

## Modeling of Air Pollutants' Dispersion by Means of CALMET/CALPUFF (Case Study: District 7 in Tehran city)

Joneidi, N.<sup>1</sup>, Rashidi, Y.<sup>2\*</sup>, Atabi, F.<sup>1</sup>, Broomandi, P.<sup>3</sup>

1. Faculty of Environment and Energy, Islamic Azad University, Science and Research Branch of Tehran, Iran
2. Environmental Sciences Research Institute, Shahid Beheshti University, Tehran, Iran
3. Department of Chemical Engineering, Masjed-Soleiman Branch, Islamic Azad University, Masjed-Soleiman, Iran

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**ABSTRACT:** The current study aims at modelling the dispersion of two pollutants, namely CO (carbon monoxide) and SO<sub>2</sub> (sulfur dioxide) released from District 7 of Tehran Municipality, from 20 main line sources, by means of CALPUFF modeling system. CALPUFF is a non-steady state puff modeling software which employs meteorological, terrain, and land-use data to effectively simulate air pollutants' dispersion from a given source. CALMET software has been applied to provide meteorological conditions within the study domain. The study has been carried out on September 30, 2012 and shows that the modeled concentrations have been below both Iranian air ambient standard and NAAQS standard for CO and SO<sub>2</sub>. It also compares the measurements from the monitoring station of Setad Bohran, showing that the simulated hourly mean concentrations of the SO<sub>2</sub> and CO do not follow similar temporal patterns for measurement values. For the absolute value, model results seem to be highly underestimated, compared to the monitored data ( $R^2 = -0.41$ ).

**Keywords:** Air pollution concentration, Iranian Ambient Air Quality Standard, Temporal pattern, CO, SO<sub>2</sub>

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### INTRODUCTION

It is vital to know about pollution and, specifically, atmospheric pollution processes in order to handle air quality problems; as a result, interpreting temporal and spatial evolution of air pollution needs detailed and extensive weather information, due to their strong relation. For conducting meteorological researches, a significant basis is provided by the measurements obtained from weather sites, surface, and upper air.

However lack of sites in every location and time (including upper air data) is biggest limitations of this basis since it is needed to know the evolution of atmospheric phenomena in detail (Hernández- Garces et al., 2015). As such, accurate meteorological models let us cover those faults. Nowadays, it is possible to choose among a large number of possible atmospheric model setups to obtain the best results, suited to the characteristics of the studied region and the phenomena. As a result, there is no universal atmospheric model setup capable of being

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\*Corresponding author, Email: [y\\_rashidi@sbu.ac.ir](mailto:y_rashidi@sbu.ac.ir)

applied on every region and phenomena, because it should be validated against monitored data to determine the degree of modeling results' accuracy and to obtain a suitable model setup (Hernández- Garces et al., 2015; Holnicki et al., 2017; Holnicki et al., 2016; Demirarslan & Doğruparmak, 2016). CALPUFF has been adopted in a number of works to model pollutants' transfer and dispersion.

In Christchurch (New Zealand), Varna and Gimson (2002) used CALPUFF to simulate the inter suburb dispersion of particulate matter pollution during a wintertime particulate pollution episode. Also, CALPUFF was applied by Levy et al. (2002) on meteorological data from the National Oceanic and Atmospheric Administration's rapid update cycle model to study the impacts of primary and secondary particulate matter across a grid in the Midwest, USA, released from a set of nine power plants in Illinois. The impacts of roadway proximity on ambient concentrations of three dangerous air pollutants was studied by Cohen et al. (2005) who developed a regression model to approximate and determine the simulated concentrations of CALPUFF. A back trajectory method, using CALPUFF model, was employed by Jiang et al. (2003) in a reverse diffusion mode to study the details of ozone formation within the Puget Sound area in western Washington State, USA. The ambient air quality around an industrial estate was investigated in order to predict the ground level concentration of SO<sub>2</sub> under different scenarios by means of industrial source complex short term (ISCST3) in India (Bandyopadhyay, 2009). The usage of CALMET/CALPUFF is well-known which as a well-established Lagrangian simulating system, with several validation tests being published (Demirarslan et al., 2017; Cohen et al., 2005; Dresser & Huizer, 2011; Fishwick & Scogie, 2011; Ghannam & El-Fadel, 2013; Levy et al., 2003; Protonotariou et al., 2005; Yau et al., 2004;

Holnicki et al., 2016; Affum et al., 2016; Affum et al., 2015). as in Similar to operational scenarios, limited available pollution and meteorological datasets draw uncertainties both in measurements and models results and it is expected that the models will display a worse performance (Khamsimak et al., 2012). The current study employs a CALMET diagnostic model to get both surface and upper air data. Also, it has applied the CALPUFF to model the local dispersion of CO and SO<sub>2</sub>, released from 20 main line sources in District 7 of Tehran Municipality, comparing the measurements from monitoring station of Setad Bohran for both air pollutants on September 30, 2012.

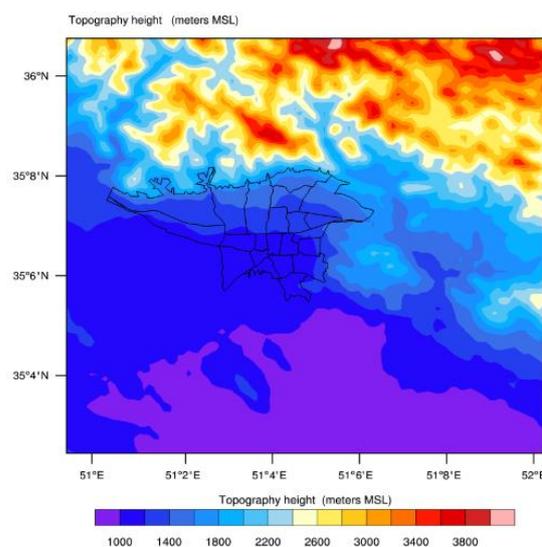
## **MATERIAL AND METHODS**

Tehran, capital of Iran, is located on the southern slope of the Alburz mountain range (35° 41' N - 51° 25' E), 1000-1800 meters above the mean sea level (Figure 1), generally having a moderate to dry climate. The significant urban expansion of the city during the last 3 to 4 decades has been due to the high rate of rural-urban migration, population growth, strong tradition of centralization, and dense urban infrastructure. Therefore, an over increasing trend in energy consumption can be seen in the capital. Located in some valleys, Tehran is surrounded on the north, northwest, east, and southeast by high to medium-high (3800-1000 m) mountains. More rainfall and vegetation cover is witnessed at northern part which is about 600-700 meter higher than the southernmost one, bordering central deserts of Iran (Madanipour, 1999; Ketabi, 2004; Malakooti, 2011). These geographical features keep influencing the meteorological fields in Tehran which has a population of 8.5 million (in contrast to the two hundred thousand people living in the city in 1920), with an estimated area of 780 km<sup>2</sup>. More often than not, daytime population exceeds 12 million inhabitants on workdays, showing the highly dynamic

temporal and spatial distribution of population in Tehran Metropolis. Huge amount of air pollutants are released by a very large population of motor vehicles (more than two million), fuel and electricity consumption, and many factories in this area. As a result, it is reported that air pollution has significant impact on the quality of urban inhabitant's life, simultaneously worsening urban environment and climate (Malakooti, 2011). The PSI (Pollutant Standards Index) system, developed by the EPA (National Air Quality and Emissions Trends Report, 1997), has been adopted by Tehran Air Quality Control Company (AQCC) to report daily air quality. It is capable of providing a simple number on a scale of 0-500 related to the health effects of the air quality levels. PSI values during recent 18 years show that air quality often fell in the "moderate" category ( $50 < \text{PSI} < 100$ ) and exceeded the threshold values ( $\text{PSI} = 100$ ) in 75 to 169 days (20 - 46%) annually. The share of Carbon Monoxide is 89% (with an average concentration beyond 4.5 ppm for 8 hours) and the share of PM10 is 19% (with an average concentration more than  $75 \mu\text{g}/\text{m}^3$  for 24 hours) in critical pollutants, responsible for the majority of unhealthy days in Tehran. This work used CALPUFF to predict  $\text{SO}_2$  and CO dispersion in District 7 of Tehran Municipality (Figure 2), comparing the model simulation with measurement results from Setad Bohran Monitoring Station, located in District 7 on September 30, 2012 to evaluate prediction accuracy. The highest PSI values of CO were recorded in November 2012 and the highest PSI values of  $\text{SO}_2$  belonged to January 2012. But the lowest PSI values of CO was seen in March and the lowest PSI values of  $\text{SO}_2$  was recorded in May 2012.

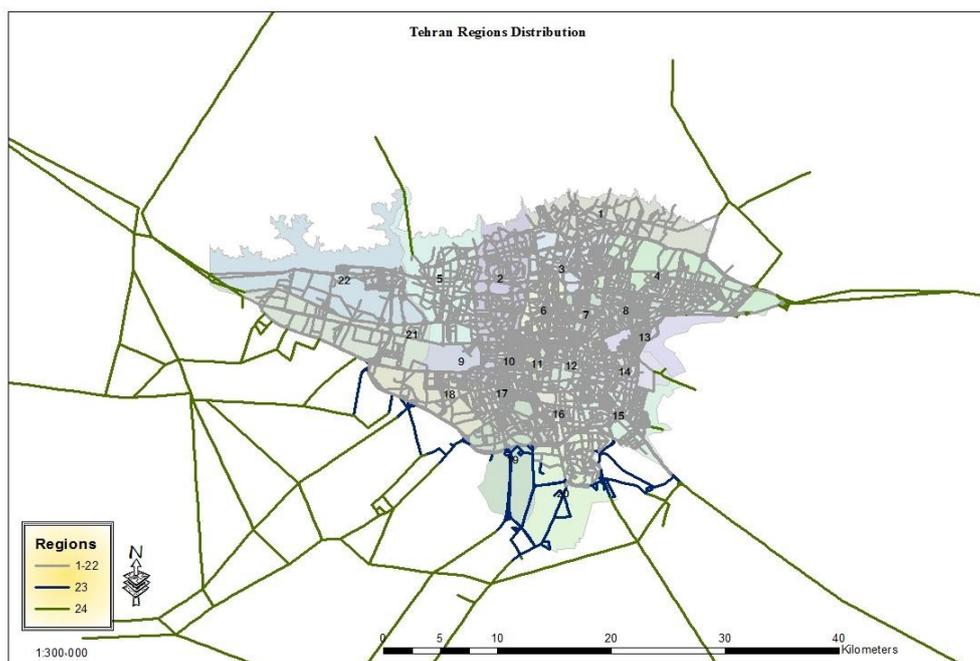
The air pollutants' dispersion is not only affected by the terrain, but is also altered by the wind vectors. Therefore, surface and upper air meteorological data were used in the modeling. The surface meteorological

data were taken from the Mehrabad Meteorological Station ( $35^\circ 41' 21'' \text{ N}$ ,  $51^\circ 18' 49'' \text{ E}$ ). The chosen set of data belonged to September 30, 2012. Initially, this date was selected as there were full sets of meteorological data available. Also, the final choice would depend on whether the full sets of upper air data were available or not. Afterwards, these surface meteorological data were converted to a specific format which would produce an output so that the surface meteorological data could be incorporated into CALMET program. Data for upper air attributes were acquired from Mehrabad station ( $35^\circ 41' 21'' \text{ N}$ ,  $51^\circ 18' 49'' \text{ E}$ ), which had been chosen thanks to its geographically closeness to the surface station as well as the point of interest.



**Fig. 1. Topography of Tehran city, being surrounded by the Alborz Mountains on the north and east side**

Keeping the date, used to retrieve the surface data, at a constant variable, upper air data was extracted from the website database. The meteorological data were converted into a format that could be used in conjunction with CALMET processor. Once more, the upper data were chosen for the specific date, based on their availability in this database along with the aforementioned surface meteorological database.



**Fig. 2. Location of districts in Tehran city**

As a meteorological model, CALMET is capable of generating hourly temperature and wind fields in the studied area. It contains two modules, namely the micrometeorological and the diagnostic wind field module, used for the analysis of overland and overwater regions (Abdul-Wahab et al., 2014; Abdul-Wahab et al., 2016). The geophysical and other prognostic or observed data as inputs are required for the diagnostic module with the observational data including mainly upper air and surface meteorological data. As aforementioned, before they could be used as input into CALMET model, they needed to be processed in a particular file format. The data can then be imputed in three different ways: an initial guess field, step one wind field, or as observational data (Abdul-Wahab et al., 2014; Abdul-Wahab et al., 2016).

CALPUFF is generally run as a Lagrangian-Gaussian puff model, based on a non-steady-state procedure. In fact while it functions, it pays attention to the results from the subsequent times during the subsequent runs and can be used in modeling multi-layers and multi species of

a specific studied area. It needs the produced 3D model by the CALMET processor and also considers the spatial and temporal variations in the meteorological studied domain in the modeling period. CALPUFF generates an output that includes the varying hourly emissions of different emission sources, in concentration units, for every grid point of the meteorological domain at different heights. Frequently, the first layer of height is usually used for the results (Abdul-Wahab et al., 2014; Abdul-Wahab et al., 2016). The CALMET output is then used as an input for CALPOST processor, which as a post processor is used to process the CALPUFF output file, including meteorological data, concentrations, and deposition fluxes. The simulation results are summarized by CALPOST in descending order from the highest concentrations of dispersion to the lowest with regard to times and coordinates in the meteorological domain (Abdul-Wahab et al., 2014; Abdul-Wahab et al., 2016). Mainly, there are three types of emission sources: the point source, the line source,

and the area/volume source. For the aim of current study, because we wanted to analyze the emissions from District 7 of Tehran Municipality only, we considered only the line sources as the emission

source. There were 20 main line sources for this study, represented in Table 1. Every other emission from other types of emission sources were discarded.

**Table 1. Description of line emission sources in District 7 in Tehran city, used in the current study**

Name of line source	X_Start (Km)	Y_Start (Km)	X_End (Km)	Y_End (Km)	Emission rate of SO <sub>2</sub> (t/year)	Emission rate of CO (t/year)
Mottahari St.	539499.12	3951968.00	539428.44	3951835.75	0.01567	4.26922
Ghoddosi St.	538970.50	3952165.75	539014.50	3952381.50	0.06143	4.26922
Beheshti Str.	539592.69	3952791.25	539393.75	3952864.00	0.00337	17.16333
Ostad Hasan St.	539592.69	3952791.25	539714.44	3952745.75	0.00739	0.082103
Khoramshahr St.	539674.00	3953454.50	539883.50	3953413.00	0.04787	1.83475
Ghandi St.	540563.81	3953078.00	540602.50	3953216.75	0.02515	9.49806
Ebn yamin St.	541046.00	3952430.50	541187.38	3952608.50	0.02432	10.03318
Hoveizeh St.	541046.00	3952430.50	540908.50	3952264.00	0.00444	9.41016
Ghanbarzadeh St.	540623.69	3952524.00	540504.56	3952270.50	0.00809	1.60466
Andisheh St.	540529.06	3951807.00	540804.81	3952138.25	0.03761	2.70714
Shariati St.	540529.06	3951807.00	540097.56	3951281.50	0.01265	11.00382
Kaboli St.	540347.94	3951941.25	540006.56	3951367.75	0.02047	4.32546
Police St.	540201.88	3952020.00	540428.00	3952636.75	0.10454	6.977
Bahar St.	538759.00	3952512.50	539014.50	3952381.50	0.00352	22.999
Sanaii St.	538708.12	3952044.75	538494.25	3952129.25	0.00634	0.065074
Lotfi St.	539244.94	3953107.25	539376.94	3953472.50	0.02008	1.36931
Malayeri St.	539244.94	3952044.75	538494.25	3952129.25	0.00214	6.83074
Zohreh St.	539244.94	3953107.25	539376.94	3953472.50	0.00735	0.7096
Sabonchi St.	539244.94	3953107.25	539241.56	3952972.50	0.01228	2.1577
Golriz St.	541173.81	3951753.50	541242.31	3951236.75	0.05894	4.869

## RESULTS AND DISCUSSION

This study modeled the emission dispersions for CO and SO<sub>2</sub> in District 7 of Tehran Municipality. The period of interest was September 30, 2012. Hourly concentrations of the air pollutants (CO and SO<sub>2</sub>) were obtained from 0:00 to 23:00 with both one-hour and 24-hour intervals. The ambient concentration of CO and SO<sub>2</sub>, emitted from the studied area (District 7) were compared based on Iranian and National Ambient Air Quality Standards (EPA NAAQS) and other guidelines. The simulated concentrations were below Iranian air ambient standard and the NAAQS (EPA National Ambient Air Quality Standards) standard for both CO and SO<sub>2</sub>. The EU (European commission ambient air quality directive) and WHO (World Health Organization air quality guideline) guidelines can be used as

reference, indicating further evaluations in order to determine the possibility of a true threat to human health. As a poisonous gas, CO has got 120 times greater affinity than oxygen molecule to bind to haem protein of haemoglobin of red blood cells and produce carboxyhaemoglobin (COHb) which might be the main reason behind brain haemorrhage and thrombosis (Varon et al., 1999).

Unburned/partially burned hydrocarbons and CO are strongly associated with irritation of the eyes as well as black coughing (Pandey et al., 2013; Markandeya et al., 2016). Also, any Exposure to SO<sub>2</sub> in the ambient air contributes to reduced lung function, increased incidence of respiratory symptoms and diseases, eye irritation, nose irritation, throat irritation, and premature mortality. During the time of interest,

maximum concentrations of CO and SO<sub>2</sub> were recorded at 16:00 and 12:00, as shown in Figures 3 and 4. Also, It can be seen from the figures, that as time progresses; a larger portion of the meteorological domain gets

covered with the dispersion clouds, since 16:00 had bigger dispersion cloud of CO while 00:00 had the lowest one. For SO<sub>2</sub>, the dispersion cloud got bigger until 20:00, only to start reducing until 23:00.

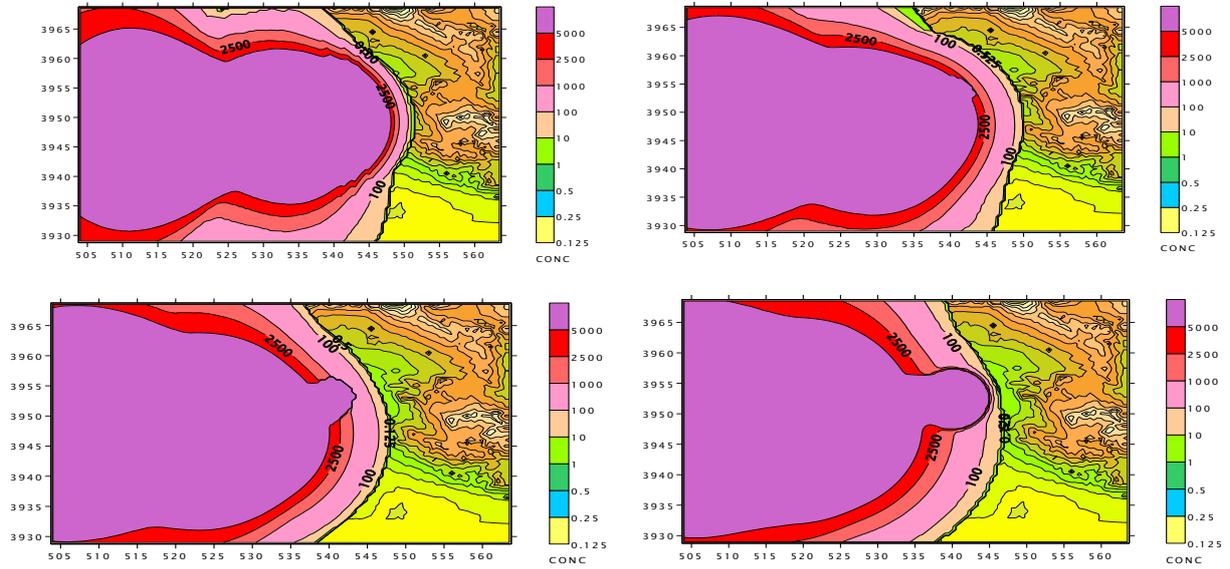


Fig. 3. Predicted spatial distribution of CO at 14:00, 15:00, 16:00, and 17:00 on September 30, 2012

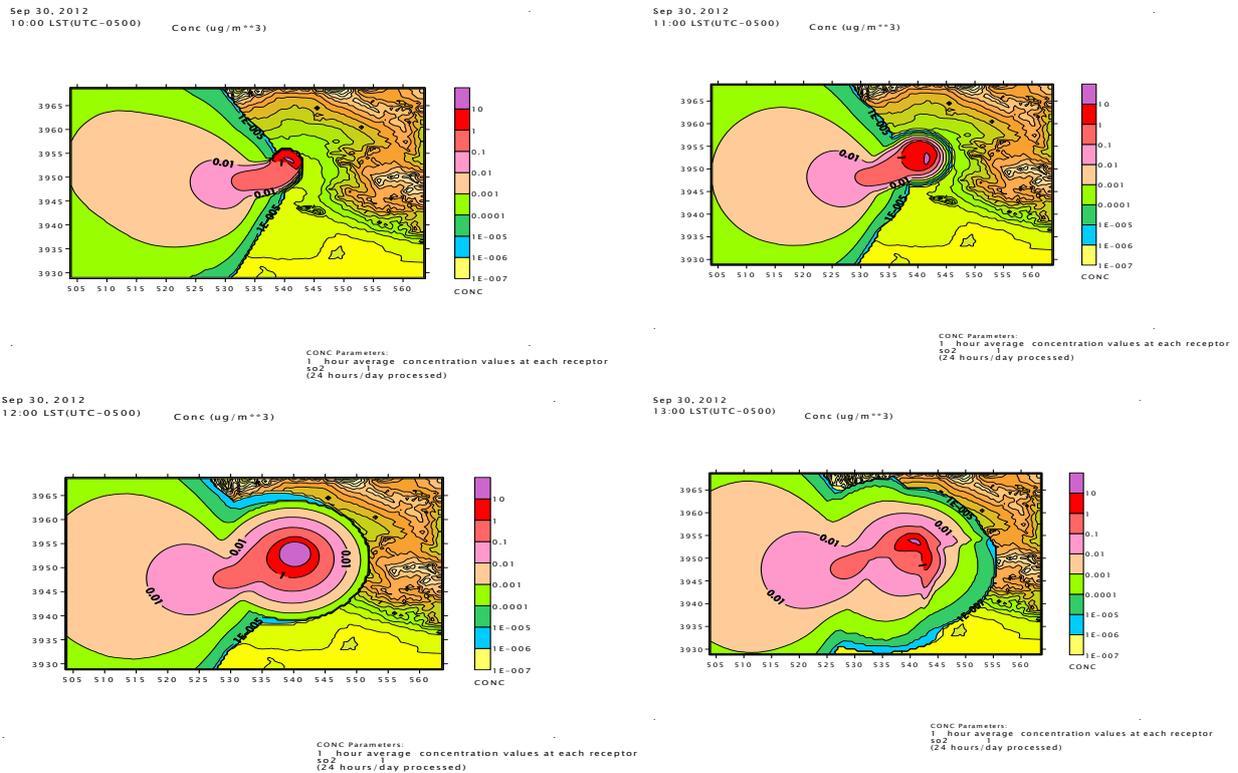
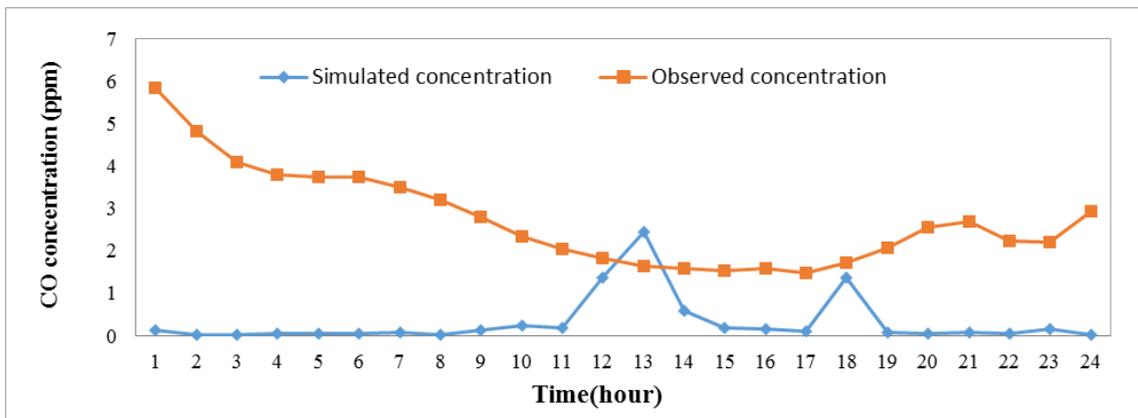


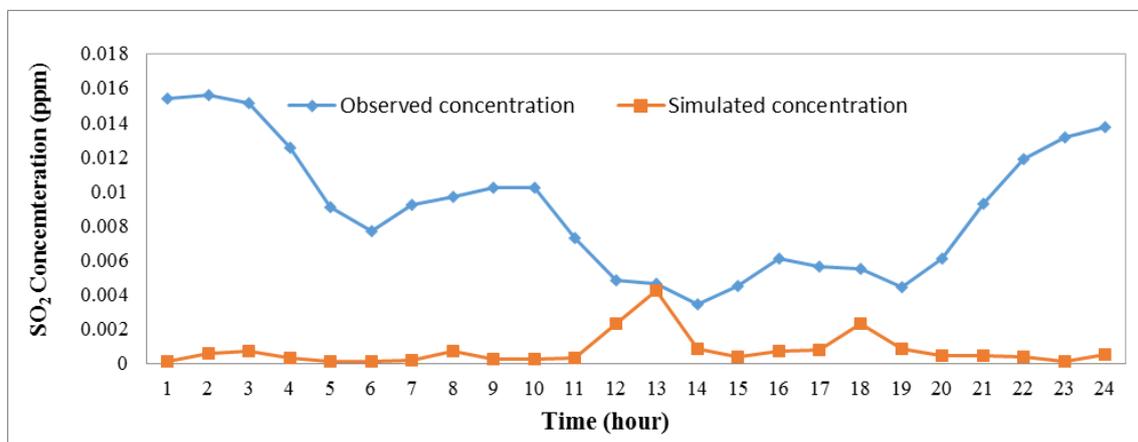
Fig. 4. Predicted spatial distribution of SO<sub>2</sub> at 10:00, 11:00, 12:00, and 13:00 on September 30, 2012

Figures 5 - 6 represent the hourly variations of CO and SO<sub>2</sub> concentrations at Setad Bohran monitoring station during the studied period, respectively. The predicted hourly average values of the SO<sub>2</sub> and CO concentrations did not seem to follow a similar temporal patterns to measurement values. For absolute value, model results seemed to be highly underestimated, compared to monitored data ( $R^2 = -0.41$ ). In a similar study, Gulia et al. (2015) validated the performance of CALPUFF

and AERMOD to assess NO<sub>x</sub> concentration, originating from steel industry. Comparison of monitored and simulated NO<sub>x</sub> concentration based on statistical analysis showed that CALPUFF performed well satisfactorily (Index of Agreement above 0.5). Also, researches showed satisfactory performance for prediction of pollutants' concentration near thermal power plant in Martin Greek, Pennsylvania (Dresser and Huizer, 2011).



**Fig. 5. Comparison between measured and predicted CO concentration (ppm) on September 30, 2012**



**Fig. 6. Comparison between measured and predicted SO<sub>2</sub> concentration (ppm) on September 30, 2012**

In addition, CALPUFF was used to predict the concentration of air pollutants with different approaches (such as PGT-ISC dispersion curve and Similarity-Theory-based dispersion) to evaluate modeling accuracy (Venkataram, 1996; Xing et al., 2007; Busini, et al., 2012). In the current study, the main reasons of

disagreement between model results and monitored data could be the assumption that air pollutant concentration was zero at 00:00 (the pollutant concentration at sampling stations was not zero due to previous concentration of air pollutants), uncertainties of measured data, and meteorological data used in the model. The

CALPUFF model appeared to be a valuable tool in evaluation of air pollutants' dispersion from air pollution sources to their proximity. Using more sampling stations to evaluate model performance, not limiting input data (especially types of emission sources) of the model, and using different approaches to evaluate the accuracy of CALPUFF modeling would lead to satisfactory results which may help authorities better understand the causes of air pollution in the affected areas. Also, they can be useful for environmental administrators to implement more effective air pollutant emissions reduction policies.

## CONCLUSION

The present study simulated sulfur dioxide and carbon monoxide dispersion from District 7 of Tehran Municipality, comparing the simulated and monitored concentrations at the Setad Bohran monitoring station. Both monitored and modeled data included hourly SO<sub>2</sub> and CO concentrations on September, 30, 2012. The predicted results were below Iranian air ambient standard as well as NAAQS standard for both CO and SO<sub>2</sub>. The predicted SO<sub>2</sub> and CO concentrations were not found to agree temporally well with the monitored data. These differences might be due to the assumption that concentration of air pollutant was zero at 00:00 (while the actual concentration of pollutant at sampling stations was not so, thanks to previous concentrations of the air pollutant), uncertainties of measured data, and meteorological data used in the model. For example, using more sampling stations for evaluation of model performance, not limiting input data (especially types of emission sources) of the model, and using different approaches to evaluate the accuracy of CALPUFF modeling would render CALPUFF model an appropriate tool for prediction of air pollutants' dispersion with approximate accuracy to its vicinity.

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