the predicted results. The chemical mechanism used in this study was the carbon bond-V gas-phase mechanism [20]. The domain contains 90 × 81 grid cells with a resolutions of 1km × 1km and 16 vertical layers. The CAMx domain was chosen based on the WRF third modeling domain and consists of a 1km grid over Tehran, from 50.94281°W to 51.92804°E and 35.27192°S to 35.99120°N. In order to feed CAMx model, initial and boundary concentrations prepared based on MOZART output data.

Meteorology

The non-hydrostatic, mesoscale Advanced Research Weather Research and Forecasting (WRF-ARW) model, version 3.4, is used as the meteorological model [21]. This mesoscale model is a state-of-the-art atmospheric simulation system based on the fifth-generation Penn State/NCAR mesoscale Model (MM5) [22] and widely used as a preprocessor in air quality modeling [23, 24]. Meteorological data for the study episode over the Tehran domain were calculated using the Weather Research and Forecasting (WRF) model with three nested domains having 9, 3, and 1km resolution, respectively (Fig. 1). The 9-3-1km domains were run together efficiently using a two-way grid nesting in WRF. WRF physical options considered for the simulation are: Grell cumulus scheme at the 9-km resolution domain and no cumulus parameterization for the smaller grids, RRTM radiation scheme, MRF PBL scheme and WSM 6-class graupel microphysics scheme with selected unified Noah land-surface model. The National Centers for Environmental Prediction (NCEP) Final Analyses (FNL) data of 1° × 1° (longitude–latitude) and a vertical resolution of 27 pressure levels was used to define the ICs and BCs. After running WRF, the WRF/CAMx preprocessor [12] was used to translate meteorological data from 1km resolution WRF output to the format required by CAMx.

Emissions Matrix

The emission data for this study were provided by the Air Quality Control Company (AQCC), and Tehran Municipality Company is responsible for the air quality monitoring of the city. The emission matrix was calculated based on the results of several studies that incorporated mobile and stationary emission sources, including a petroleum refinery located in the southeast of the city. The matrix includes CO, CH_4, NOx, SO_2, and VOC for mobile and main industrial emissions, in 106 × 73 grid cells over Tehran with a resolution of 500 m × 500 m. In order to convert VOCs to carbon bond-V VOC species, the splitting factors provided by the U.S. Environmental Protection Agency [25] were used. These emission data were converted to the CAMx modeling domain and also the UAM format, using an interface code written in FORTRAN. Contribution of main pollutants sources on total pollutant emission over Tehran in the study conducted by JICA [26] are summarized in Table 1. In this paper the used on -road vehicle emission inventory was the modified version of JICA emission inventory for on-road vehicle sources by AQCC base on traffic data for about 13 thousand roads, derived from travel demand model simulation for calendar year 2005. Hourly maximum emission data for CO, NOx, and VOC pollutants over Tehran are shown in Fig. 2.

Table 1: Contribution of main pollutants sources on total pollutant emission over Tehran.

Sector	Emission Percent					
	SOx	NOx	CO	HC	SPM	Total
Total Manufacturing	64.0	41.8	5.4	2.5	6.2	18.2
General service & Household	13.6	11.1	0.3	13.2	2.5	4.6
Energy Conversion	19.2	17.7	0.2	14.1	1.4	5.9
Transport	3.2	29.3	94.1	70.2	87.9	71.2

RESULTS

Meteorology

To evaluate the WRF model performance over Tehran, temperature at 2m altitude and wind speed and direction at 10m altitude was compared against observations at Resalat meteorological station, located at 51° 27' 40.88″ and 35° 44' 25.71″ (longitude-latitude), shown in Fig. 3. Location of Resalat station in Tehran is shown in Fig. 4. Average predictions and observations of each parameter at Resalat station and normalized mean bias (NMB) error for each were calculated and results are summarized in Table 2.Times series plots of 2m observed and predicted temperatures and also value of NMB error, which are 7% for the study episodes, respectively, show that the WRF model had good performance in modeling daily trends and hourly temperature values over the Tehran modeling domain. During selected episode, temperature values and hourly trends were well predicted by the model and just a small underestimation is seen in the daily maximum temperature in the first two days. At the end of the episode, the temperature decreased because of humidity and cloud volume increased, which led to reduction of radiation and hence rate of chemical reactions in the atmosphere. The values of wind speed were well predicted by the model. As shown in Table 2, the average wind speed in this episode was extremely low and only towards the end of the episode, on December 5, the maximum wind speed increased to about 5m/sec. The average bias of wind speed shows underestimation in the winter time episode. Value of NMB error shows good model performance in predicting wind speed. Generally, time series plots show that WRF performs acceptable in mild selected episode.

Table 2: Summary of WRF performance statistics for temperature (˚C), wind speed (m/s) and wind direction (deg.).

Temperature (˚C)			Wind speed (m/s)			Wind direction (deg.)		
Avg-Obs	**Avg-Pre**	**NMB**	**Avg-Obs**	**Avg-Pre**	**NMB**	**Avg-Obs**	**Avg-Pre**	**NMB**
November 30 to December 6								
8.78	8.69	0.07	1.67	1.34	-0.06	134.0	134.83	-0.29

Evaluating CAMx model performance

CAMx model results in the study episode compared with observations from three monitoring stations shown in Fig. 4. Concentrations predicted by the model were compared against observations at Poonak and Aghdasyeh stations, illustrated in Fig. 5 and 6. Mean average observations and predictions and values of NMB from Fig. 5 and 6 were calculated and are summarized in Tables 3 and 4. Concentrations of O_3 were not measured correctly at both stations; therefore, data from Sharif station were used for evaluating model performance in predicting O_3 concentrations. Poonak monitoring station is located in the northwest part of Tehran and Aghdasyeh monitoring station is located in the northeast part, and both of them are near the northern mountains. As showed in Fig. 5 and 6, hourly trend variation of pollutant concentrations is high at Poonak and Aghdasyeh sites. On December 3 and 4, a forced holiday was imposed on citywide operations to protect the health of citizens, but the emission reduction caused by this was not considered in the simulation. Hence, the maximum concentration of primary pollutants for the entire episode predicted by the model was mostly observed on December 4. During the last two days of the modeling episode, the relative humidity increased intensively over Tehran and precipitation occurred; this caused the level of observed and predicted pollutant concentrations to decrease dramatically. Values of NMB errors at Poonak site varied from 68 to −38% for primary pollutants, which show poor model performance at this station. At Sharif monitoring site, which is located in a high-emission area of Tehran, the maximum values of O_3 were overestimated for December 1, 2, and 3. During the last three days of the modeling episode, the level of O_3 concentration decreased and was underestimated by the model because of meteorological conditions.

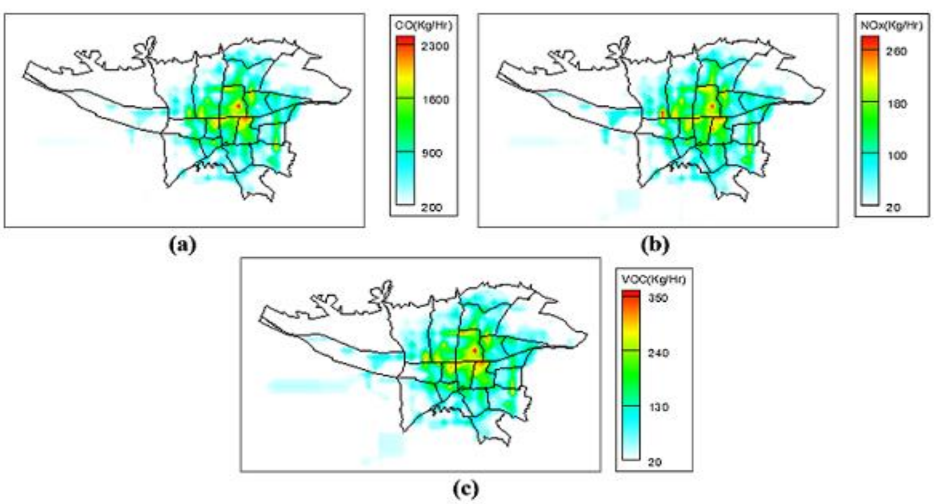


Fig. 2: Sample emission data for (a) CO, (b) NOx, and (c) VOC pollutants (kg/hr.) on the 1-km grid at 12:00 AM.

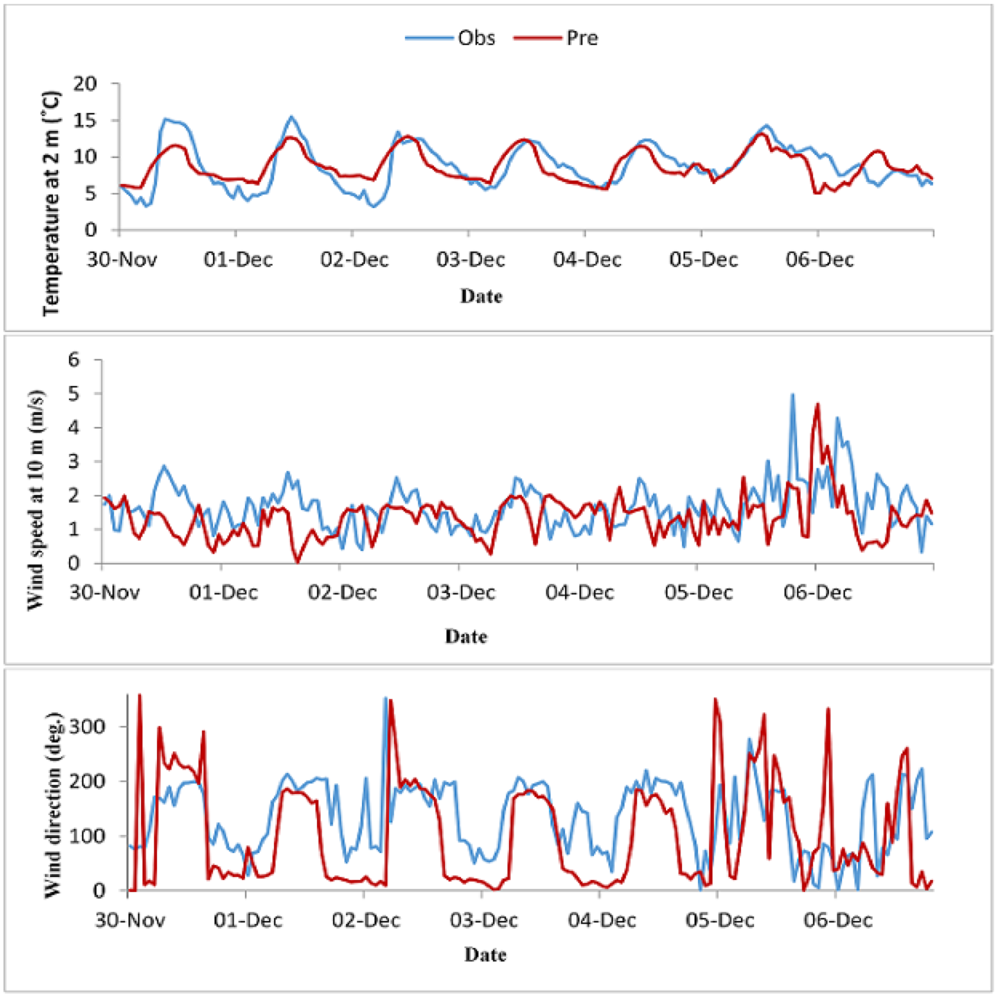


Fig. 3: Hourly time series of observed and predicted temperature at 2m, wind speed and wind direction at 10m, at Resalat site.

Table 3: Summary of CAMx performance statistics for NO (ppb), NO_2 (ppb), CO (ppm) and SO_2 (ppb) at Poonak station and O_3 (ppb) at Sharif station during November 30 to December 6, 2012.

	Observation	MOZART IC & BC	
Pollutant	**Mean-Obs**	**Mean-Pre**	**NMB**
NO	99.95	42.67	-0.54
NO_2	50.11	26.55	-0.50
O_3	8.89	6.66	-0.38
CO	3.97	1.75	-0.38
SO_2	33.44	10.44	-0.68

Table 4: Summary of CAMx performance statistics for NO (ppb), NO_2 (ppb), CO (ppm) and SO_2 (ppb) at Aghdasyeh station during November 30 to December 6, 2012.

	Observation	MOZART IC & BC	
Pollutant	**Mean-Obs**	**Mean-Pre**	**NMB**
NO	105.41	25.00	-0.72
NO_2	36.47	25.84	-0.37
CO	3.86	1.84	-0.53
SO_2	40.63	10.97	-0.73

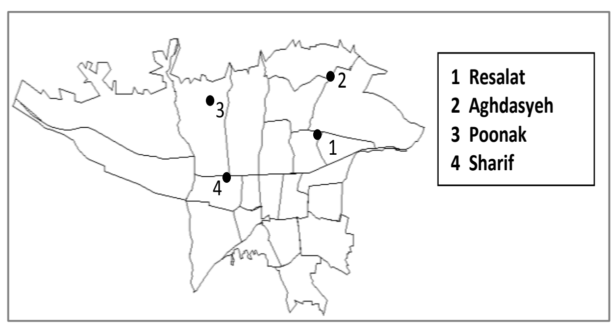


Fig. 4: Monitoring stations used for the WRF/CAMx model validation.

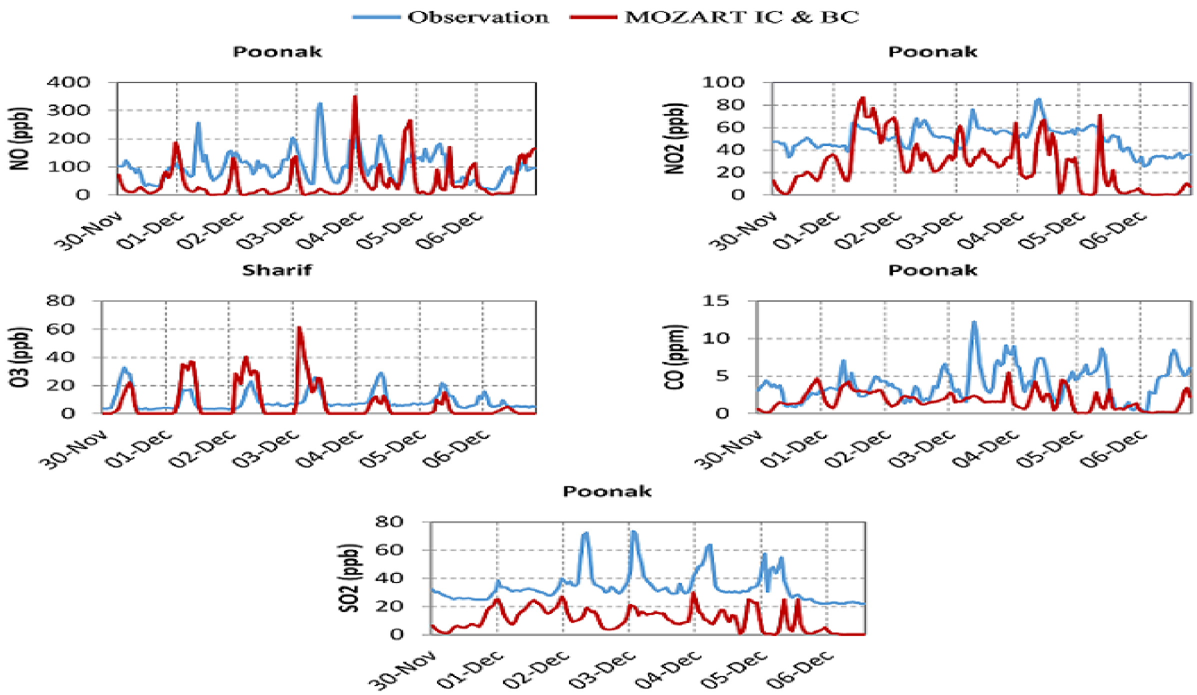


Fig. 5: Hourly time series of observed and predicted NO, NO_2, CO and SO_2 concentrations at Poonak station and O_3 concentrations at Sharif station, during November 30 to December 6. (— Observation — MOZART IC & BC).

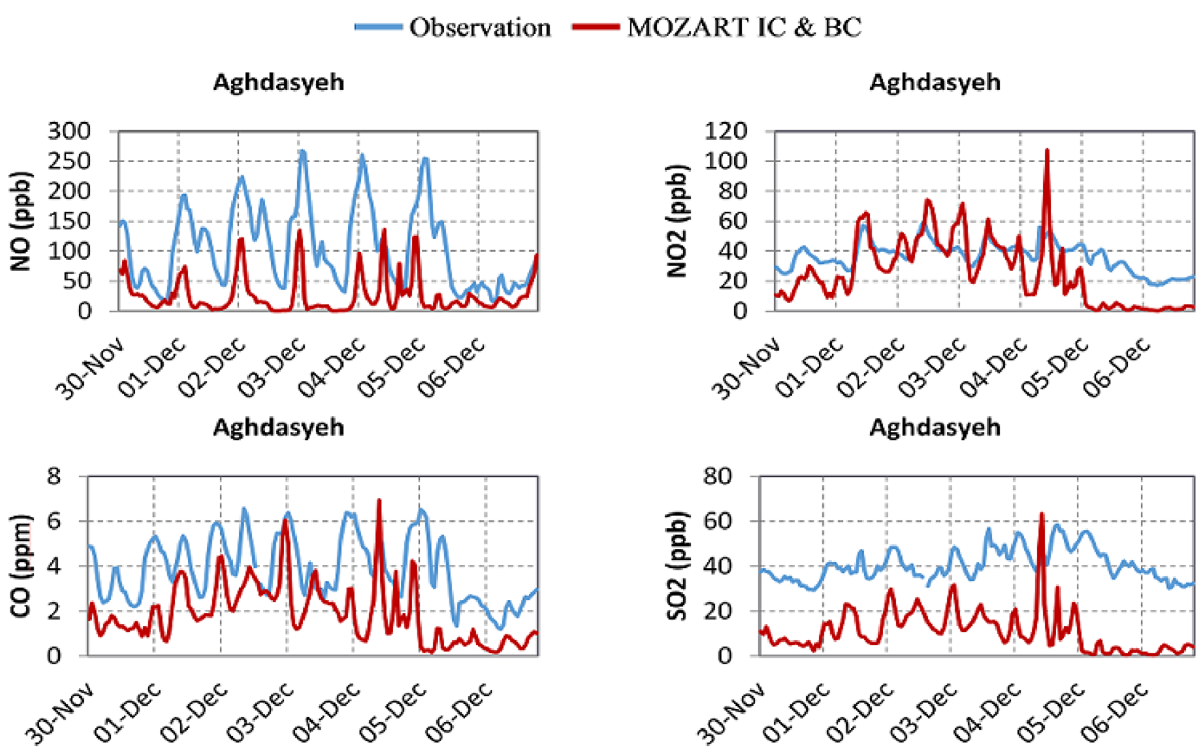


Fig. 6: Hourly time series of observed and predicted NO, NO_2, CO and SO_2 concentrations at Aghdasyeh station, during November 30 to December 6. (— Observation — MOZART IC & BC)

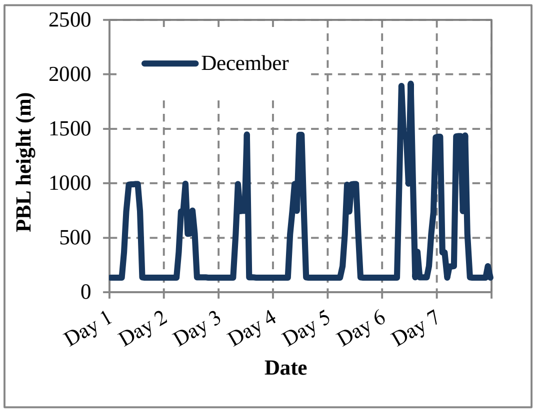


Fig. 7: Time series of simulated Planetary Boundary Layer (PBL) height for July 7 to 13 and November 30 to December 6.

Investigating the impact of meteorological conditions

CAMx simulation in the study episode was used to analyze the influence of meteorological conditions on pollutant concentrations. Pollutant concentrations and daily trends can be greatly affected by changes in local meteorological conditions such as solar radiation, wind direction, wind speed, relative humidity, and temperature over the Tehran area. Here the impact of meteorological parameters such as planetary boundary layer (PBL) height, temperature, wind, and relative humidity in the study episode was analyzed. Fig. 7 shows the hourly variation of PBL height during the episode. Figs. 8a, 8b and 8d show the spatial distribution of the 2 m temperature, the 10 m wind, and relative humidity at the lowest level of the WRF in the 1km domain at 12:00 UTC on December 2, 2012, respectively. Also, Fig. 8d shows the spatial distribution of relative humidity at 24:00 UTC on December 5. The study episode was characterized by low temperatures, wind, and PBL height, with most of the Tehran area dominated by easterly and southeasterly winds. The spatial distribution of relative humidity, shown in Figures 8c and 8d, indicates that the humidity in the selected episode was generally high, especially on December 5 and 6. Because of increased cloud volume and the occurrence of precipitation, the relative humidity increased dramatically. The average distribution of predicted NO, NO_2, CO, O_3, and SO_2 concentrations in the CAMx lowest level over the Tehran modeling domain for November 30–December 6, 2012, are illustrated in Fig. 9.

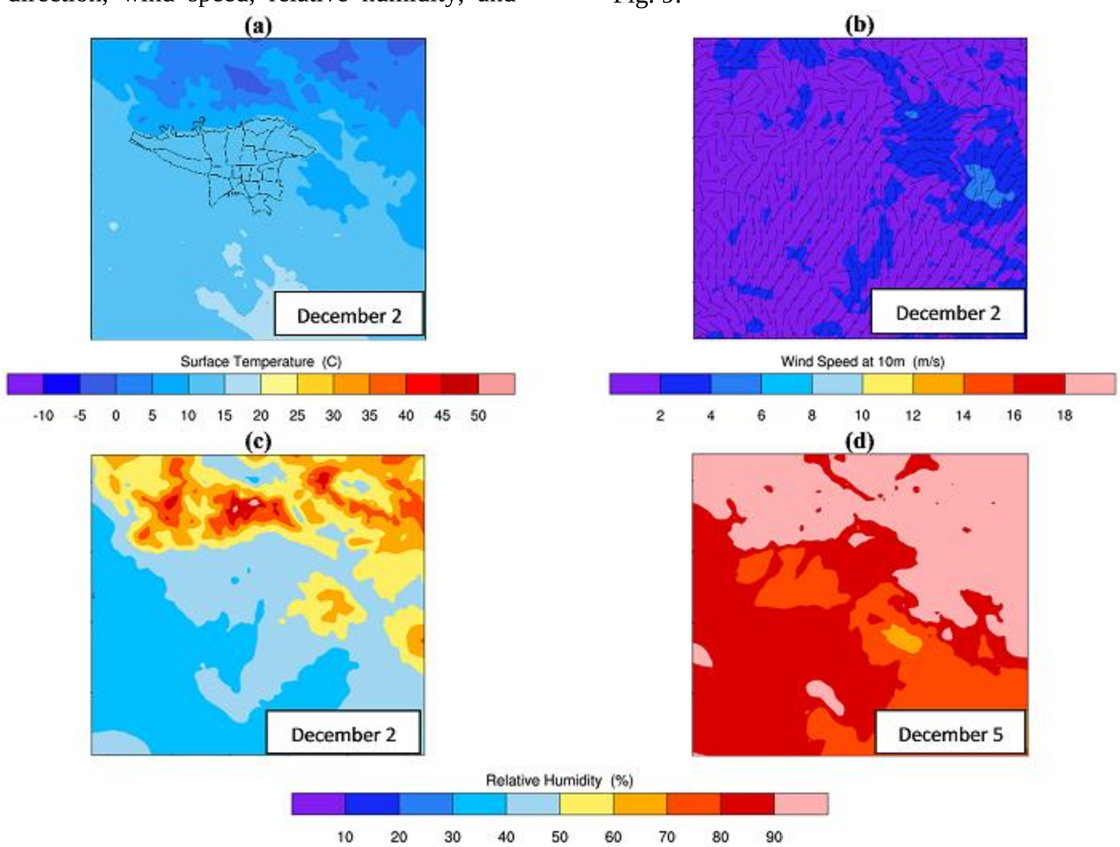


Fig. 8: WRF simulated (a) 2-m temperature, (b)10-m wind, WRF-simulated (c & d) relative humidity (%) at the lowest model level in Domain 3 at 12:00 UTC for (a), (b), (c) and 24:00 UTC for (d).

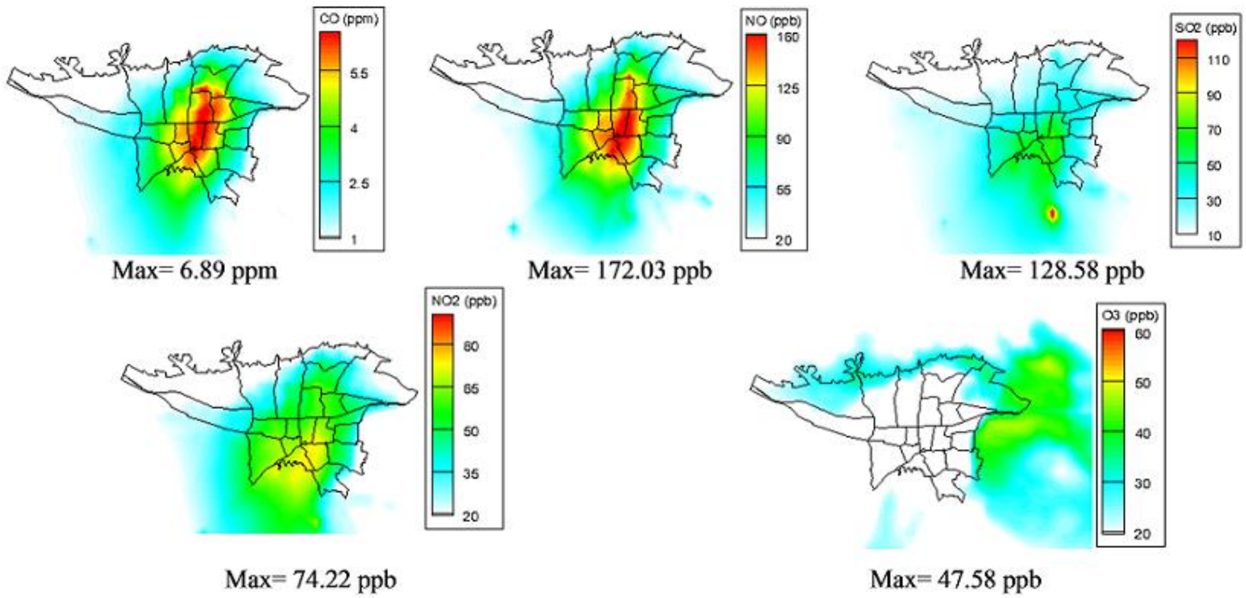


Fig. 9: Average distribution of CO, NO, NO_2, O_3 and SO_2 concentrations over Tehran during November 30 to December 6 (right), 2012.

DISCUSSION

Observed high hourly trend variation of pollutant concentrations can be due to the effect of the northern mountains, which affect wind field in the northern parts of Tehran [4, 27, and 28]. Values of average bias and time series plots for the entire winter episode at Poonak and Aghdasyeh sites show an underestimation in prediction of all pollutants concentrations, which led to an increase in NMB errors. In similar study Maciejewska [29] showed that in general, WRF-CAMx modelling system underestimated the measured pollutant concentrations. For both O_3 and particulate matter in various averaging time series have been fulfilled at a satisfactory level, based on the analysis of the fractional error (FE) skill criteria, fractional bias (FB) and, the benchmark of index agreement (IA). In current study, the main reason for WRF-CAMx modelling system underestimation is insufficient emission data at the site position used for the simulation because some of the main pollution sources at the western area of Tehran, such as the Tehran-Karaj highway and Mehrabad airport, were not considered in the emission data [29]. Underestimation of nighttime O_3 emission may have been caused by the vertical diffusion coefficient calculated by the WRF model, emission data, or chemistry. Differences between CAMx results and observations may be related to insufficient emission data used for the simulation [11]. The data are old, and do not reflect emissions from some main pollution sources such as entranceways in the west, east, and southern parts of city, the airport, stationary sources, and roads and streets that have been added to the city as a result of city expansion during recent years. This may have caused an underestimation of pollutant concentrations at background stations and regions far from the city center [12]. In addition, inaccurate speciation, meteorology, and local impacts at the monitoring stations used for model validation may have impaired results. Small domain used for CAMx model simulation without using nesting option caused boundary concentrations affecting more on model results. Hence, further studies should be conducted in order to investigate the impact of domain number, size and resolution on model results. Also, during the last three days of the episode, increased cloud volume over Tehran led to a decrease in radiation and hence rate of chemical reactions in the atmosphere [30]. Obvious impact of meteorological conditions is seen in the simulated spatial distribution, location, and magnitude of the predicted pollutant concentrations. In the selected episode, the maximum level of concentrations was more dispersed over Tehran because of meteorological conditions, mainly lower levels of wind speed and PBL height, which impact vertical mixing and horizontal transportation of pollutants. These conditions led to the maximum levels of NO, CO, and SO_2 primary pollutants to become dramatically high. In the center of the city, higher rates of NOx emission led to consuming O_3 in chemical reactions. Hence, minimum O_3 concentrations are seen in the high-emission areas of Tehran. During the episode, the dominant daytime wind direction caused O_3 to be mostly produced in the eastern part of Tehran. During the episode, limitations in horizontal transportation and vertical mixing resulted in average concentrations of primary pollutants more dispersed over the city from north to south [24, 9, 31]. CAMx modeling for the Europe domain using input data for meteorology, emissions, and boundary conditions under predicted the concentration trends for all pollutants both in summer and winter, except for SO_2, which generally had little bias. They illustrated that any changes in emission inventory, boundary conditions and metrological input data have an important role in the air quality model performance. Further studies on separating the influences of emissions from meteorology and boundary conditions on model performance, based on the simulation of the response to emission changes over time, modeling different years which are separated by emission reductions in response to control strategies are needed [19]. In addition, further investigations based on the Comprehensive Air-quality Model with Extensions (CAMx) modeling to simulate the relative contribution of local and regional sources of surface pollutants like ozone [32] to determine how chemistry and emissions within the domain can affect the production, loss, lifetime, and transport of trace gases are required.

CONCLUSION

In this paper, the WRF/CAMx modeling system was used as an analytical tool to study pollutants emission and dispersion over Tehran modeling domain in a wintertime episode in order to introduce a useful tool for Tehran air pollution researches. The selected episode took place in December 2012, during which high measured concentrations of gaseous pollutants were caused by meteorological conditions. The performance of WRF/CAMx modeling tool was evaluated through using air quality monitoring station data for a set of gaseous pollutants. Predicted meteorological parameters and average spatial distribution of pollutants over Tehran shows that during the study episode over the city of Tehran domain, given the complex terrain of the city, gaseous pollutants accumulate mostly because of the absence of removal mechanisms such as advection. Gaseous pollutant concentrations increase dramatically during such episodes, which could lead to unhealthy and dangerous levels. Results shows the need of further calibrations and tuning of parameters of the model more precisely, such as preparing more accurate emission inventory data from different type of sources within the area, sensitivity analysis of results to model setup parameters consists of domain numbers, size and resolution, number of vertical levels and initial and boundary concentrations, before using the system for daily air quality forecasts and awareness.

ETHICAL ISSUES

Ethical issues such as plagiarism have been observed by authors.

CONFLICT OF INTEREST

There was no conflict of interest.

AUTHORS’ CONTRIBUTION

All authors contributed equally.

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