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Impact of Meteorological Parameters on Dispersion Modeling of Sulfur Dioxide from Gas Flares (Case Study: Sirri Island)

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P A P E R I N F O

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A B S T R A C T

In this study, in 2011 for the duration of two months, the dispersion of a major air pollutant, sulfur dioxide from gas flares of an oil field, in Iran, was investigated. Due to the complexity of meteorological parameters in modeling area, California Puff (CALPUFF) model was used in this study. CALPUFF is a more advanced model than AERMOD which considers the effects of meteorological parameters in coastal areas, which was applied with meteorological and geophysical parameters produced by the Weather Research and Forecasting (WRF) model for the selected days of modeling period to investigate the impact of these parameters on modeling results. Since there is no option in the model for flares, flare parameters including emission rate and effective height and diameter were calculated based on EPA method to simulate better the real condition of flaring. Simulation results revealed that CALPUFF model could adequately express the effect of meteorological condition on results of modeling in each hour of the simulation period. The results of the simulation showed that low-height flares have the most impact on the ground level concentration of air pollutant on the island. The effects of elevated flares were at a far distance from flaring activity and mostly occurred outside of the island. CALPUFF model showed excellent compatibility with meteorological data produced by WRF and could properly account for the effect of meteorological and terrain parameters on dispersion modeling.

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INTRODUCTION

Flaring is a conventional and reliable means for disposal of waste gas from oil and gas facilities. This process is an indispensable part of oil and gas production, which require safe disposal of flammable waste gases [1]. Despite the broad application of flaring, this process unleashes a huge amount of air pollutants to the environment. The diversity and types of released pollutants are governed by the composition of inlet gas to the flares and the combustion efficiency, which depends on several factors including temperature, wind speed, the velocity of gas exiting flare and so forth [2]. Major air pollutants released from gas flares are sulfur dioxide, nitrogen oxide, carbon monoxide, non-methane volatile organic compounds, particulate matter, methane, and carbon monoxide [3]. SO_2 can be emitted from flares if the sulfur component exists in the flared waste gas. NO_X production is strongly dependent on temperature and formed by the fixation of the molecular nitrogen from the air. Emission of CO from the flare is due to incomplete combustion. Iran is a significant exporter of oil, and its economy, growth and Policy are highly dependent on oil production. Gas flaring is a considerable amount and results in various environmental impacts including climate change, acid rain, agricultural destruction, and especially adversely affected on human health. Detailed study of the dispersion of the air pollutants from gas flares is a vital process to specify the air quality of oil field and regions close to them and find solutions to moderate their attendant impacts. The application of air dispersion models has been increased rapidly in recent years, and these models with applying monitoring activities become an effective method in air quality evaluation. The main features of air dispersion models are their low-cost application and acceptable results which incorporate the impacts of meteorology, topography, source type in a particular broad area [4]. Dispersion models are in general based on Gaussian approximation of horizontal and vertical profiles of concentration. They contain algorithms to include the effect of sources, topology, wind speed and direction and chemical reactions [5]. One of the most commonly used models by regulatory agencies in this area is CALPUFF. The performance of the CALPUFF modeling system has been evaluated in several studies [6, 7, 8, 9, 10]. Modeling the dispersion of air pollutants emitted from gas flares in locations like those that Islands require considering additional factors such as complex meteorological and terrain parameters. Incorporating all these

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factors with the lack of meteorological data in locations such as islands requires a thorough study that is a necessity for locations like Iran, which account for a significant amount of flaring in the world and have several flaring sites on islands. Coupling dispersion models with prognostic meteorological models is an efficient way for locations with a lake of meteorological data. This method was used in some recent studies:

Kesarkar et al. [11] mentioned that AERMOD requires hourly surface and upper air meteorological observations for simulating the pollutant dispersion. The required meteorological parameters are derived from high-resolution prognostic simulations using WRF model to overcome this difficulty. The methodology for coupling of air quality model (AERMOD) with regional weather prediction model (WRF) was discussed. The methodology of coupling a prognostic regional weather model with an air pollution model for simulating pollutant dispersion has shown encouraging results, and the system has potential to overcome the limitation of unavailability of required local meteorological observations. Abdul-Wahab et al. [12] investigated the transport and dispersion patterns of SO_2 originating from Mina Al-Fahal refinery, in the Sultanate Oman by employing California Puff (CALPUFF) dispersion modeling system. The CALPUFF modeling system was coupled with WRF to obtain the meteorological fields of the study area. The results of the study indicated that the performance of the CALPUFF was better than that of ISCST. Abdul-Wahab et al. [12] applied CALLPUFF and MM5 model to study the dispersion pattern of SO_2 emission from a refinery in Oman. The results of study well matched with observation data with minor differences in magnitudes. Also, a comparison between modeling data and the regulatory limits was carried out. The results determined that the concentration of SO_2 was lower than regulatory limits in communities nearby refinery.

Ghannam and El-Fadel [13] investigated the role of different sources to ground-level concentrations of carbon monoxide (CO), nitrogen dioxide (NO_2), and PM_{10} in a coastal urban area by considering emissions from an industrial complex with multiple stacks, quarrying activities, and a nearby highway. In this study, a coupled CALPUFF/MM5 model was used. In another recent study, dispersion modeling of PM_{10}, SO_2 and NOx were conducted by application of combined WRF/CALPUFF model for Benxi city in China [14]. The result of this study has shown that the predicted concentrations by the CALPUFF model were in good agreement with monitoring sites data. By reviewing the works were done on this topic, it is evident that few works were carried out for modeling of gas flares. Furthermore, modeling of gas flares is different from other point sources like regular stacks and requires calculation of flare parameters before applying dispersion models. Also, lack of meteorological data in remote areas like islands could be significant uncertainty in modeling activity. Coupling metrological models with dispersion models were tested in some recent works and the results in most cases showed good agreement between modeling results and observational data from monitoring stations. Consequently, application of air pollution dispersion models with metrological models like WRF, which is the next generation of mesoscale numerical weather prediction systems, could be a useful tool in the prediction of pollutants concentrations in areas around gas flares.

In this work, modeling the dispersion of SO_2 from gas flares on an island will be done with CALPUFF model by embedding calculated parameters for gas flares in the model. This modeling will be performed by application of CALPUFF-WRF coupled model for certain days to investigate the effect of coastal area and related meteorological parameters on modeling results.

MATERIALS AND METHODS

Study area

Sirri Island has been selected for this study. This island is in the Persian Gulf, which belongs to Iran and situated at about 75 km off the coast of Iran. The island located in 76 km of Bandar Lengeh and administered by Hormozgan Province. It covers an area of 17.3 kilometers squared. Sirri Island has hot and humid weather. The average temperature of the island ranges from about 40 degrees centigrade in July to about 12.5 degrees centigrade in the coldest month of the year [15]. The highest point on this island is about 24 meters above the sea level, and most of the island is flat. The oil production of the island is more than 100,000 barrels per day [16]. There are multiple oil and gas exploration and production facilities on this island. These oil and gas facilities produce a considerable amount of air pollutants. Flares are one of the significant sources of air pollution in this region. Figure 1 shows the location of major flares on the island.

Dispersion modeling

CALPUFF is an advanced dispersion model, which applies Lagrangian puff Gaussian algorithm to predict concentrations of air pollutants downwind of emission sources. In this regard, CALPUFF requires 3D meteorological fields [17]. It could be possible by application of surface observation and upper air meteorological data or prognostic meteorological models, like MM5 and WRF. The first choice is not available in many parts of Iran because of inconsistent meteorological data from weather stations. The second approach also has limitations due to high computational requirements. These limitations could be resolved by the support of related organization and agencies. In this study, WRF model will be used to produce meteorological input data for CALPUFF modeling system. MMIF is an interface software that recently released to construct the required input meteorological parameters for CALPUFF model [18]. This software is used in this investigation, to prepare the 3D meteorological input of CALPUFF with WRF output data.

Meteorological modeling

The Weather Research and Forecasting (WRF) model is a system that used for numerical weather forecasting and atmospheric conditions studies in both operational and research applications. The WRF model contains various physics and dynamic schemes that provide several choices for applying different combination of physics and dynamics to the desired area. Finding optimum configuration for WRF model requires several runs of the model for different physics and dynamic that needs high computational time and power. Azadi et al. [19] applied six different configurations of

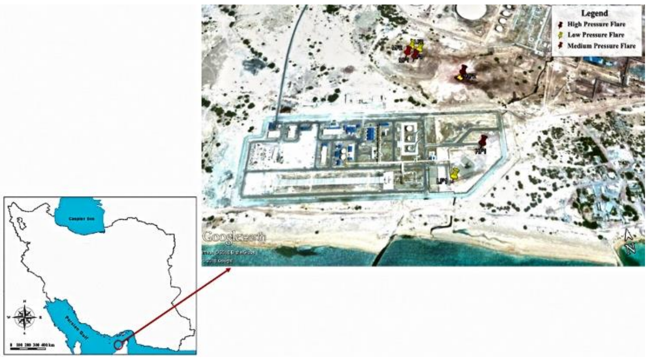


Figure 1. Location of major flares in Sirri island

physics and dynamics to find the most appropriate combination for forecasting of daily precipitation over Iran. In this study, the physics and dynamic configuration [19]) will be used to run WRF model on Sirri Island. Three domains were considered for WRF configuration with 12, 4 and 1.33-kilometer resolutions for horizontal grid respectively and 27 levels in the vertical direction (Figure 2). The center coordinates of domains are 25.914259° N and 54.527322° E that is located on Sirri Island.

The WRF model was run for two five days' period from 29 January 2011 to 2 February 2011and 20 October to 24 October 2011. The output of WRF was compared with observational data from Sirri Island weather station to evaluate the result of the model with observed meteorological data. The following statistical functions were used for assessing the performance of WRF model:

Mean Average Error (MAE):

$$MAE=\sum_{i=1}^{n}\frac{|M_i-O_i|}{n} \qquad (1)$$

where M_i is the modeled value for cell i, O_i is the observed value for cell i, and n is the number of values analyzed.

Root Mean Square Error ($RMSE$):

$$RMSE=\sqrt{\sum_{i=1}^{n}\frac{(M_i-O_i)^2}{n}} \qquad (2)$$

Root Mean Square Error ($RMSE$) is similar to MAE but more sensitive to occasional significant errors due to its quadratic term.

Bias ($BIAS$):

$$BIAS=\sum_{i=1}^{n}\frac{(M_i-O_i)}{n} \qquad (3)$$

Bias provides information on the trend of the model to overestimate or underestimate a variable.

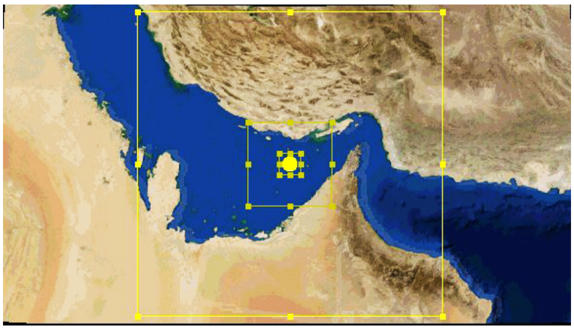


Figure 2. Three domain selected for running WRF

The coefficient of Determination (R^2):

The coefficient of determination detrmines how well data points fit a statistical model. The general definition of the coefficient of determination is:

$$R^2=1-\frac{SS_{res}}{SS_{total}} \qquad (4)$$

where SS_{res} is the sum of squares of residuals and for when observed value is shown by y_i and modeled value with f_i, it could be represented by:

$$SSres=\sum_i (y_i-f_i)^2 \qquad (5)$$

SS_{total} is the total sum of squares and when the mean of the observed data represent by $\bar{y}$, it can be expressed by Equation (7).

$$SS_{total}=\sum_i (y_i-\bar{y})^2 \qquad (6)$$

$$\bar{y}=\frac{1}{n}\sum_{i=1}^{n}(y_i) \qquad (7)$$

Source parameters

Flares are considered as point sources; however, a flare option is not available in CALPUFF model. Therefore, calculation of plume rise and effective stack diameter based on the heat release from flare require being done. This difference is due to a flare releases heat at the stack top and also heat loss by radiation [20].

Effective release height and effective diameter can be calculated based on EPA guideline from Equation (8) through Equation (10) [21]:

$$H_{effective}=H_{actual}+0.00456\left(\frac{H}{4.1868}\right)^{0.478} \qquad (8)$$

$$d=9.88\times10^{-4}\times Q_H^{\,0.5} \qquad (9)$$

$$Q_H=(1-F)H \qquad (10)$$

where, $H_{effective}$ is effective stack height (m), H_{actual} is actual stack height (m), H_r is net heat release rate (J/s), H is total heat release rate (Cal/s), Q_H is source heat release (Cal/s), F is radiative loss factor (%), d is diameter (m). The assumption in Equation (10) is that 55% of total heat released from the flare is lost by radiation that is the maximum heat loss suggested by Leahey and Davies [22].

Calculation of the emission of SO_2 is based on the sulfur content of input gas to the flare and combustion efficiency. The emission is calculated by Equation (11):

$$SO_2\left(\frac{g}{S}\right)=\text{combustion efficiency}\times\frac{\text{MW } SO_2}{\text{MW Sulphur Content}} \qquad (11)$$

The calculated parameters for flares in the study area is represented in Table 1.

CALPUFF Model

As mentioned before, CALPUFF requires three-dimensional meteorological and geophysical parameters that are created by CALMET preprocessor. MMIF program was used as an alternative for CALMET program to construct these parameters for CALPUFF model. CALPUFF which is the central processor of CALPUFF modeling system calculates the concentration of pollutant based on the puff Gaussian algorithms and 3D meteorological and geophysical parameters. The CALPro, the GUI for CALPUFF model, was used in this study to calculate the concentration of pollutants with meteorological and geophysical parameters produced by

TABLE 1. Calculated emission rate, effective height and diameter for flares in Sirri Island

Flare Type	Emission Rate SO_2 (g/s)	Effective Height (m)	Effective diameter (m)
Low Pressure	125.939	10.6	3.1
Low Pressure	125.939	10.6	3.1
Low Pressure	125.939	10.6	3.1
Low Pressure	42.461	21.1	3.1
Medium Pressure	0.183	12.5	3.3
Medium Pressure	0.183	12.5	3.3
High Pressure	2.698	87.8	4.5
High Pressure	412.198	107.7	5.4

MMIF program. Since there is no option in CALPUFF model for modeling flare sources, the modified parameters of height and diameter of the stack with a calculated emission rate of pollutant were used as source input parameters for CALPUFF model. CALPUFF model was run for two five days period from 29 January 2011 to 2 February 2011 and 20 October 2011 to 24 October 2011. Short-term time averages of 1, 24-hour and total period was investigated to study the effect of hourly meteorological parameters on results of modeling. Also, modeling was carried out separately for both short and elevated flares to consider the contribution of these flares on ground level concentration. CALPUFF results were used by CALPOST to produce the average concentration of pollutants for desired time average. Figure 3 shows the data flow in CALPUFF modeling in this study.

RESULTS AND DISCUSSION

WRF outputs

WRF model was run for two five days' period starting from 29 January 2011 to 2 February 2011 and 20 October 2011 to 24 October 2011. The comparison of WRF output results with observed values that were taken from Sirri's weather station is shown for wind direction, wind speed, temperature and pressure in Figure 4.

WRF outputs show good agreement with observed wind direction, wind speed, temperature and pressure. The observed values of these parameters were recorded for every 3 hours, starting from 3 am to 15 pm in each day in Sirri's weather station. Average of statistical functions including Mean Average Error (MAE), Root Mean Square Error (RMSE), and bias with coefficient of determination (R^2) were

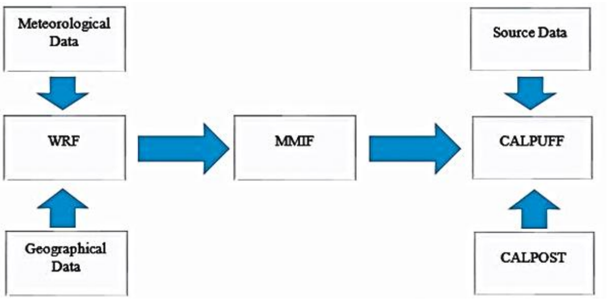
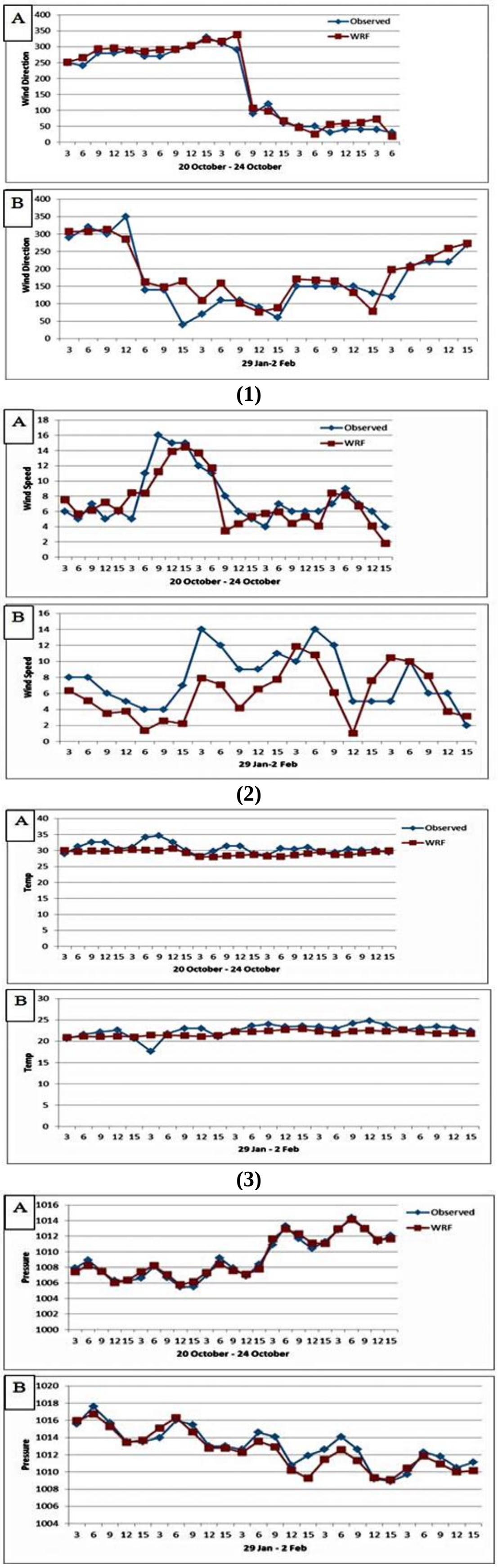


Figure 3. Data flow in CALPUFF modeling system



(1)

(2)

(3)

(4)

Figure 4. Comparison of Observed and WRF computed values of wind direction (1), wind speed (2), temperature (3) and pressure (4); for A) 20 October 2011 to 24 October 2011 B) 29 January 2011 to 2 February 2011

calculated and represented in Table 2 for wind direction, wind speed, temperature, and pressure of each period for better representation the comparison of the output results from WRF model and observed meteorological parameters.

Table 2 proves that WRF model had an acceptable prediction of meteorological parameters. Prediction of wind direction is similar to observed values and especially in the period from 29 January to 2 February, the predicted, and observed values have a high dependency, and the amount of error is acceptable. Wind speed, temperature, and pressure also have the same pattern, and as the value of Bias shows, the model underestimates these parameters except for pressure in the period from 20 October to 24 October with the amount of lower than 2m/s for wind speed, 1.5℃ for temperature and 0.5 mbar for pressure. Except for temperature in 20 October to 24 October, all other parameters have high coefficient of determination, which shows the good replication of observed values with model predictions. Although temperature has low, value of R^2 but its error is lower than 1.5℃, which could be considered acceptable. The overall performance of WRF model in prediction of meteorological parameters for application in CALPUFF dispersion model was satisfactory and could be a great asset to investigating the dispersion of air pollutants in each hour with different meteorological conditions that occur during a day.

CALPUFF outputs

The CALPUFF model was run in this study by using WRF output data as input meteorological and geophysical parameters for two five-day periods starting from 29 January 2011 to 2 February 2011 and 20 October 2011 to 24 October 2011to investigate the effect of hourly meteorological parameters on the dispersion of sulfur dioxide emitted from flares. The modeling was carried out for 1hour; 24 hour and full period averages and the result of simulation for highest predicted values of each averaging period with the highest total period are represented in Table 3.

TABLE 2. Average of statistical functions for wind direction and speed, temperature and pressure

Parameter	MAE	RMSE	BIAS	R^2
Wind direction 29 Jan -2 Feb	26.03	41.19	-	0.79
Wind direction 20 Oct – 24 Oct	15.04	18.69	-	0.98
Wind speed 29 Jan -2 Feb	1.61	1.99	-0.50	0.38
Wind speed 20 Oct – 24 Oct	2.68	3.46	-1.63	0.70
Temperature 29 Jan -2 Feb	1.65	2.08	-1.51	0.38
Temperature 20 Oct – 24 Oct	1.15	1.40	-0.75	0.23
Pressure 29 Jan -2 Feb	0.72	0.92	-0.48	0.97
Pressure 20 Oct – 24 Oct	0.38	0.45	0.03	0.87

TABLE 3. First rank of highest 1, 24 and total period average concentration of SO_2

Pollutant	Period (year/month/day, start time)	Average period (hour)	Peak value (µg/m^3)
SO_2	2011/1/30 18:00	1	1394.01
	2011/10/22 08:00		1014.28
	2011/1/29 23:00	24	137.63
	2011/10/20 23:00		525.69
	2011/1/ 29 00:00	Period	59.96
	2011/10/20 00:00		28.59

Figure 5 represents the wind vectors with the terrain of modeling domain for the highest value of 1 hour average period of SO_2 on 29 January to 2 February period. As it is shown, the wind speed is lower than 5 m/s and in the range of 0.01 to 5.01 m/s which by a clear sky of this region conditionally stable condition was existed. Figure 6 Shows the stability of atmosphere in this condition with the distribution of SO_2 around flares.

In these hours, the mixing height was as low as 140 m, and by considering elevated flares release height on the island, the

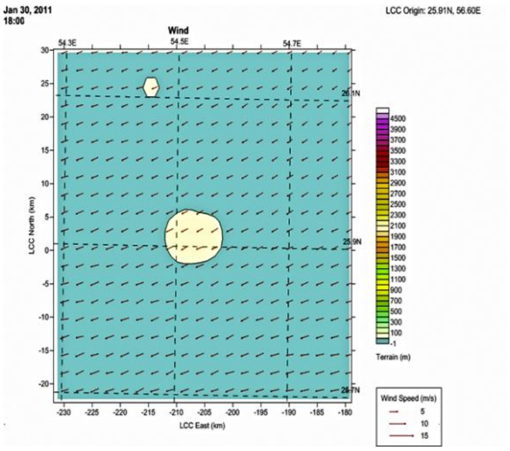


Figure 5. Wind vectors and terrain of modeling domain at 30 January 2011, 18:00

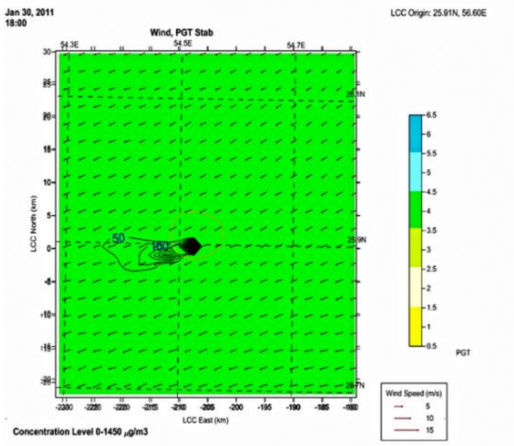


Figure 6. Contours of SO_2 concentration with stability 30 January 2011, 18:00

dispersion of SO_2 must occur above the mixing height. This situation caused high ground level concentration around flares that caused by flares with a lower elevation. To illustrate this condition better, CALPUFF model was run for two cases, first only for flares with short heights and the second one, for flares with high elevation. Figure 7 represent these two cases.

The emission from elevated flares is distributed in different directions in comparison with two low-height flares. It can be understood that by considering the direction of the wind in higher elevations as shown in Figure 8, the maximum concentration was mostly caused by low-height flares and distribution of pollutant concentration is not far from sources. Also, maximum concentration occurred in about 400 meters from low-height flares since the stable condition reduces horizontal and vertical dispersion of SO_2. This condition also existed near sunrise in October. As it is represented in Figure 9, low-height flares had the most impact on maximum concentration around flaring activity. In this condition like maximum concentration in January period, when the pollutant released from low-height flares, it cannot disperse well in both horizontal and vertical directions. It caused by stability

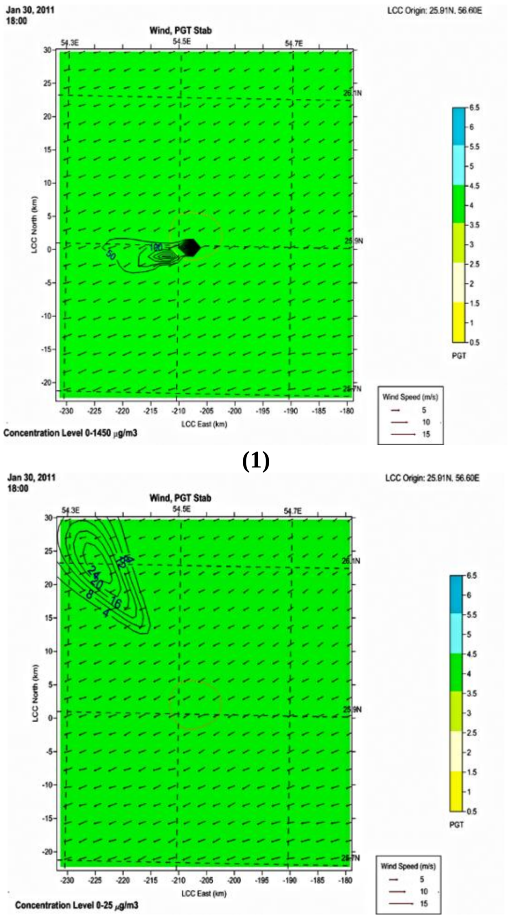


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Figure 7. Contours of SO_2 concentration distribution for considering only (1) short flares and (2) elevated flares, 30 January 2011, 18:00

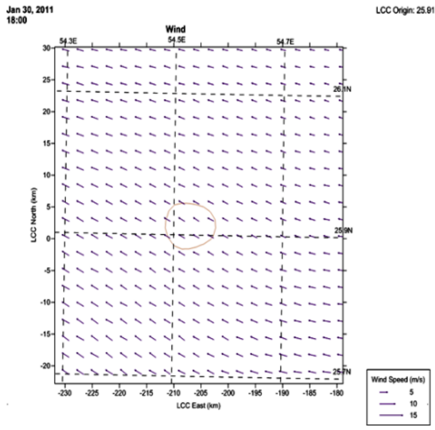
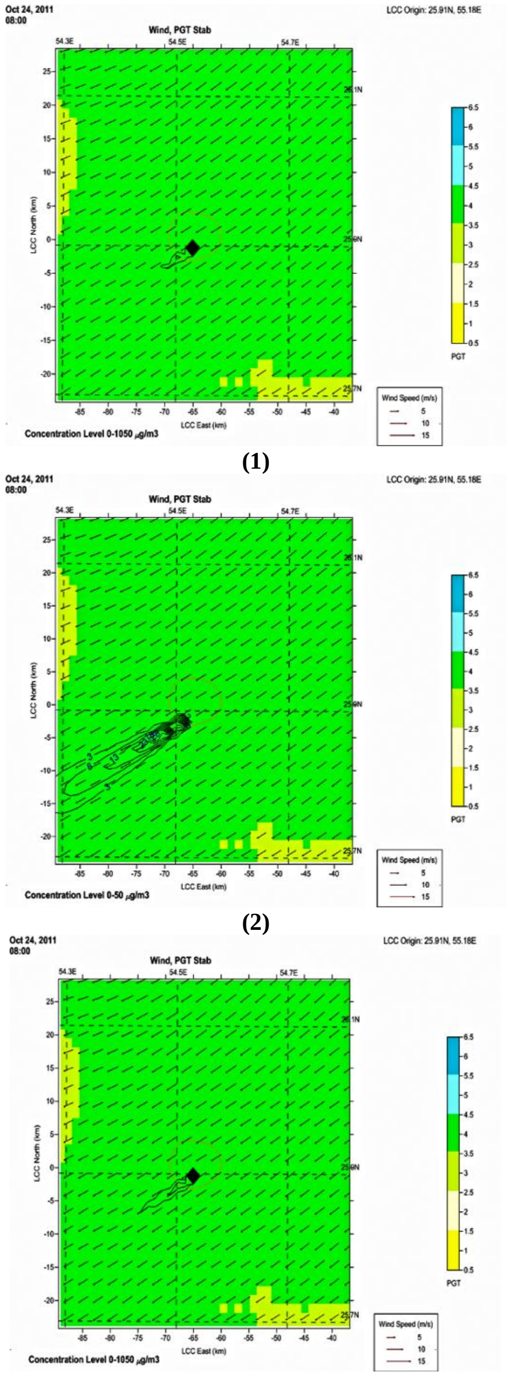


Figure 8. Vectors of wind at 160-meter height



(1)

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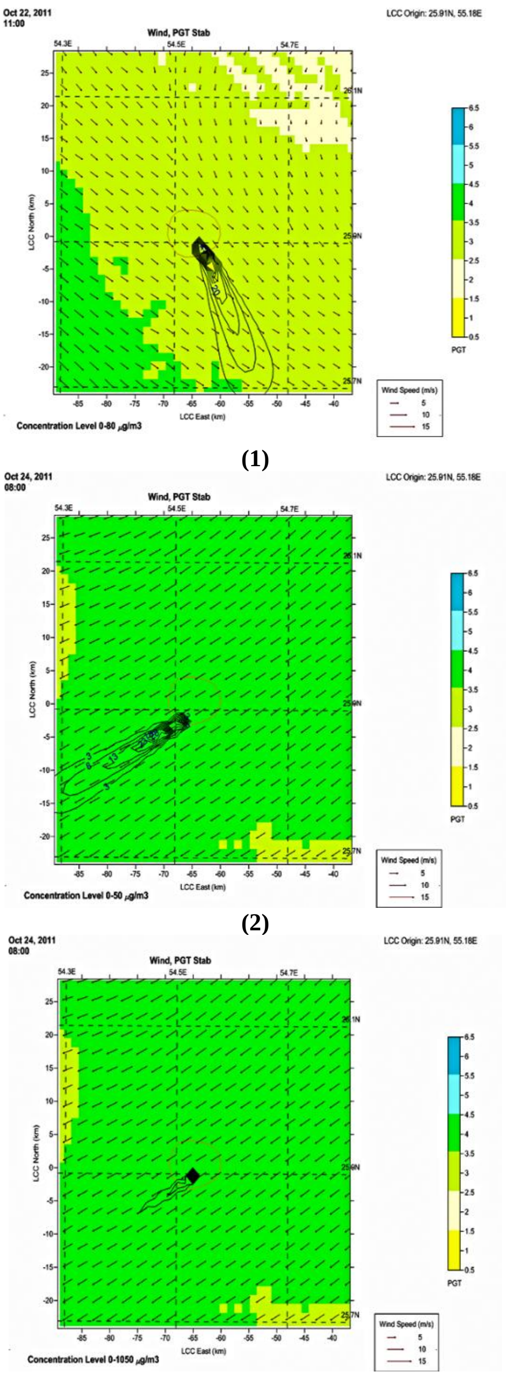
Figure 9. Contours of SO_2 concentration distribution for (1) only short flares, (2) only elevated flares, (3) both elevated and short flares, 24 October 2011, 8:00

and mixing height, so it reached the ground reached the ground level in a shorter distance, and because of low dispersion in horizontal and vertical directions that means lower dilution of pollutant with air, the concentration would be high.

The impact of stability and mixing height could be shown better when comparing the maximum and minimum conditions. For better representation of the effect of atmospheric stability and mixing height on the dispersion of air pollutant from flares, the contours of SO_2 concentrations distribution for two cases were shown in Figure 10.



(1)

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Figure 10. Contours of SO_2 concentration distribution for (1) only short flares, (2) only elevated flares, (3) both elevated and short flares, 22 October 2011, 11:00

As it is depicted in the above figures, by increasing the instability of the atmosphere and mixing height, emission from low-height flares was also dispersed in both horizontal and vertical directions, which causes lower ground level concentration around flaring.

By comparing the maximum ground level concentration of SO_2, which occurs in relatively stable condition and the unstable condition, it can be understood that most of the ground level concentration of air pollutant from flares caused by flares with low height. The impact of elevated flares are at longer distances from flaring activity, and in this study, their effect is mostly out of the island.

CONCLUSION

In this study, dispersion of an air pollutant, sulfur dioxide from gas flares on an island in Iran, which is one of the primary oil fields in the Persian Gulf, was investigated by application of CALPUFF model for two months of the year 2011. The effect of the terrain of modeling domain was considered in modeling. Since there was no option in this model for flares, modified flare parameters including emission rate and effective diameter and height of flare were calculated based on EPA guideline to represent better the actual flaring condition. The CALPUFF dispersion model, which is an unsteady state Lagrangian Gaussian model, was applied to investigate the effect of complex meteorological and terrain parameters that exist in locations like islands. The modeling was carried out with meteorological and geophysical data were provided by WRF prognostic meteorological model. The result of the study showed that the maximum concentrations mostly occur near flaring zone and cover a part of the industrial area. The objective of this study was the application of CALPUFF modeling system to investigate the effect of stability and mixing height on results of modeling. The result of modeling showed an excellent coupling of WRF model and CALPUFF modeling system. CALPUFF model could adequately express the effect of meteorological condition on results of modeling in each hour of the simulation period. The results of the simulation showed that low-height flares have the most impact on the ground level concentration of air pollutant on the islands. The effects of elevated flares were at a far distance from flaring activity and mostly occurred outside of the island.

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Persian Abstract

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چکیده

در این مطالعه ، در سال ۲۰۱۱ به مدت دو ماه، پراکندگی یکی از آلاینده‌های اصلی هوا یعنی دی اکسید گوگرد از شعله‌های گاز یک میدان نفتی، در ایران مورد بررسی قرار گرفت. با توجه به پیچیدگی پارامترهای هواشناسی در منطقه مدل‌سازی، از مدل California Puff (CALPUFF) استفاده شده است. CALPUFF یک مدل پیشرفته‌تر از AERMOD است که اثر پارامترهای هواشناسی در مناطق ساحلی را در نظر می‌گیرد، که با پارامترهای هواشناسی و ژئوفیزیکی تولید شده توسط مدل تحقیقات آب و هوا و پیش‌بینی آب و هوا (WRF) برای روزهای منتخب دوره مدل‌سازی به کار برده شده تا تأثیر این پارامترها را بر نتایج مدل‌سازی بررسی کند. از آنجا که هیچ گزینه‌ای در مدل شعله‌های آتش وجود ندارد، پارامترهای شعله‌وری از جمله میزان انتشار و ارتفاع و قطر موثر بر اساس روش EPA برای شبیه‌سازی بهتر شرایط واقعی شعله‌وری محاسبه شد. نتایج شبیه‌سازی نشان داد که مدل CALPUFF می‌تواند تأثیر شرایط هواشناسی را بر نتایج مدلسازی در هر ساعت از دوره شبیه‌سازی بیان کند. نتایج همچنین نشان داد که شعله‌های کم ارتفاع بیشترین تأثیر را در غلظت سطح آلاینده هوا در جزیره دارند. تأثیرات شعله بلند در فاصله بسیار دور از فعالیت شعله‌وری بوده و بیشتر در خارج از جزیره رخ داده است. مدل CALPUFF سازگاری بسیار خوبی با داده‌های هواشناسی تولید شده توسط WRF نشان داد و می‌تواند به درستی تأثیر پارامترهای هواشناسی و زمینی را در مدل‌سازی پراکندگی نشان دهد.