CERTIFICATION OF APPROVAL

CFD MODELLING FOR HYDROGEN SULFIDE EMISSION FROM MALAYSIA GAS GATHERING STATION

by

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Approved by,

____

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September 2012

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

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Praise to Allah SWT as His willingness, I have successfully completed Final Year Project (FYP) entitled Computational Fluid Dynamic (CFD) Modelling For Hydrogen Sulfide Emission From Malaysia Gas Gathering Station. This project could not be finished to its fullest without Dr. Risza Rusli, who served as my supervisor, as well as one who challenged and encouraged me throughout my time spent studying under her. Her guidance and supports truly help. She would have never accepted anything less than my best efforts, and for that, I thank her. Deepest thanks to Dr. Usama guiding me and giving advice to handle the project. Without her continued efforts and supports, I would have not been able to bring my project to a successful completion. I thank my family especially my parents for giving support throughout the project. And not to forget, most gratitude to all of my friends who willing to give cooperation while completing the task. The knowledge and information shared are really appreciated. Last but not least, thanks again to everyone who keenly helped and support me to complete the project. May god bless all of us.

Muzammil Munir

ABSTRACT

Nowadays, the release of hydrogen sulfide from storage capacity of oil and gas industries have become serious threat to lives and property near the leakage source. The storage capacity of natural gas containing hydrogen sulfide is large and widely distributed. Thus, an efficient, low cost tool needs to be available in order to analyze the dispersion. Computational Fluid Dynamic (CFD) Fluent has been proposed to study the emission of hydrogen sulfidein oil and gas industries especially from gas gathering station. This method contains four steps: firstly, set up a CFD model and monitor points, the data are taken from Malaysia Gas Gathering Station; secondly, solve CFD equations and predict the real-time concentration field of toxic gas releases and dispersions: thirdly calculate the toxic releases according to gas concentration by using modified Pasquill-Gifford (PG) approach. Lastly, analyze both results from CFD and modified PG approach. Comparison from both results will determine the efficiency of CFD tool for the study of toxic gas exposure. The result from this study can be used for further evaluation of counter-measure of hydrogen sulfide hazard in Malaysia Gas Gathering Station and to study the risk associated at the site.

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CHAPTER I
INTRODUCTION

1.1 BACKGROUND

Major toxic gas accident in oil and gas demonstrate the urgent of a systematic risk analysis method. There is investigated accident reports of hydrogen sulfide emission associated with oil and gas development. The storage of natural gas containing hydrogen sulfide is large and widely distributed in oil and gas processing plant. The release of hydrogen sulfide in processing plant imposes serious threats to individual and assets around the leakage. Health Safety and Environment of United Kingdom reported 35 on-shore hydrogen sulfide exposure in industry from 1990-2003. Half of the incidents listed mostly from leaking of hydrogen sulfide equipment (F, R, M, & J, Analysis of H2S-incidents in geothermal and other industries, 2009). One of the most severe cases related is the sour gas blowout containing hydrogen sulfide occurred in Kaixian, China on December 23, 2003. About 64,000 residents are affected and 243 deaths along with 9000 hospitalization(Yang, Chen, & Renjian, 2006). This recent accident that happened demonstrates that the analysis of toxic gases emission is very important.

This project focuses on a study to simulate and visualize the magnitude and extent of hydrogen sulfide dispersion. The event of hydrogen sulfide accidental released is assumed to happen in a gas gathering station of a high-sulfur gas field. Due to the erosion caused by hydrogen sulfide and carbon dioxide, the leakage mostly released at flanges, valves, pipes etc. Computational fluid dynamics (CFD) FLUENT systematic approach have been proposed to study the toxic gas exposure. The simulation is increasingly being used to study a wide variety of gas release and dispersion problems. For example the application of CFD Fluent to simulate one of the tests in the “Falcon” series of LNG spill tests (Gavelli, Bullister, & Kytomaa, 2008). CFD is considered as the most convenient method to properly representing the wind-flow field in complex industries structure and complex topography. Complex structure can disturbed the dispersion behavior of releases.

1.2 PROBLEM STATEMENT

For recent study of emission of toxic gases there are few conventional tools being used such as CALPUFF, FLACS, Breeze ISC with ISCST3X PC version 3.2.3 and FLUENT etc.Some of the tools may not giving reliable result with realistic conditions. Thus, to provide a more comprehensive study on dispersion problem of toxic gases, CFD Fluent has been proposed.The complex structure and uneven topography around the gas gathering station had also cause problems to analyze the emission of toxic gases. For this project, the focus is on conventional CFD Fluent tools to study the emission of hydrogen sulfide around the gas gathering station. The data from CFD will be compared with the modified Pasquill-Gifford approach.

Hydrogen sulfide is very toxic, quickly reactive, and cause serious accidents. There are high risks of industries related to hydrogen sulfide. These include:

- Industries handling sulfides or other sulphuric substances
- The oil and gas industries
- Workplace where fermentation and other anaerobic decomposition of organic material (F, R, M, & J, Analysis of H2S- incidents, 2009).

It is proposed to focus on the gas gathering station in Malaysia since high population around the site. The real data from choosen site will be recorded and analyze using CFD. Furthermore, the result from this project will be relevant for further study of the threats and the consequences towards individual workers and environment. The counter measure can be proposed to prevent the threat.

1.3 OBJECTIVES

Objectives are an outcome that can be reasonably achieved within an expected timeframe and with available resources. Therefore, for this project the main objective to be achieved is CFD modeling as reliable method to analyse the dispersion of Hydrogen

Sulfide from Malaysia gas gathering station. The method is feasible to analyse the dispersion of Hydrogen Sulfide from gas gathering station in Malaysia.

1.4 SCOPE OF STUDY

The scope of this project is to study the toxic substance exposure in oil and gas industries, specifically at gas gathering station. During operation at gas gathering station, toxic substance may be released, routinely or accidently, at extraction, storage or processing stage. For this study, the emission rate is taken from flanges at storage point, oil storage tanks.

Contaminants present in natural gas, which need to be extracted at processing plant, include water vapor, sand, oxygen, carbon dioxide, nitrogen, rare gas such as helium, neon and hydrogen sulfide (Skrtic, 2006). However, only hydrogen sulfide is considered for the subject in this study. CFD Fluent tool are being used to analysis the emission rate of hydrogen sulfide from point of release. The structure and topography of the gas gathering station are also considered during the analysis. CFD technique is being selected because the advantage to predict gas concentration at any point of structure including complex structure and complex topography. There are four scope of study to be achieved in this project:

- To conduct study on the consequences and threats of hydrogen sulfide towards individual around gas gathering station.
- To measure the emission rate of hydrogen sulfide by using CFD Fluent
- To validate the result from CFD by using Pasquill-Gifford approach
- To demonstrate for gas release and dispersion problems, CFD approach has advantage in high speed and capable of providing complete information whether at ideal or realistic conditions

CHAPTER II

LITERATURE REVIEW

2.1 HYDROGEN SULFIDE- GENERAL DESCRIPTION

Hydrogen Sulfide had been studied in the early times since the 1600s. In the 19th century, Petrus Johannes Kipp had invented device to generate hydrogen sulfide and hydrogen. Hydrogen Sulfide (H_2S) is a colorless gas with rotten egg smell, soluble in various liquids including water and alcohol.The structure is similar to the water.

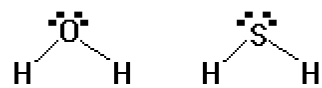


Figure 1 : Hydrogen Sulphide structure

The density of hydrogen sulfide is 1.393 g/L at 25C and 1 atm: which is 18% greater than ambient air. The melting point is -85.5C while boiling point is -60.7C. Based on the report, the average ambient air hydrogen sulfide was estimated to be 0.3µg/m^2 (0.0001 ppm) under clear conditions. Some common names for the gas include sewer gas, stink damp, swamp gas and manure gas. It can be formed under conditions of deficient oxygen, in the presence of organic material and sulfate (Hydrogen Sulfide, 2000).

2.2 HYDROGEN SULFIDE IN OIL AND GAS INDUSTRIES.

Hydrogen Sulfide naturally produces from crude oil and natural gas. The thermal conversion of Kerogene produced oil and natural gas (Skrtic, 2006). High sulfur Kerogene also produced hydrogen sulfide during decomposition which then trapped inside the well. Natural gas consists largely of methane and ethane, with also propane and butane, some higher alkenes, nitrogen, oxygen, carbon dioxide, hydrogen sulfide and sometimes valuable helium(Wan Abu Bakar & Ali). The exploration of oil and gas can release naturally occurring hydrogen sulfide into ambient air. Some of the natural gas deposit contain up to 42% hydrogen sulfide. In Canadian province of Alberta, there are heavy concentration of high-sulphur content oil and gas field(Guiddoti, 1996)

Chemical Name	Chemical Formula	Percentage (%)
Methane	CH_4	70-90%
Ethane	C_2H_6	
Propane	C_3H_8	0-20%
Butane	C_4H_{10}	
Carbon Dioxide	CO_2	0-8%
Oxygen	O_2	0-0.2%
Nitrogen	N_2	0-5%
Hydrogen sulphide	H_2S	0-5%
Rare gases	A, He, Ne, Xe	trace

Table 1: Typical composition of Natural Gas

In Malaysia, the production is sour natural gas. The Environmental Protection Agency (EPA) classifies natural gas as sour when hydrogen sulfide presents greater than 5.7 milligrams per normal cubic meters (Wan Abu Bakar & Ali).

Chemical Name	Chemical Formula	Percentage (%)
Methane	CH_4	40-50%
Ethane	C_2H_6	5-10%
Propane	C_3H_8	1-5%
Carbon Dioxide	CO_2	20-3-%
Hydrogen sulphide	H_2S	0-1%

Table 2 : Chemical composition in crude natural gas offshore of Terengganu, Malaysia

Most of crude natural reserves in Malaysia are located at offshore Peninsular Malaysia, Sarawak and Sabah.

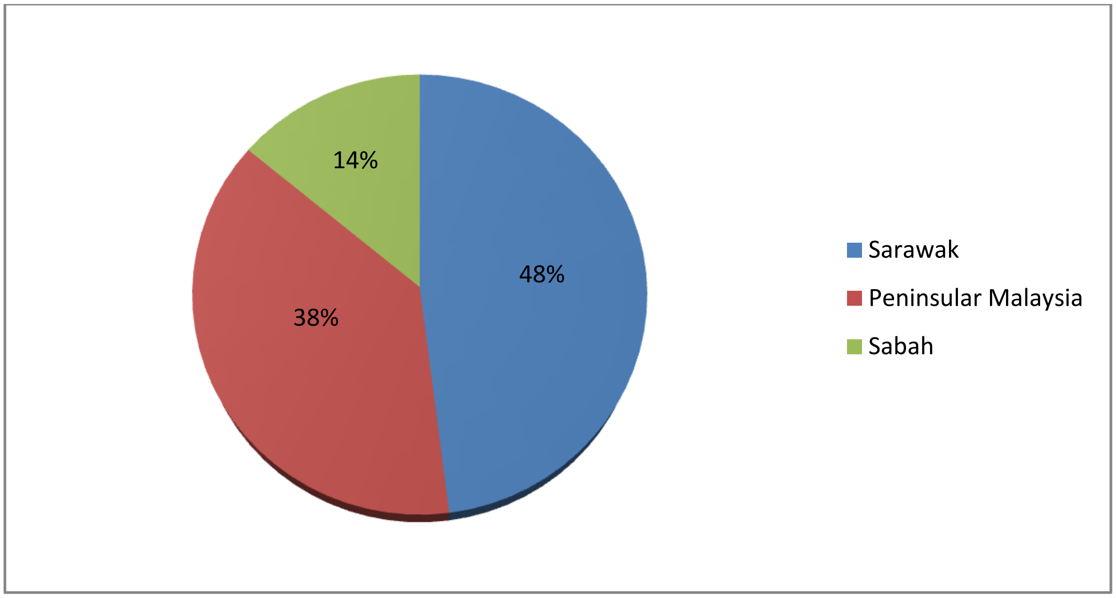


Figure 2 : Natural gas reserve in Malaysia

Hydrogen sulfide is the primary chemical hazard of natural gas production. It is classified as contaminants present in natural gas, which need to be removed at processing facilities called desulfurization plants. Ninety five percent of desulfurization process involves absorption using amine solution while other method includes carbonate processes, solid bed absorbents, and physical absorption.High corrositivity of Hydrogen Sulfide can cause corrosion to oil and gas pipelines. This will impose serious threat to process drilling, well completion, perforating, gas test, exploiting and transportation. Recently, a number of leakage accidents of hydrogen sulfide-bearing natural gas are recorded, as shown in Table 3(Jianwen, Da, & Wenxing, 2011).

Time	Address	Institution	Consequence
1992.9.28	The Zhao 48# well 700meters away from the north of Song town, Gezi village, Zhao county, Hebei province	20th team of underpit operation corporation, Petroleum Administration Bureau of North China	Causing 6 residents surrounded killed and 24 people poisoned
2003.12.23	The 16# gas well of Northeast Gas Field in Gaoqiao town, Kai Xian, Chongqing	China National Petroleum Corporation	243 people died from poisoning, 2142 people hospitalized and 65000 people were evacuated in this accident. Direct economic losses are amounted to 6400 million yuan [5].
2006.3.25	The Luo 2# well of Sichuan Oil & Gas fields	China National Petroleum Corporation	About 10000 people surrounded were evacuated

Table 3 : The leakage accidents of hydrogen sulfide related to oil and gas industries in China.

2.3 HYDROGEN SULFIDE- OCCUPATIONAL HAZARD

Hydrogen sulfide toxicity is a known risk for workers in the petroleum, sewer, maritime and mining industries. Based on EPA documented accident releases, the sources of emission of hydrogen sulfide that have serious impact the public are well blowouts, line releases, extinguished flares, collection of sour gas in low-lying areas, line leakage, and leakage from idle or abandoned wells(EPA, 1993).The lower lethal concentration of hydrogen sulfide is 600ppm. The acceptable concentration of inhalation is 20 ppm on 8h averaged basis. Additionally hydrogen sulfide may be released accidentally or routinely released into atmosphere at gas gathering station or natural processing plant. For example, the release of hydrogen sulfide release with concentration of 6 ppm inside the Ardiyah sewage treatment plant in Kuwait (Al-Shammiri, 2004).

Hydrogen sulfide poses serious inhalation hazard. Hydrogen sulfide is heavier than air and may travel along the ground. The effects to human health are based on the concentration of the gas and the length of exposure.The organs and tissue with exposed mucous membranes and with high oxygen demand is the main target of hydrogen sulfide. The gas is rapidly absorbed by the lungs but absorption through skin is minimal. The gas can penetrates deeply into the respiratory tract because low solubility and capable of causing alveolar injury leading to acute pulmonary oedema. In addition, the exposure also affects the eyes

Hydrogen Sulfide enters the circulation directly across the alveolar- capillary barrier, it dissociate into sulfide ion at this area. Some remains as free hydrogen sulfide in blood and it dissociate with metalloproteinase, disulphide- containing proteins, and thio-S-methyl- transferase, forming methyl sulfides (Hydrogen Sulfide, 2000).At the beginning of the release, people can notify the presence of rotten egg odor at low concentration in air. However, continuous low level exposure can cause olfactory paralysis: the inability of nose to detect concentration of 150-250 ppm. Hydrogen Sulfide paralyze the olfactory nerve, preventing the nose to detect the smell.

Below is the effect at various exposure levels (CCOHS):-

Concentration (ppm)	Human health effect
0.001 – 0.13	Odour threshold
1-5	Moderately offensive odour, possibly with nausea, or headaches with prolonged exposure
20-50	Nose, throat and lung irritation, digestive upset and loss of appetite, sense of smell starts to become fatigued, odour cannot be relied upon as a warning of exposure
100-200	Severe nose, throat and lung irritation, ability to smell odour completely disappears.
250-500	Potentially fatal build-up of fluid in the lungs in the absence of central nervous system effects especially if exposure is prolonged
500	Severe lung irritation, excitement, headache, dizziness, staggering, sudden collapse, unconsciousness and death within 4-8 hours, loss of memory for period of exposure
500-1000	Respiratory paralysis, irregular heartbeat, collapse, and death.

Table 4 : Effect of Hydrogen Sulphide towards human health

2.4 CFD FLUENT

CFD FLUENT are increasingly being applied to study the toxic gas short range dispersion. In addition, CFD FLUENT have advantage to analyse complex topography and dispersion around building. Fluent, Inc and the US EPA national Exposure Research laboratory are working together to demonstrate CFD simulation as the applied tool for environmental assessment studies (Tang, Huber, Bell, & Schwarz, 2006). By solving conservation equation related to convection and diffusion of the chemical species, CFD FLUENT can models the mixing and transport of the species. Steady state Reynolds-averaged Navier-Stokes (RANS) equations with k-ε turbulence model are being used since it is practical for routine application today. The wind inlet boundary values of turbulent kinetics energy k and the corresponding one to its dissipation ε are given by the following equations:

$$k = \frac{1}{\sqrt{C}} U^2$$

$$\varepsilon = \frac{1}{k}\frac{u^2}{z}$$

For the study of hydrogen sulfide inside CFD FLUENT can be described as "species mixing problem without reactions". The FLUENT take account the equation below:-

$$\frac{\partial}{\partial t}(\rho Yi) + \nabla.(\rho v Yi) = -\nabla Ji + Ri + Si$$

Y*i* is the local mass fraction of each species through convection –diffusion equation for *i*th species. R*i* is the net rate of production of species *i* by chemical reaction. In this project the reaction are consider zero since there are no reaction involved. S*i* the rate of creation by addition from the dispersed phase plus any user-defined sources.J*i* is the dispersion flux of species *i*. For turbulent flow, J*i* is computes using the following equation:

$$Ji = -\left(\rho Di, m + \frac{\mu t}{Sci}\right) \nabla Yi$$

Di,m is the diffusion coefficient for species I in the mixture. Sci is the turbulent Schmidt number. $\mu t$is turbulent viscosity.

The main factor to modeling the plume dispersion is the simulation of the atmospheric boundary layer. Other factor that will determine best result for modeling is the mean flow field. A two dimensional (wind along x, vertical direction z) are used to setup the boundary layer. The data required to setup the boundary conditions are friction velocity, roughness height and mass flow rate. The outcomes of the vertical profile are pressure, temperature, mean velocity (U), turbulence kinetic energy (TKE), and turbulent dissipation rate (ε).

Later, the generated boundary layers are used as the inlet profiles for the dispersion simulation of three dimensional. An important parameter is the turbulent Schmidt number (Sc) which characterizes the relative diffusion of momentum and mass due to turbulence:

$$Sc = \frac{\mu}{\rho D}$$

$\mu$is the turbulent viscosity and D is the turbulent diffusivity. The default for Sc is 0.7.

For this project, the simulation will be run under steady state and assuming constant wind speed and wind direction. The reference for wind speed is based on Norwegian Meterological Institute and the Norweign Broadcasting Corporation (Stower, 2012). The normal wind speed around the Kerteh Gas Gathering Station which located nearby the Samui waters is 4-7 m/s. The wind directions mostly have direction of south and south-southwest.

2.5 MODIFIED PASQUILL- GIFFORD (PG) APPROACH

Pasquill -Gifford approach is the classical method for analysis of dispersion pattern.

$$C(x,y) = \frac{Q}{\pi \sigma_y \sigma_z u} \exp(-0.5 \frac{Y^2}{\sigma_y^2})$$
$$\times \left\{ exp\left[-0.5\left(\frac{z-H}{\sigma_z}\right)^2\right] + exp\left[-0.5\left(\frac{z-H}{\sigma_z}\right)^2\right]\right\}$$

Based on the equation, the ratio of predicted to measured concentration should be close as to approve PG model is an accurate predictor of downwind concentrations. However, based on the studied made by Mahesh A. Rege and Richard W. Tock (Rege & Tock, 1996) the PG model is found to overpredict the downwind concentration especially in the case of heavy toxic such as hydrogen sulfide. The standard PG model also were developed using experimental data beyond 100m gases other than hydrogen sulfide. Figure 3 show the PG model performance compared with the real data (Rege & Tock, 1996).

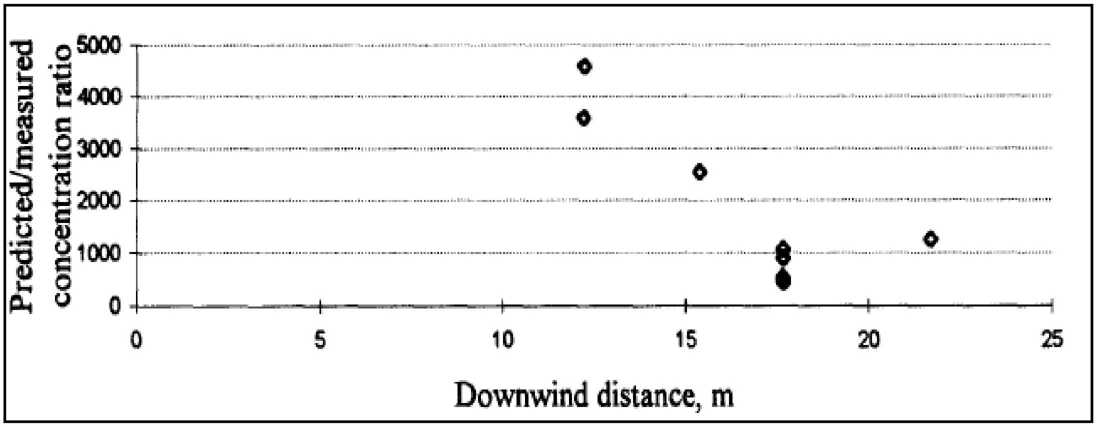


Figure 3: PG model predictions of downwind hydrogen sulfide concentration compared with experimental data

In order to obtain more reliable estimates of downwind concentration an empirical correction was implemented. These concentrations were then used to back calculate the emission rate. The calculations are based on the definition of residual of the concentration.

$$d = \ln(Cp) - \ln(Cm)$$

Cp is PG model-predicted concentration and Cm is the measured concentration. A linear regression of the residual data provides a functional form to define the correction function for the PG model. The correction function F(x) was defined as

$$F(x) = \exp[-(a + bx)]$$

And b are parameter obtained from linear regression and x the downwind distance. The value of this parameter are listed in Table 5.

Type of gas	*a*	*b*
H_2S	10.68	−0.22
NH_3	4.56	−0.14

Table 5: Parameter for corrected function

The corrected form for the PG model for gases at ground level became

$$C(x, y) = \frac{Q}{\pi \sigma_y \sigma_z u} \exp(-0.5 \frac{Y^2}{\sigma_y^2})\, F(x)$$

Where y is the crosswind distance is the wind speed, σy is the plume standard deviation in lateral direction and σ_z the plume standard deviation in vertical direction. By using the modified PG approach, the results of predicted concentration are within 20% of the actual emission rate. However the modified PG is valid for the distance of below 30m. It become more conservative as the crosswind distance increased.

2.6 RISK ANALYSIS

The toxicity of a chemical or physical agent is a property of the agent describing its effect on biological organisms (Crowl & Louvar, 2002). A toxicological studies aim is to quantify the effect on target organism. Before further studies, the toxicant must be identified in term of its chemical composition and physical state. For this studies, the factor that need to be identified is the dose units and the period of the simulation. The dose unit is determined in milligram of toxic gas per cubic meter of air (mg/m^3). Acute toxicity is the effect of single exposure close together in short period of time (Crowl & Louvar, 2002).

After the analysis of emission complete, the project continues with analysis of the risk related to the hydrogen sulfide. One approach is to use dose response model. For single exposure the probit method is suitable to be applied.

$$P = \frac{1}{(2\pi)^{0.5}} \int_{-\infty}^{Y-5} \exp\left(\frac{-u^2}{2}\right) du$$

The probit variable Y can be expressed as follows:

$$Y = A + B \ln V$$

V represents toxic dose while A and B for hydrogen sulfide are constant of -31.42 and 1.4 respectively. For estimations of instantaneous, time varying release, the toxic dose is estimated by integration or summation over several time increments (Bo & Guo-ming, 2010).

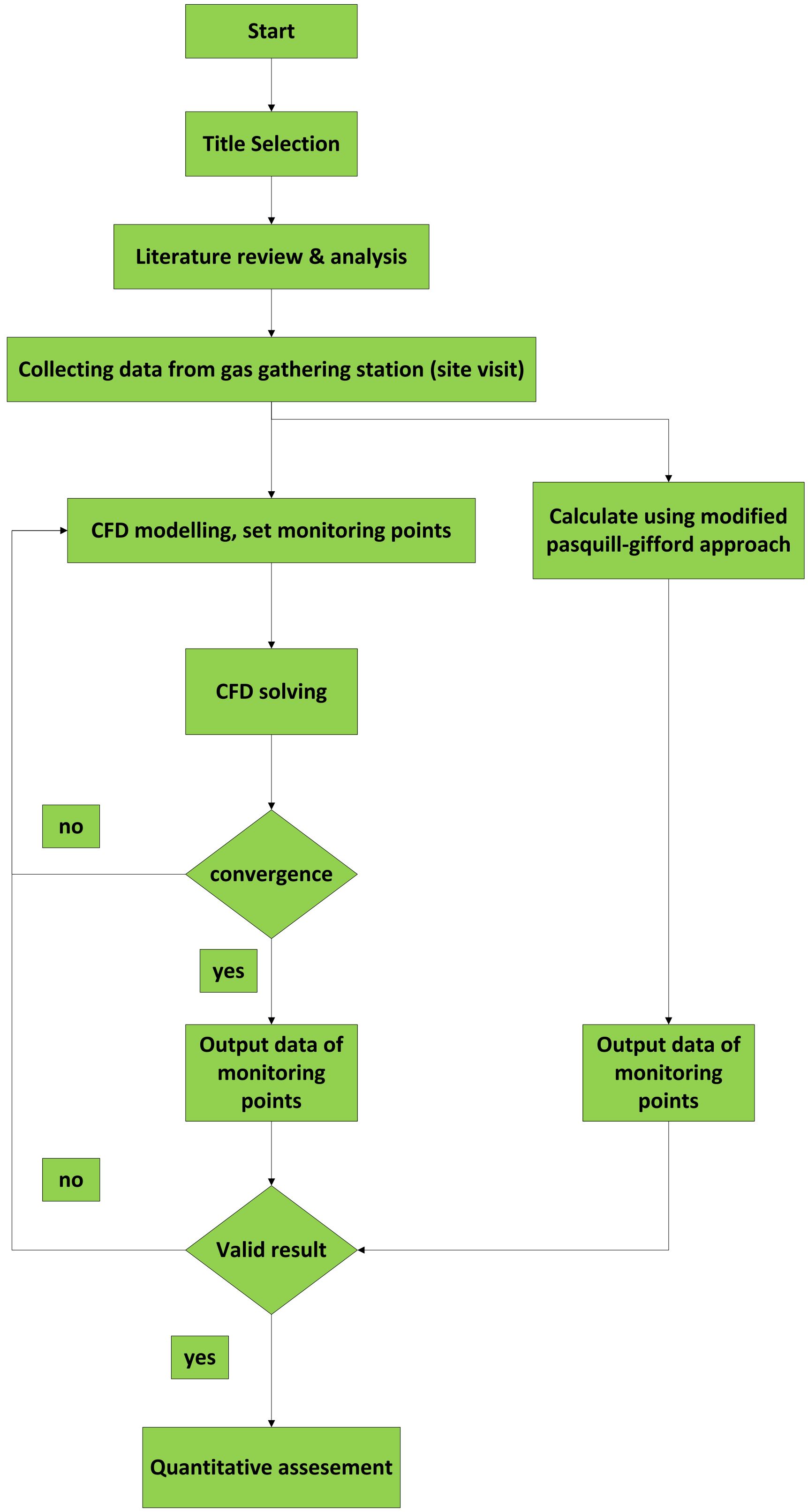
$$V = \int_{t\,0}^{t\,end} C^n dt$$

n for hydrogen sulfide is 1.43

CHAPTER III
METHODOLOGY

3.1 OVERALL METHODOLOGY

A CFD Fluent tool has been proposed as the tool to analyse the hydrogen sulfide dispersion. The start of the project is done by selecting the title of the project. The project continues with the articles research and literature study. In order to relate the situation to a real case, a site visit has been done to few of Malaysia gas gathering station. During the visit, the real data of hydrogen sulfide emission had been collected. A survey regarding incident and hydrogen sulfide threat also had been done during the site visit. For confidential reason, the details of the site are not stated. The data for the input of the analysis are being adjusted as to have the same situation for most of the site. There are four general steps to complete the analysis of hydrogen sulfide exposure from release point by using CFD Fluent. Firstly, set up appropriate two dimension CFD models which consider plant dimension, topography, and structure. Secondly, setup the meshing part. Thirdly, setup the condition by considering the wind velocity, temperature and pressure. Next, setup the monitor points in the CFD model to investigate the toxic gas dispersion. Finally, completed data from the CFD Fluent are being used for further comparison with modified pasquill-gifford method.


Start
Title Selection
Literature review & analysis
Collecting data from gas gathering station (site visit)
CFD modelling, set monitoring points
Calculate using modified pasquill-gifford approach
CFD solving
no
convergence
yes
Output data of monitoring points
Output data of monitoring points
no
Valid result
yes
Quantitative assesement

3.2 SETTING UP CFD FLUENT MODEL

Computational geometry should be setup before the analysis of the dispersion gas being done. The data of the geometry should be referred to the real layout of the Malaysia Gas Gathering Station. The setting of the x-direction is horizontal refer to west to east direction; while the y-direction is horizontal refer to the north to south. For high sulfide natural gas dispersion, the computational geometry should be setup larger than the site as to consider the ambient wind impact. The model can be created by using workbench. The gas gathering station has a length of 250 m and width of 120 m (Bo & Guo-ming, 2010).

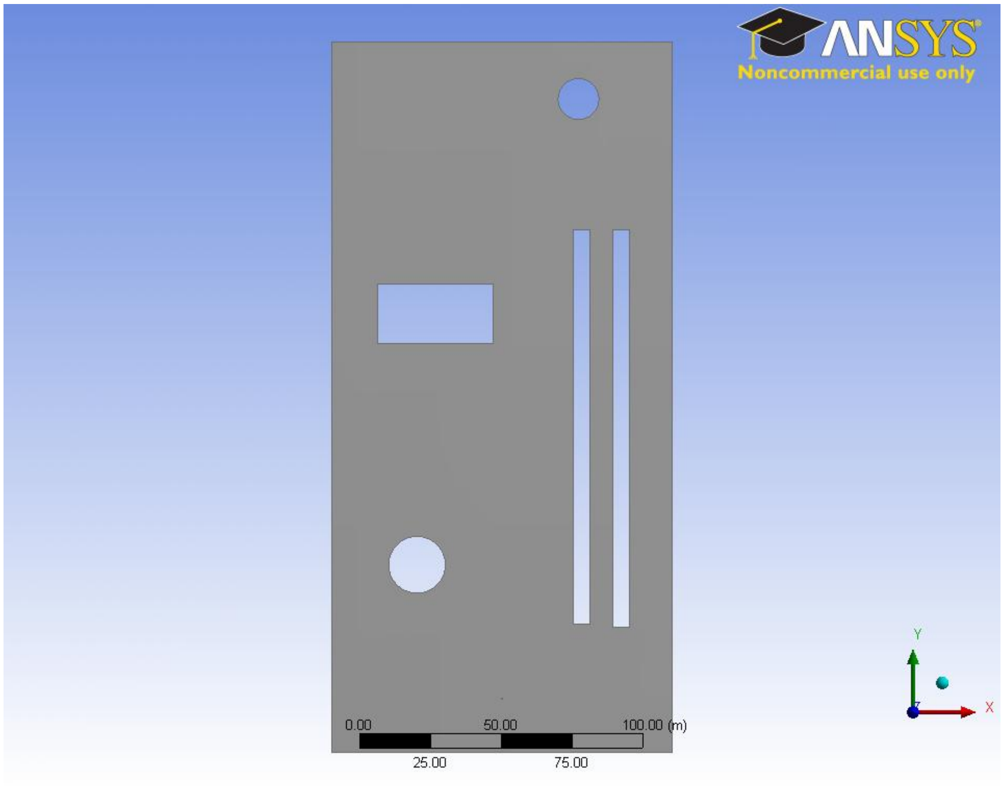


Figure 4: Gas gathering station geometry

Next, the determination of the leakage source. . Due to the erosion caused by hydrogen sulfide and carbon dioxide the leakage is likely to happen in flanges, valves and pipes. An acute threat to the human will occur since the released gas contains hydrogen sulfide. This can be predicted based on the report or accident cases happened at the site. For this project the assumption on the leakage source is at the flange. The leakage source is around flange with a diameter of 48cm. Leakage direction is the same as wind direction of positive Y-axis with different flow rate of 5.0kg/s and 10kg/s. The released natural gas contains methane, hydrogen sulfide and carbon dioxide with mole composition of 76.2, 15.16 and 8.64% respectively. Figure 5 is the mesh generation near the leakage source. A much more refined mesh at the leakage source. For mesh generation, the unstructured grid can be used.

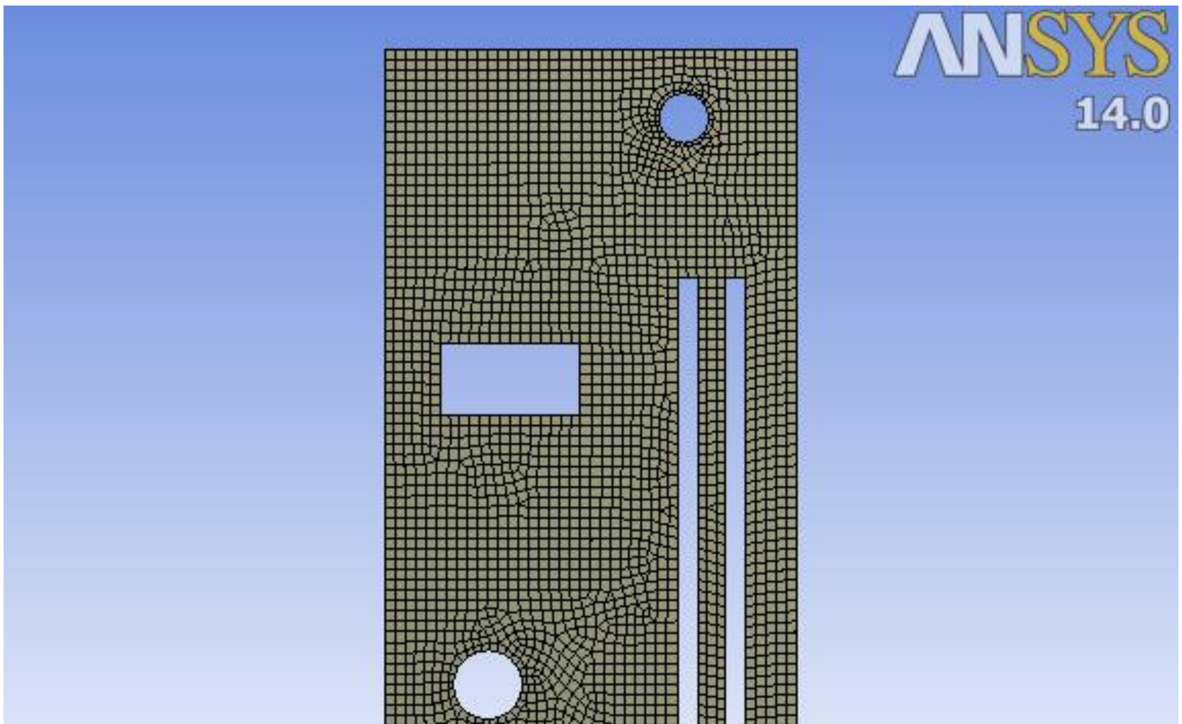


Figure 5: Mesh Generation

Next, the setting for the domain condition. Wind speed is one of the significant parameter of the domain condition. It determines the rate of the released gas diluted with ambient air. The wind inside the computational domain is corresponding to the law of the wall (Bo & Guo-ming, 2010). The other parameter related is the selection of turbulence model. This project had choose to use RANS since it can provide sufficient accuracy and computation cost.

Lastly, is the setup of the monitor points. There are several monitor points being placed according to the flow of dispersion. The monitor points are used to determine the molar concentration over the distance from the leakage point. The areas which have presence of workers likely to inhale the released gas are considered as monitor points such as control room.

3.3 CFD COMPUTATION APPROACH

An unsteady state condition is being setup by implementing k-ε model. For gas dispersion there is no reaction happen between the gas during leakage. The leakage source set to be "mass flow inlet" with 10 kg/s for 2.5 minute. The time step is set to be 0.5 sec with 300 time step. The process is repeated with different approach of mass flow inlet of 5kg/s and 1kg/s.

3.4 GANTT CHART OF FYP

Gantt chart FYP I

No.	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	First meeting with coordinator and supervisors	■	■						Mid-semester break							
2	Preliminary Research Work		■	■	■	■										
3	Submission of Extended Proposal Defence						●									
4	Proposal Defence									■	■					
5	Project work continues											■	■	■		
6	Submission of Interim Draft Report														●	
10	Submission of Interim Report															●

● Suggested milestone

■ Process

Gantt chart FYP II

No.	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14	15
1	Project Work Continues	■	■	■	■	■	■	■									
2	Submission of Progress Report									●							
3	Project Work Continues									■	■	■	■	■			
4	Pre-SEDEX								Mid-Semester Break				●				
5	Submission of Draft Report													●			
6	Submission of Dissertation (soft bound)														●		
7	Submission of Technical Paper														●		
8	Oral Presentation															●	
9	Submission of Project Dissertation (Hard Bound)																●

● Suggested milestone

■ Process

CHAPTER IV

RESULT & DISCUSSIONS

3.5 DISPERSION OF HYDROGEN SULFIDE WITH MASS FLOW INLET OF 10 KG/S

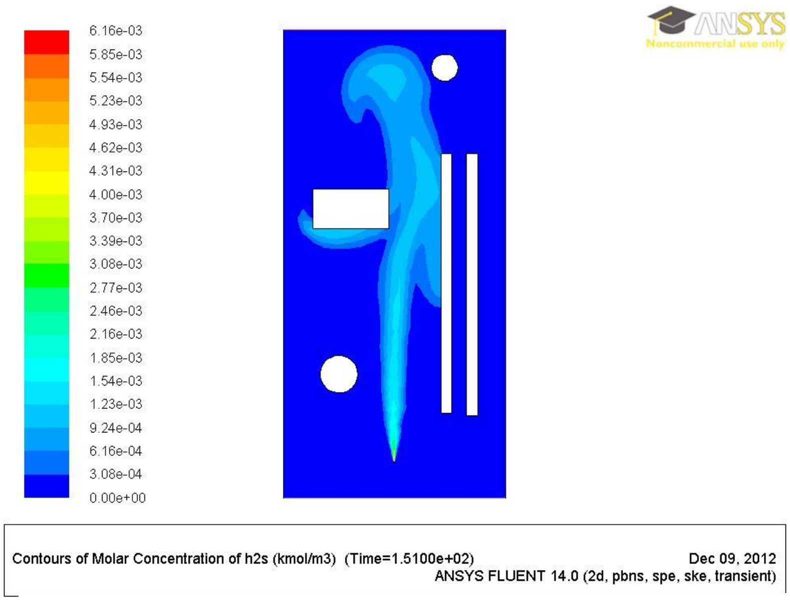


Figure 6 : Contour with the mass flow inlet of 10 kg/s

The picture above show the contour of hydrogen sulfide gas with mass flow inlet of 10 kg/s for 2.5 minute duration. The dispersion came into contact with the control room situated 125 meter from leakage source. The dispersion also passes through the pipe one which is the operation side.

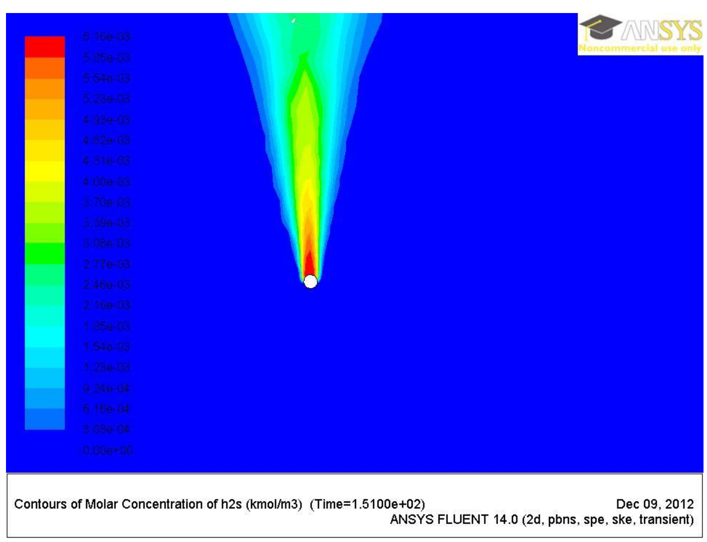


Figure 7: Contour of leakage point with diameter of 48 cm at flange.

Figure 7 show closer view on the release point. The red colour at the centre of the leakage point show the maximum molar concentration of hydrogen sulfide. The dark blue colour indicates the lowest molar concentration which is zero concentration.

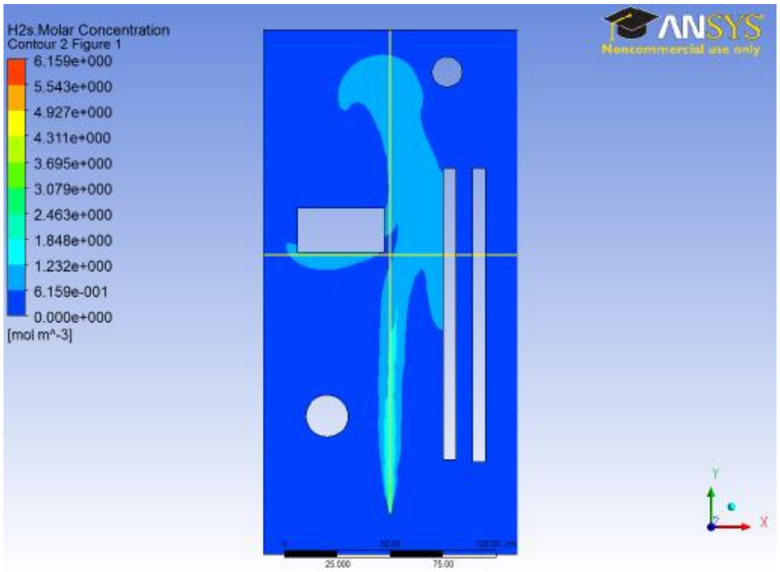


Figure 8: Contour with concentration line

To have a detail on the concentration dispersion, a line is constructed along the dispersion start from leakage point (X=60 cm, Y=20 cm) towards end of the domain (X=60 cm, Y=250cm). A line also was constructed in front of the control room to determine the highest concentration around the building from point (X=0 cm, Y=143cm) towards (X=120 cm, Y=143cm).

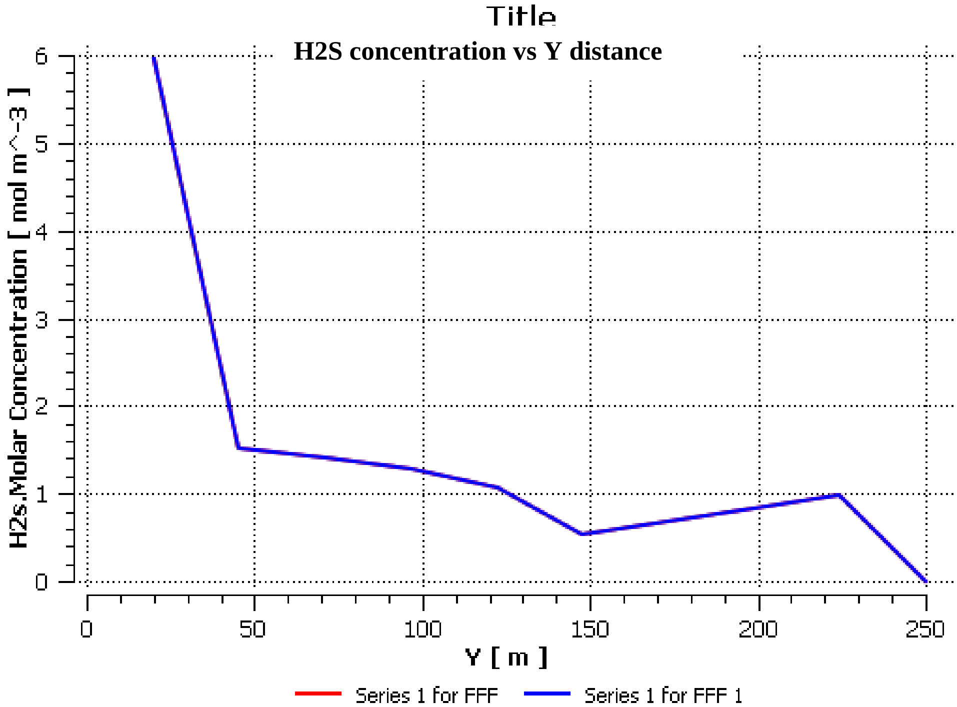


Figure 9: H2S concentration vs Y distance

Distance (m)	Concentration (kmol/m^3)
20	0.0060
45.5556	0.0015
71.1111	0.0014
96.6667	0.0013
122.222	0.0011
147.778	0.0005
173.333	0.0007
198.889	0.0008
224.444	0.0010
250	0.0000

Table 6: Concentration along Y distance

based from the Figure 9, the lowest concentration recorded are 0.009454 mol/m^3 while the highest concentration is 6.158579 kmol/m$^{3.}$ The concentration decreases along the Y distance.

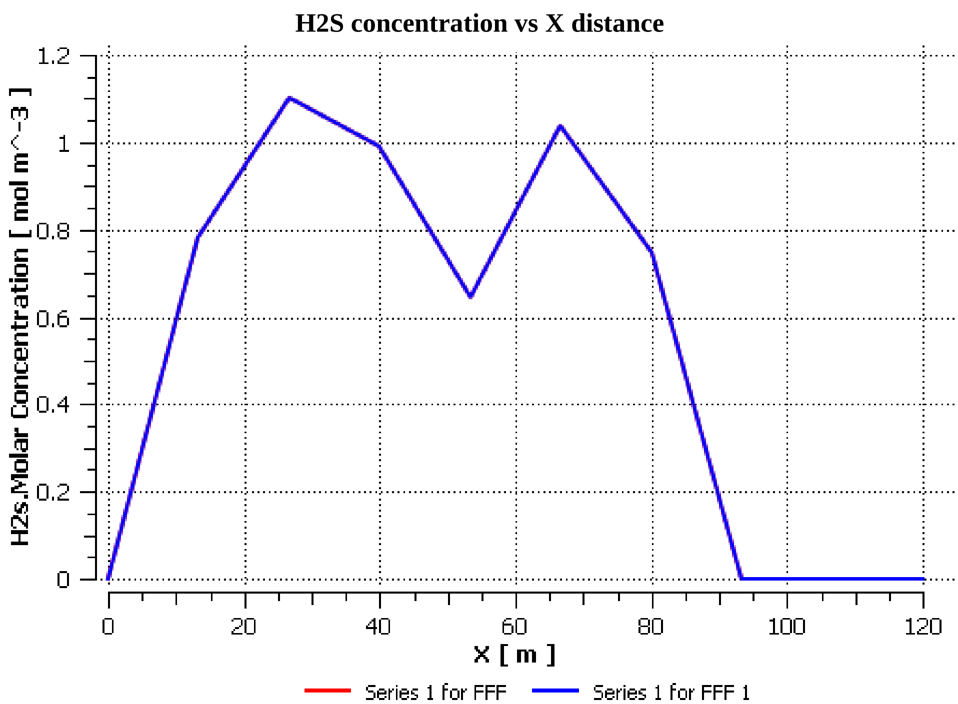


Figure 10: H2S concentration vs X distance

Distance (m)	Concentration (mol/m^3)
0	2.06E-05
13.3333	0.782809
26.6667	1.10173
40	0.989505
53.3333	0.646037
66.6667	1.03918
80	0.745207
93.3333	0
106.667	0
120	0

Table 7: Concentration in front of control room

Graph in Figure 10 indicate the hydrogen sulfide concentration in front of control room. The highest concentration surrond the building is 1.10173 mol/m^3.

3.6 DISPERSION OF HYDROGEN SULFIDE WITH MASS FLOW INLET OF 5 KG/S

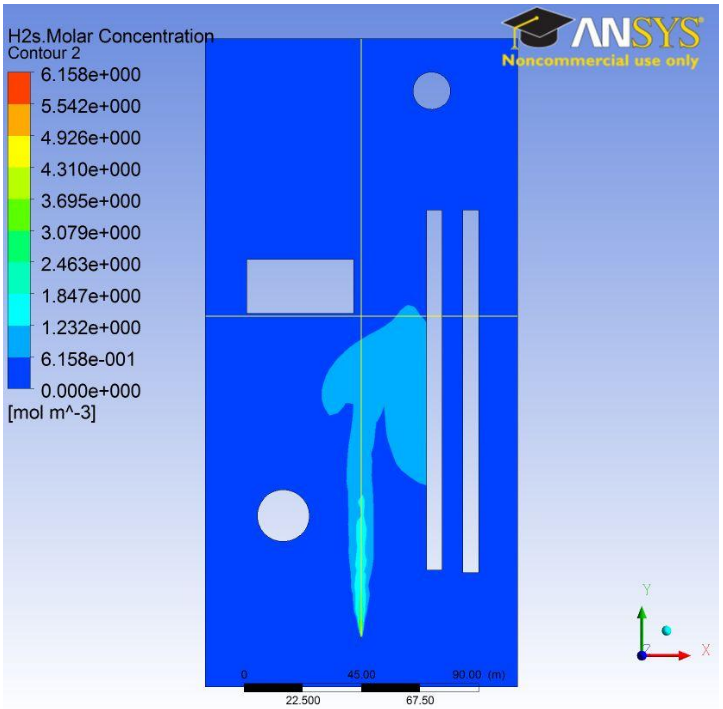


Figure 11: Contour with mass flow inlet of 5kg/s

Figure 11 indicate the dispersion of hydrogen sulfide does not reach the area of control room but come into contact with pipe one. Graph of hydrogen sulfide concentration along the Y axis as shown in Figure 12show the highest concentration is 6.158 mol/m^3. For X axis the highest concentration is 0.781087 mol/m^3.

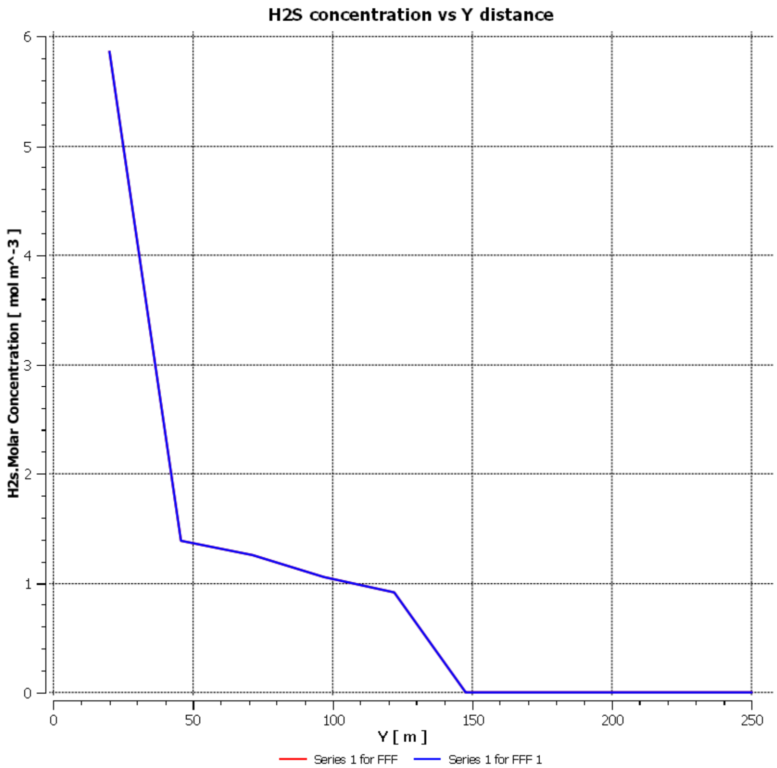


Figure 12: H2S concentration vs Y distance

Distance (m)	Concentration (mol/m^3)
20	5.86205
45.5556	1.3909
71.1111	1.25292
96.6667	1.05817
122.222	0.913781
147.778	0.000332
173.333	7.44E-07
198.889	0
224.444	0
250	0

Table 8: Concentration at Y distance

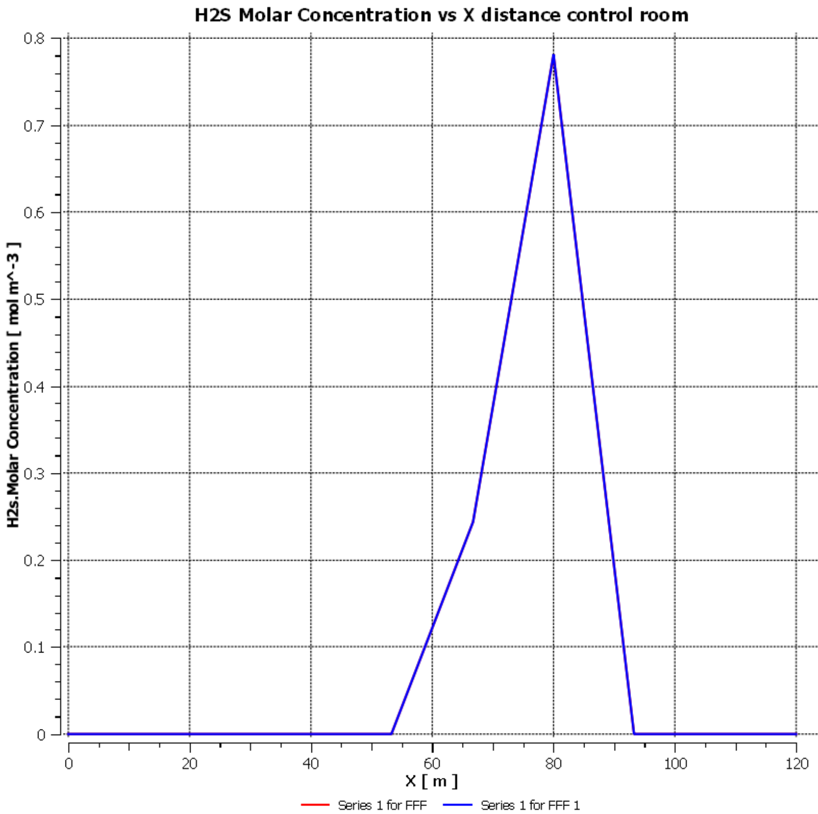
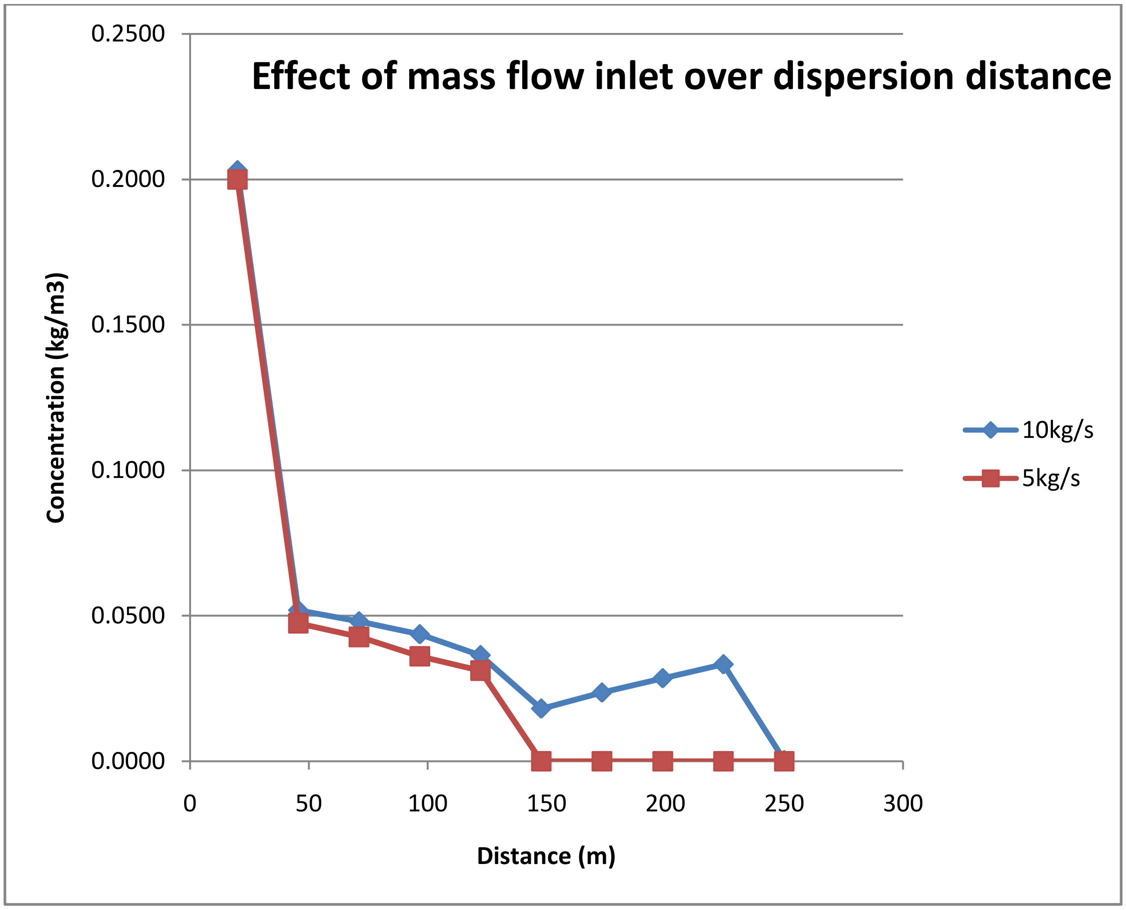


Figure 13: H2S concentration vs X distance

Distance (m)	Concentration (mol/m^3)
0	1.33E-18
13.3333	6.60E-14
26.6667	0
40	9.54E-10
53.3333	0.000196
66.6667	0.243836
80	0.781087
93.3333	0
106.667	0
120	0

Table 9: Concentration in front of control room

3.7 THE EFFECT OF MASS FLOW INLET OVER AREA OF DISPERSION



The higher the amount of release will affect the dispersion distance. Mass flow inlet with 10kg/s already reaches the control room area within 2.5 minute. The concentration amount also increases with increasing mass flow inlet.

3.8 COMPARISON STUDY

3.8.1 Comparison Conventional Pasquill-Gifford Method with CFD Fluent

A comparison analyse had been done to indicate the data from the CFD Fluent are valid for hydrogen sulfide dispersion. For pasquill gifford approach, the situation being used is plume with continuous steady state source at ground level and wind moving in y direction at constant velocity u. The concentration along the centerline of the plume downwind is given at y=z=0:

$$C(x,0,0) = \frac{Q}{\pi \sigma_y \sigma_z u}$$

$\sigma_y(m) = 0.08x(1 + 0.0001x)^{-0.5}$

$\sigma_z(m) = 0.06x(1 + 0.0015x)^{-0.5}$

Q = 10 kg/s

U = 6m/s (Class D wind speed)

Assumption for the atmospheric stability classes is neutrally stable, thus class D is the most suitable class. The concentration along the centerline of the plume downwind is given at y=z=0.

Distance (m)	PG (kg/m^3)	CFD(kg/m^3)
20	0.2808	0.2031
45.5556	0.0552	0.0519
71.1111	0.0231	0.0481
96.6667	0.0127	0.0436
122.222	0.0081	0.0364
147.778	0.0056	0.0181
173.333	0.0042	0.0236
198.889	0.0032	0.0285
224.444	0.0026	0.0333
250	0.0021	0.0003

Table 10: Concentration from PG and CFD Fluent

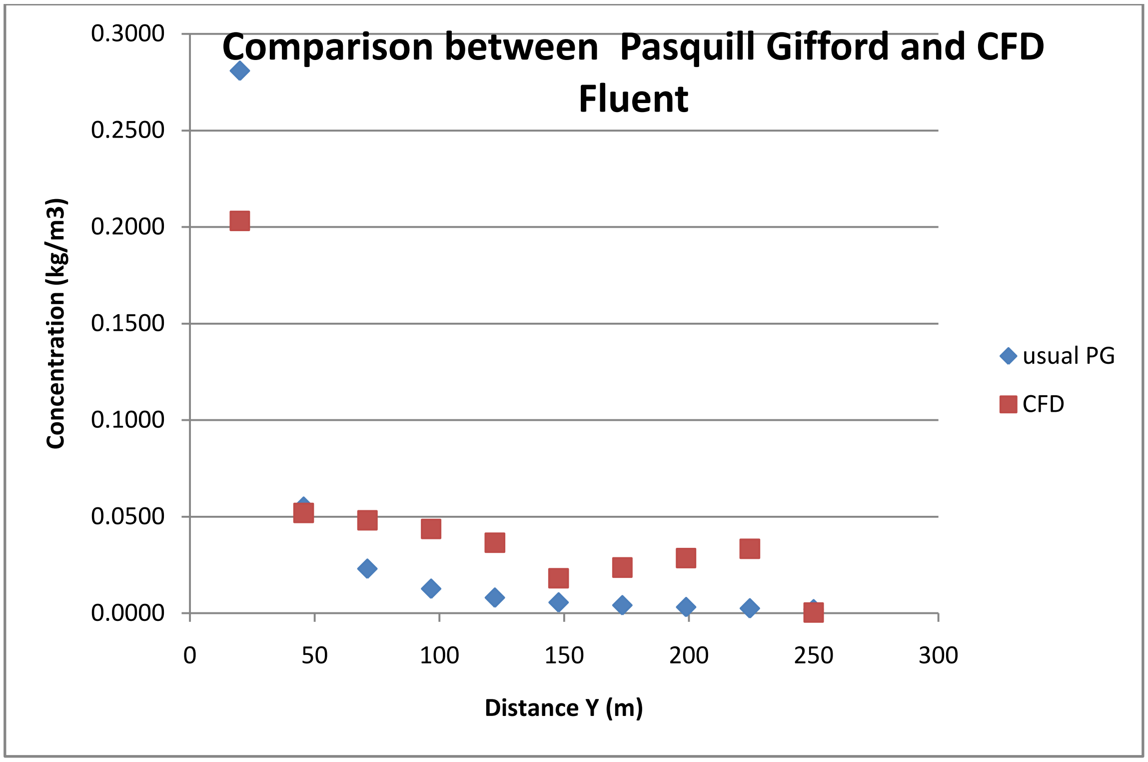


Figure 14: Comparison between Pasquill Gifford and CFD Fluent

From the Figure 14, the PG results have close results with CFD Fluent. The result show CFD Fluent result is valid for data with the distance at 50m and above. Result at 20 m show a large different thus show that PG have overpredict the dispersion.

The cause of large different of the result at the downwind may be due to the accumulation of hydrogen sulfide with atmosphere. But there is no evidence of accumulation hydrogen sulfide in atmosphere (Rege & Tock, 1996). Another speculation of this overpredicts is because of the transformation of hydrogen sulfide to sulfur dioxide which will sink to the ground. The overprediction also may be attributed of large error in the estimation of standard deviations of the plume. This standard deviation was developed by using other gas than hydrogen sulfide.

To overcome the large difference and overprediction, this project estimation of concentration with distance below 30 m need to use modified PG method.

3.8.2 Comparison Modified Pasquill-Gifford Method with CFD Fluent

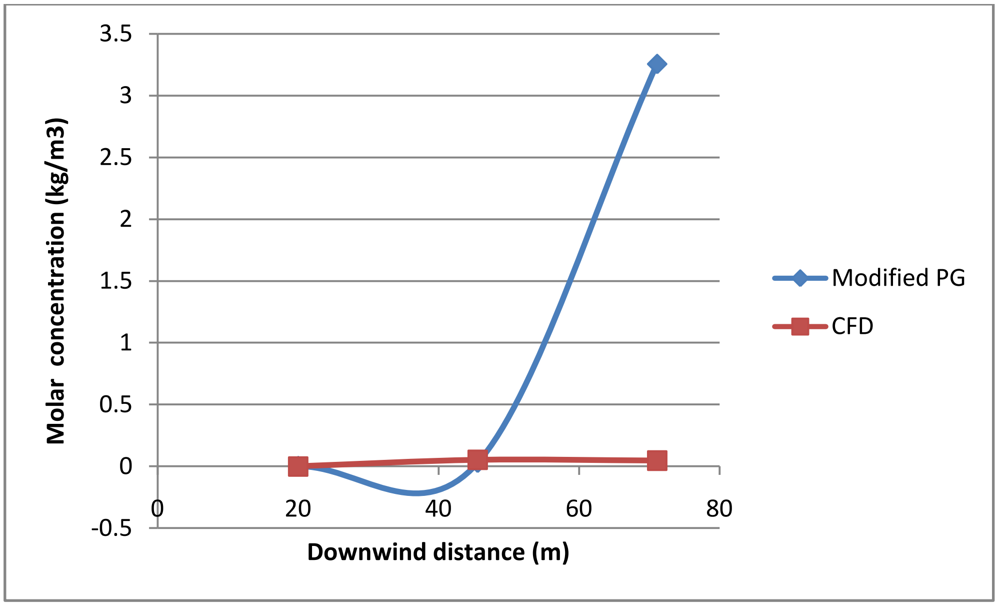


Figure 15 : Comparison of Modified PG and CFD with distance below 50 m

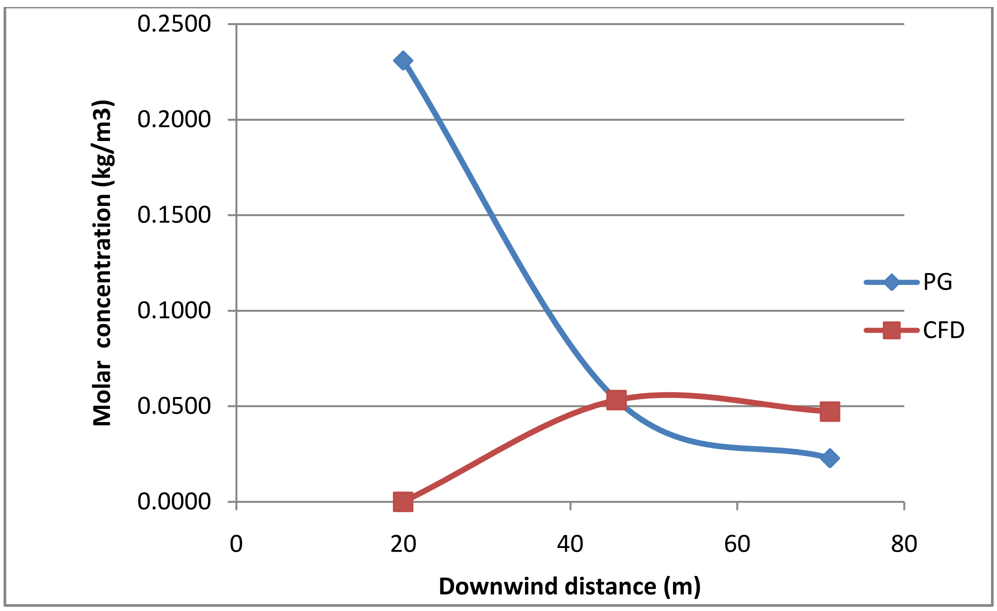


Figure 16 : Comparison of concentration of PG and CFD with distance below 50 m

The mean difference of concentration in Figure 15 is 0.0351. The mean difference of concentration in Figure 16 is 0.0967. The lower mean differences in concentration show Modified PG has more reliable result in downwind concentration below 50 m. However as the crosswind distances of the sample increased, the emission rate by the corrected model often exceeded factor of two (Rege & Tock, 1996). Hence the applicability of corrected model is only valid for direct downwind distance with y=0. There are limitations of PG approach since it only applies only to neutrally buoyant dispersion of gases. The dominant features of dispersion are related to the turbulent mixing. It is valid for distances of 0.1-10 km from the release point (Crowl & Louvar, 2002).

3.9 RISK ANALYSIS

For risk analysis the analysis focuses on the area near to the control room which has high population of human. Table 11 indicate the concentration around the control room at 2.5 minute.

Distance (m)	Concentration (mg/m^3)
0	7.0246E-13
13.3333	2.6694E-08
26.6667	3.7569E-08
40	3.3742E-08
53.3333	2.203E-08
66.6667	3.5436E-08
80	2.5412E-08
93.3333	0
106.667	0
120	0

Table 11: Concentration in front of control room

The highest concentration detected is 3.7569E-08 mg/m^3. The concentration does not exceed the limit of threshold limit values (TLV). For hydrogen sulfide the TLV is 10 ppm or 14 mg/m^3.

If the duration of the release increases, the concentration may increase and can cause threat to the worker. In reality the workers would not stay inside the dispersion area if there is leakage of toxic gas. This is happening if the detector of hydrogen sulfide is malfunctioning and the dose exceeds 100 ppm which will cause human smell loss. Workers need to quickly evacuate the dispersion area and enter the control room where there is breathing apparatus are stored.

CHAPTER VI
CONCLUSIONS

The major objective of this study is to evaluate the reliability of CFD Fluent as a tool for the analysis of hydrogen sulfide. Modified PG method had been proposed to validate the early distance of emission. Result from CFD Fluent is compared with modified PG. Even though, the result from modified PG give different result from CFD but the result are more favorable than the result from simple PG. The empirical correction provided for the early emission had improved the result of emission for neutral conditions of atmospheric stability and downwind distances up to 30m. For further improvement of this corrected PG model is to establish the horizontal and vertical dispersion standard deviations. The dispersion coefficient for short distance is usually unknown for PG model. These modified PG model gives an alternative for short range atmospheric dispersion. Simple PG methods are further used to calculate the theoretical concentration for distance more than 30 m.

CFD Fluent method is reliable to evaluate the emission rate of toxic gas such as hydrogen sulfide in Malaysia gas gathering station. It can be widely used for risk analysis of toxic gas exposure and consequences. Moreover, these methods are more safe and low cost than simulation of real experiment. It is low risk method and provides high speed and complete information.

Further study on this subject is on the evaluation of Malaysia gas gathering station safety equipment. The toxic gas detection and alarm system and emergency evacuation need to be evaluating for safer environment and precautions.

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