Environ Monit Assess (2023) 195:1272
https://doi.org/10.1007/s10661-023-11879-2

RESEARCH

Assessment of air quality using AERMOD modeling: a case study in the Middle East

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Received: 8 September 2022 / Accepted: 13 September 2023 / Published online: 5 October 2023

Abstract Emissions of greenhouse gases from industrial facilities, such as refineries, are one of the most significant environmental problems in many countries. This study aimed to assess the present status of emission sources near a gas refinery region, and the contribution of sources to air pollution was estimated by monitoring CO for a year at a fixed station. This descriptive-analytical study was conducted between January and December 2020. A simulation of CO gas distribution and pollutant concentration prediction was carried out. The results show that the maximum concentration of CO in the 1-h period was 2260 μg/m^3, which corresponds to the peak concentration in spring, and in the 8-h period, it was 573 μg/m^3, which corresponds to the peak concentration in winter. The studied area's maximum pollutant concentration was also compared to national and international standards for clean air. In all four seasons, the maximum simulated CO concentrations were lower than the Iranian and EPA standards for clean air. Maximum concentrations have occurred in the southern slopes of the study area's heights, and, due to the appropriate wind speed, maximum concentrations in the northeastern mountain peaks occurred at a more considerable distance due to the high altitude of the mountains and the lack of suitable conditions for pollutant escape. Furthermore, because of the height of smokestacks and flares from the ground and the effect of wind on the release height, the concentration of pollutants at the foot of the stacks is low and decreases gradually over a certain distance. Finally, the distribution and deposition of pollutants in the pathway of the smoke were influenced by the type of topography.

Keywords AERMOD · Carbon monoxide · Gas refinery · Air pollution modeling

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Introduction

The release of numerous organic compounds into the atmosphere is linked to the activities of oil refineries and petrochemicals, which are significant sources of air pollution (Abdelrasoul et al., 2010; Moridzadeh et al., 2020). Carbon monoxide, sulfur dioxide, nitric oxide, and particulate matter are all common pollutants these industrial plants emit (Eslamidoost et al., 2022; Shubbar et al., 2019). Carbon monoxide is emitted into the atmosphere by around 2600 million tons each year, 60% of which is emitted by manufacturing activities (Almetwally et al., 2020) that have a greenhouse impact of two to three times that of CO_2 (Atabi et al., 2014; Vali et al., 2021).

Air dispersion models are commonly used in this context to investigate the distribution and behavior of air pollutants in industrial locations and to estimate possible health hazards (Freddy Kho et al., 2007). Air pollution modeling aids in the prediction of pollutant concentrations and distributions, as well as the understanding of key aspects of air pollution and their application to air pollution management (Gulia et al., 2015). The AERMOD model is a steady-state smokestack model that distributes air at appropriate scales depending on the boundary layer turbulence structure. AERMOD is a permanent state distribution model that can be used to determine the concentrations of various pollutants in urban and rural areas, smooth and uneven surface emissions, and at the height of point, volumetric, and various types of surface sources, which are mostly for the distribution of pollutants up to 50 km (Kesarkar et al., 2007).

Several studies have demonstrated that the AERMOD model, with its characteristics, is appropriate for atmospheric dispersion research and a helpful tool for analyzing atmospheric dispersion (Macêdo & Ramos, 2020; Saqer & Al-Haddad, 2010). However, according to recent studies, no codified research has been done on modeling the emission of air pollutants from stacks and flares using the AERMOD model. Hence, we probe its utility in the prediction of CO levels. Therefore, this study aims to evaluate the dispersion of carbon monoxide pollution from stationary sources to test and disclose the features of the AERMOD application. The distribution of carbon monoxide in one of the gas refining companies in the Middle East was predicted and compared over 1 year in this study using AERMOD software.

Materials and methods

Study area

This descriptive-analytical study was conducted between January and December 2020. The gas refinery company has been exploited for gas purification of gas fields since 1988, with an approximate recoverable reserve and an estimated recoverable volume of seven hundred twenty billion cubic meters of gas.

Measurement of flue gases

The emissions of pollutants from refinery stacks were monitored once per season using a Gas Analyzer TESTO 350 in four seasons: spring, summer, fall, and winter. The device's standard operating type is defined using EPA-CTM030-41 and ASTM D 6522–00. The device probe was measured at a standard point on the stack, 8d from the bottom and 2d from the top (Chavoshi et al., 2011). The months of flue gas measurement were chosen depending on the refinery's highest activity in each season, with winter (March), spring (June), summer (September), and fall (November) being the months of choice. The measurement time for each stage was about 10 to 15 min, and the number of samples taken in this period for each stack was 2 to 5 samples (average of 3 measurements), with the highest concentration and emergency conditions for modeling selected after calculating the average, maximum, and minimum concentrations measured. Exhaust gas was measured in the winter from 16 operational smokestacks, in the spring from 12, in the summer from 14, and in the fall from 14, respectively. Finally, after calculation, the emission rate in grams per second was used in the model's information section on the characteristics of pollutant emission sources. The gas refinery's total number of stacks is 25, and its total number of flares is 3. Also, the equipment used in the study has been calibrated and is accredited in accordance with ISO 17025.

Set-up of receiver networks

The receivers were estimated as a network system using typical Cartesian network tools in AERMOD 8.9.0 software due to the necessity of exhaust gas dispersion and measurement of pollutant concentrations at various distances from the refinery. A total of 441 network acceptors were established in Cartesian coordinates throughout a 2500 km^2 region, with a set network distance in each of the two directions, *X* and *Y*, so that the distribution of pollutants across the whole modeling range could be shown clearly.

Meteorology data

The AERMET processor organizes and processes meteorological data into a format that can be used with the AERMOD 8.9.0 distribution model (Jafarigol et al., 2016). The AERMET preprocessor's needed and accepted meteorological data must be in the form of 1-h measurements. Because the heights of the refinery and the city are similar and there is little variation in post and altitude between the two regions, the meteorological data from the city airport, which is the nearest meteorological station to the refinery and is located 20 km away, were utilized. The National and Provincial Meteorological Department provided meteorological data from the synoptic station in the research region, including rainfall, temperature, cloud cover, pressure, humidity, wind direction, and wind speed (Iran Meteorological Organization [Internet], 2020). The hourly data were split and translated into an appropriate SAMSON format before being put into the AERMET module using Excel.

The wind rose area was also produced using the WRPLOT program. A wind rose is a graph that uses a central coordinate system to depict the speed and frequency of winds in a particular region. The meteorological data file for the upper atmosphere with the PFL extension and the meteorological data file for the surface with the extension SFC, utilized as the input of the AERMOD model, are contained in the two output files of the AERMET processor. The meteorological station is described in detail in Table 1.

Topographic data

Digital files of 1:25000 maps of the surveying organization, including elevation points and level lines at a distance of 20 m, are extracted from DGN files (30 sheets) and a digital elevation model (DEM) in ArcMap 10.3 software prepared with a size of 10 m pixels. In contrast, DEM designed in a particular module of topographic data processing (AERMAP), which is considered in the software, was processed and entailed in front of the AERMAP processor to increase modeling accuracy. Finally, by supplying the necessary data, modeling of the distribution of CO emissions from the stacks for periods of 1 h and 8 h was completed. The research area has been set at 2500 km^2 around the refinery to determine the impact of this pollutant on the health of refinery staff and locals. Modeling has been done for receivers 1.5 m above ground level and at ground level (breathing height). In AERMOD 8.9.0 software, Fig. 1 displays the DEM map of the area in 3D view mode.

Results

Meteorological measurement

Figure 2a depicts the research area's geographical directions and the wind rose and wind direction. The percentage of direction distribution is as follows: winds are blowing from the southwest at 25%, from the south at 17%, 10% from the northeast, and 8% from the northwest. Due to the biggest proportion of winds, the predominant wind rose is the wind from the southwest throughout the region. On the right-hand legend of Fig. 2a, the wind speed range is classified by different colors. Figure 2b depicts the percent and wind speed of the study region, which reveals that roughly 4.4% of total winds are serene and 44.7% of winds have a speed (0.5–2.10 m/s), with an average wind speed of 4.8 m/s.

Evaluation of CO effects by AERMOD v8.9.0

The model's results were in the form of alignment curves to CO pollutant concentrations in the receiver network and defined geographical regions. We report the following findings from the AERMOD modeling:

Table 1 Meteorological station information of the study area

Meteorological station	Distance to source	Meteorological parameters
City Airport Meteorological Station	20 km	Air temperature, air pressure, humidity, rainfall, wind speed, wind direction, and cloud cover

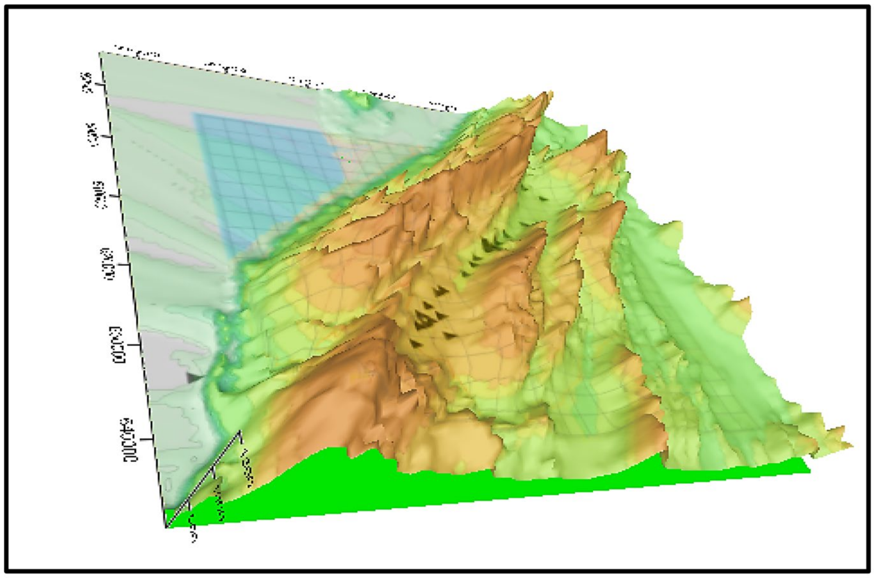


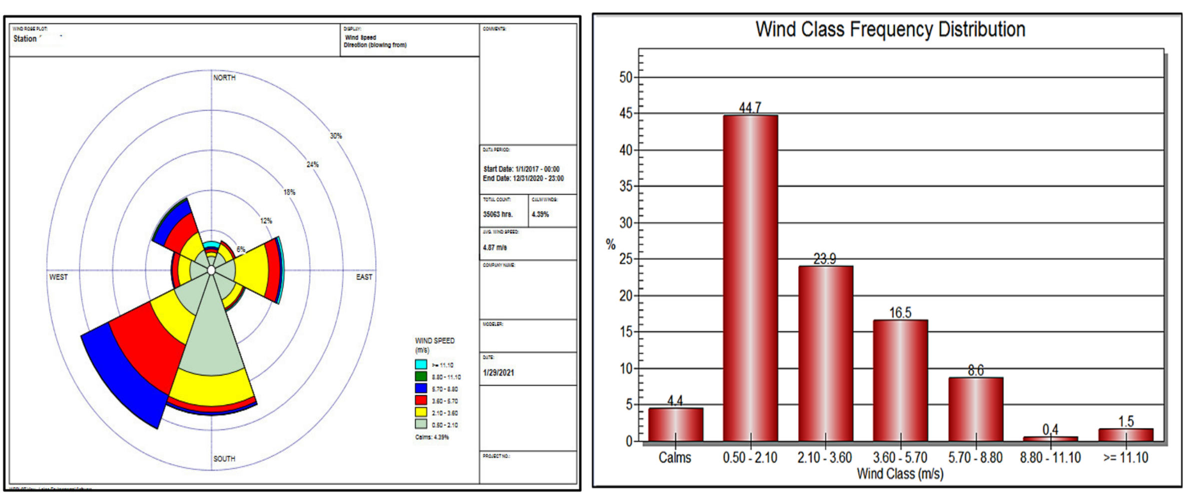
Fig. 1 DEM of the study area in 3D view mode in AERMOD software

Alignment curves obtained from simulation of 1-h CO concentration

Figure 3a depicts the distribution of CO concentrations throughout 1 h in winter, with the greatest value of 2235 μg/m^3. Figure 3b shows the distribution of 1-h CO concentrations in spring, with a top value of 2260 μg/m^3. Figure 3c depicts the distribution of 1-h CO concentrations in summer, with a maximum value of 1440 μg/m^3. Figure 3d represents the distribution of 1-h CO concentrations in fall, with the highest value of 1476 μg/m^3.

Alignment curves obtained from simulation of 8-h CO concentration

Figure 4a depicts the distribution of CO concentrations during 8 h in winter, with a high of 573 μg/m^3. Figure 4b shows the range of 8-h CO concentrations in the spring, with a top value of 437 μg/m^3.



a **b**

Fig. 2 Wind rose in the study area (**a**) and wind frequency distribution (**b**)

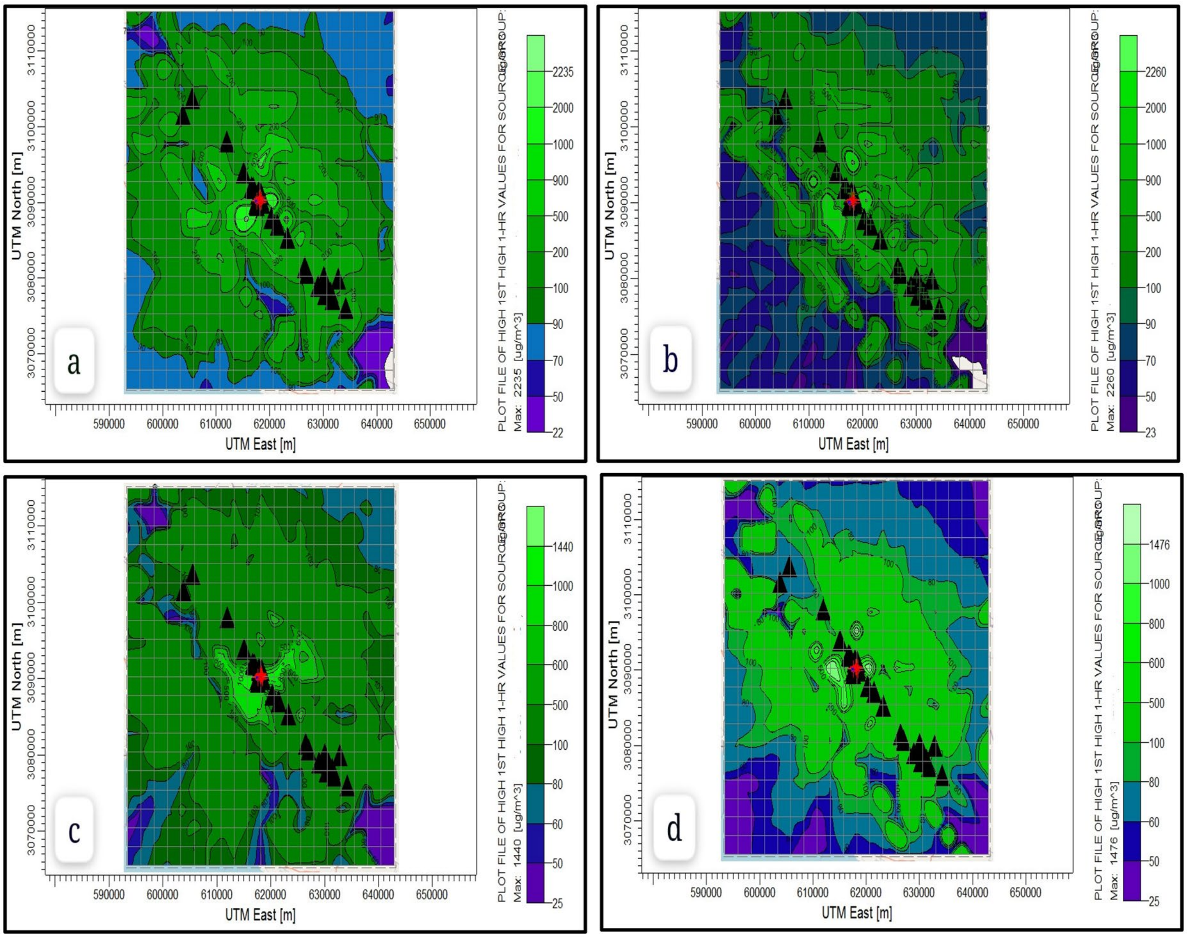


Fig. 3 The distributed 1-h concentrations of CO pollutants during four seasons (**a**–**d**)

Figure 4c shows the summer distribution of 8-h CO concentrations, with a maximum value of 440 μg/m^3. Figure 4d depicts the distribution of 8-h CO concentrations in fall, with the highest value of 419 μg/m^3.

The pattern of fluctuations in 1-h CO pollutant concentrations from the refinery (zero point of the horizontal axis) to the village (20 km upstream of the refinery) is examined in Fig. 5a, with the maximum and lowest concentrations corresponding to summer and fall, respectively. The pattern of pollutant concentrations from the refinery to the village (20 km upstream of the refinery) was compared to the clean air standard in Fig. 5b, and the findings revealed that the CO pollutant concentrations are lower than the standard in all seasons. Figure 5c depicts the progression of CO pollutant concentrations from the refinery (zero point of the horizontal axis) to the village (24 km downstream of the refinery), with the highest and lowest concentrations corresponding to summer and fall, respectively. The pattern of pollutant concentrations from the refinery to the village (24 km downstream of the refinery) was compared to the clean air standard in Fig. 5d, and the findings revealed that CO pollutant concentrations are lower than the standard in all seasons.

Figure 6a depicts the trajectory of CO concentration fluctuations over 8 h from the refinery (zero point of the horizontal axis) to the village (20 km upstream of the refinery). Summer and fall have the highest and lowest concentrations in this figure, respectively. The pattern of CO pollutant concentrations from the refinery to Hossein Abad village was compared to the clean air standard in Fig. 6b, and the findings indicated that CO pollutant concentrations are lower than the standard in all seasons. Figure 6c depicts the

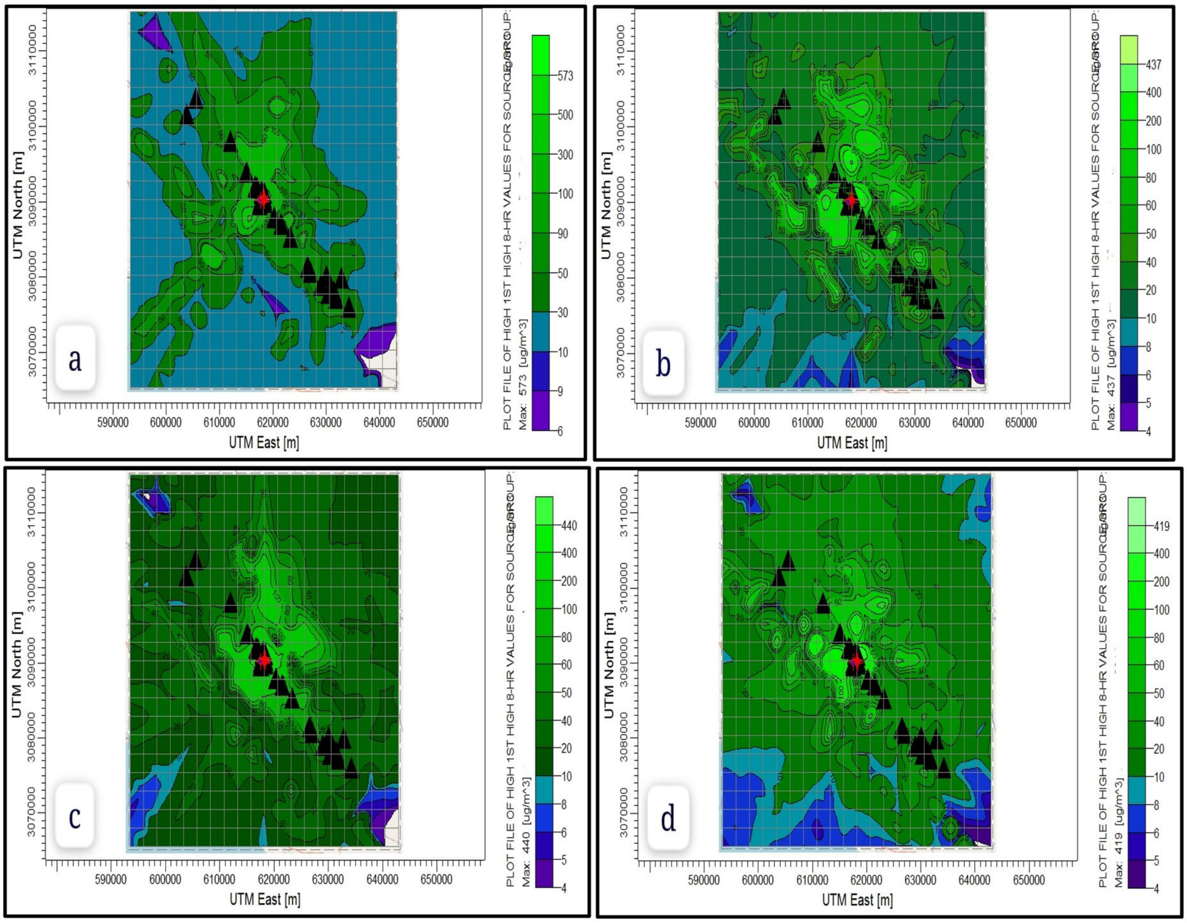


Fig. 4 The distributed 8-h concentrations of CO pollutants during four seasons (**a**–**d**)

pattern of variations in CO pollutant concentrations during an 8-h period from the refinery to the village (24 km downstream of the refinery). Summer and fall have the highest and lowest concentrations, respectively, in this figure. The pattern of pollutant concentrations from the refinery to the village (24 km downstream of the refinery) was compared to the clean air standard in Fig. 6d, and the findings revealed that CO pollutant concentrations are lower than the standard in all seasons.

Discussion

The maximum CO emission in 1-h and 8-h periods is 40,000 and 10,000 μg/m^3, respectively, according to Iran's clean air and EPA standards. When the quantity of CO emitted from the refinery is compared to the clean air standard, it can be concluded that the maximum emission concentrations of 1 h and 8 h of CO are lower in all studied seasons. The findings of this study agree with those of Afzali et al., who used the AERMOD model to calculate the emission of different contaminants from an incineration facility. This investigation revealed that pollutant concentrations on the ground are lower than their standard levels at various time averages (Afzali et al., 2014). It also aligns with a study conducted in 2020 by Zakaria and Aly, which found that CO distribution was lower than the ambient air quality standard (Zakaria & Aly, 2020). Tartakovsky et al. conducted a study in 2013 to predict the concentration of total suspended particles (TSP) from a rock mine using two atmospheric dispersion models, CALPUFF and

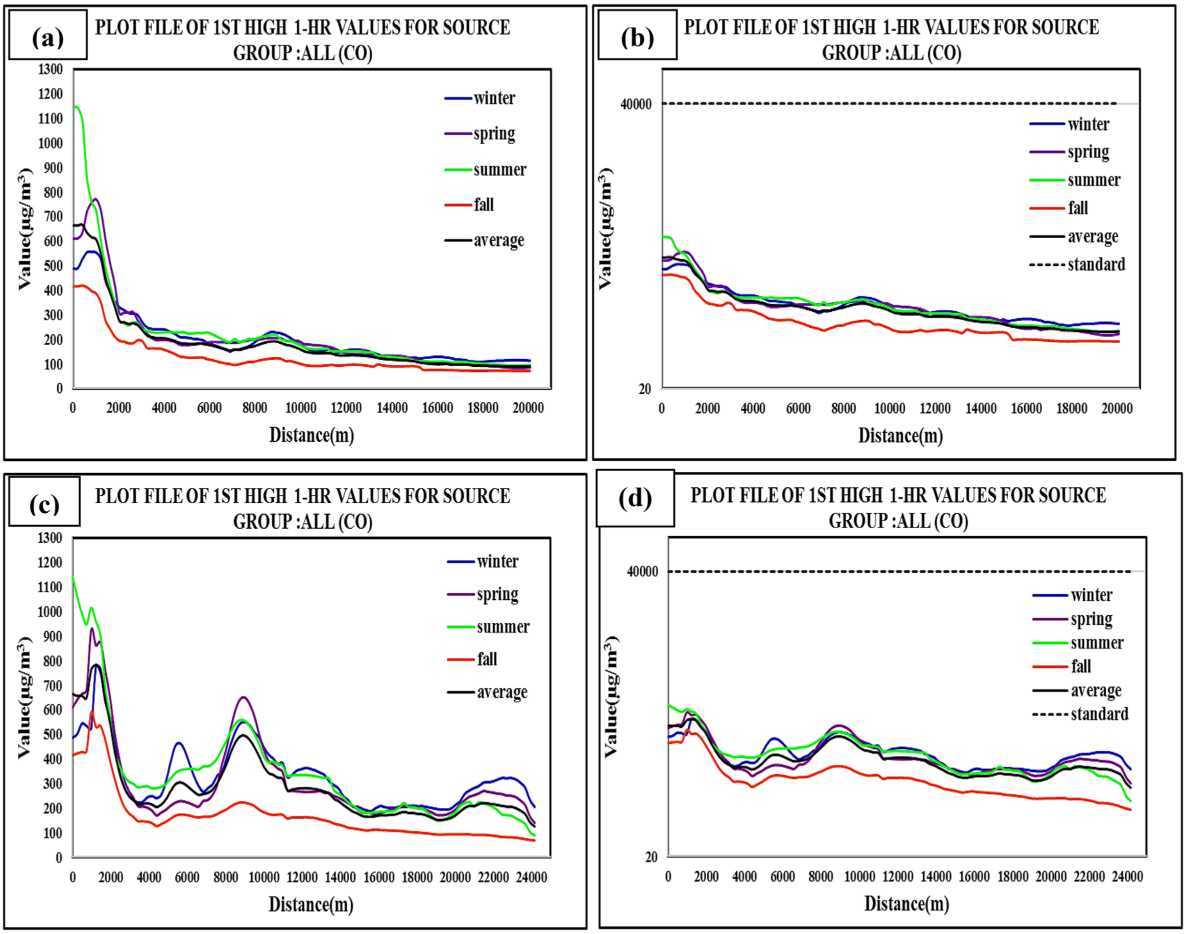


Fig. 5 Trend of 1-h concentration of CO pollutants from the refinery to the last residential area upstream (**a**) and downstream (**c**) and comparison with clean air standards (**b**, **d**)

AERMOD. They concluded that AERMOD predictions were more consistent with the measurements than CALPUFF predictions and that meteorological data were required for reliable scattering calculations in a complex area (Tartakovsky et al., 2013). This was completely considered in the current study, and all meteorological data from the meteorological organization of the entire country and province were received in 10-min intervals, totaling 261/191 thousand points, with AERMOD software being utilized in the AERMET module. Measurements from 25 emission sources were modeled over 1 year in this study. While the measurements were taken within a week and 12 points from the source of emissions in the study conducted by Seangkiatiyuth et al. on the emission of NO_2 from a cement complex, the greatest concentrations were observed at a distance of up to 5 km from the source of emissions. The findings of these studies indicate that combining AERMOD with long-term data from pollution sources in the study region can give more valuable and reliable information for identifying high-pollution locations for development impact assessment (EPA) and emission control guidelines to enhance air quality. Our work, on the other hand, found that the direction and speed of wind impact the dispersion of pollutants and that pollutants are spread in the direction of the wind, as well as land characteristics and topographic conditions, which is consistent with the findings of the current study (Seangkiatiyuth et al., 2011).

The topographic conditions of the study area and meteorological conditions, which include seven

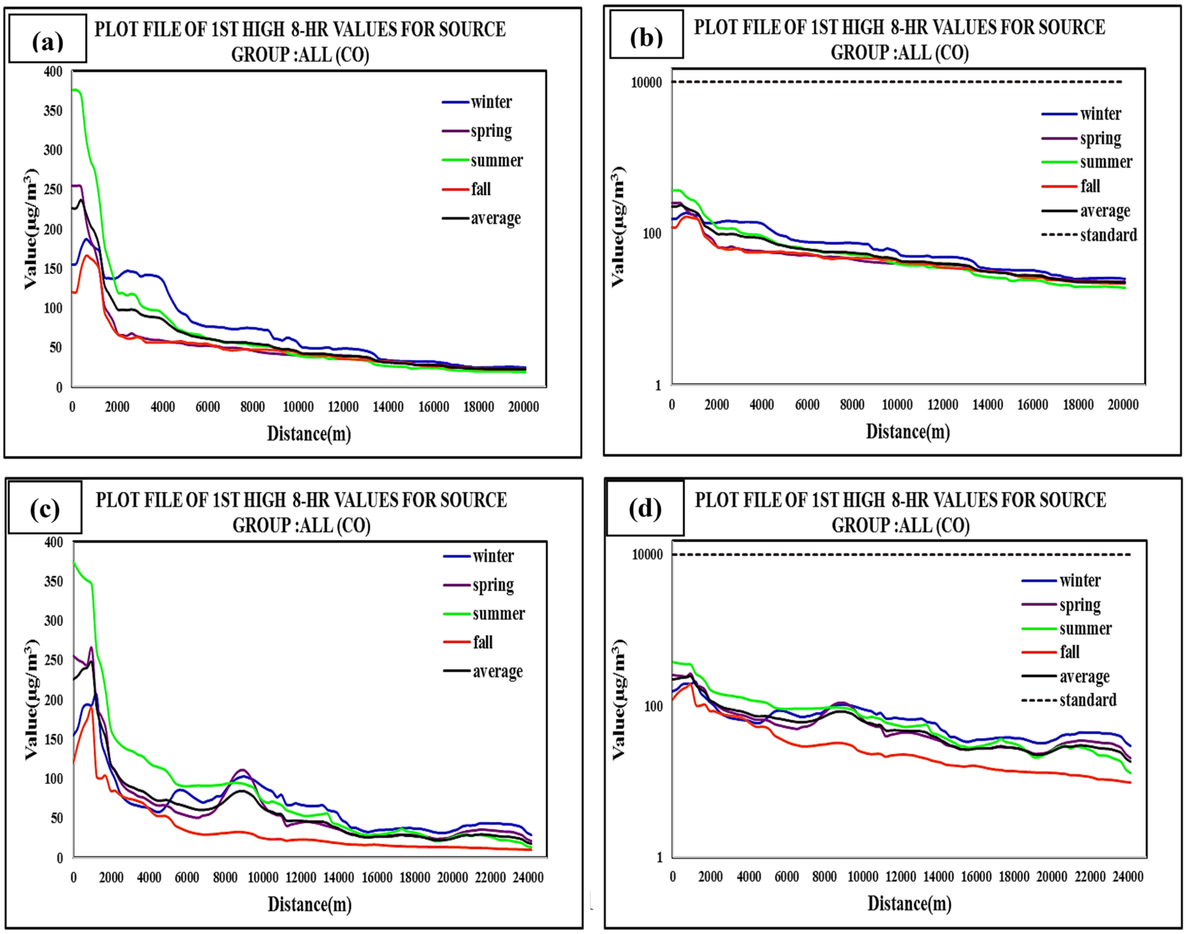


Fig. 6 Trend of 8-h concentration of CO pollutants from the refinery to the last residential area upstream (**a**) and downstream (**c**) and comparison with clean air standards (**b**, **d**)

necessary items, have the most significant effect on the spread of pollution, according to the equilibrium curves of the simulated concentrations in this study, which is consistent with Macêdo et al.'s study of 2020. The simulations revealed that air pollutants were dispersed due to Aracaju, Brazil's climatic and topographic circumstances (Macêdo & Ramos, 2020). The climatic and topographic parameters of the research region were found to be quite efficient in the dispersal of pollutants in this study. As a result, the AERMOD model is ideal for atmospheric dispersion research and is a helpful tool for analyzing atmospheric dispersion. Rowangould's investigations on software capacity to evaluate modeling capabilities are also consistent. According to the findings of a 2015 study that used the AERMOD model to determine and model the amount of particulate matter emitted from car exhaust in Los Angeles and California, air quality assessment using this model can be useful in identifying solutions, saving time and money, protecting public health, and ensuring proper planning (Rowangould, 2015). In addition, Rashidifard et al. conducted a study titled Comparison of AERMOD and CALPUFF models in CO emission modeling (Steel Plant). The results revealed that the AERMOD model outperformed the CULPUFF model (Rashidifard et al., 2018).

Overall, we can suggest that the simulation performed in this work, despite the intrinsic deficiencies every simulation has (i.e., simplification of the complex real world), is of relatively high accuracy and hence of significant value to the livelihood and safety of workers and inhabitants of the region.

Conclusion

The maximum carbon monoxide concentration in the research region for 1 h and 8 h periods is lower than the quantity of clean air introduced in Iran and the EPA requirement. The southern slopes of the area presented the majority of the highest concentrations. The distance between the source and the foot of the stack, as well as the influence of wind on the release height, have resulted in low concentrations of pollutants at the foot of the stack, which gradually decrease with increasing distance. The terrain also influences the distribution and deposition of pollutants in the path of the smoke. High concentrations are more common when there is a stable boundary layer, mild winds, and little mixing and turbulence. The maximum amount of CO concentration has occurred in the foothills of the western and southwestern mountains due to the climatic conditions and topography of the region (higher altitude and longer length of the southwest mountains than the northeast mountains) and pollutant emission rate, as well as low wind speed and no pollution displacement. They assess the distribution power of resources, topographic circumstances, and climatic factors of the region to aid in better understanding pollutant behavior in these situations. A general analysis of air pollution maps and land use in the area shows that urban, agricultural, and pasture land uses are unaffected by direct pollution from the refinery. The highest concentration of CO pollutants in the central parts and areas close to the company is expected not to be alarming, with concentrations in all studied areas falling below the national and international standards.

Acknowledgements This research with project number 21506 was conducted in the Department of Environmental Health Engineering, Shiraz University of Medical Sciences.

Author contribution Zahra Eslamidoost: conceptualization, methodology, and validation. Mohammad Reza Samaei: conceptualization, supervision, validation. Hasan Hashemi: data curation. Mohammad Ali Baghapour: reviewing and editing. Morteza Arabzadeh: methodology and investigation. Samaneh Dehghani: reviewing and editing. Saeed Rajabi: reviewing and editing

Availability of data and material The datasets generated and analyzed during the current study are available from the corresponding author upon reasonable request.

Declarations

Ethical approval All authors have read, understood, and have complied as applicable with the statement on "Ethical responsibilities of Authors" as found in the Instructions for Authors and are aware that with minor exceptions, no changes can be made to authorship once the paper is submitted.

Consent for publication This manuscript does not contain any person's data.

Competing interests The authors declare no competing interests.

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