Comparison of CALPUFF and AERMOD Modeling systems for predicting SO_2 emissions from a gas refinery

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Abstract

Nowadays, air pollution is one of the major challenges in Assaluyeh, therefore, in the present study, according to the importance of the fourth refinery gas as the largest gas refinery in the region, the amount of emissions from Stacks and flares has been initially determined and then the distribution has been identified in the region. In this research, AERMOD and CALPUFF models have been used as the tools for the predition of SO_2 emissions of Stacks and flares of 4^{th} South Pars gas refinery located in Assaluyeh. First, SO_2 emissions from refinery Stacks and flares have been obtained by field measurements and emission coefficient respectively in four seasons of 2013. Then, the distribution of these emissions has been examined using dispersion models AERMOD and CALPUFF in an area of 50 × 50 km in each direction x and y in the one-year period of 2013 to the average time of 1, 3, 8, and 24 and the amounts resulting from the performance of the models have been compared to the results of field measurements at 9 receiving stations as a separate receptors in the model. Review of charts and statistical parameters has shown that, according to the evaluation of predictions made, performance of both models to predict the concentration of pollutants in the region can be generally considered acceptable.

Keywords: SO_2, AERMOD model, CALPUFF model, gas refinery

Introduction

Entering pollutants and also the rate of releasing pollutants into the atmosphere have an effect on air pollution. Pollutants may be released periodically or continuously from a point or non-point source or sources. The dispersion of pollutants also depends on the way entering the atmosphere. Lack of information on the distribution of pollutants makes the determination of their emissions difficult outside the site and the surrounding residential areas. Because of the focus on oil and gas industry, Assaluyeh is the spotlight of many professionals of Environmental Sciences and air pollution is considered one of the challenges facing this industrial area. Hence, better and more effective control and reduction of air pollutants has been the agenda of the relevant organizations. In this study, SO_2 Emissions from a gas refinery in South Pars Gas Complex located in Assaluyeh have been estimated by two common atmospheric dispersion models AERMOD and CALPUFF.

Generally, Sulfur oxides SO_x are the maximum amount of gases discharged into the air in addition to nitrogen oxides NO_x around gas refineries. Sulfur dioxide is one of the important atmospheric pollutants, which is a major cause of urban air quality problem (1). In fact, many studies have emphasized that the critical concentration of SO_2 emitted from industrial facilities in the area countries can seriously affect air quality in the region (2, 3). The comparison of the predicted 24-hour concentrations of pollutant SO_2 with 24-hour standards WHO, EPA and Iran National standards shows that results in many areas have been higher than the desired standards.

CALPUFF model has been approved by Environmental Protection Agency as a model for the non-steady and complex flow modeling including cases that are in the complex terrain and also in places where the stationary and reverse flow are important. Modeling system consists of three main parts CALMET, CALPUFF and CALPOST. CALPUFF is actually a non-uniform Lagrangian-Gaussian model of fluid motion which has subroutines for networking of time changes, the meteorological conditions in the three dimensions, and effects of Terrain, wetland and dry land subsidence, diffusion and dispersion on the marine environment, building downwash. CALPOST is used for post-processing the output results and processing simulation files.

AERMOD model is able to simulate the floating plume. In general, Gaussian models are limited to flows through simple surface, but AERMOD model uses a simple method to approximate the flows passing through the ups and downs(4). This model is formed from a meteorological preprocessor called AERMET and a geological preprocessor called AERMAP in addition to the main processor AERMOD(5).This study examines the performance of each model AERMOD and CALPUFF in such circumstances for the first time. Performance Estimation of the Models has been conducted in two ways in the study: First, by comparing the observed data and model output, modeling accuracy at any point in the desired time period has been achieved in the designated recipient points for models (based on the coordinates UTM). In the second stage, the performance accuracy of the models in comparison with each other has been examined.

Methods:

Study area

The port city of Assaluyeh is a huge industrial area at Bushehr in southern Iran. Fourth South Pars gas refinery is located in the South Pars region in southeast of Bushehr. The refinery consists of two phases of sea and land and has been designed in three phases with harvesting and processing capacity of 110 million cubic meters and 36.7 million cubic meters for each phase. It has 33 Stacks and 8 flares that are the major sources of air pollution caused by emissions from Stacks and flares. Generally, the concentration and diffusion of SO_2 in the region have been modeled and predicted by AERMOD and CALPUFF models and healthy and unhealthy areas have been specified in the region according to the maximum concentration and the results of the two models together with the results of field measurements have been verified using statistical relationships.

Model input data

In this study, upper atmosphere data and synoptic stations have been used through Iran Meteorological Organization to verify the initial studies of climate and to provide input data of meteorological model CALMET and AERMET. The surface meteorological data required has used recorded and quality-controlled data by the Meteorological Organization in 2012-2013 for Airport Station Assaluyeh which is the nearest station to the study area(6). A dominant wind direction is from the northwest to southeast in the station.

Seasonal changes, especially changes in atmospheric parameters such as the size and direction of wind, temperature, boundary layer height and relative humidity in the area in different seasons will have a significant effect on the propagation direction of pollutants (plume) and will affect air pollution. Therefore, the modeling has been done in four seasons to investigate the changes.

Receptors in two separate and network system have been presented to the model to cover all the resources in the domain of modeling studies, centralize of the desired source and also include the area where it can express topographical and meteorological features of the area. Network receptors have been defined in Cartesian coordinates within an area of 50 × 50 square kilometers in each direction x and y respectively, and the location of the monitoring stations has been introduced in the model as distinct receptors. Arrangement of all receptors to the center of a stack in the phases 6, 7, 8 has been selected so that it can cover all sources and express atmospheric phenomena in an intermediate and micro-scale as well as the effects of topography and land use. Modeling for the receptors has been done at a height of 1.5 meters above ground level (breathing).

After the review of the production process and determine the sources of emissions during field visit to the region, measurement of SO_2 from working Stacks has been done by Testo 350 XL at specific points sampled from the Stacks in four seasons, spring, summer, autumn, winter in 2013 and 3 times per season. Since the diffusion coefficients indicate production and emissions in normal operating conditions of a process, the sampling has been done in normal operating conditions of the system and refused in the abnormal conditions such as repairs or out- of - service equipments that affect the performance of the process(7). Environmental emissions sampling has been also performed in 9 receptors by LSI Lastem Babuc A that has interchangeable electrochemical sensors made in Italy to verify the model results.

Validation of the model

In the present study, evaluating the results of modeling has been done By AERMOD and CALPUFF models with the values of field measurements for the desired receptors using the statistical parameters proposed by EPA America. These parameters are:

- The correlation coefficient (CCOF)

According to equation (1), Parameter CCOF shows the relationship between the model results and field measurements and as much as it is closer to 1, it shows the desired accuracy of the results of the model.

$$CCOF = \frac{\sum_{i=1}^{N}(X_i - \bar{X})(Y_i - \bar{Y})}{\left(\sum_{i=1}^{N}(X_i - \bar{X})^2 \sum_{i=1}^{N}(Y_i - \bar{Y})^2\right)^{1/2}} \qquad \text{Equation (1)}$$

- Fractional bias (FB)

Based on the framework provided by Olesen(8) statistical performance of the results has been expressed by fractional bias parameters (Fractional Bias), which represents tendency of the model to predict more or less than the actual value in this study. The amount of fractional bias -0.67 has been equal to over prediction by a factor of 2 and 0.67 equal to under prediction by a factor of 2. The deficit bias 0 indicates that the prediction of model is complete. A good model performance should have a fractional bias less than 0.3.

$$FB = \frac{\bar{C}_O - \bar{C}_P}{0.5(\bar{C}_O - \bar{C}_P)} \qquad \text{Equation (2)}$$

Research findings

In this study, the characteristics of each of the two models CALPUFF and AERMOD have been first evaluated. Since CALPUFF and AERMOD models have been proposed for large (more than 50 km) and small ranges respectively they have been selected for better comparison of an area with dimensions of 50 × 50 km and then the data of output concentration of these models have been compared with each other.

In general, evaluation of Figure 1 to Figure 4 shows that SO_2 simulated concentrations have been greater in comparison with maximum concentration measured and smaller in comparison with lowest concentration measured. Both models showed good agreement compared with the median values. The CALPUFF model output has been also more consistent with the measured values. The average value of the fractional bias (FB) for pollutants SO_2 in AERMOD and CALPUFF models has been 0.53 and 0.001 respectively. FB values indicate that CALPUFF has done relatively precise predictions. The average values of CCOF for pollutants SO_2 in AERMOD and CALPUFF models have been 0.84 and 0.85 respectively. FB values indicate that CALPUFF has done relatively precise predictions.

Performance investigation of dispersion models can be always performed by comparing model output with measurements made. Therefore, AERMOD model results have been compared with measured values for the maximum 1-hour average concentration of 9 receptors in this study. Statistical parameters CCOF and FB have been shown in Table 1. The correlation coefficient values for pollutants SO_2 have been 0.88 for spring, 0.60 for summer, 0.96 for autumn and 0.94 for winter.

Table 1. Validation of AERMOD model results

Statistical parameters	2013 Spring	2013 summer	2013 autumn	2013 winter
CCOF	0.88	0.60	0.96	0.94
FB	0.69	0.69	0.25	0.48

The maximum one-hour SO_2 concentration has been compared with standard to assess the impact on air quality and found that the concentrations predicted have been above the ambient air quality standard. Statistical parameters CCOF and FB have been shown in Table 2 for CALPUFF model validation. The correlation coefficient values for pollutants SO_2 have been 0.75 for spring and summer, 0.95 for autumn and winter. Maximum SO_2 daily concentration dispersion has happened in autumn and winter. Considering these factors, the used model has shown reasonably satisfactory results to predict the distribution of SO_2 concentration.

Table 2. Evaluation of CALPUFF model results

Statistical parameters	2013 Spring	2013 summer	2013 autumn	2013 winter
CCOF	0.75	0.75	0.95	0.95
FB	-0.04	0.09	-0.03	-0.01

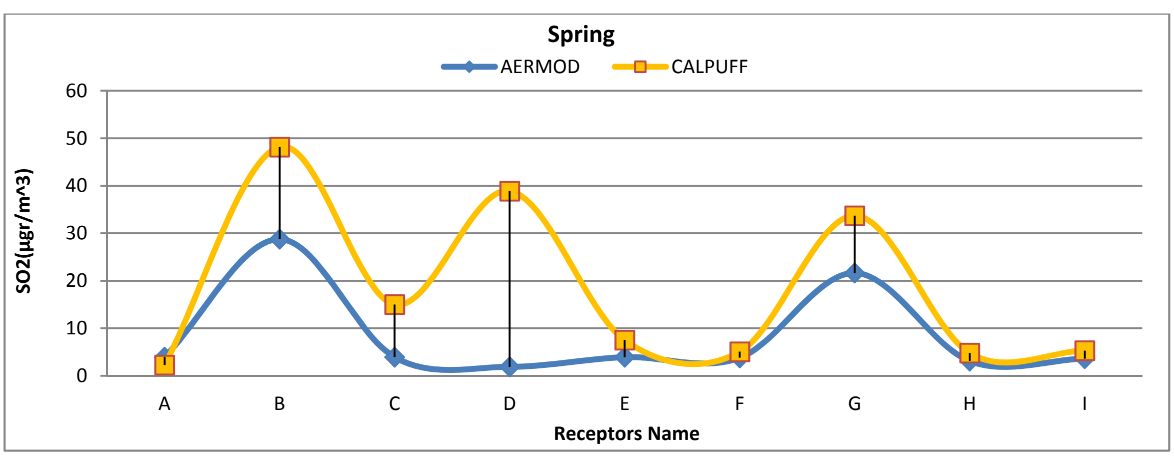

Figure 1.Comparison of the two CALPUFF and AERMOD model results at 9 receptor stations in spring

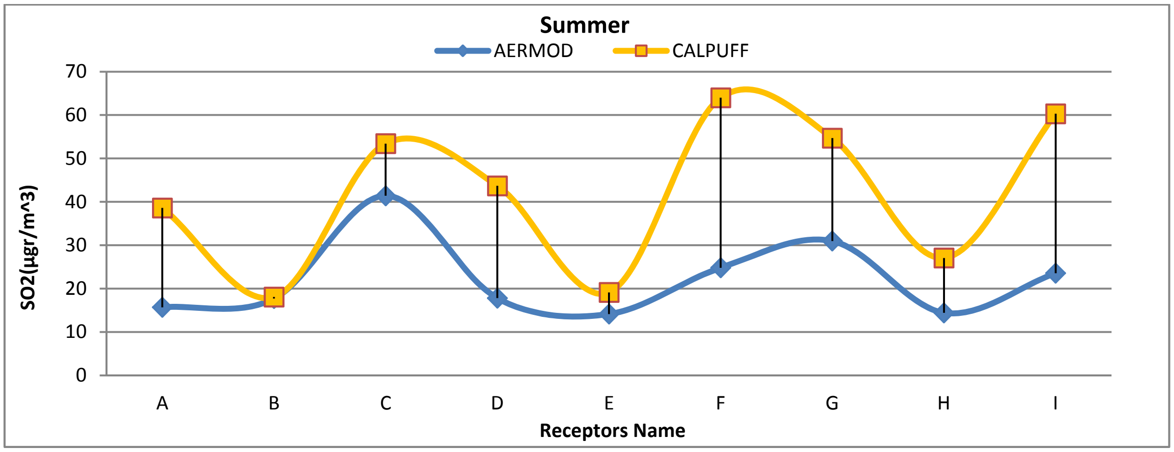

Figure 2. Comparison of the two CALPUFF and AERMOD model results at 9 receptor stations in summer

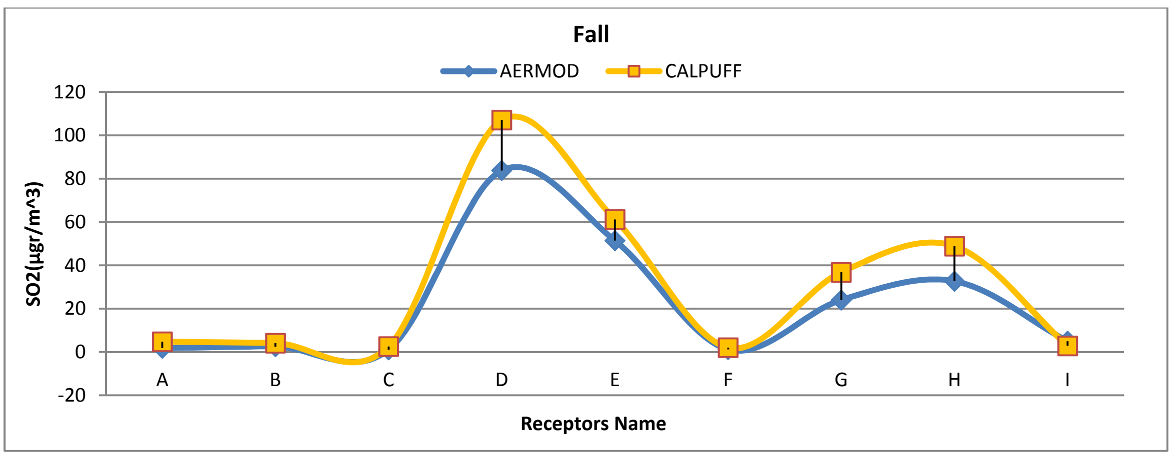

Figure 3.Comparison of the two CALPUFF and AERMOD model results at 9 receptor stations in autumn

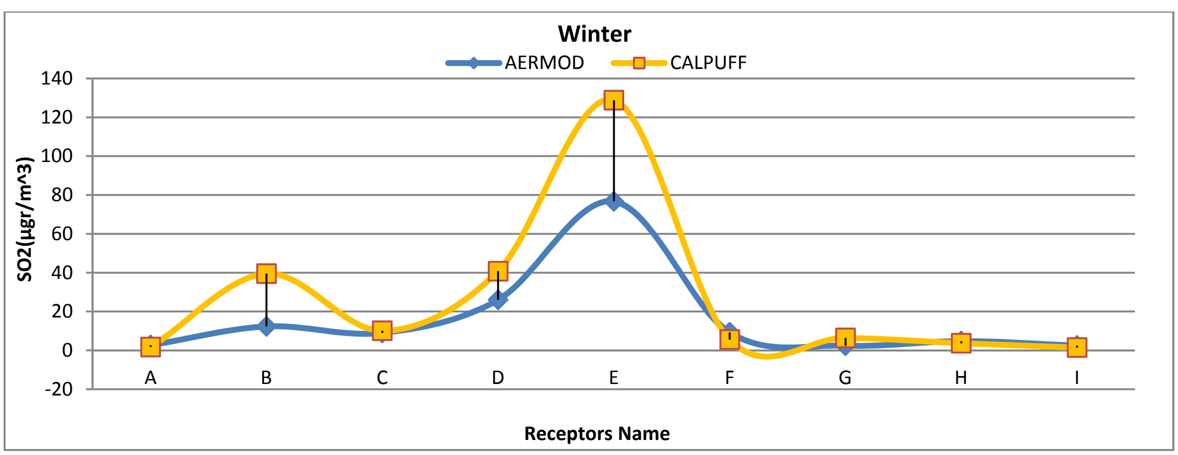

Figure 4.Comparison of the two CALPUFF and AERMOD model results at 9 receptor stations in winter

Discussion and Conclusion

In this study, studies and analysis have been firstly carried out about the performance of AERMOD and CALPUFF models and determination the limits and capabilities of both models. Then, all the information on the measured seasonal values of SO_2 pollutants and meteorological parameters measured at the meteorological station Assaluye has been collected and the information required to implement the AERMOD and CALPUFF models have been provided. Then, using the database including meteorological parameters, topography, a list of sources of emissions and SO_2 pollutant concentrations, first, AERMOD model and then CALPUFF model has been implemented for the four seasons in 2013. The results of the models have been compared with the values measured by environmental monitoring stations and evaluated using a set of statistical relationships in order to verify the models.

It can be generally said that calculation and accurate determination of the major air pollutants in industrial areas have been always considered as a major step for decision making in relation to air quality management programs to prevent environmental degradation. According to the various comparisons and statistical measures in this study, the overall performance of CALPUFF model has been superior to AERMOD model. AERMOD model does not apply to dry or wet depositions of gases and includes dry deposition using a reflecting algorithm. In general, prediction of AERMOD has been less than reality. High levels of ambient concentrations measured in comparison with the modeled values can be revealed that not only point sources of emissions, such as stacks and flares have an effect on the emissions but also moving emission sources such as vehicle could also play a role in this case. According to the results of modeling, different output concentrations have been mainly obtained from the comparison of the Gaussian model (AERMOD) and Lagrangian model (CALPUFF). To air quality management including development of control strategy and assessment of potential pollutant transmission in the region, the amount and distribution of pollutants should be considered in the region.

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