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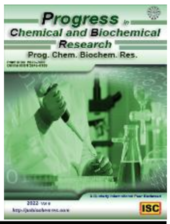

Original Research Article

Modelling of Emission Dispersion Pattern of Nitrogen Oxide (NOx) in Steel Production Unit in Iran by Using Phast Software

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ABSTRACT

Background: For each industry, especially those that produce a lot of gases, investigating air pollution problems is so important these days. To control and reduce emissions-related outcomes, it is necessary to model and investigate concentration rates of emissions.

Methods: In the present paper, the dispersion pattern of NOx emissions from a steel production unit located in Iran was modelled by using PHAST (process hazard analysis software tool) software in F class atmospheric conditions. It is the first time that an investigation of air pollution, NOx, has been conducted in this industrial area. Hence, the dispersion ranges of emissions, durability period, the maximum ground-level concentration, and other outcomes were examined.

Results: The results demonstrated that the health of the villages' inhabitants surrounding the factory was exposed to risk within 5.5 km. Besides, the emission concentration was extremely annoying and unhealthy for all people up to the radius of 9.6 km and for sensitive people, the elderly, and children up to the radius of 16 km. Therefore, it is recommended to the studied factory take some measures in terms of promoting control technologies and reduce emissions to extend safe boundaries up to a radius of at least 7. Moreover, a monitoring program should be done more precisely and rigorously to reduce the environmental outcomes and damages resulting from the emissions to the minimum rate.

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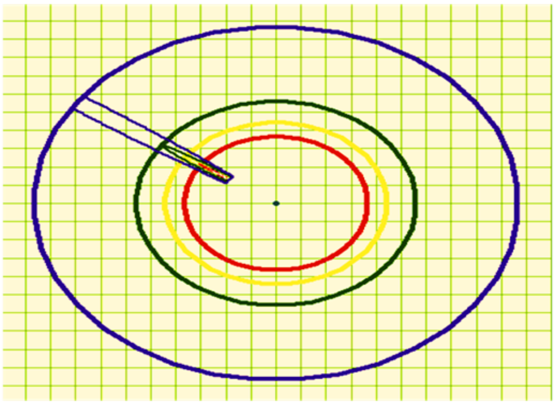
GRAPHICAL ABSTRACT



1. Introduction

Since the advent of the industrial revolution up to now, a large amount of chemicals has been produced into the atmosphere by humans, mainly in the form of particulate and gaseous emissions, which negatively influenced their health and also the environment [1]. Among the various achievements of the industrial revolution, the Steel industry has been known as one the most important industrial development indicators of countries in the world. The tendency to establish steel production units has increased in response to the population growth and demand for industrial activities. Despite the effective and useful achievements of this strategic commodity which leads to the easier life and well-being for human beings, there are many unwanted outcomes and potential dangers such as environmental impacts, air pollution, and related problems such as global warming, climatic changes, acid rains, etc. which has turned to one of the most important challenges of the present era [2-5]. Broadly speaking, Steel production is one of the most pollutant-emitting processes [6] contributing to a variety of air pollution problems and greenhouse gas (GHG) emissions [7,8]. One of the most important and toxic emissions generated by steel production units is Nitrogen oxide (NOx) which is emitted at very high temperatures during steel production processes. In the steel industry, the condition for the NOx emission is ideal due to high temperature. Nitrogen monoxide and nitrogen dioxide (known as NOx) remain in the atmosphere for successive days and produce nitric acid, nitrates, and nitrites through chemical reactions and cause acid rain. Besides, they cause chemical light smog and proxy acetyl nitrate generation (PAN), which are environmentally essential to be considered [9-13]. Indeed, the family of Nitrogen oxide (NOx) (NO, NO_2, N_2O, etc.) adversely influences not only the human health, but also the environmental function in a wide range [14]. Therefore, it is crucial to take measures for assessing and predicting toxic emissions such as NOx and their dispersion pattern in the region, or any changes in concentration at different times and places to keep them at a standard level and ultimately eliminate or minimize their adverse impacts on human health and environment. Considering the mentioned points, many studies have been conducted to evaluate emission rates of different toxic gases such as NOx, CO, particulate matter, etc. from various sources by adopting different methods. After reviewing different studies, it was figured out that one of the most practical and reliable methods for assessing the emission rate of toxic substances and gases isophase (Process Hazard Analysis Software Tool) software. This software is capable of assessing the risk, developing consequence models, and modeling the emission rates and dispersion patterns of toxic gases including carbon monoxide, methane, chlorine, nitrogen oxides, etc. released by industrial or oil production activities. A majority of the studies based on Phast software have been concerned with assessing risks or modeling emission rates for gases such as carbon monoxide, methane, chlorine, etc. (not only nitrogen oxides) from various sources including industrial activities, steel production units, activities related to oil and combustion, petrochemicals, etc. which demonstrate the wide range of Phast usability. Hence, it is instructive to review some of the recent studies that have been done with different aims based on Phast software, which prove its reliability and capability in achieving the desired goals.

Esfandian *et al.* (2021) conducted their research based on Phast software to assess the risk of gas tank and toxic emissions in different scenarios. They could determine the strength of the radiation or pressure wave, and the safe distances by using Phast software [5]. Khorram (2020) made an attempt to examine the emission rate of chlorine gas and its impact on a target population in a worst scenario by the use of Phast software and ERPGs, IDLH, and STEL criteria in a nuclear power plant located in Iran to utilize the outcomes in an emergency response program [15]. Kouidri *et al.* tried to present an experimental environmental study in an industrial city of HassiR'mel. They have conducted their research in nine sections and have devoted part 4 to simulate the NOx dispersion and some other gases by using phast software. They figured out that the CO and NOx contents are influenced by improving or modifying the burners [16]. Shahpari *et al.* drew attentions to Phast software as one of the most practical and reliable software for modeling and assessing the dispersion and emission of gases in oil and gas industry [17]. In another study, Naemnezhad *et al.* (2017) adopted Phast software to assess the consequences of oil production platform operation in Iran. Besides, they studied the dispersion pattern of the emitted substances through and beyond the facility, the distance traveled, area covered by released material, and their impact on `human, and the environment [18]. Si *et al.* (2011) investigated the energy efficiency assessment at a steel company by using Phast software. They regarded steel industry, which extremely contributes to greenhouse gas emissions [8].

As a result of the above-mentioned points, the objective of this article is to assess and predict the emission rate of NOx, one of the most poisonous gases produced during still production. We calculated and modeled NOx concentration and dispersion in all points of the region by using PHAST (Process Hazard Analysis Software Tool), a software package in the F class, to assess the emission rate of NOx in a steel production unit located in Iran. It was a new activity in this industrial location to perform environmental controls. The Phast results were compared with AQI (air quality index), which is a prominent and developed Index or a rating scale for determining the pollution rate of the air. Hence, based on Phast' results and AQI, the hazardous and sensitive districts, which were exposed to the most poisonous contaminants, were recognized. The outputs can be considered by regional planners during planning and decision-making process to overcome the problems associated with the air quality, human health, and environmental pollution caused by industrial operations.

1.2. NOx emission

NOx is produced by several mechanisms both within and after flame combustion [19]. Nitrogen oxides (NOx) are worldwide consequences of high-temperature combustion operations and are harmful pollutants in the air. Indeed, they are ubiquitous in air chemistry. Hence, their emission reduction should be critical in both stationary and mobile planning [20-22]. The nitrogen oxides (NOx) family including nitric oxide or nitrogen monoxide (NO), nitrogen dioxide (NO_2), nitrous oxide (N_2O), and their compounds, do indeed have a wide variety of health and environmental effects. Besides, given limited solubility in water, nitric oxide (NO) permeates all parts of the respiratory system. Nitrogen oxides infiltrate effectively into the lungs' alveolar cells (epithelium) and surrounding capillary vessels, affecting the alveolar structures and their efficiency in an adverse way [23]. Thus, a brief exposure to NOx causes respiratory morbidity, including weakened host defenses, increased lung inflammation, and reduced lung efficiency [24,25].

The concentration of nitrogen oxides has been evaluated in several ways in recent years, especially in countries with high NOx production potential. Zhang *et al.* (2020) evaluated NOx emission during the Covid-19 pandemic. Their evaluation demonstrated a significant decrease in NOx emission during quarantine [26]. Krzywański *et al.* (2017) introduced another way of estimating NOx emission from a circulating fluidized bed combustor by the use of the Artificial Neural Network Approach [27]. Provataris *et al.* (2017) developed a new model for predicting NOx emissions and investigated its capability and reliability for NOx emissions from two automotive DI Diesel engines. Their results showed a satisfactory performance of their newly developed model in assessing NOx emissions [28]. In another paper, Mijling *et al.* (2013) used an algorithm to build a monthly NOx emission time series in ages between 2007 and 2011 in provinces located in the East of china and the countries around it [29]. Krzywański *et al.* (2011) presented another newly developed computer program to assess several emissions including NOx from the combustion of solid fuels [30].

1.3. Air quality index (AQI)

Related to the aforementioned illness effects and destructive environmental impacts of nitrogen oxides, many studies have drawn attention to developing standard criteria for the released rate of NOx and other emissions to keep them at the standard level. Therefore, a plausible index is required to define the standard limits of inhaling poisonous substances and emissions. Van den Elshout *et al.* (2008) reviewed the existing air quality indicators in their paper [31]. Cogliani (2001) utilized a regression model to anticipate air pollution in cities by using an air pollution index that was closely associated with meteorological data [32]. Goyal *et al.* (2006) conducted research in Delhi on daily air quality prediction of air contaminants by using ARIMA and multiple linear regression (MLR) models [33]. The following is one of the important indices developed and used in a wide range of evaluating the emission processes. In 1999, the U.S. Environmental Protection Agency introduced another index called the air quality index (AQI), which states whether the air is polluted or clean and demonstrates the effect of polluted air on human health [34,35]. The air quality index (AQI) is used to indicate the quality of air in a specific place. To calculate the AQI, an air pollutant concentration from a monitor or model is essential. The way of converting air pollutant concentration to AQI differs contaminant by contaminant and varies between nations' ministries, the values of the air quality index are separated into ranges, and each range is given a description and a color code. As displayed in Figure 6, the AQI splits into six degrees of health hazard. AQI aims to help people realize the effects it might have on human health (Technical Assistance Document for the Reporting of Daily Air Quality). Table 1 presents a sample set of features and rules applied to the Context Rule base for the IQA. Based on the above aforementioned points, the AQI was utilized in the present paper to assess the air quality around an industrial park which is the main source of toxic gases such as NOx.

Table 1. AQI and features [36,37]

Levels of health concern	AQI values	NO2 (ppm) 1-hour	Description	Action	Colour
Air quality status are:	When the AQI is in this range:	When NO2 is in this range:	Features in this rate is:	The action required in this rate:	As represented by this colour
Good	0-50	0-0.053	The air quality is satisfactory, but for some contaminants, there may be a moderate health issue for a few numbers.	No precautionary instructions	Green
Medium	51-100	0.054-0.100			Yellow
Unhealthy for sensitive groups	101-150	0.101-0.360	Members of vulnerable populations may suffer health consequences.	Very sensitive people should reduce prolonged or strenuous activity if possible.	Orange
Unhealthy	151-200	0.361-0.64		People with lung diseases such as asthma, the elderly, and children should reduce the prolonged or strenuous outdoor activities if possible.	Red
Very unhealthy	201-300	0.65-1.24	Members of vulnerable populations may suffer more significant health consequences.	People with lung diseases such as asthma, children, and the elderly should avoid any physical activity outside the home. Other people should reduce outdoor activities.	Purple
Dangerous	301-400	1.25-1.64	When a trigger causes a health change, everyone may encounter more significant health consequences.	People with lung diseases such as asthma, children, and the elderly should not leave home and minimize their activities. Other people should avoid outdoor activities.	Maroon
Very dangerous	401-500	1.65-2.04	Causes health alerts of emergency situations to be issued.	People with lung diseases such as asthma, children, and the elderly should not leave home and minimize their activities. Other people should avoid outdoor activities.	Maroon

2. Methodology

A scenario was selected based on the geographical, metrological, and climatic conditions of Guilan Province, where the steel factory is located [38]. Next, PHAST software was used to analyze the NOx emissions dispersion and their impact on air quality and the ecosystem. By the use of Phast, the critical points, and the maximum ground level concentration of emissions are determined in the target regions [39-41].

In the following, the adopted procedure for conducting the study is further explained:

2.1. Case study

Guilan Province is one of the 31 provinces of Iran. It lies along the Caspian Sea. The studied steel factory is located in the industrial park in one of the rural areas of Guilan Province, which is 15 km to the southeast of the urban area. The rural areas surrounding the industrial park constitute 1.5% of the rural population of this province and seven of the most important villages around the industrial park are shown in Figure (1) as A, B, C, D, E, F, and G. The factory ends to natural lands in both north and south and there are many villages around it. The prevailing wind blows in the northwestern direction in the cold seasons of the year and directly affects the industrial park including the steel factory in the surrounding villages.

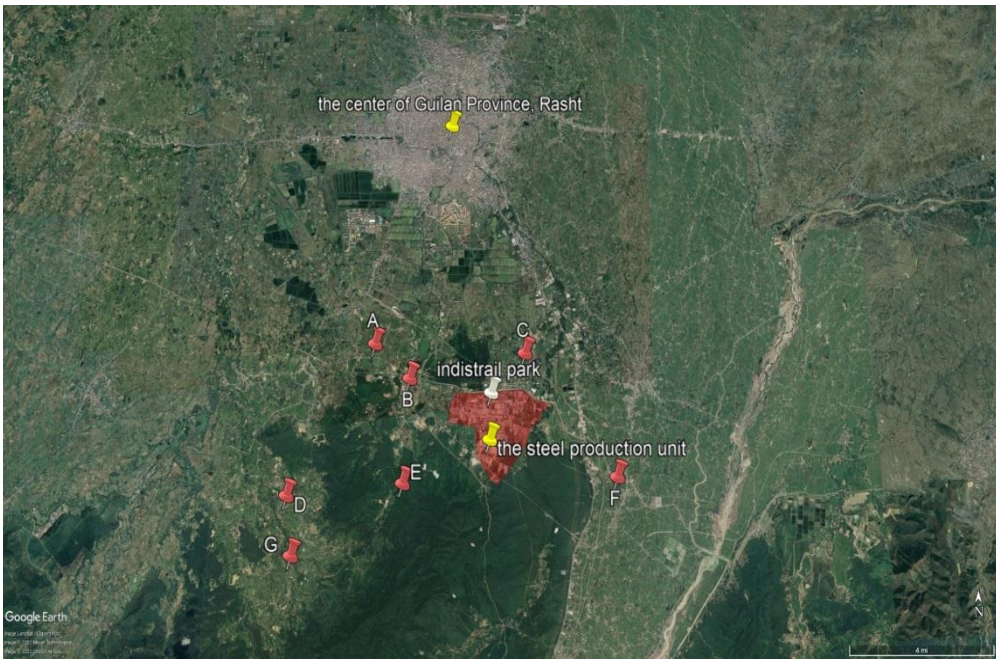


Figure 1. Location of steel production unit

2.1.1. Scenario selection

To define the scenario, the most stable atmospheric condition was considered. Hence, the resulting outcomes and damages could be predictable and controllable in the case of the occurrence of such critical conditions. The scenario was defined on a winter evening when the temperature was 5 °C, the wind speed was 1 m/s, and it was completely cloudy (F class atmospheric conditions) with a relative humidity of 87%. Besides, a smoked column containing emissions of nitrogen oxides from the flue of the studied steel production unit with a height of 18 m and diameter of 3 m was dispersed to the surrounding environment [38].

2.1.2. Using Phast software

Phast software is one of the most practical and reliable programs for assessing and simulating various gas emissions and dispersions in the oil and gas industry. Broadly speaking, it is concerned with poisonous gas release, explosion, and fire. It is used by over 300 organizations globally due to its reliability and technological competence [17,18,42-45]. It examines and quantifies the severity of situations that might endanger personnel, facilities, or the environment. Det Norske Veritas (DNV) Software widely acknowledged as the world leader in the field of industrial accident risk assessment, developed PHAST as part of a product line. Generally, many top worldwide companies and governments have accepted it as a vital element for decision support in industrial risk and public safety [46]. In the present study, given the capability and reliability of Phast, it was selected to model NOx emissions from the steel production unit in F-class atmospheric conditions. Then, hazardous and sensitive regions were identified concerning the concentration of emissions in different regions by using Phast software.

2.2. Data collection

Two kinds of data were required as inputs into Phast software and were collected through the environmental agency of Guilan province:

A) Data related to metrological and climatic condition which are listed in Table 2.

B) Data related to the studied steel production unit and factory's flue and analysis of the outlet gases are presented in Table 3.

Table 2. Data related to the metrology and climatic condition [47]

Variable	Data measured
Ambient temperature	5 °C
Wind speed	1 m/s
Relative humidity	87%
Region	Rural (Relatively flat)
Stability level	F

Table 3. Data related to the studied factory's flue [47]

Flue height	18 m
Flue diameter	3 m
Temperature of the outlet gas	30 °C
Mass of outlet NOx emissions	729.4 kg
Intensity of release from flue	0.2026 Kg/s
Discharge speed of emissions	2.62 m/s
Time for discharge	3600 S

3. Results and Discussion

3.1. Threatened regions based on AQI

Given that NOx emissions are majorly important in terms of environmental degradation and health-related levels, thus experiments were performed to investigate the threatened regions in terms of AQI. Four hazardous regions surrounding the factory were identified and summarized in Table 4 [35]. Accordingly, the dangerous index of each area was identified that was based on AQI, so there are fourth areas where demonstrate levels of health concern. By using this tool, environmentalists can determine the dangerous rate of each reaction at each zone of pollution, and solve problems caused by air pollution if they can.

By entering the input data (data related to metrology, climate condition, steel production unit, and the flue) and map of the region into PHAST software, a diagram of the threatened regions was obtained in terms of different distances, as depicted in Figures 2 and 3. The results show that the pollutant concentration gradually decreases by increasing in distance. Specifically, with ending the third hazardous region (6.9-16.2 km), the NOx concentration has significant decrease. Besides, it is observed that most of the rural areas are located in these regions, which are known as "unhealthy," and "unhealthy for sensitive" groups, as listed in Table 1. In these areas, the vulnerable populations with more significant health consequences may suffer from emissions so that an applicable solution is required to be implemented through steel factories, regional planners, and environmental agencies.

It is north worthy that calculation was done in F class which is the worst possible scenario to model NOx emission in the worst condition. The performed model in normal atmospheric conditions was in a good agreement with the information provided by Environment Agency and the sensitivity was plausible. Hence, the results of phast software and assessing based on AQI were compared with the information obtained from the environment Agency, which was physically collected and demonstrated an acceptable accuracy.

Table 4. Hazardous regions surrounding factory

Regions	Distances	The emission rate of pollutant based on AQI	Levels of health concern	Colour
1. The first region	4499.27 m	AOI (401-500) 60 min= 2.04 ppm	Very dangerous	Maroon
2. The second region	5500.27 m	AOI (301-400) 60 min= 1.64 ppm	Dangerous	Maroon
3. The third region	6900.27 m	AOI (201-300) 60 min= 1.24 ppm	Very unhealthy	Purple
4. The fourth region	16200.3 m	AOI (101-150) 60 min= 0.36 ppm	Unhealthy	Red

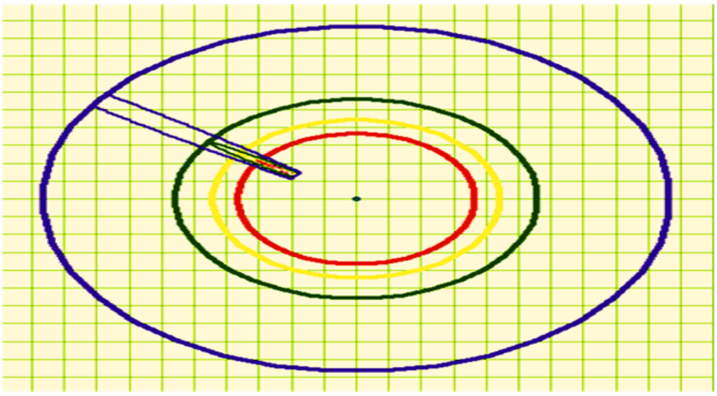


Figure 2. Threatened regions in terms of distance

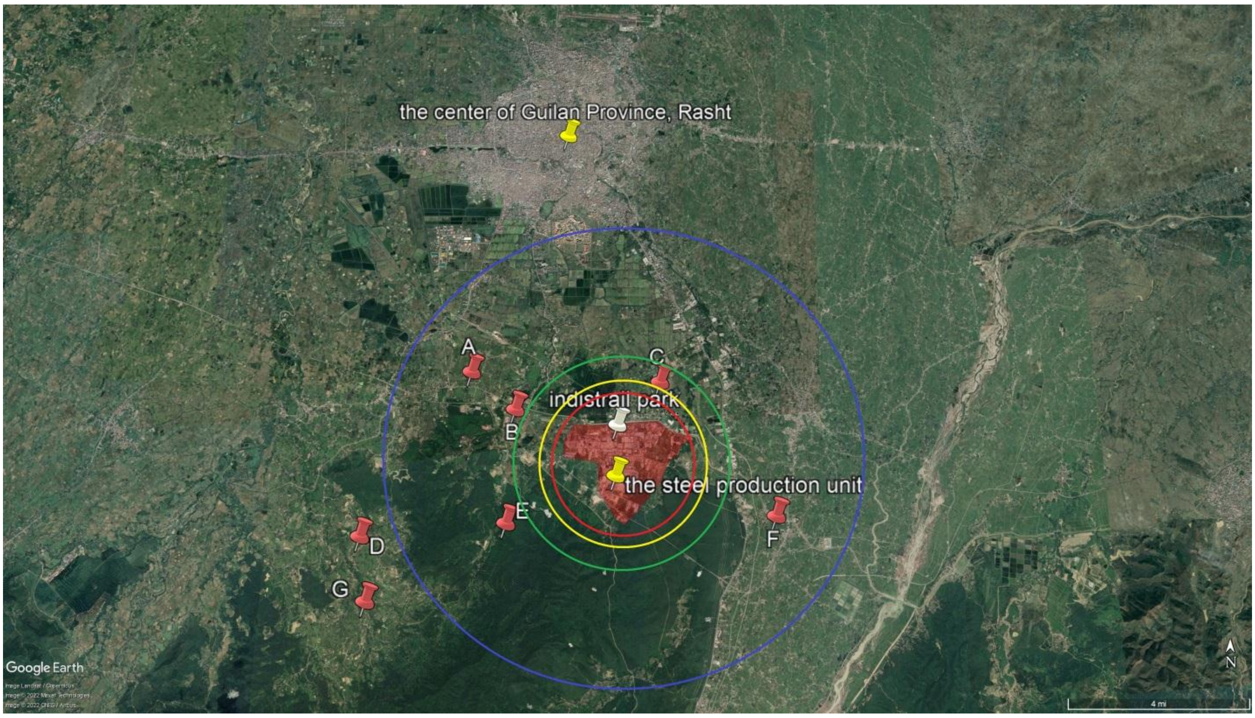


Figure 3. Threatened regions in terms of distance

3.2. Evaluating dispersion range of emissions

Figures 4 and 5 demonstrate the side and top view of emission dispersion. As can be observed, the emissions exited from the flue at the height of 18 m above the ground level and were dispersed at the height of more than 90 m above the ground level and a radius of 16.200 km from the source. Most of the rural points in the studied area are located in the fourth distance. Hence, it can be claimed that the location of the industrial park and steel production unit was relatively selected in a proper way to have the minimum adverse effect on humans and the environment. However, the region is going to be affected somehow during the steel factory's operation, and special Interventions are required.

According to the presented figures, emissions with a concentration of 2.04 ppm were recognized as a very dangerous level and continued to be dispersed up to the radius of 4.5 km from the source for 1.77 h at the ground level. Fortunately, there is no rural area in this region. Likewise, the interventions should be implemented for employees and workers of the industrial park and those who are temporarily traveling to this area. According to Figure 3, they covered an area of about 4.80 km^2. Emissions with a concentration of 1.64 ppm were known as dangerous levels. They were dispersed up to a radius of 5.5 km at the ground level for 1.8 h and covered approximately 7.50 km^2. Besides, the concentration gradually decreased over time. The emissions with a concentration of 1.24 ppm were identified as dangerous levels, were spread up to the radius of 6.9 km from the source at the ground level for 2.026 h, and covered an area of about 1246.43 km^2. Emissions with a concentration of 0.36 ppm as unhealthy levels were spread up to the radius of 16.2 km from the source for 3.16 h and affected the radius of 16.200 km. The performed modeling in the normal atmospheric conditions was in a good agreement with the information provided by Environment Agency and the sensitivity was plausible.

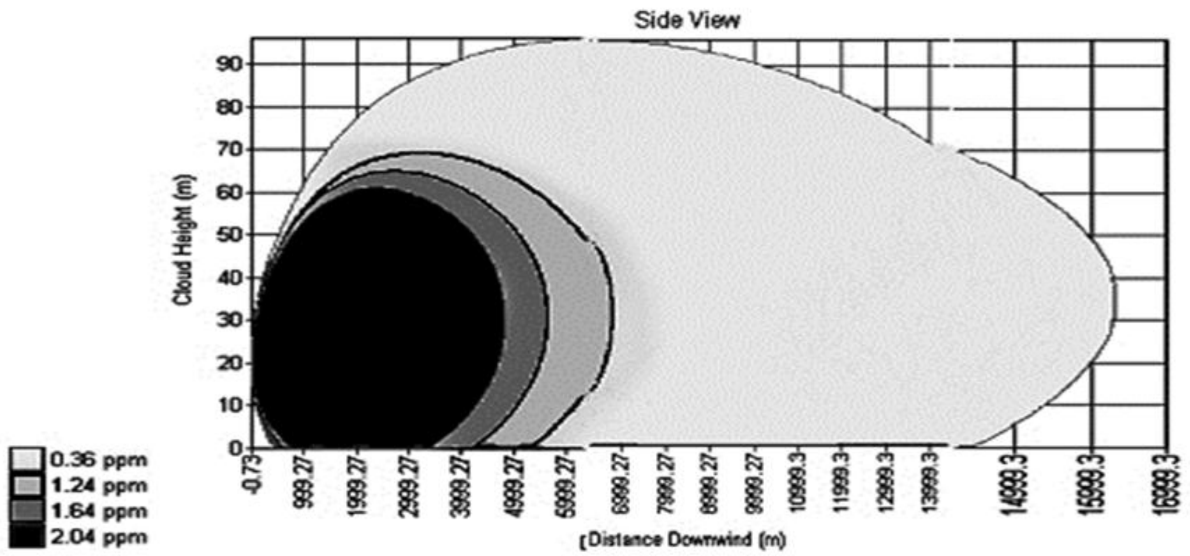


Figure 4. Side view of the emissions dispersion

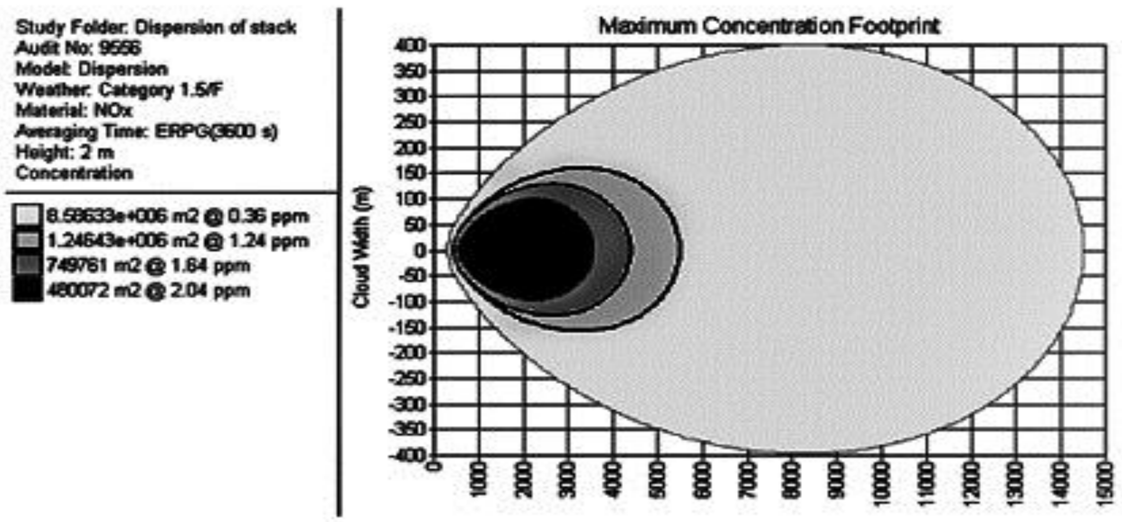


Figure 5. Top view of the maximum concentration dispersion of emissions at the ground level

4. Conclusion

Obviously, through investigating the threatened regions, the concentration of emissions would be higher than 2.04 ppm up to the radius of 4. 5 km from the source. Residents around the studied factory would be exposed to risks such as increased met hemoglobin in the blood, intensification of respiratory allergies, increased number of respirations, and decreased lung capacity. On the other hand, it would cause dangerous and carcinogenic tumors by producing photochemical oxidants. Plant growth would be disrupted and leaf tissues would be damaged due to the concentration increase of these emissions. In addition, up to the radius of 5.5 km from the source, the concentration of the emissions would exceed 1.64 ppm and residents would be exposed to the annoying odor of emissions and outbreak of irreversible, serious risks such as asthma, acute bronchitis, and nitrosamine production. At both mentioned levels, the experts emphasize that children, asthmatic patients, and patients with cardiovascular or pulmonary diseases should not leave home and others should also avoid outdoor activities [35].

The concentration of emissions would exceed 1.24 ppm up to a radius of 6.9 km from the source that is unhealthy for all people and the odor of emissions is annoying. It also irritates the throat and causes coughing and shortness of breath. Furthermore, it accelerates primary reactions of respiratory problems such as asthma. Nitrogen dioxide irritates the mucous, and thereby increases respiratory infections in children and respiratory complaints such as coughing and sputum in adults. Complications of air pollution with nitrogen dioxide include weight loss, reduced immunity to infectious diseases, and susceptibility to bacteria and probably viral infections [48,49]. In such circumstances, the experts recommend children, asthmatic patients, and patients with cardiovascular or pulmonary diseases avoid outdoor activities. The other people should also reduce their heavy activities [35]. The concentration of emissions would exceed 0.36 ppm up to the radius of 16.2 km from the source, which is unhealthy and annoying for unhealthy and susceptible people. It irritates the lungs and reduces the resistance of the respiratory system to diseases such as the flu. People who have asthma would suffer from breathing the air containing nitrogen dioxide. The experts recommend sensitive groups, especially those with cardiovascular or pulmonary diseases, the elderly, and children avoid prolonged outdoor activities [35].

Therefore, it is recommended to the studied factory take some measures for promoting control technologies and reducing emissions to extend safe boundaries, especially for the surrounding residents of the industrial part up to a radius of 7 km. Moreover, environmental monitoring program should be done more accurately and rigorously so that the outcomes of the emissions would be reduced to a minimum level.

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