



## Consequence Modeling for Accidental Events of SO<sub>2</sub> Release in a Detergent Manufacturing Company



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### ABSTRACT

**Background:** Chemical industries and facilities pose the risk of potential hazards in case of accidents, which lead to injuries and financial losses due to the spread of materials in the surroundings of the accident. These materials often have harmful properties (e.g., toxicity or flammability), and their release could cause secondary accidents (e.g., fire, poisoning, and explosion). The present study aimed to assess the effects of toxic sulfur dioxide (SO<sub>2</sub>) in a suffocation unit.

**Methods:** A possible scenario of SO<sub>2</sub> emission was selected using the matrix presented by the researchers. Afterwards, the hazard and operability study method was used to analyze the conditions. The modeling and evaluation of the outcomes of the selected scenario for SO<sub>2</sub> gas emission from the gas pipeline were carried out using the PHAST7.11 software.

**Results:** The worst scenario was observed in the employees within the approximate distance of 10 meters and height of two meters from the gas leakage (100 mm leakage diameter) and gas diffusion angled from horizontal impingement.

**Conclusion:** About 1.84 seconds after the leakage of toxic SO<sub>2</sub> (distance: 10 meters, height: 1.39 m), the concentration was approximately 39,339 ppm, which was the worst scenario in August, with the possible mortality risk of 49%.

## 1. Introduction

Due to the lack of attention to safety regulations and regular inspection, adverse incidents are witnessed in various regions of the world each year. Process industries are the industries in which raw materials are converted into intermediate or final products through physical or chemical processes or other operations. Process industries are associated with potential hazards in chemical industries and facilities, which may cause injuries, death, and financial losses. In addition to the loss of materials from the source, such incidents lead to the spread of materials in the surrounding areas. These materials often have hazardous properties (e.g., toxicity or flammability), and their release

to secondary accidents (e.g., fire, toxicity, and explosion). These incidents could occur due to failure in process design, technical malfunction of equipment or human errors [1].

Some of the main contributing factors to adverse incidents in industries include problems in the safe design of activities, wrong design, hardware and software errors, defective system of work license, inappropriate management of changes, defects in identifying hazards, inappropriate reaction in emergencies, use of inappropriate materials for construction leading to corrosion and failure), improper distribution of responsibilities among individuals, ineffective communication, and inattention to the learned experiences from past events [2].

In order to prevent industrial accidents, it is essential to



evaluate industrial facilities based on various scenarios. Consequence analysis is a tool used by process engineers to assess industrial activities to determine the extent of the risks and possible casualties caused by accidents [1]. In the present study, the consequences of possible process events from the furnaces and transmission pipelines of sulfur dioxide (SO<sub>2</sub>) gas have been investigated using the PHAST7.11 software.

SO<sub>2</sub> is a colorless gas, which reacts on the surfaces of many solids and airborne particles. It is non-explosive and has a suffocating odor, weighing almost twice as air. SO<sub>2</sub> is soluble in water and raindrops and could convert into sulfurous acid. Furthermore, sulfur trioxide (SO<sub>3</sub>) is combined with water vapor and forms sulfuric acid. It is estimated that SO<sub>2</sub> remains in the air for 2-4 days on average [3,4]. Sulfur oxides are among the most important atmospheric pollutants, which are produced through the combustion of combustible materials (especially in fossil fuel power plants), causing damages to humans, plants, animals, objects, and equipment [5]. Some of these injuries in humans include allergic rhinitis, lung inflammation, lung cancer, dyspnea, coughing, sneezing, and decreased lung capacity [6].

Considering the severe toxicity of SO<sub>2</sub> gas, the present study aimed to evaluate the consequences of SO<sub>2</sub> discharges from pipelines during the processing and transfer of SO<sub>2</sub> gas.

## 2. Materials and Methods

### 2.1. Study Design

The methodology of the present study was based on the guidelines of the American Society of Chemical Engineers (AIChE) to assess the consequences of the release of chemicals. Various methods that are used to evaluate these consequences often have a relatively similar framework, with some differences in the details and stages. In the current research, in addition to visiting the industrial site and studying the production process, the knowledge and experiences of the employees and records of the previous accidents in the industrial unit were exploited to select the proper scenario. After scenario selection, the hazard and operability study (HAZOP) technique was used to analyze the conditions. After screening the results, the worst and most likely scenarios were selected. Finally, the modeling and evaluation of the consequences of the selected scenario of SO<sub>2</sub> emissions from the production transmission pipelines were carried out using the PHAST software.

### 2.2. Study Area

A large-scale detergent production company was selected as the location of the study. In this industrial complex, the sulfur was required to be solidly integrated into the refinery, which would enter the furnace in the liquid form after melting. Combustion would occur in the furnace (sulfur, air, and flame), resulting in the production of the SO<sub>2</sub> gas, so that the produced SO<sub>2</sub> would be transferred by pipes for the next stage of the process. To model the SO<sub>2</sub> emissions using the software, basic data were required, which are described in detail in the following sections.

#### 2.2.1. Technical and Process Data for the Studied Equipment

The required technical information of the equipment used to produce and transfer SO<sub>2</sub> for modeling included the pipe length, internal diameter of the pipe, number of the flanges connected to the pipe, number of the welding points in the pipe path, and reservoir height. In addition, the important process data for modeling were the internal pressure of the pipe and internal temperature of the pipe (Table 1).

#### 2.2.2. Climate Data

A digital anemometer (model: MASTECH 61-650 CE) was used to collect the data on the wind speed, humidity, and temperature in each month of 2017. Moreover, the data on the wind rose were collected from the Meteorological Organization, and the atmospheric stability conditions were also evaluated, including six classes (A-F). Consequently, the F stability was considered as the worst condition (Table 2).

#### 2.3. Consequences of the Toxicity of the Released Materials in the Environment

The threshold limit value-short-term exposure limit (TLV-STEL) criteria were used to evaluate the toxicity of the SO<sub>2</sub> emissions. The SO<sub>2</sub> amount of the TLV-STEL within the occupational exposure limits is 0.25 ppm [7]. Many of the methods that are used for consequence assessment often have a relatively similar framework, with the differences mainly in the details and stages [8].

##### 2.3.1. First Step: Scenario Selection

Four scenarios were applied for the two-ton transmission pipeline to evaluate the consequences of SO<sub>2</sub> release.

**Table 1:** Technical and Process Information of Studied Equipment

No	Study Areas	Technical information of equipment				Process information of equipment		
		length of the pipe (m)	Height of the tank(m)	The inner diameter of the pipe (cm)	Number of flanges connected to the pipe	Number of boiling points in the pipe path	Internal pressure of the pipe(bar)	Internal temperature of the pipe (°C)
1	2- ton transmission pipeline	15	-	25	2	8	0.9	625
2	1- ton transmission pipeline	14	-	25	3	15	0.9	625
3	furnace 2	-	5	-	-	-	0.9	625
4	furnace 1	-	5	-	-	-	0.9	625
1	2- ton transmission pipeline	15	-	25	2	8	0.9	625

**Table 2:** Data on Atmospheric Conditions of Study Area

Month	Summary of annual weather conditions			Stability
	Average temperature (°C)	Average relative humidity (%)	Average wind speed (m /s)	
April	24	29	2.2	F Stable
May	24	34	2.2	F Stable
June	26	36	2.1	F Stable
July	33	45	2.0	F Stable
August	37	46	1.6	F Stable
September	36	46	2.4	F Stable
October	23	36	3.1	F Stable
November	19	31	3.3	F Stable
December	10	17	3.5	F Stable
January	5	15	3.5	F Stable
February	4	15	3.7	F Stable
March	20	30	3.6	F Stable

As is shown in Table 3, the criteria for scenario selection were based on the previous studies conducted by DNV specialists [9]. The selected scenarios for the two-ton transmission pipeline were as follows :

- First scenario: Continuous release from a rupture with the diameter of five millimeters ;
- Second scenario: Continuous release from a rupture with the diameter of 25 millimeters;
- Third scenario: Continuous release from a rupture with the diameter of 100 millimeters;
- Fourth scenario: complete pipe rupture

For the scenarios with the diameter of five, 25, and 100 millimeters, six different directions were considered for gas release (Table 4), including horizontal, horizontal impingement, horizontal angle, horizontal impingement angle, down-impinging on the ground, and vertical.

*2.3.2. Second Step: Analysis of the Conditions*

For the accurate analysis of the cause of incidents, the HAZOP method was used to assess the risk of the SO<sub>2</sub> production and transfer processing operations. In addition, the consequences and causes of SO<sub>2</sub> emissions were investigated based on the selected scenarios (Table 5). The HAZOP technique is a specific structure for hazard identification and assessment in process units by a team consisting of various engineering expertise. The method has been acknowledged as the basis for the identification of the process risks in the design and operation of industrial units [10]. After the process evaluation, an experienced team in HAZOP was formed in the presence of several experts, including technicians, electrician and instrumentation administrators, production administrators, chemical engineering personnel, and health and safety executives. Regular meetings were organized with the team, and the

**Table 3:** Selected scenarios based on equipment indicators

Dimensions of studied rupture	Equipment
5 mm and complete rupture	Pipes with a diameter of less than 1.5 inches
5 mm, 25 mm and complete rupture	Pipes with Cascade 2 to 6 inches
5mm, 25mm, 100mm and complete rupture	Pipes with 8 to 12 inches
Full rupture of inlet and outlet lines and sudden discharge	Tanks
Depending on the diameter of the inlet and outlet pipes, the leakage of the sealant with a diameter of 5 mm, 25 mm, 100 mm	Pumps

HAZOP method was used to investigate and identify the hazards. In this evaluation, the P&ID map was applied to identify the parameters involved in the process, as well as the causes of the deviation based on these parameters. Finally, the consequences of the deviations were identified.

*2.3.3. Third Step: Modeling of the Incident*

The simulation of the incidents was carried out after considering all the influential factors in the incidents based on the HAZOP method and described details in the previous sections. The modeling of the release of toxic SO<sub>2</sub> was performed based on various parameters, such as the technical features of the furnace and pipes, process features of the furnace and pipes, and atmospheric conditions. Moreover, the PHAST 7.11 software was used to evaluate the toxic effects of SO<sub>2</sub> emissions and their modeling [9].

After the modeling, the effects of the incidents were evaluated. To this end, the amount of the casualties and losses resulting from the outcomes of the scenario was calculated. The purpose of the evaluation was to determine the mortality rate in the study. The mortality rate of the individuals affected by the gas poisoning scenario was obtained by calculating the Y-factor variable using Equation 1.

Equation (1):

$$P = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{Y-s} \exp\left[-\frac{u^2}{2}\right] du$$

**Table 4:** List of studied scenarios for SO<sub>2</sub> gas pipelines

No	Scenario type	Gas emission modes	Scenario location
1	Complete rupture of 2- ton transmission pipeline	Catastrophic rupture	SO <sub>2</sub> gas transmission pipeline
2	Catastrophic rupture Diameter 100mm- leak 5mm- leak 25mm- leak leak-disc rupture	1-Horizontal impingement 2-Horizontal impingement 3-Angeled from Horizontal 4-Angeled from Horizontal impingement 5-Down-impinging on the ground 6-Vertical	SO <sub>2</sub> gas transmission pipeline

**Table 5:** Identification of scenario hazards with the Hazop method

Scenario	Guide Word	Parameter	Deviation	Causes	Consequences
SO <sub>2</sub> emission scenario due to complete catastrophic rupture-Leak leakage with a diameter of 5 ,25 and 100 mm	more	temperature	Increase temperature	The entry of excessive molten sulfur into the furnace	Perforation of boiling points - Gas leakage
	Less	Air flow rate	Increase temperature	Low air flow rate. Inlet to the furnace	Perforation of boiling points - Gas leakage
	more	Moisture	Increase temperature	Raising the moisture inside the furnace due to the air entering the furnace	Perforation of boiling points - Gas leakage
	more	pressure	increases the pressure	Eclipse the air outlet path inside the furnace	Perforation of boiling points - Gas leakage
	more	air	Increase temperature	The inappropriateness of the size or weight of the furnace stones makes it possible to reject and add more air inside the furnace, which increases the furnace temperature.	Perforation of boiling points - Gas leakage

**2.3.4. Fourth Step: Evaluation of Damage**

At this stage, the outputs of the software simulation were interpreted and matched the findings based on the map of the geographical locations of the study area and combining other data, such as the number of the workers at the site, distance from the point of emission (Table 6), and amount of the damage caused by leakage (e.g., possibility of death/injury).

**3. Result and Discussion**

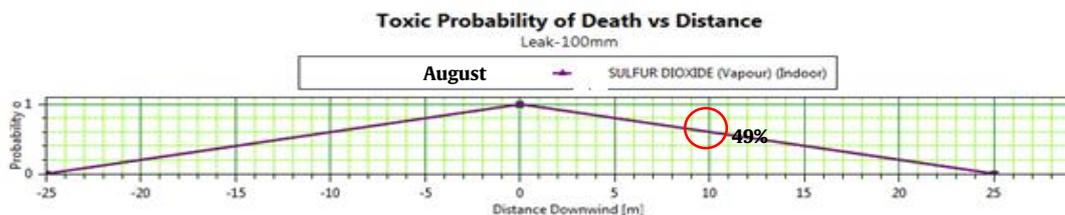
According to the data on the climatic conditions and technical specifications of the equipment in the four scenarios modeled in the present study, per 15 employees who were working at approximately 10 meters of length and height of 1-5 meters, the gas leak scenario with the diameter of 100 millimeters and gas emission with the horizontal impingement angle mode was associated with the worst conditions and most significant consequences. Approximately 1.84 seconds after the gas leak and SO<sub>2</sub> emission at the distance of 10 meters and height of 1.39 meters, the concentration was approximately 39,339 ppm in August, which represented the worst conditions compared to the other seasons of the year. In this scenario, the possibility of death was estimated at 49%, which equaled almost seven individuals (Figure 1).

Air temperature, wind speed, and atmospheric stability are among the most important influential factors in the dispersion of released gas. Depending on weather conditions and atmospheric stability, warm seasons were observed to have the highest SO<sub>2</sub> emission concentration in the present study, so that the highest concentration of released gas was observed in August. According to the current research, the main consequences of the emissions of toxic SO<sub>2</sub> to the environment were toxicity to humans and damage to plants, animals, objects, and equipment [9]. The TLV-STEL criteria are fundamentally used for the evaluation of the consequences of gas emissions based on the guidelines of the American Conference of Governmental Industrial Hygienists (ACGIH).

These guidelines show the highest concentration of chemicals in the air, to which individuals could be exposed for 15 minutes with a 60-minute interval four times per day without causing eye/throat injuries or irreversible health effects. The standard TLV-STEL for SO<sub>2</sub> is 0.5 ppm [7]. Some of the main signs of exposure to this gas include pulmonary reactions and stimulation of the lower respiratory tract. Based on the scenarios in the present study, the leakage of the gas from the transmission pipeline caused its release in various ways, which affected the individuals, plants, animals, and equipment that were in the distribution pathways, leading to consequences such as death, plant destruction, and damage to animals and equipment [11].

**Table 6:** Modeling results of SO<sub>2</sub> emissions in the 100mm- leak scenario

Gas release mode from the pipeline	Month	Distance to work place(m)	Height to work place (m)	Highest concentration (ppm)	Time to reach to work place (Sec)
Down-impinging on the ground	June	10.40	1.59	59666	1.77
	August	10.45	1.41	61051	1.78
	October	10.38	1.67	58002	1.84
	March	10.33	1.81	56066	1.87



**Figure 1:** Possibility of Death at Various Distances

## 4. Conclusion

According to the results, the gas leakage scenarios with the diameter of 100 millimeters, distance of 10 meters, and height of 1-5 meters were hazardous and considered to be the worst scenarios as they lead to various consequences after emission. In this regard, the observance of the principles and safety rules, installation of emergency gas alarm announcements, and implementation of overhaul program for permanent care and maintenance are highly recommended.

## Authors' Contributions

Gh.S., supervised the project, M.I., drafted the manuscript with the support of Gh.S., Both authors read, revised, and approved the final manuscript.

## Conflict of Interest

The Authors declare that there is no conflict of interest.

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