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Research Article

SIMULATING DISTRIBUTION PATTERN OF EMISSION FROM CRACKING FURNACE FLUE OF VINYL CHLORIDE UNITE

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ABSTRACT
Controlling and decreasing the outcomes resulted by the dispersion of pollutants require modeling the distribution pattern of these gasses from their sources and investigating their dispersion scope and environmental effects. In this study, destructive effects of air- and environmental-polluting gases were studied and dispersion manner of these pollutants was examined in industrial environments with high population density. In the present paper, the case study was performed on the dispersion of emissions from cracking furnace flue of vinyl chloride monomer (VCM) unit, Bandar Imam Khomeini Petrochemical Complex, using PHAST software.

Keywords: *Outcome Control, Vinyl Chloride Monomer, Bandar Imam Khomeini Petrochemical Complex, Flue Outlet, Cracking Furnace*

INTRODUCTION
Studying and identifying the behavior of flue emissions during dispersion lead to obtaining the complex functions of time-depending concentrations at different points with different distances from the dispersion location. These equations result in obtaining a series of logical data, through which the effects of chemicals, after spilling on people and environment, can be investigated. Moreover, the effect of concentration in open and closed areas on the equipment and surrounding environment can be examined. Using these calculations, better information can be achieved about the design and safety of industrial environments; thus, considering the risk level, designs are performed in the safest possible manner (SalehiArtimani, 2012).

Goals
- Determining expansion scope of emissions such as carbon monoxide, nitrogen dioxide, and sulfur dioxide
- Showing expansion scope of emissions considering the abnormal operation scenario of the studied flue
- Identifying risks arising from harmful concentrations on the personnel of Bandar Imam Khomeini Petrochemical Complex and its surrounding industrial environments
- Investigating whether the topology of the industrial unit has been correctly done and the safety limit has been observed or not
- Proposing solutions for controlling and reducing outcomes of the dispersion of emissions in petrochemical industry

Selecting the Scenario
To define the possible scenario according to the title of this study, dispersion pattern of these gases from the flue of Site 3 was constantly investigated as the main scenario. Also, owing to the importance of this problem, in addition to the normal operation of Flue 3 of VCM unit, an abnormal scenario (the combination of different percentage of emission from the flue) was also considered and its related studies were conducted. Selected gases for the present research included carbon monoxide (CO), nitrogen dioxide, and sulfur dioxide (NO_x).
Dispersion manner of these three gases was measured considering two different weather conditions in warm and cold seasons and the combination of these conditions with the normal and abnormal conditions

of flue operation. Also, more information about the behavior of pollutants would provide better understanding about the concept of emission dispersion.

Analyzing the Conditions

In this section, attempts are made to identify all the physical conditions which affect the incident; i.e. factors that influence the formation and development of the outcomes of the scenarios should be determined. Emergence of different environmental outcomes is not predictable and avoidable in most cases. Predicting these outcomes at different times and places requires identifying and evaluating risky locations and also investigating the expansion scope of the effects of pollutants and the governing situation and conditions.

The studied place was Bandar Imam Khomeini Petrochemical Complex, which was located with the area of 270 ha in the northwest of Persian Gulf in Khuzestan province, with 160 km distance to the southeast of Ahvaz and 84km to east of Abadan in Bandar-eImam Khomeini Port (Shahrui *et al.*, 2014).

Figure 1: A view of Bandar Imam Khomeini Petrochemical Complex

MATERIALS AND METHODS

- ***Data and Information***

Below, process information, physical specifications of the model, and weather conditions of Bandar Imam Khomeini petrochemical area, which were used for modeling gas dispersion, is provided.

- ***Process Information and Physical specifications of Flue 3 with Normal Operation***

Process information and specifications were related to Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex with normal and abnormal operations and a represented in Tables1 and 2.Also, the combination of normal percentage and abnormal scenario is given in Tables3 and 4.

Table 1: Process information and specifications of Flue 3 of VCM unit with normal operation

Parameter	Flue diameter	Mass flow ofCO	Mass flow of So_2	Mass flow of NO_2	Totalmass flow of emission in standard conditions	Height of flue	Temperature of emission	Speed of emissions
Unit	Cm	gr/s	gr/s	gr/s	m^3/s	M	C^0	m/s
Value	153	0.126	0.144	0.351	3.233	25	210	201

Table 2: Process information and specifications of Flue 3 of VCM unit with abnormal operation

Parameter	**Flue diameter**	**Mass flow of CO**	**Mass flow of So_2**	**Mass flow of NO_2**	**Total mass flow of emission in standard conditions**	**Height of flue**	**Temperature of emission**	**Speed of emissions**
Unit	Cm	gr/s	gr/s	gr/s	m^3/s	M	C^0	**m/s**
Value	153	0.181	0.828	0.474	3.233	25	210	**201**

Table 3: Information of the combination of normal percentage of emission from Flue 3 of VCM unit

Weight percent	**Mole percent**	**Existing gases**
33.98475	41.45108	O_2
0.002308	0.003216	CO
65.99808	58.52673	CO_2
0.006444	0.008683	NO_2
0.002643	0.001608	SO_2
0.000166	0.003216	H_2
0.005615	0.000643	H_2S

Table 4: Information of the combination of abnormal percentage of emission from Flue 3 of VCM unit

Weight percent	**Mole percent**	**Existing gases**
20.08924	26.5	O_2
3.320109	5.00322	CO
52.68459	50.53	CO_2
8.725336	8.0055	NO_2
15.18005	10.0016	SO_2
0.000153	0.0032	H_2
0.000517	0.00064	H_2S

- ***Weather Conditions***

According to the documents presented by the synoptic website of Weather Station, two different weather conditions (one in summer and another is winter) were considered for simulating the dispersion of emissions from Flue 3 of vinyl chloride unit. Based on the available standards for determining different weather conditions, these two states were selected so that, not only the dominant average, but also all the possible weather conditions of the studies region would be covered.

1. Summer with slow wind blow (temperature: 50°C, wind speed: 1 m/s, moisture: 85%, atmospheric stability: completely stable)
2. Winter with slow wind flow (temperature:7°C,wind speed:1m/s, moisture:70%,atmospheric stability: completely stable)

In this project, surface roughness of the areas surrounding Bandar Imam Khomeini Petrochemical Complex was considered to be 1 m.

- ***Using PHAST (Process Hazard Analysis Software Tool) software for modeling***

PHAST is a universal analysis instrument and one of the most conventional tools for modeling the dispersion of toxic gases and air pollutants in European countries. This software is easy to use and

flexible and allows users to analyze different values for a vast range of model parameters. Amount of dispersion and its situation based on the given information can be determined in the software on Google Earth and GIS (Geographic Information System) maps and warning is made if needed. Figure 1shows a combination of the predicted parameters along with the results obtained by the software for analyzing the dispersion of dangerous materials in this location (Pandya *et al.*, 2012; Patra, 2006).

- ***Modeling***

Modeling Dispersion of CO Emission from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex (Normal Operation Scenario of the Flue)

In modeling CO emission from the flue, the data and information of the tables were used as the input of PHAST6.7 advanced software. As can be seen in Fig. 1, by referring to AQI Tables, four concentration levels with separate colors (for better recognition) were determined for the CO concentration, which included: concentration of 2.2 ppm in blue indicating Index 50 and good region in terms of health level; another layer with concentration of 12.5 ppm in green showing Index 150 and unsafe region for sensitive people in terms of health; the following concentration level of 15.5 ppm in yellow showing Index 200 and unsafe region for healthy; finally, the closest layer to the flue in red with the concentration of 30.4 ppm, showing Indices 300 to 500 that is very unsafe or even dangerous region. Since the gas concentration was different in different seasons, only the results of selected concentrations are demonstrated in Figure 1.

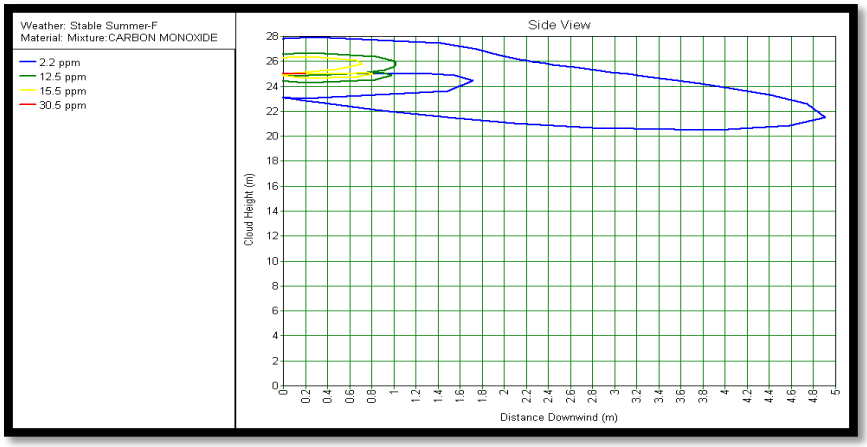


Figure 1: Side view of CO dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex in summer

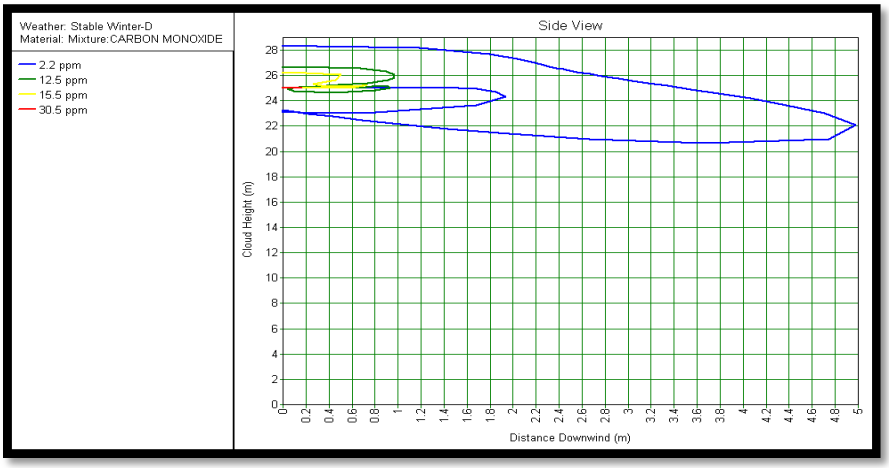


Figure 2: Side view of CO dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex in winter

Results of modeling in Figures 1 and 2 for summer and winter weather conditions showed that, considering the 25 m height of the flue, CO gas ultimately descended to the height of 22 m after dispersion; thus, it did not reach the ground level, the main reason of which can be that this gas is lighter than air. As is clear in Figures 1 and 2, dangerous weather conditions only existed in the area with the height of more than 23m and it can be said that good weather condition existed up to the height of 28m and distance of 5 m from the flue. The important result is that, even in the worst condition, no concentration of CO could reach the ground level and the flue designers of VCM unit have shown suitable performance in terms of using the tools for air pollution reduction and also selecting proper height of the flue. According to these appropriate measures, humans and other creatures around the industrial environment would not be exposed to the risk of such gases.

Modeling Dispersion of SO_2 Emission from Flue 3 of VCM Unit in Bandar Imam Khomeini Petrochemical Complex (Normal Operation Scenario of the Flue)

SO_2dispersion from the flue depended on weather conditions, flue specification in the factory, gas flow, combination of gas percent, and so on, as mentioned in Figures 5-8. here, influence range of SO_2produced from the factory flue was determined for hot and cold seasons and also the concentrations of 0.144, 0.225, 0.305, and 0.605 ppm corresponding to Indices 100, 150, 200, and 500, which indicated average, unsafe for sensitive people, unsafe, and dangerous health levels, respectively. Since this gas is heavier than air, it is expected to get closer to the ground after emission from the flue and passing some distance. Results of SO_2modeling are shown in Figures 3 and 4.

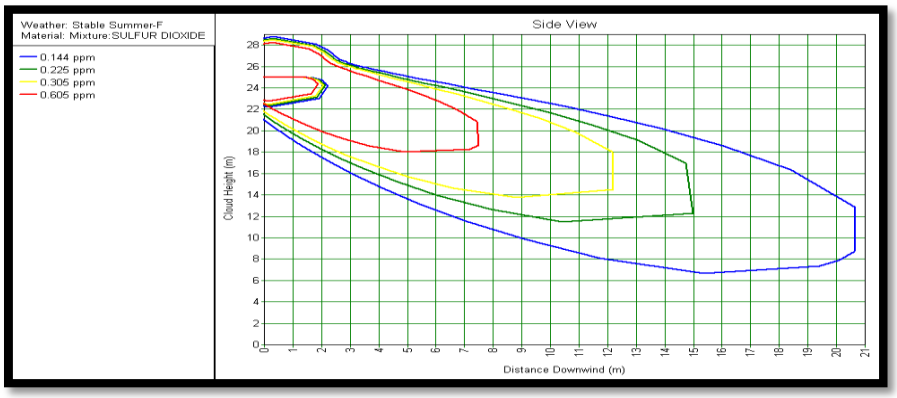


Figure 3: Side view of SO_2 dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex in summer

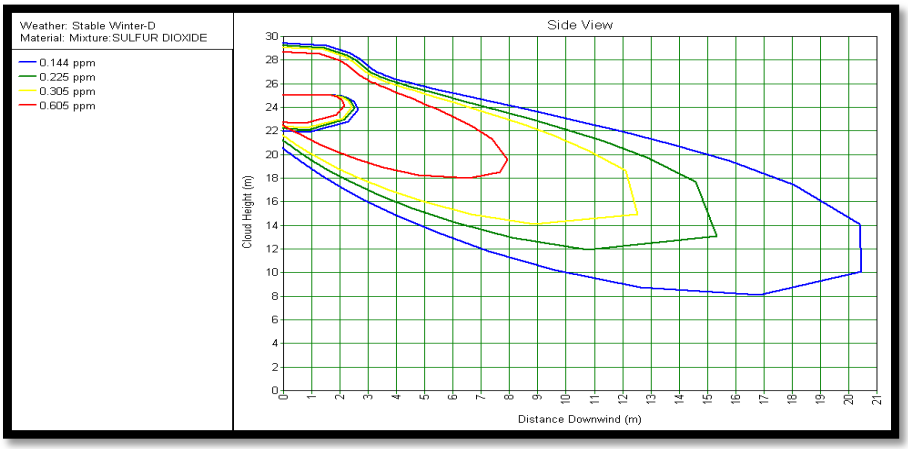


Figure 4: Side view of SO_2 dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex in winter

According to the results obtained from Figures 3 and 4, it can be mentioned that, after dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex, SO_2 was descended up to the height of 6 m in summer and 8 m in winter. Also, in normal operation condition of the flue, it would reach the ground level neither in summer nor in winter. Although this gas is heavier than air, due to low concentration of the emission from this flue, the gas present in air was diluted and did not reach the ground level.

Modeling NO_2 Dispersion from Flue 3 of VCM Unit in Bandar Imam Khomeini Petrochemical Complex in summer

As is clear in Figures 5 and 6 and Map 1, in modeling NO_2 emission from the flue, four concentration levels of NO_2 were determined in four different colors (for better recognition) as follows: Concentration of 0.1 ppm in blue represents Index 100 and average region in terms of healthy level; another layer with the concentration of 0.36 ppm in green showing Index 150 and unsafe region for sensitive people in terms of health; the following concentration level of 0.65 ppm in yellow showing Index 200 which is completely unsafe; finally, the most dangerous region that is the closest to the flue with the concentration of 1.25 ppm and Index 500 representing dangerous region.

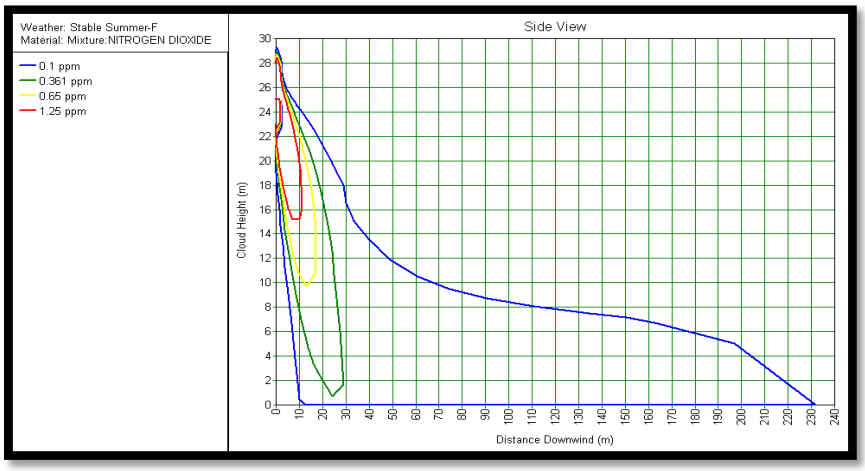


Figure 5: Side view of NO_2dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex in summer

Map 1: Dispersion of NO_2 from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex in winter

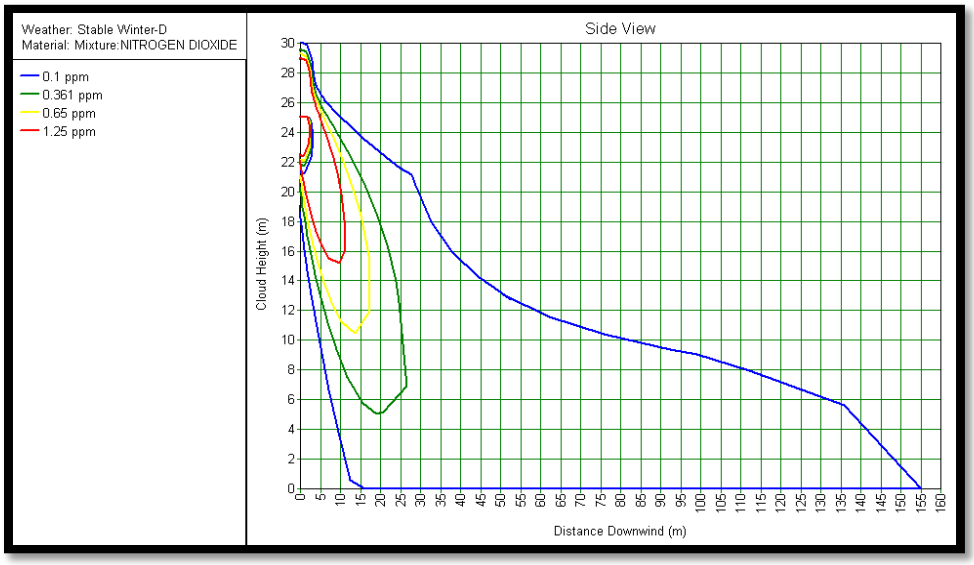


Figure 6: Side view of NO_2dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex in winter

According to Figures 5 and 6 and Map 1demonstrating the result of modeling NO_2 from Flue 3 of VCM unit, this gas reached 10 and 15 m distance from the ground level in winter and summer, respectively, after dispersion from the flue with the height of 25 m. The concentration with which it reached the ground was equal to 0.1 ppm and based on AQI Table, it was at average health level. In other words, NO_2 is heavier than air and, if its flow exceeds the permitted limit, it would reach the ground level.

Since any incident may occur in the processing unit, in this study, a scenario was considered for the abnormal operation of Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex; in this case, the concentration of pollutants with acute condition (i.e. high concentration) was modeled.

Modeling CO Dispersion from Flue 3 of VCM Unit in Bandar Imam Khomeini Petrochemical Complex (Abnormal Operation Scenario of the Flue)

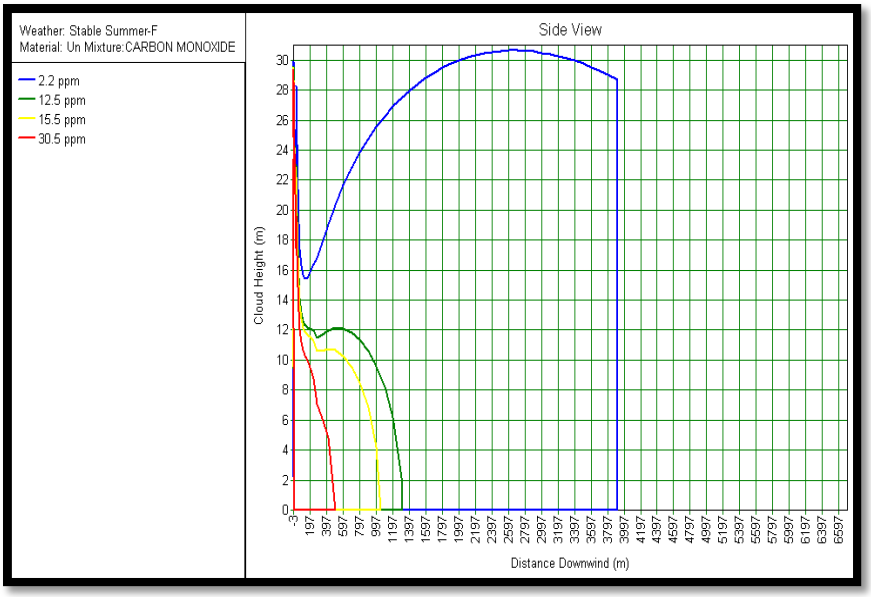
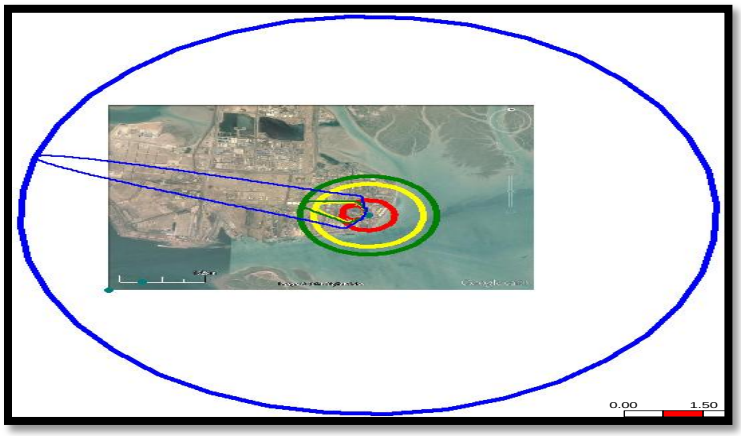


Figure 7: Side view of CO dispersion from Flue 3 (with the combination of abnormal percentage) in VCM unit of Bandar Imam Khomeini Petrochemical Complex in summer



Map 2: NO_2 dispersion from Flue 3 (with abnormal percent) in VCM unit of Bandar Imam Khomeini Petrochemical Complex in summer

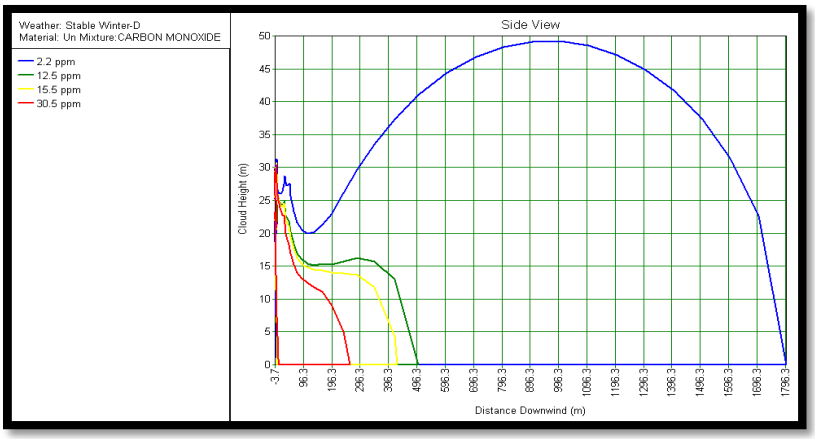
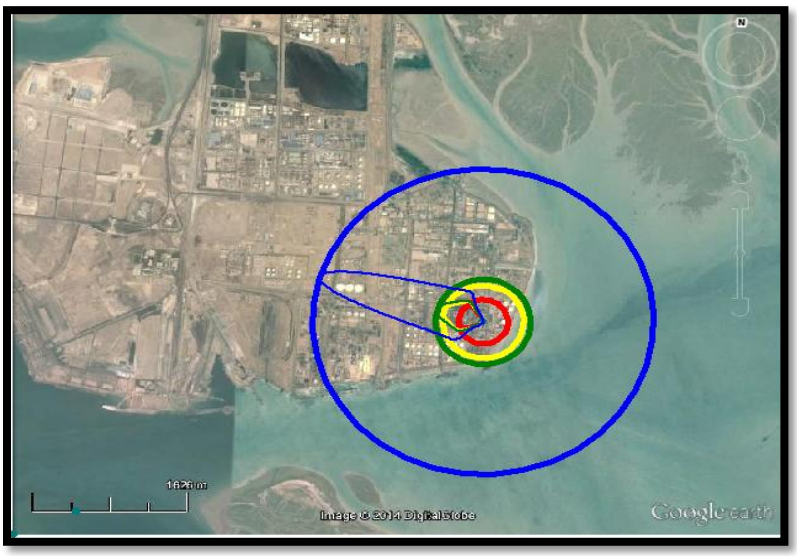


Figure 8: Side view of CO dispersion from Flue 3 (with abnormal percent) in VCM unit of Bandar Imam Khomeini Petrochemical Complex in winter



Map 3: NO_2 dispersion from Flue 3 (with abnormal percent) of VCM unit in Bandar Imam Khomeini Petrochemical Complex in winter

By modeling the abnormal operation scenario for the studied flue, as observed in Figures 7 and 8 and Maps2 and 3, all the concentration levels of Co for both summer and winter reached the ground level; in the case of occurrence, such a scenario can be very dangerous.

Modeling SO_2 Dispersion from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex (Abnormal Operation Scenario of the Flue)

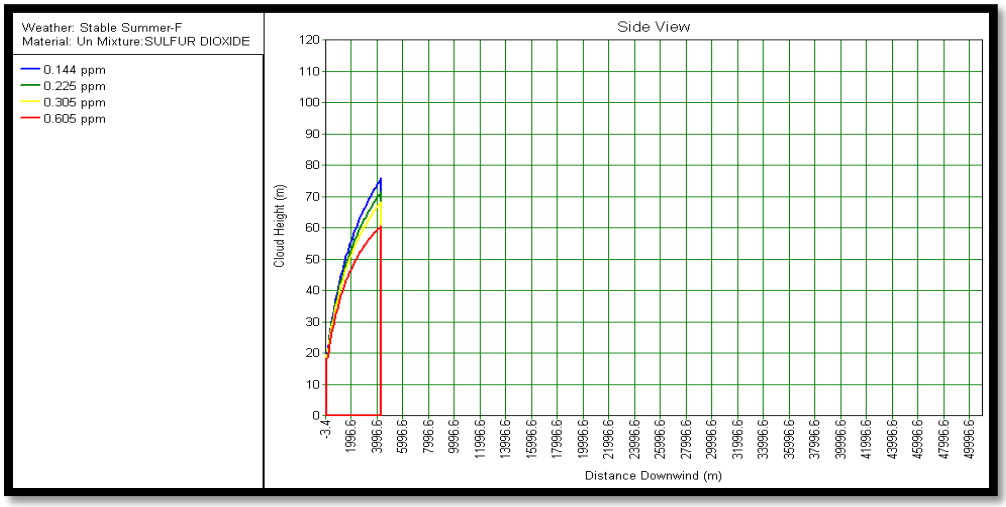


Figure 9: Side view of SO_2 dispersion from Flue 3 of VCM unit (with abnormal percent) in Bandar Imam Khomeini Petrochemical Complex in summer

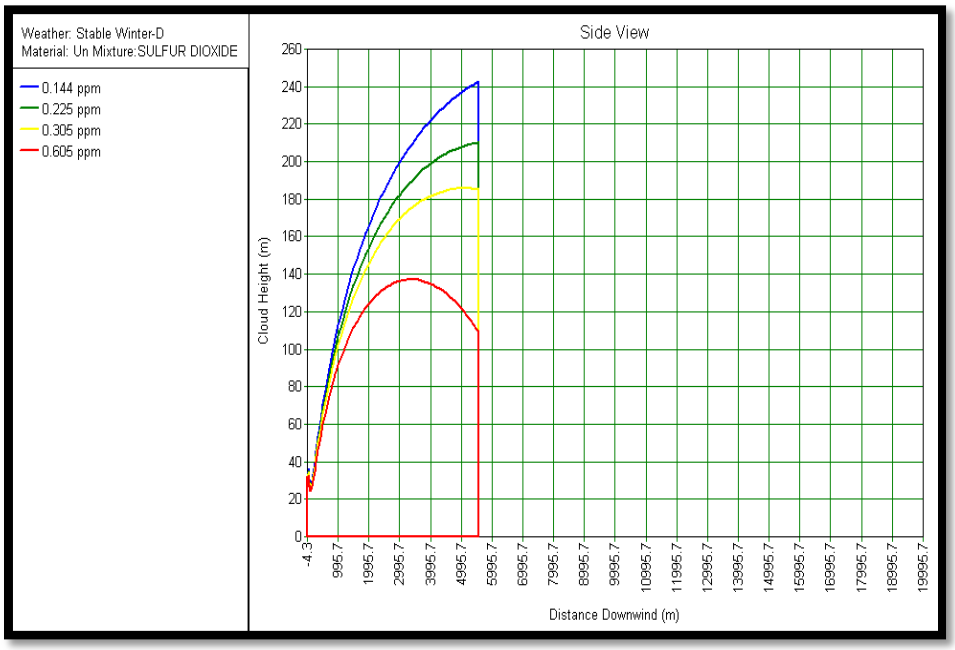


Figure 10: Side view of SO_2 dispersion from Flue 3 of VCM unit (with abnormal percent) in Bandar Imam Khomeini Petrochemical Complex in winter

Using the results of modeling the outcomes of the abnormal scenario of SO_2 emission from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex, it was concluded that all the concentration levels of SO_2 reached the ground level, which can be challenging. The results obtained from Figs. 9and 10 evidently indicate the results obtained from the occurrence of abnormal operation scenario of the flue.

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Modeling NO_2 Dispersion from Flue 3 of VCM Unit in Bandar Imam Khomeini Petrochemical Complex (Abnormal Operation Scenario of the flue)

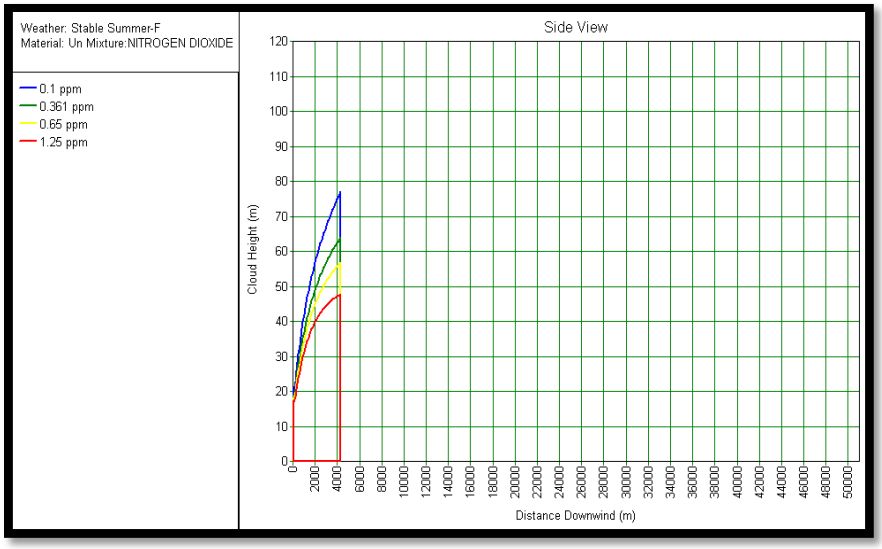

Figure 11: Side view of NO_2 dispersion from Flue 3 (with the combination of abnormal percentage) in Bandar Imam Khomeini Petrochemical Complex in summer

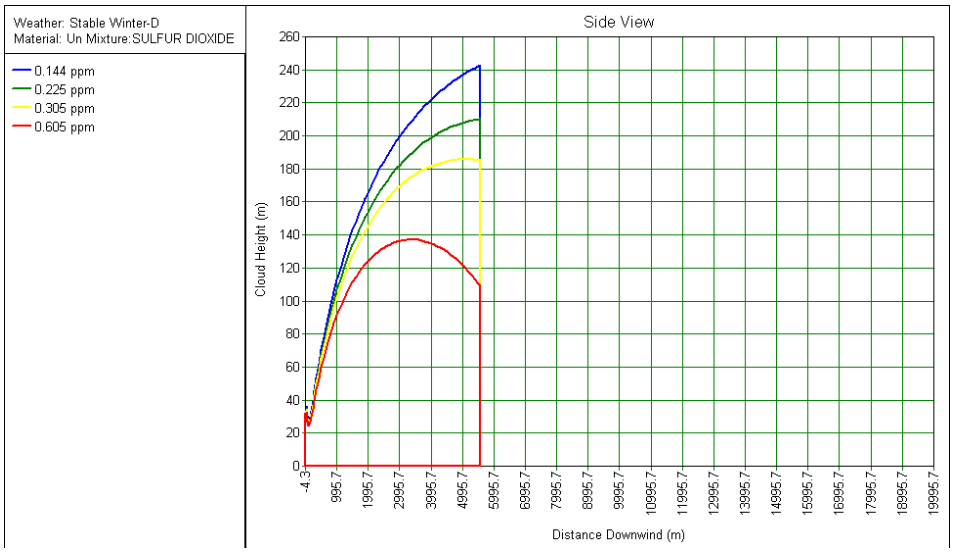

Figure 12: Side view of NO_2 dispersion from Flue 3 (combination of abnormal percentage) in Bandar Imam Khomeini Petrochemical Complex in summer

Through modeling, outcomes of NO_2emission obtained by the abnormal operation scenario of the studied flue in Figures 11 and 5-12 were clearly obtained. Considering the results of this study, concentration of the levels of AQI Table for the occurrence of abnormal operation scenario would reach the ground level, which is very dangerous.

Discussion and Conclusion

Analysis of Results

Results of modeling are shown in Tables4 and5. It should be mentioned that the numbers and concentrations related to health levels were selected based on the definitions in AQI Table.

Table 4: Summary of results of modeling the dispersion of pollutants (NO_2,SO_2,CO) at flue level for normal scenario in summer (height of 25 m)

Name of pollutant	Average health level to distance from flow downstream (m)	Undsafe health level of sensitive people to distance from flow downstream (m)	Unsafe health level to distance from flow downstream (m)	Dangerous health level to distance from flow downstream (m)
CO	5	1.2	1	0.2
SO_2	10	8	5	4
NO_2	12	10	8	4

Table 5: Summary of results of modeling the dispersion of pollutants (NO_2,SO_2,CO) at flue level for normal scenario in winter (height of 25 m)

Name of pollutant	Average health level to distance from flow downstream (m)	Undsafe health level of sensitive people to distance from flow downstream (m)	Unsafe health level to distance from flow downstream (m)	Dangerous health level to distance from flow downstream (m)
CO	5	1	0.6	0.2
SO_2	8	5	4	3
NO_2	15	8	7	6

Results of modeling the outcomes of the dispersion of emissions from Flue 3 of VCM unit of in Bandar Imam Khomeini Petrochemical Complex showed the fact that, in the normal operation condition of this flue and its related furnaces, concentration of no pollutant would endanger the surrounding environment, indicating the suitable design of flue and observation of appropriate environmental points by the authorities of this complex. But, as far as the abnormal operation of the flue or its attached furnaces was concerned, it should be mentioned that, in the case of such a scenario, a very dangerous atmosphere would dominate the complex and its adjoining units; in such a situation, not only the lives of the staff would be at risk, but also the company's credit would be threatened.

Discussion

Existence of pollutants and the inseparable role of global industrialization in this regard have challenged humans to find a solution for minimizing or modifying the dispersion of industrial pollutants. Thus, destructive roles of SO_2,CO, and NO_2areespecially fundamental. To precisely investigate and control air pollution, sufficient information should be available about dispersion sources of pollutants, their distribution in the environment, and finally effects of pollutants. So, it is essential to present dispersion models of pollutants and investigate their environmental effects.

As explained in the previous sections, one of the most important dispersion sources of pollutants is flues of petrochemical industry. Iran's petrochemical industry as one of the largest industries plays a special role in its cultural and economic development, which necessitates the need for observing environmental and safety requirements for this industry. Iran's petrochemical industry is developing; this claim has been proven in recent years by increased rate in terms of production, quality, and product diversity. In spite of its admirable capabilities, this industry could not be excluded from other industries in terms of air pollution.

Therefore, after modeling important pollutants of this industry and examining results of such modeling, some solutions were proposed for reducing the pollutants of petrochemical industry, which have been generally considered and used by Bandar Imam Khomeini Petrochemical Complex and can be helpful in terms of utilization, topology and construction of other factories.

Solutions for Air Pollution Reduction during Different Steps of Production in Industry

- Training to increase the awareness level of staff of this industry about environmental and air pollution issues and making these issues their concerns
- Selecting suitable consumable fuel for factories
- Precisely controlling combustion conditions such as changing the amount of extra oxygen by computer control systems
- Properly designing the flare in furnaces
- Using furnaces with high thermal efficiency to minimize CO_2 gas, which is inevitably produced during the combustion of hydrocarbons and CO
- Observing safety limits for polluting industries
- Preparing and presenting environmental standards during different steps of factory construction and also production
- Completely observing environmental standards

Cooperation of all people of the society along with all the legal and administrative measures of governmental institutions in this regard will promise the achievement of a pollution-free environment (Ghiassedin, 2006; Omidkhah and ParishanNadaf, 2006; Bryson, 1998).

Conclusion

Considering the studies and calculations performed in this research, after modeling the distribution of emissions from Flue 3 of VCM unit in Bandar Imam Khomeini Petrochemical Complex, it was concluded that the flue and furnaces of this unit have been correctly designed. Although it was true that emissions from this flue did not adversely affect humans, these pollutants can seriously end anger the environment. So, managers and authorities of large industries should pay more attention to decreasing environmental emissions from industrial flues.

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