PREDICTION OF NO\textsubscript{2} CONCENTRATIONS IN A GAS REFINERY USING AIR DISPERSION MODELING

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Abstract. Nitrogen dioxide (NO\textsubscript{2}) is considered as one of the most important ambient air pollutants in gas refineries. In this study, AERMOD dispersion model was applied for prediction of NO\textsubscript{2} ambient concentrations and dispersion patterns from point sources, including 13 stacks and six flares in a gas refinery located in Asaluyeh, Iran. For this purpose, the NO\textsubscript{2} concentrations exhausted from the stacks were measured by a portable emission analyzer and the NO\textsubscript{2} concentrations resulted from the flares were estimated using the emission factors. Moreover, the amounts of ambient NO\textsubscript{2} concentrations in 10 monitoring stations were measured in four seasons. Then, the ambient NO\textsubscript{2} concentrations and dispersion patterns were predicted using the AERMOD model within a domain of 10 × 10 km\textsuperscript{2}, in 1-hr and 12 months averages and the unhealthy zones in the study area were defined. The results revealed that for both annual observed and predicted values, ambient NO\textsubscript{2} concentrations were higher than WHO standard limits but they did not exceed the US EPA standard limits. However, the hourly observed and predicted concentrations were lower than the standard levels. Statistical methods were used for comparing the predicted and observed NO\textsubscript{2} concentrations. Simulation results indicated that the predicted concentrations were underestimated by a factor of 20\% in comparison to the measured ones which revealed the estimated contribution of other sources including mobile sources and neighbor sources located in the vicinity of the gas refinery.

Keywords: AERMOD, air quality, emission, performance, point source

Introduction

Air pollution will adversely affect the quality of life and human health. Therefore, it has been widely concerned by environmental experts in the world.

The World Health Organization (WHO) has reported that about 2.7 million people die due to the health effects of air pollution annually (WHO, 2014). The minimum concentrations of gasses in the atmosphere could be essential in determining the health status of the societies (Shooter et al., 1993). Meanwhile, the air quality management policies are important in order to reduce the acute effects of air pollutants. Identifying the emissions due to different sources and assessing their adverse effects are important for appropriate air quality management (Bhanarkar et al., 2005).

The NO\textsubscript{2} concentrations exhausted from the gas refinery usually increase with rising ignition temperature that leads to producing NO, and then oxidized to nitrogen dioxide (NO\textsubscript{2}) in the presence of oxygen in the atmosphere. NO\textsubscript{2} is an air pollutant with a 1–3 days
lifetime in mesoscale. Ambient NO\textsubscript{2} concentrations have been regulated by the U.S. EPA as one of the six primary air pollutants. Respiratory tract infections due to the pollutant’s interaction with the immune system may be increased by NO\textsubscript{2} exposure. Furthermore, it has been associated with slight respiratory symptoms at low NO\textsubscript{2} concentrations and with death in indoor locations (Chen et al., 2007). It is caused throat, eyes and nose irritation for inhalation in human (Perkins, 1974). Direct effects of nitrogen oxides can be considered as the creation of smog and photochemical ozone components (Akdemir et al., 2013). The U.S. EPA (2010) has determined that the hourly average ambient NO\textsubscript{2} concentrations should not exceed 200 µg/m\textsuperscript{3}. In order to meet the regulation goals and for minimizing the adverse effects of air pollutants, it is essential to study the disperions of air pollutants which are affected by several factors including atmospheric stability, orography, obstacles, roughness, maximum mixing height, wind speed and wind direction, and height of the release above ground level (Crowl and Louvar, 2002; Seangkiatiyuth et al., 2011).

Various methods including measurement, emission inventory and simulation studies are applied to assess air pollution impacts due to pollutants released into the atmosphere and to monitor whether pollutants’ concentrations exceed the standard limits (Capelli et al., 2013). Air quality dispersion modeling is important for predicting the pollutants’ concentrations, simulating the emission distribution patterns and the spatial allocation of outdoor air pollutants (Holmes and Morawska, 2006; Zhang et al., 2010). On the other hand, dispersion models are effective tools for predicting the contributions of emissions due to various pollutant sources including traffic, industry, residential and commercial sectors (Cimorelli et al., 2005). Advanced dispersion models such as American Meteorological Society/Environmental Protection Agency Regulatory Model (AERMOD) were often applied for predicting the air quality after a long time, e.g. at least 10 years (Ma et al., 2013).

As AERMOD model can combine various concepts and complex algorithms, it has been used for evaluating the ambient concentrations and dispersion patterns of some pollutants, including SO\textsubscript{2}, PM\textsubscript{10}, VOCs, hydrogen cyanide (HCN), and sulfur hexafluoride (SF\textsubscript{6}) (Bhardwaj et al., 2005; Orloff et al., 2006; Venkatram et al., 2001, 2004, 2009; Zou et al., 2009, 2010).

Moreover, AERMOD can be used for simulating the dispersion of heavy metals, such as chromium and mercury (Sax and Isakov, 2003; Mazur et al., 2009). When upper climatological data are not accessible, AERMOD can be integrated with meteorological models such as MM5, WRF, and RAMS, etc (Caputo et al., 2003; Isakov et al., 2007; Kesarkar, 2007).

Some studies were carried out regarding prediction of NO\textsubscript{2} concentrations and dispersion patterns with AERMOD. The dispersion of NO\textsubscript{2} emitted from four cement plants in Thailand were studied using AERMOD model. In this study, the predicted ambient NO\textsubscript{2} concentrations were compared with the observed values in 12 receptors. The results showed that simulated and observed concentrations were in better agreement within 1-5 km than those at receptors situated in 5 km further away from the reference point. Moreover, the results revealed that both observed predicted ambient NO\textsubscript{2} concentrations were not exceed the limit values set by the National Ambient Air Quality Standards (Seangkiatiyuth et al., 2011). Furthermore, AERMOD was used for modeling of NO\textsubscript{x} , PM\textsubscript{2.5} and SO\textsubscript{2} emissions from point and line sources in Halifax, Nova Scotia, Canada in 50 × 50 km\textsuperscript{2} domains over 1-hr, monthly and annual periods averages. The evaluation of model performance was done by applying...
statistical parameters and the results showed poor agreement among the observed and simulated results (Gibson et al., 2013). In another study, Cohan et al. (2011) examined the dispersion and predicted concentrations of NO\textsubscript{x} and PM\textsubscript{2.5} in port communities in California using AERMOD. The correlation coefficients for NO\textsubscript{x} and PM\textsubscript{2.5} were 50% and 43%, respectively (Cohan et al., 2011). AERMOD model was also used to simulate the NO\textsubscript{2} and SO\textsubscript{2} concentration in Beilun area. The results demonstrated that the ambient average concentrations of NO\textsubscript{2} and SO\textsubscript{2} were equivalent to 16.7%~58.3% and 26.7%~53.3% of the clean air quality standard respectively. However, concentrations of NO\textsubscript{2} and SO\textsubscript{2} were relatively higher in the upper air of Beilun region. NO\textsubscript{2} and SO\textsubscript{2} gasses in the upper air were a reason for the high potential of acid rain on Beilun region (Hasson et al., 2013).

In order to study the performance of applying emission control devices, AERMOD modeling system was applied for predicting the air pollution in Xuanwei, an important industrial city in China, and it was concluded that AERMOD can be used properly for simulating NO\textsubscript{x} and SO\textsubscript{2} emissions (Ma et al., 2013). The emission, transport, dispersion, and concentration analysis of PM emitted from a big industrial complex in Malagueño city, Argentina, were also conducted using AERMOD model. The model was applied to 224 emission sources. The performance of the model was evaluated by comparing the simulated results with the observed Total Suspended Particulate matters (TSP) at two monitoring sites for 62 continuous days in winter. The results showed the impact of the industrial activities on the local PM concentrations, from which stockpiles and unpaved industrial roads were the main emission sources, straightly affecting two of the nearest neighborhoods in the study area (Abril et al., 2016). In another study, AERMOD model was used to predict SO\textsubscript{2}, CO, NO\textsubscript{x} and PM\textsubscript{10} emissions impacts at receptors due to calcining processes including handling and storage of raw petroleum coke in Argentina. The observed and predicted ambient pollutants’ concentration levels were compared with public health standards. The results revealed that the exposures of the simulated NO\textsubscript{x}, CO, PM\textsubscript{10} and SO\textsubscript{2} concentrations were lower than the air quality standards. However, the PM concentration level was higher than the standard limits (Singh et al., 2015).

The exposures of various pollutants including NH\textsubscript{3}, CH\textsubscript{4}, CO, CO\textsubscript{2}, H\textsubscript{2}S, NO\textsubscript{2}, N\textsubscript{2}O, SO\textsubscript{2} and organic dust were estimated for populations residing in close vicinity to ten poultry concentrated animal feeding operations (CAFOs ) located in Central Poland. AERMOD model was used to predict the pollutants’ concentrations in order to compute the Hazard Index (HI) for a mixture of chemicals. Results presented that the estimated hazard indexes which were less than unity; therefore there was low potential for adverse health consequences for the surrounding society for the combined mixture of chemicals (Pohl et al., 2016).

A comparative study regarding the health effects of emissions due to vehicles and industries were conducted in China and Pakistan. In this study, ambient CO, NO\textsubscript{2}, and SO\textsubscript{2} concentrations were measured and compared with U.S. EPA, WHO and national clean air standards in China and Pakistan (Niaz et al., 2015).

The performances of ISCST-3, AERMOD, and CALPUFF models for NO\textsubscript{x} and CO emissions in point, line and area sources were compared together using statistical analysis in Körfez. The results revealed that AERMOD predictions for NO\textsubscript{x} concentrations were lower than those predicted by ISCST-3, and CALPUFF models. Meanwhile, CO concentrations predicted by AERMOD were among the concentration levels simulated by CALPUFF and ISCST-3 (Demirarslan and Doğruparmak, 2016).
The main goal of the present study was to simulate the ambient concentrations and dispersion patterns of NO$_2$ emitted from stacks and flares in a sour gas refinery located in a complex industrial region with special climatological and topographical conditions and to determine the contribution of the gas refinery in NO$_2$ emissions using AERMOD dispersion model.

In this study, ambient NO$_2$ concentrations in a gas refinery situated in Asaluyeh was measured seasonally in 10 receptors in and around the refinery from June 2014 to May 2015. Thereafter, the 1-hr and annual ambient concentrations and dispersion patterns of NO$_2$ were simulated by applying AERMOD dispersion model in the area of 10×10 km$^2$. Moreover, the predicted concentrations in receptors were compared with the measured ones using statistical methods. Then, unhealthy zones were determined in the study region using contour plots of the seasonal NO$_2$ distribution patterns. Finally, the contribution of emissions due to point sources in this refinery was determined.

**Materials and Methods**

**Study Area**

Asaluyeh, a sub-city of Kangan, belongs to Boushehr Province, which locates in the southwest of Iran. The desired gas refinery as shown in *Figure 1*, is situated on 27° 30’ to 27° 31’ north latitude and 52° 34’ to 52° 36’ east longitude in Asaluyeh. It was commissioned with a refining 50 million cubic meters per day sour gas and 80,000 barrel per day gas condensate to supply for the Iran’s local strategic demand.

**Figure 1. The study area, the point sources and monitoring stations**
Field Measurements

Emission Sources

The point sources in the gas refinery included 13 stacks and six flares. The exit velocity of the flue gas and concentrations of NO\(_2\) emitted from the stacks were measured by a portable emission analyzer (TESTO 350 XL), in four seasons (June 2014 - May 2015) and four times in each season (ASTM, 2011a). The emission rate of NO\(_2\) resulting from the flares was also determined by emission factors according to EPA/AP-42 method.

The required AERMOD inputs data were including emission height (m), flue gas temperature (°C), inner diameter of stack (m), flue gas velocity (m/s), geographical coordinates (X,Y) and elevation above the ground level (m) (Table 2). The locations of point sources are illustrated in Figure 1. In the current study, the maximum NO\(_x\) emission for the continuous operation has been considered. The total NO\(_2\) emission rate from 19 point sources which evaluated according to Tier2 in AERMOD guidelines (US EPA, 2009, 2010a) was 270 g/s.

Table 2. Characteristics of point sources in the gas refinery

<table>
<thead>
<tr>
<th>Sources*</th>
<th>Cartesian Coordinates</th>
<th>Diameter</th>
<th>Height</th>
<th>Flue Gas Temperature</th>
<th>Flue Gas Velocity</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>X (m)</td>
<td>Y (m)</td>
<td>(m)</td>
<td>(m)</td>
<td>(°C)</td>
</tr>
<tr>
<td>BO-1</td>
<td>0</td>
<td>0</td>
<td>3</td>
<td>42.7</td>
<td>160.5</td>
</tr>
<tr>
<td>BO-2</td>
<td>-17</td>
<td>-10</td>
<td>3</td>
<td>42.7</td>
<td>154</td>
</tr>
<tr>
<td>BO-3</td>
<td>-33</td>
<td>-26</td>
<td>3</td>
<td>42.7</td>
<td>159</td>
</tr>
<tr>
<td>BO-4</td>
<td>-49</td>
<td>-35</td>
<td>3</td>
<td>42.7</td>
<td>154</td>
</tr>
<tr>
<td>GTG-1</td>
<td>-183</td>
<td>145</td>
<td>4</td>
<td>30</td>
<td>550</td>
</tr>
<tr>
<td>GTG-2</td>
<td>-167</td>
<td>130</td>
<td>4</td>
<td>30</td>
<td>550</td>
</tr>
<tr>
<td>GTG-3</td>
<td>-153</td>
<td>111</td>
<td>4</td>
<td>30</td>
<td>550</td>
</tr>
<tr>
<td>GTG-4</td>
<td>-139</td>
<td>94</td>
<td>4</td>
<td>30</td>
<td>550</td>
</tr>
<tr>
<td>GTC-1</td>
<td>311</td>
<td>-110</td>
<td>3.15</td>
<td>17.3</td>
<td>520</td>
</tr>
<tr>
<td>GTC-2</td>
<td>325</td>
<td>-129</td>
<td>3.15</td>
<td>17.3</td>
<td>520</td>
</tr>
<tr>
<td>GTC-3</td>
<td>339</td>
<td>-129</td>
<td>3.15</td>
<td>17.3</td>
<td>520</td>
</tr>
<tr>
<td>X-1</td>
<td>129</td>
<td>-266</td>
<td>2.1</td>
<td>117</td>
<td>592</td>
</tr>
<tr>
<td>X-2</td>
<td>31</td>
<td>-138</td>
<td>2.1</td>
<td>117</td>
<td>500</td>
</tr>
<tr>
<td>F-1**</td>
<td>998</td>
<td>221</td>
<td>0.48</td>
<td>142.8</td>
<td>800</td>
</tr>
<tr>
<td>F-2**</td>
<td>1057</td>
<td>474</td>
<td>0.48</td>
<td>142.8</td>
<td>800</td>
</tr>
</tbody>
</table>

* BO: Boiler, GTG: Gas Turbine Generator, X: Incinerator, GTC: Gas Turbine Compressor, F: Flare
**According to Iowa Procedure the modified diameter and height were used for flares.


**Ambient NO$_2$ Concentrations**

Measurements of 1-hr average of ambient NO$_2$ concentrations were performed using a mobile device (LSI-Lastem Babuc A) in four seasons and four times in each season from June 2014 to May 2015 in 10 receptors (ASTM, 2011b). The locations of receptors from reference point (BO-1) have been presented in *Table 3*.

*Table 3. Cartesian coordinates of the receptors*

<table>
<thead>
<tr>
<th>Receptor</th>
<th>Cartesian Coordinates</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>X (m)</td>
</tr>
<tr>
<td>A</td>
<td>402</td>
</tr>
<tr>
<td>B</td>
<td>-127</td>
</tr>
<tr>
<td>C</td>
<td>-286</td>
</tr>
<tr>
<td>D</td>
<td>-460</td>
</tr>
<tr>
<td>E</td>
<td>-201</td>
</tr>
<tr>
<td>F</td>
<td>-13</td>
</tr>
<tr>
<td>G</td>
<td>55</td>
</tr>
<tr>
<td>H</td>
<td>594</td>
</tr>
<tr>
<td>I</td>
<td>904</td>
</tr>
<tr>
<td>J</td>
<td>691</td>
</tr>
</tbody>
</table>

**Meteorological Data**

All Surface and upper-air weather data (wind speed, wind direction, temperature, cloud cover, dew point temperature, pressure at sea level, rainfall and humidity, solar radiation) in eight time steps (0:00, 3:00, 6:00, 9:00,12:00, 15:00, 18:00, 21:00) in a day were provided as meteorological inputs for AERMOD from June 2014 to May 2015 (IRIMO, 2015). The annual wind rose was produced based on data received from Asaluyeh Weather Station (*Figure 2*). The prevailing wind direction in this station was from NW to SE in all seasons. The AERMET was employed to simulate the climatically conditions using the values of Bowen ratio, surface roughness length and Albedo parameters based on the types of the surrounding vegetation and land use in the study area. The values of these parameters have been presented in *Table 1*.

*Table 1. The surface specifications according to meteorological data*

<table>
<thead>
<tr>
<th>Sector Number</th>
<th>Beginning Direction (Degree)</th>
<th>Ending Direction (Degree)</th>
<th>Albedo</th>
<th>Bowen Ratio</th>
<th>Roughness Length (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0</td>
<td>150</td>
<td>0.28</td>
<td>6</td>
<td>0.3</td>
</tr>
<tr>
<td>2</td>
<td>150</td>
<td>300</td>
<td>0.14</td>
<td>0.1</td>
<td>0.0001</td>
</tr>
<tr>
<td>3</td>
<td>300</td>
<td>360</td>
<td>0.28</td>
<td>6</td>
<td>0.3</td>
</tr>
</tbody>
</table>
Figure 2. The annual wind rose in the study area

Elevation Data

In order to predict the NO$_2$ concentrations at receptors, elevation data was required as model input. In this study, the required digital elevation files were provided from Iran National Cartographic Center. The 3D view of topography in the study region produced by GIS with a resolution of 90 m has been shown in Figure 3.

Figure 3. The 3D view of topography in the study region
**AERMOD Modeling System**

AERMOD dispersion model developed by the U.S. EPA is a steady-state Gaussian model for predicting air pollutants’ concentrations and dispersion patterns due to various emission sources. AERMOD model consists of three sections: Meteorological Preprocessor (AERMET), Terrain Preprocessor (AERMAP) and AERMOD Gaussian Plume Model (US EPA, 2004a, 2004b, 2009). It is necessary to provide all emission rates due to various sources (point, line, area, and volume sources) and the meteorological and topographical data to predict pollutants’ concentrations and dispersion patterns in rural and urban areas, calculating building downwash effect, terrain adjustment, etc. at short-range (up to 50 km) (Cimorelli et al., 2005; Perry et al., 2005). AERMOD makes distribution estimations by utilizing the meteorological characteristics of the study region, including stack diameter and height; stack temperature, flue gas velocity, wind direction and wind speed (Mokhtar et al., 2014; Huertas et al., 2014; Stein et al., 2007).

In this study, simulations for NO\textsubscript{2} ambient concentrations and dispersion patterns were performed for the total study area of 100 km\textsuperscript{2}, where a grid of 50 m \times 50 m was built.

**Evaluation of AERMOD Performance**

In order to evaluate the model performance, the results of field measurement and model simulation were compared together using statistical methods. Statistical Parameters suggested by U.S. EPA (U.S. EPA, 2003, 2005) including: “correlation coefficient (COR)“, “Normal Mean Bias (NMB)“, “Normal Mean Error (NME), “fractional bias (FB),” and also “Index of Agreement (IOA)“ (Luhar, 2003) were applied (Equations 1 ~ 5). According to Eq. (1), parameter COR indicates the relationship between the Simulated and the measured results. The more the value of COR is closer to 1, the performance of the model is more satisfactory.

\[
COR = \frac{\sum_{i=1}^{N} (S_i - \bar{S})(M_i - \bar{M})}{\left(\sum_{i=1}^{N} (S_i - \bar{S})^2 \sum_{i=1}^{N} (M_i - \bar{M})^2\right)^{1/2}} \quad \text{(Eq. 1)}
\]

NMB and NME parameters were applied to evaluate the model performance for simulating NO\textsubscript{2} concentrations. The variation ranges for COR, NMB and NME were (-1 \sim + 1), (-1 \sim + \infty), (0 \sim + \infty), respectively (U.S. EPA, 2003).

\[
\text{NMB} = \frac{\sum_{i=1}^{N} (S_i - M_i)}{\sum_{i=1}^{N} M_i} \times 100 \quad \text{(Eq. 2)}
\]

\[
\text{NME} = \frac{\sum_{i=1}^{N} |S_i - M_i|}{\sum_{i=1}^{N} M_i} \times 100 \quad \text{(Eq. 3)}
\]

FB indicates the tendency of the model to predict values more or less than the measured concentrations in this study (Olesen, 2001). The acceptable value for FB was less than 0.3 (Ghannam and El-Fadel, 2013).
IOA is sensitive to differences between the measured and simulated results means as well as to certain changes in proportionality (Luhar, 2003). The variation range for IOA was (0,1).

\[ IOA = 1 - \frac{\sum_i^N (S_i - M_i)^2}{\sum_i^N (S_i + M_i - \bar{S} - \bar{M})^2} \]  

(Eq. 5)

Where, \( S_i \): simulated concentrations, \( M_i \): measured concentrations, \( \bar{S} \): average simulated concentrations, \( \bar{M} \): average measured concentrations, \( N \): the total number of measurements.

Results and Discussion

Experimental Results

The 1-hr averages of ambient NO\(_2\) concentrations in 10 receptors in four seasons from June 2014 to May 2015 have been illustrated in Figure 4. For all receptors except B in summer 2014, the measured ambient NO\(_2\) concentrations were lower than the clean air U.S. EPA standard for 1-hr ambient concentration levels. However, in all seasons the simulated ambient NO\(_2\) concentrations in all receptors were lower than the standard limit (200 \(\mu\)g/m\(^3\)). Based on the safety regulation for hourly NO\(_2\) concentrations (200 \(\mu\)g/m\(^3\)) published by the WHO Guideline, NO\(_2\) emissions from the gas refinery showed no significant health effects on personnel. However, the average annual concentration was 87 \(\mu\)g/m\(^3\) which was higher than the WHO standard limit (40 \(\mu\)g/m\(^3\)) and they have not exceeded the U.S. EPA standard limits (100 \(\mu\)g/m\(^3\)) (WHO, 2017; U.S. EPA, 2010b).

![Figure 4. Ambient NO\(_2\) concentrations in 10 receptors at 1-hr average period](image-url)
The 1-hr averages of ambient NO\textsubscript{2} concentrations measured in 10 receptors varied from 46.4 to 97.6 \(\mu\)g/m\textsuperscript{3} in summer 2014, from 47 to 375 \(\mu\)g/m\textsuperscript{3} in autumn 2014, from 54.5 to 120.2 \(\mu\)g/m\textsuperscript{3} in winter 2015 and from 78.9 to 125.8 \(\mu\)g/m\textsuperscript{3} in spring 2015. As a result, the highest observed NO\textsubscript{2} ambient concentration was measured in autumn and the lowest amount was measured in summer for 1-hr average period. However, in all seasons the predicted ambient SO\textsubscript{2} concentrations in all receptors were lower than the US EPA clean air standard levels except for B monitoring stations in autumn 2014, due to the direction of prevailing wind (from NW to SE) and the neighboring refineries.

The simulated results also showed that the variations of NO\textsubscript{2} concentrations were ranged from 21.2 to 83.03 \(\mu\)g/m\textsuperscript{3} in summer 2014, from 35.7 to 162 \(\mu\)g/m\textsuperscript{3} in autumn 2014, from 34.5 to 87 \(\mu\)g/m\textsuperscript{3} in winter 2015, and from 73 to 114.5 \(\mu\)g/m\textsuperscript{3} in spring 2015, which presented the highest concentration in the autumn and the lowest value in the summer. Meanwhile, in all seasons the simulated ambient NO\textsubscript{2} concentrations in all receptors were lower than the clean air standard levels.

A comparison among the results of measured 1-hr average NO\textsubscript{2} concentrations and the simulated values for 10 monitoring stations (receptors) in four seasons in the study area is presented in Figure 5. As shown, the simulated ambient NO\textsubscript{2} concentrations were less than the measured ones for all receptors. The variations among the simulated and measured ambient NO\textsubscript{2} concentrations in D, I and J receptors were higher than those in other receptors. These receptors were situated on the border of the study area with other refineries and it might be resulted from emissions due to other neighboring refineries and other industries. The observed and simulated results were in good agreement. The values and locations of maximum simulated ambient NO\textsubscript{2} concentrations at 1-hr and annual averages are presented in Table 4.
Figure 5. Comparison among measured and simulated 1-hr averages of ambient NO$_2$ concentrations for 10 receptors

Table 4. Maximum simulated amounts of ambient NO$_2$ concentrations based on the average periods in a 10×10 km$^2$ domain

<table>
<thead>
<tr>
<th>Time Scale</th>
<th>Max. Concentration (μg/m$^3$)</th>
<th>hour</th>
<th>day</th>
<th>month</th>
<th>X (m)</th>
<th>Y (m)</th>
<th>Z (m)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1-hr</td>
<td>10544.1</td>
<td>19</td>
<td>21</td>
<td>11</td>
<td>1650</td>
<td>2050</td>
<td>1.5</td>
</tr>
<tr>
<td>Annual</td>
<td>217.4</td>
<td>-</td>
<td>-</td>
<td>-</td>
<td>2550</td>
<td>1050</td>
<td>1.5</td>
</tr>
</tbody>
</table>

The NO$_2$ distribution maps based on annual simulated results among the four seasons are presented in Figure 6. In this figure, the areas with intensive color were more affected by NO$_2$ emissions and defined as unhealthy zones. As shown in the figure, the unhealthy zones were located in the right part of the simulating domain.

a) Summer 2014  
b) Autumn 2014
1-hr maximum concentrations of the simulated and measured values were used for the statistical analysis for evaluating the model performance. The values of correlation coefficients (COR) for NO$_2$ concentrations were 0.89 in summer 2014, about 0.87 in autumn 2014, about 0.67 in winter 2015 and about 0.73 in spring 2015. The results are shown in Table 5. As a result, there were acceptable ranges for statistical parameters and the model simulation indicated that the simulated concentrations were underestimated in compare to the measured ones.

**Table 5. The results of statistical analysis**

<table>
<thead>
<tr>
<th>Season</th>
<th>COR (0,1)</th>
<th>NMB ≤%15</th>
<th>NME ≤%30</th>
<th>IOA (0,1)</th>
<th>FB &lt;0.3</th>
</tr>
</thead>
<tbody>
<tr>
<td>Summer (2014)</td>
<td>0.89</td>
<td>-16</td>
<td>16</td>
<td>0.86</td>
<td>-0.017</td>
</tr>
<tr>
<td>Autumn (2014)</td>
<td>0.87</td>
<td>-38</td>
<td>28</td>
<td>0.70</td>
<td>-0.047</td>
</tr>
<tr>
<td>Winter (2015)</td>
<td>0.67</td>
<td>-21</td>
<td>25</td>
<td>0.61</td>
<td>-0.023</td>
</tr>
<tr>
<td>Spring (2015)</td>
<td>0.73</td>
<td>-22</td>
<td>22</td>
<td>0.63</td>
<td>-0.025</td>
</tr>
</tbody>
</table>

Since there are some limitations for applying AERMOD modeling system, the simulation results may not be quite accurate. The limitations are such as: lack of module for considering NO$_2$ deposition reactions; high sensitivity of AERMOD to various time scales (Zou et al., 2010; Bhardwaj, 2005); lack of considering the dynamic emission rates (U.S. EPA, 2009); lack of considering the substantial time intervals for wind velocities less than 1 m/s; errors due to monitoring devices (Drew et al., 2007); complexity in topographical structure of the study area (El-Fadel et al., 2009), coastal evaporation, and the geographical effects (Yao et al., 2011).
A comparison made among the measured and predicted ambient NO$_2$ concentrations. The results indicated that the predicted concentrations were underestimated by a factor of 20% in comparison to the measured ones which indicated the contribution of other sources including mobile sources and the neighboring gas refineries and other industries.

Conclusions

In the present study, ambient NO$_2$ concentrations in a gas refinery located in Asaluyeh was measured in 10 receptors in and around the refinery and the 1-hr and annual ambient NO$_2$ concentrations and dispersion patterns were simulated by AERMOD model in 10×10 km$^2$ domain. Then the unhealthy zones were determined in the study area using contour plots of the seasonal NO$_2$ distribution patterns. It was found that the hourly observed and predicted concentrations of NO$_2$ were lower than the U.S. EPA clean air standard except in receptor B in autumn 2014. However, there was no health risk due to NO$_2$ emissions for short time (1-hr) exposure in the gas refinery. Furthermore, a comparison made among the measured and the simulated NO$_2$ concentrations in 10 receptors. The results indicated the performance of the modeling was quite satisfactory with little disagreement in the values of predicted results. The discrepancy between the average simulated and measured concentrations varied from 2% to 56%; however the average predicted concentrations were underestimated by a factor of 20% in comparison to the measured ones.

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REFERENCES


Minabi et al.: Prediction of NO₂ concentrations in a gas refinery using air dispersion modeling

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