

**TOXICITY STUDY OF CO<sub>2</sub> RELEASE IN BIOGAS  
PROCESS USING COMPUTATIONAL FLUID  
DYNAMICS MODELING**

By

AHMAD FAHMY BIN YAHYA

Dissertation submitted in partial fulfillment of  
the requirements for the  
Bachelor of Engineering (Hons)  
(Chemical Engineering)

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CERTIFICATION OF APPROVAL

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Approved by,

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UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

September 2013

## **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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AHMAD FAHMY YAHYA

## ABSTRACT

Biogas processing technologies have been widely applied in industries due to the limitation of non-renewable energy as a source of energy. Together with the biogas production, the emission of carbon dioxide gas from the product also brings the major concern on how safe the carbon dioxide gas concentration from the biogas industry could be. In fact, accidental release of carbon dioxide may cause severe damage and losses during the biogas production. Example of biogas production is landfill gas (LFG) that produces by anaerobic condition through the degradation of municipal solid waste by microorganism. The ability to predict foreseeable accidental scenarios and investigate their consequences is a fundamental aspect in the assessment of the risk of a process or technology. However, due to the limited operational experience in biogas, the process to identify the hazard especially toxicity associated with a larger scale process like biogas become more difficult and complicated. This paper presents an early investigation on how the carbon dioxide gas will react and disperse to the atmosphere due to the leaking in biogas process. Besides, the most important part for this project is to find out the toxicity safe distance on carbon dioxide release in biogas process base on its concentration. Thus, a Computational Fluid Dynamic (CFD) modeling is used to simulate the dispersion behavior of biogas from pressurized release into the atmosphere. CFD is the well-known tool used to investigate the behavior of released substance especially liquid and gas. CFD also equipped with a branch of fluid mechanics that involve algorithm and numerical method to solve the problem related with the fluid flow. In comparison with the natural gas, biogas will shows higher concentration of carbon dioxide because of the low carbon dioxide content in the natural gas. Hence, it proof that biogas is more toxicity than natural gas in term of carbon dioxide release.

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# CHAPTER 1

## PROJECT BACKGROUND

### 1.1 Introduction

As the total population of the world increase, the demand for the energy also increases. From the very basic thing like lighting on the bulb to the most complex job like turning on the engine, all of these need energy. However, the continuity of the supply energy is still in a big worry. Based on the statistic release from BP Global in 2012, reserve world oil amount is 1,386 billion barrels that approximately will last long up till 46 years (Anderson, 2012). Natural resources for energy like coal, crude oil and natural gas need thousands of years to form naturally and cannot be replaced as fast as they are being consumed (Depletion of Oil Energy Resources, 2010). To make it worst, the world oil consumption increase by roughly 600,000 barrel per day. According to this figure, it is crucial for the people to explore and find another source of energy as the substitute energy for the non-renewable source that can last longer.

A renewable resource is a natural resource that can restore with the passage of time, either through naturally repeated process or biological reproduction. Due to this reason, this is why the demand for the renewable energy suddenly increases. Beside the availability, the reduction on the pollutant produce also gives a good value on the renewable energy. As been reported in RenewableEnergyWorld.com, the President of the United State of the America had announced the addition of three manufacturing hub for the green energy generation (Williams, 2013). From this, it is agreed that if more government start promoting the renewable energy, the reliant on the non-renewable energy will be reduce.

Recently, there is a lot of renewable energy that had been generated and produced. One of the energy is biofuels energy. Biofuels is a fuel that produce from renewable biological resource such as plant biomass and treated municipal and industrial waste. Among the common products that produce from the biofuel are biodiesel, bioethanol, solid biofuel and biogas. All of this output is known as first generation of biofuels (Walker, 2008). For the biogas, it is typically refer to a gas that formed by the breakdown of the organic matter in the absence of the oxygen. The two main type of biogas are landfill gas and digester gas that produced from the domestic waste and bioreactors respectively (Dupont, 2006). Usually, the major component of the biogas is methane gas that has 50% to 75% of volume in the biogas. However, this composition highly dependent on the waste nature of the raw material and the way it is being process (Naskeo, 2009).

Biofuels have been around since the cars exist. In the early 20<sup>th</sup> century, Henry Ford was fueled his Model Ts with ethanol that derived from the peanut oil (Biofuel, 2011). However, the huge exploration on petroleum makes the biofuel largely forgotten. Fortunately, with the sudden rise in oil price as well as public concern on the global warming caused by the carbon dioxide emission, the biofuel now is back on demand. Due to this arising impact, there are a lot of biogas plant are constructed in this world. Together with the plant production, the plant process safety also gives the big impact to the human population.

The plant process safety is the most important criteria that need to be focusing when involve with the plant operation. Like other plant, the biogas plant also gives high risk associated with hazard to its operators. Besides its flammability, toxicity of high concentration of CO<sub>2</sub> that comes from biogas also gives high risk due to its property that displaces oxygen in atmosphere. Furthermore, the biogas produce from the animal manure also bring the same hazard as the biogas plant. Incident like farmer dead after been trapped in the confine space always related with the hazard of the biogas. Severe injuries and death from exposure to a biogas is not common occurrence in biogas industry, but even one death happened, it still can raise the awareness to the people especially when it can be prevented (Aldrich, 2005).

## 1.2 Problem Statement

There is nothing as important as safety that we cannot take time to practice it especially in plant operation. However, no matter how many years the worker has been experienced with the industry, the accident still can be occurring. The Star on May 2012 reported that a worker died and 23 others were injured in an explosion at a PETRONAS Gas processing Plant in Kerteh (Zolkepli, 2012). The cause for the incident might come from the hazard of the vapor cloud of the hydrocarbon but still, it involves the human errors.

From this statement, it is strongly recommended for the employees especially the chemical engineers to learn and know the properties and hazard of the chemical that they handle with. Biogas plant produce a lot of flammable and toxic gas like methane ( $\text{CH}_4$ ) that lead to fire, explosion or suffocation hazards in case the equipment and the control operation fail to function properly (Steiglechner, 2011). This is mainly because of the component that make up the biogas is Methane ( $\text{CH}_4$ ) and  $\text{CO}_2$  that produce from anaerobic process. Despite all of this information, there is still big question on how safe the biogas plant operation will be especially during unforeseen incident happen. This is because the data or the information on the hazard of the biogas is not abundant especially in term of biogas toxicity. The risk analysis study on the toxicity of biogas become more complicated when there is no data present to illustrate how far the toxicity of this biogas can travel in certain period of time.

Besides that, the variation of the biogas composition also gives the researcher hard time to study how toxic the biogas can be according to its physical and chemical properties. In addition, the lack of case studies on biogas toxicity based on real event also makes the investigation become harder. Serious incident such as Bhopal 1984 highlight the significance of planning and modeling for emergencies to reduce the probability and consequences of toxic release (Chemical Process Safety, 2011).

Hence, to study on the dispersion of  $\text{CO}_2$  toxicity release from the biogas, Computational Fluid Dynamic (CFD) tools can be used for the studies. Living the fact that not much toxicity dispersion modeling has been develop, this is the reason why CFD is used to examine the effect of the  $\text{CO}_2$  toxicity from biogas in this study.

### **1.3 Objective**

To study on the dispersion of toxicity release from the biogas, this project will be done by fulfill the following objectives:

- To identify the safe distance for CO<sub>2</sub> release from biogas using Computational Fluid Dynamic (CFD) tool.
- To study on the behavior of CO<sub>2</sub> release from biogas process.

### **1.4 Scope of Study**

This project will be focus more on the generation of dispersion model from biogas source using CFD-FLUENT modeling. The scope of research for this project will be narrow down by study on the CO<sub>2</sub> gas release behavior from the biogas process instead of study on the other composition of biogas like methane. Other than that, this project will be run with the variation of the wind speed to see the comparison and relate it with turbulence effect. Besides, the difference between CO<sub>2</sub> concentrations during discharge is another case that will be study for this project.

## CHAPTER 2

### LITERATURE REVIEW

#### 2.1 Hazard of Biogas

The production of the biogas is the process where organic substances are split into the methane and carbon dioxide. Due to its process, biogas plant can be classified as one of the chemical plant. Based on Table 1, the most common accident that relates with the chemical plant is fire, followed by explosion and toxic release (Chemical Process Safety, 2011).

Table 2: Three Types of Chemical Plant Accidents (Chemical Process Safety, 2011)

Type of Accident	Probability of Occurrence	Potential for Fatalities	Potential for Economic Loss
Fire	High	Low	Intermediate
Explosion	Intermediate	Intermediate	High
Toxic Release	Low	High	Low

Biogas composed mainly of methane (CH<sub>4</sub>) gas and carbon dioxide (CO<sub>2</sub>). However, the biogas also contains other traces of compound like hydrogen sulfide (H<sub>2</sub>S) and organosulphur (mercaptans) in small amount (Dupont, 2006). Methane gas that contains 50% to 75% from the total biogas volume will create the explosive mixture when mix with air and can produce serious hazardous explosion. For the methane gas, the Lowest Explosion Limit (LEL) and the Upper Explosion Limit (UEL) is 4.4% and 16.5%

respectively (Siemens, 2010). Hence, it is crucial to always check the value for the explosive limit of methane gas so that its composition in air will never fall into this range.

Beside explosion, methane gas can also bring hazard to human in term of choking. Methane is inert, colorless, odorless gas that has  $0.66\text{kg/m}^3$  in density (Chrebet, Martinka, 2012). Based on the density value, methane gas is lighter than air and will accumulate at the roof space. At low concentration, methane gas can act as narcotic and the victim may not be aware because of asphyxiation. At the high concentration, methane can result in suffocation due to the oxygen displaced in atmosphere. According to the Jefferson Lab Policy, 19.5% amount of oxygen in atmosphere is considered to be hazardous Oxygen Deficient Atmosphere compare than its normal value which is 21% (Oxygen Deficiency Hazard, 2008).

Other than methane gas, hydrogen sulfide ( $\text{H}_2\text{S}$ ) gas also can give the hazardous impact to the workers even it contain 0% to 3% in the biogas volume.  $\text{H}_2\text{S}$  gas is a flammable gas that can be identify by the smell of rotten eggs at the concentration of 0.03ppm to 0.15ppm in air. (Horak et al., 2007). As the concentration increase, the  $\text{H}_2\text{S}$  gas will become odorless and poisonous that can cause death.

## 2.2 Toxicity of CO<sub>2</sub>.

A basic principle of toxicology is there is no harmless substances, only harmless ways of using the substances (Chemical Process Safety, 2011). Based on this statement, the CO<sub>2</sub> is not a very toxic gas if we know how to handle it properly. Every day, human being live in the atmosphere that contains certain amount of CO<sub>2</sub> and drinks a tin of carbonated drink but still, no hazard occurs. Unfortunately, 107 people were intoxicated while 19 of them were hospitalized after been exposed to CO<sub>2</sub> gas that accidentally release from the fire system in Monchengladbach, Germany (Harper, 2011). The big question arise here is how the CO<sub>2</sub> can be so hazardous and toxic.

Based on Material Safety Data Sheet (MSDS) that provide by the Airgas Company, CO<sub>2</sub> is non-flammable gas, inert, colorless as well as odorless gas. It has density around 1.98 kg/m<sup>3</sup> that makes CO<sub>2</sub> gas heavier than air (Thomas, Martinka, 2012). From here, we can conclude that at high concentration, CO<sub>2</sub> gas will displace oxygen in air to the low dangerous level and cause asphyxiation (deficient supply of oxygen). According to Dr. Peter Harper (2011), CO<sub>2</sub> gas will give sudden threat to the human body at concentration of 15% in air while at 50%, it will give immediate danger to life by decrease the oxygen concentration in air. However, at 50% concentration in air, a reason a person dies is not clear whether because of oxygen depletion or effect of inhalation cause by CO<sub>2</sub> toxicity, but still the outcome is death.

CO<sub>2</sub> gas will undergo the process of sublimation which is the phase change from solid to gas at the temperature of -78.51<sup>0</sup>C at atmospheric pressure (Moe, 2012). Even in the solid phase, CO<sub>2</sub> gas also can give threat to human life according to its concentration. There is case which been reported that a 59-year old man were found dead after entered a recently repaired walk-in freezer that contained dry ice which is the solid form of carbon dioxide. After investigation, physician had confirmed that the cause of death was because of inhalation of CO<sub>2</sub> gas and reduced O<sub>2</sub> gas (Dunford et., al 2009). Hence, the issue here is not the phase of the CO<sub>2</sub> gas that will give danger to human live, but the amount of the concentration and period of time that someone been exposing to CO<sub>2</sub> gas.

“All substances are poisons, there is none which is not poison. Only the dose permits something not to be poisonous.” (Paracelcus, 1493 – 1541). Based on this, it explain why the people should know the safe concentration value for certain chemical compound especially carbon dioxide. According to NIOSH (2009), Short Time Exposure Limit (STEL) for CO<sub>2</sub> gas in 15 minutes is 30000 ppm (3% in air) while Time Weight Average (TWA) in 10 hours is 5000 ppm (0.5% in air). So, the CO<sub>2</sub> gas will not give any toxic behavior if the concentration is less than 3% in air but if more than 5%, CO<sub>2</sub> gas will irritate the respiratory tracts (Thomas, Martinka, 2012).

To assess on how toxic the CO<sub>2</sub> gas concentration effect with exposure time, Health and Safety Executive (HSE) has constructed the assessment of Dangerous Toxic Load (DTL) (Harper, 2011). Under this assessment, there are two assessments which are Specify Level of Toxicity (SLOT) and Significant Likelihood of Death (SLOD) that can be used as the benchmark to study on the CO<sub>2</sub> gas toxicity for this project. Table 3 illustrates how the assessment looks alike.

Table 3: Concentration vs Time Consequences for CO<sub>2</sub> Inhalation. Health Safety Executive (HSE)

<b>Inhalation Exposure Time</b>	<b>SLOT: 1% - 5% Fatalities</b>		<b>SLOD: 50% Fatalities</b>	
	<b>CO<sub>2</sub> Concentration in Air</b>		<b>CO<sub>2</sub> Concentration in Air</b>	
60 min	6.3 %	63 000 ppm	8.4 %	84 000 ppm
30 min	6.9 %	69 000 ppm	9.2 %	92 000 ppm
20 min	7.2 %	72 000 ppm	9.6 %	96 000 ppm
10 min	7.9 %	79 000 ppm	10.5 %	105 000 ppm
5 min	8.6 %	86 000 ppm	11.5 %	115 000 ppm
1 min	10.5 %	105 000 ppm	14 %	140 000 ppm

Other than human, biogas also has possibility to give negative impact to equipment. The high concentration of CO<sub>2</sub> together with the hydrogen sulfide (H<sub>2</sub>S) can create the highly corrosive environment when it is not dried (Eekelen, 2011). With this environment, the tendency of the equipment especially in piping during biogas transfer to leak is high.



However, the behavior of CO<sub>2</sub> toxicity dispersion model from biogas process is not available yet. Even most of its chemical and physical properties are known, there is still no enough data on how much the concentration of CO<sub>2</sub> will be disperse and travel through atmosphere from certain discharge point.

### 2.3 Oxygen (O<sub>2</sub>) Deficiency.

Normally, oxygen content in air is around 21% by volume under normal atmospheric pressure. Typically, human being will feel the effect when the oxygen concentration decreases around 1 or 2 %. This can be pictured when people hiking the highest mountain or peak where the oxygen level is low. According to Naranjo (2007), healthy people will unable to walk actively and their body movement will be affected if the oxygen in environments is around 15% to 19%.

Typically, a lot of reasons can cause the oxygen deficiency to happen. An incident like loss of primary containment cause by leaking equipment is one of the factors that contribute to this issue. Release gas like methane and carbon dioxide that produce from the biogas process from the leaking equipment can accumulate at certain area and will displace the oxygen content in the atmosphere. Most famous case in which this situation always occur is in the confine space like storage of animal manure.

The summary for the effect of O<sub>2</sub> deficiency is shown below in Table 4:

Table 4: Effects of oxygen deficiency. Data from CCOHS

<b>Volume of O<sub>2</sub> in Air</b>	<b>Effect to Human Body</b>
12% - 16%	Breathing and pulse rate are increased, with slight muscular incoordination
10% - 14%	Emotional upsets, abnormal fatigue from exertion, disturbed respiration
6% - 10%	Nausea and vomiting, inability to move freely, collapse, possible lack of consciousness
< 6%	Convulsive movements, gasping, possible respiratory collapse and death

## 2.4 Biogas versus Natural Gas

Other than biogas, natural gas is also one of the main contributors to the world source of energy. Besides the way its produce, natural gas also different in term of its composition with biogas. As stated before, biogas is produce mainly from the decomposed of organic compound without the presence of oxygen. Usually, biogas has 50 – 65% of methane, 25 –50% of carbon dioxide, 0 – 1% of hydrogen sulfide and small amount of hydrogen (Thyo, Wenzel, 2007). The overall comparison between biogas and natural gas composition can be seen in Table 5:

Table 5: Comparison between Natural Gas and Biogas. Data from Eekelen, 2011

COMPOSITION	NATURAL GAS	BIOGAS
CH <sub>4</sub>	81%	55 – 70%
CO <sub>2</sub>	< 1%	30 – 45%
C <sub>2</sub> H <sub>6</sub>	2.85%	-
C <sub>3</sub> H <sub>8</sub>	3.41%	-
N <sub>2</sub>	1.35%	0 – 5%
O <sub>2</sub>	0.01%	0 – 6%
H <sub>2</sub> S	0 – 1 ppm	10 – 2000 ppm
OTHERS	Mercury	H <sub>2</sub> , NH <sub>3</sub> , Siloxane, Halogens
HUMIDITY	15 – 25%	70 – 100 %

As shown in Table 5, the concentration for CO<sub>2</sub> in biogas is higher than natural gas. This is one of the reasons why the biogas is chosen as a subject to study for this project. For the early prediction, the different composition between these two gases will exhibit different result on the dispersion model.

## 2.5 Biogas Behavior

Biogas will be transport in liquid form during the transportation. When leaking occurs, biogas in pipeline will be dispersed from high pressure pipeline into lower pressure atmosphere. Biogas is a floating gas which is different with the dense gas properties that tends to accumulate near to the ground level. The buoyancy effect of the biogas will dilute its concentration which makes the gas cloud less concentrated to the air. So, it is important to investigate the relation of biogas buoyancy with its dispersion behavior.

Transportation and storage of biogas will be more favorable in liquid form in order to save the area needed and makes the transportation process easier. There will be two phases of release when the pressurized liquid leaked because of the difference between higher pressures in the pipeline compare to the atmosphere. Aerosol will be produced when the liquid evaporates faster and takes energy from itself and surrounding to cool itself. If the mass of the leakage is large, the gas will accumulate and evaporate to produce a discharge gas that will act like a dense gas. The cooling of pressurized liquid will condense ambient humidity which then produces vapor cloud.

When biogas released into atmosphere, it can be dispersed by turbulence due to the fact that atmosphere is always in process of motion caused by eddies. According to Schulze, if there is a leak from pipeline, maximum concentrations downwind will occur in stable condition which means that the turbulence will be least with very minimum wind. On the other hand, in unstable atmosphere with windy condition, rapid dilution will occur at which elevated releases will bring worst case concentrations.

# CHAPTER 3

## METHODOLOGY

### 3.1 Research Methodology

#### 3.1.1 Computational Fluid Dynamics (CFD)

CFD is the state-of-the-art computer program for modeling fluid flow and heat transfer in complex geometries (Siddiqui and Jayanti, 2012). The CFD core solver has been validated for numerous industrial problems and in a large number of academic papers. As this project will relate to a lot of case studies like variation of wind speed and point of release, CFD is a good choice of tool to simulate the dispersion modeling for this purpose. According to Kunwar (2009), the elements of CFD are:

#### PRE-PROCESSOR

- To input the problem geometry, volume mesh generation, define the flow parameter and boundary requirement to the code.

#### FLOW SOLVER

- To solve the related equation of the flow subjects to the condition provided. 4 different methods that will be use is finite difference method (FDM), finite element method (FEM), finite volume method (FVM) and spectral method.

#### POST PROCESSOR

To deliver the data and show the result in graphical form. Make the user easy to read the format.

This simulation project will be based on 3-d Reynolds –averaged Navier Stokes equations. By using CFD-FLUENT, the dispersion of biogas from pipeline with the function of time can be simulated and the safe distance for toxicity of carbon dioxide can be determined.

### 3.1.2 Project Flow

The project flow is as shown in Figure 1:

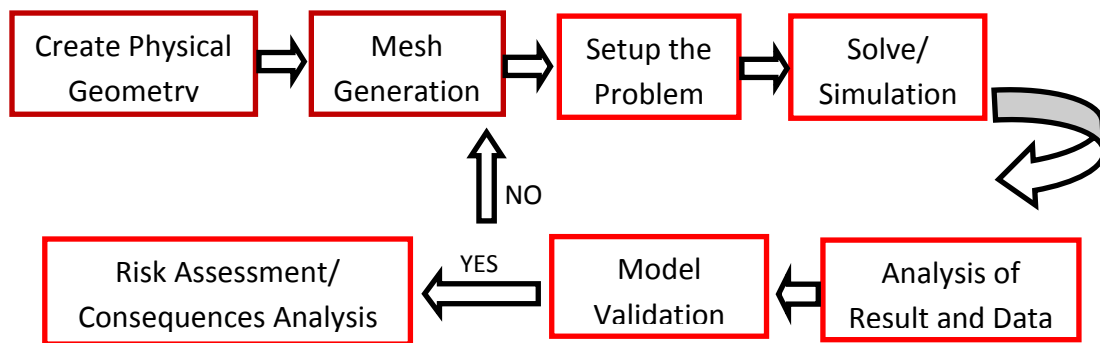


Figure 1: The Project Flow

The project flow can be described as below:

- Determine the composition of biogas and natural gas
- Create physical geometry as representative of environment area
- Generate mesh suitable with computational method and time frame of the project
- Setup the problem by input the environment condition like wind speed and obstacle.
- Solve the simulation.
- Analyze the data and the result obtain.
- Validate the model by comparing with the literature review model done by other researchers.
- Assessment of safe distance study by using the standard provide by NIOSH and other HSE regulations.
- Case study using PHAST.

## 3.2 Simulation: CFD ANSYS-Fluent

### 3.2.1 Physical Geometry

The simulation model will be developed by using Design Modeler provided by the CFD ANSYS-FLUENT. The geometry will be chosen based on the 2D XY plane for more easily computational time. The geometry will be an area of 10m wide and 5m high as a symbol of environment area. For the point of discharge, pipe leaking scenario is selected for this project and will happen at ground level which is on axis X of the plane. Generally, the pipe leaking size is influenced by lot of factors like mechanism, stress level and the material properties .However, 10mm leaking size will be chosen based on the IP Model Code (2005) that used as the reference. Figure 2 show the image of the physical geometry create for this project:

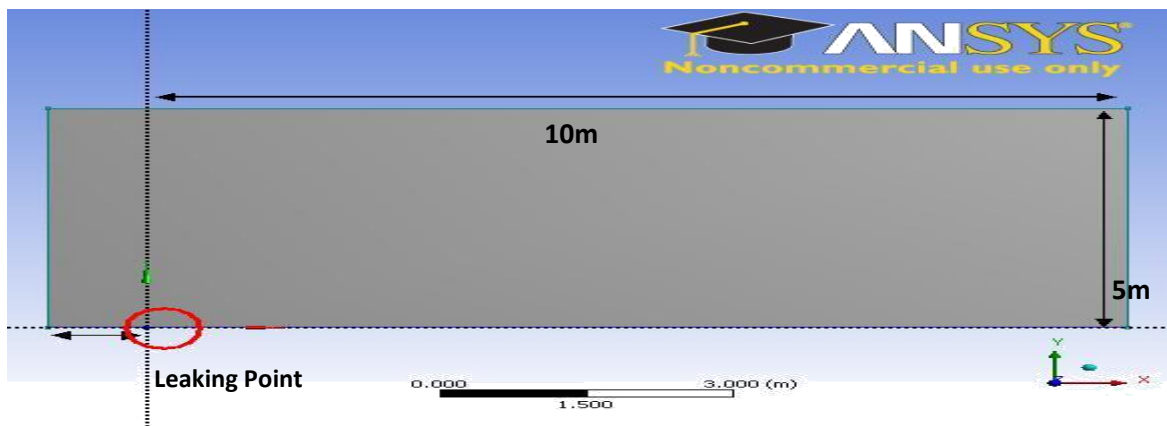


Figure 2: Physical Geometry

### 3.2.2 Meshing

The objective of meshing is to indicate and balance up the quality of the mesh and computational time. A good mesh will give better precision and accuracy on the result produces. In order to determined which one is the good mesh, several simulation will be done with a variation of meshing and compared it with theoretical result that produced by other researchers and standard. The poor meshing will produce low quality of grid that will cause inaccurate solutions and slow convergence (Tauseef, Rashtchian, and Abbasi, 2011).

Table 6: Mesh 1 Condition

Relevance center	Coarse
Smoothing	Low
Span angle center	Fine
Curvature Normal Angle	18 degree
Refinement	Off
Inflation	Off

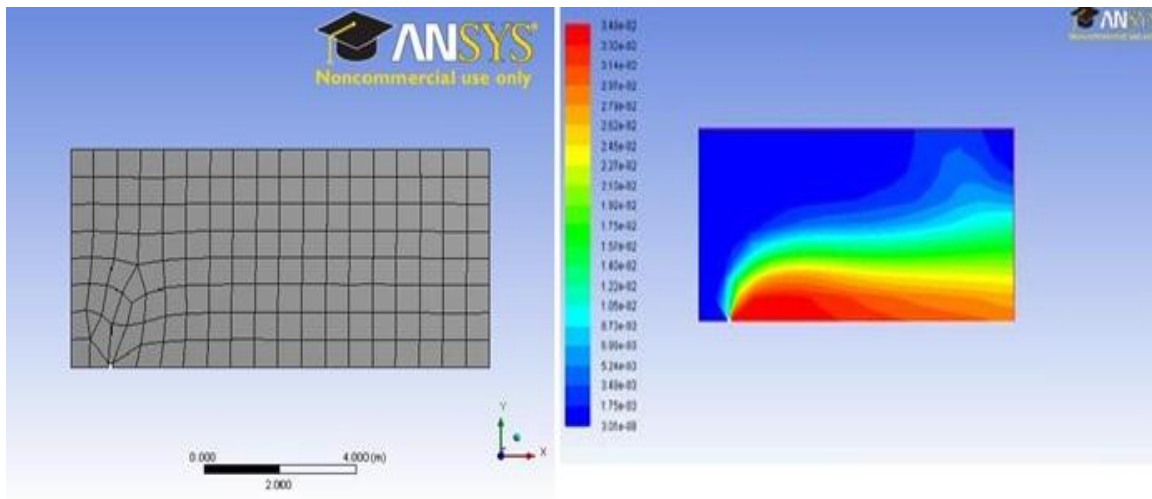


Figure 3: Mesh 1

For the Mesh 1, the mesh was constructed by using default mode as specified in Table 7. No specific changes had been made. The result in Figure 3 show the biogas release not diluted with the surrounding air when it flows upward. The biogas leaking is expected to be at high velocity as it is highly pressurized in the transmission pipeline. So, the mesh needs to be highly refined at the pipeline leaking area.

Table 7: Mesh 2 Condition

Relevance center	Fine
Smoothing	High
Span angle center	Fine
Curvature Normal Angle	10 degree
Refinement	On
Inflation	Program Controlled
Nodes	7094
Elements	7011
Minimum Mesh Metrics	0.53
Maximum Mesh Metrics	0.99
Average Mesh Metrics	0.99

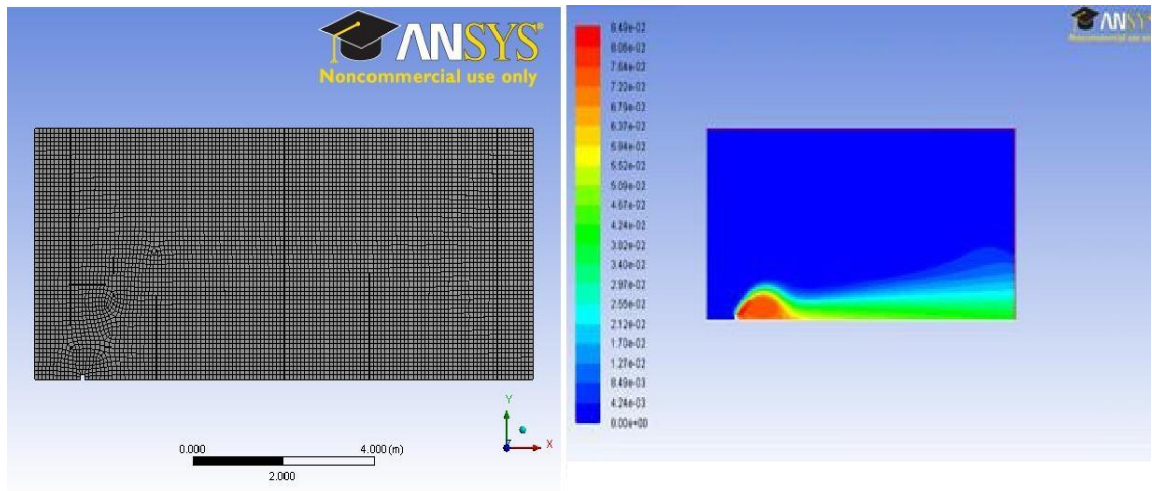


Figure 4: Mesh 2

After did some changes on the mesh condition as summarized in Table 8, the result shown for Mesh 2 in Figure 4 indicates the biogas concentration is more diluted when flows upward compare than Mesh 1. The latest result looks more reliable as the concentration of the biogas will decrease when flow upward because diluted with surrounding air



### 3.2.3 $k-\varepsilon$ Turbulence Model

The  $k-\varepsilon$  turbulence model is the most validated and most common model based on the Reynolds averaged Navier-Stokes equations for CFD simulation (Scargiali et al., 2011). The  $k-\varepsilon$  model transport equations offer two significant parameters, one for  $k$ , the turbulent kinetic energy, and the other one is for  $\varepsilon$ , the turbulence dissipation rate. The  $k-\varepsilon$  equation assumes that the turbulence viscosity is the function correlated with the turbulence kinetic energy and dissipation. The  $k-\varepsilon$  model provides excellent performance for flows that involve rotation, separation and recirculation. This model will be suit for this project because it provides the gas dispersion that related to release to atmosphere.

### 3.2.4 Boundary Condition

The problem setup will be done by input the dispersion condition that will be simulated. The boundary condition that will be used is as below:

Table 8: Boundary Condition

<b>BOUNDARY</b>	<b>TYPES</b>	<b>EXAMPLE</b>
Wind inlet boundary	Velocity inlet	Mass flow, temperature and turbulence value.
Wind outlet boundary	Pressure inlet	Constant pressure outlet surface
Gas inlet boundary	Mass flow inlet	Mass flow, temperature and turbulence value for inlet gas flux
Top boundary	Pressure outlet	Constant pressure outlet surface
Ground Boundary, Building wall	wall	No slip condition, roughness, fixed temperature

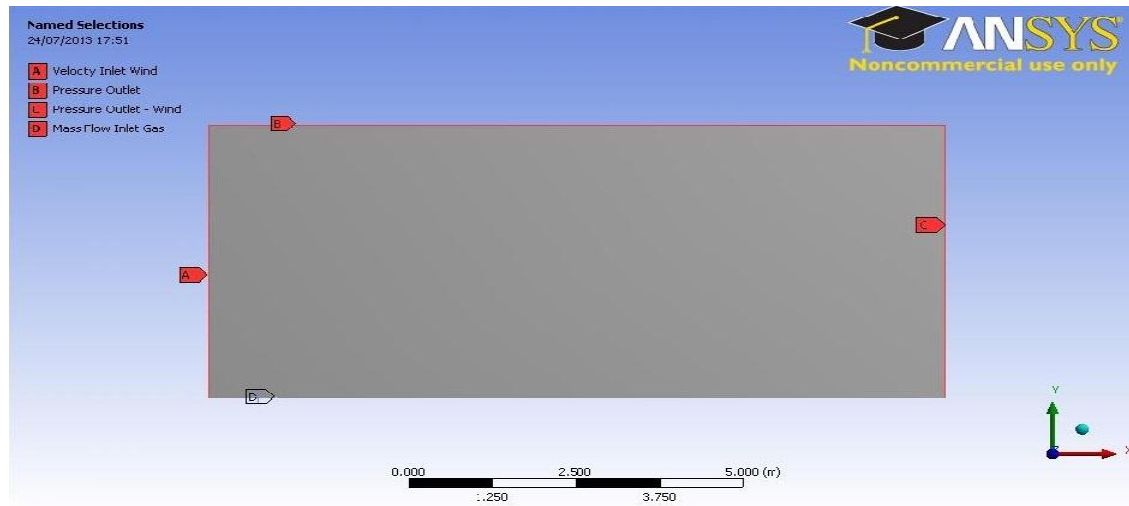


Figure 5: Boundary Condition

### 3.2.5 Model Validation

In order to make the simulation model look reliable, the output for this project will undergo validation process by comparing it with other establish standard provided. One of the standards is by comparing the result produce from this simulation project with the experimental data obtain from the Kit Fox Experiment. Kit Fox Experiment is design to study on the effect of the ground roughness of industrial process plants and meteorological condition on the formation and extend of the CO<sub>2</sub> gas cloud (Papanikolaou, Heitsch and Baraldi, 2011). Even though the setup for Kit Fox Experimental study is totally different with this project, but the CO<sub>2</sub> gas concentration release from the experiment is certified and accurate to be used in order to assess the accuracy for this project.

### 3.3 Model Dispersion Study

#### 3.3.1 Type of gas

Two type of gas that will be uses is biogas and natural gas. Initial assumption will be made by state that the phase of the gas will be in gas phase rather than multiphase. The assumption is done in order to makes the simulation simpler. For biogas, it is made up of 70% of methane and 30% of carbon dioxide gas. The CO<sub>2</sub> content in the biogas is higher than natural gas. CO<sub>2</sub> content in natural gas is less than 1% and this is one of the reasons why biogas is chosen as a subject for this project.

#### 3.3.2 Wind speed

In term of wind speed on the gas dispersion, the wind speed will flow from left to the right and parallel to the X-axis. The wind speed at surrounding atmosphere will be affected by the intensity of the atmospheric turbulence. Logically, with the higher atmospheric turbulence, it will dilute the concentration of the biogas and reduce the hazard risk probability. The standard used to identify the atmospheric stability is by using the Pasquill atmospheric stability classes which classified the amount of atmospheric turbulence into six classes as shown in Figure 2.

STABILITY CLASS	DEFINITION	STABILITY CLASS	DEFINITION
A	Very unstable	D	Neutral
B	Unstable	E	Slightly stable
C	Slightly Unstable	F	Stable

Figure 6: Pasquill-Gifford stability categories.

#### 3.3.3 Obstacles

Another important factor for this simulation is the presence of obstacle. The leaking point for this modeling will be at origin which is  $XY = (0, 0)$ . Obstacle can give turbulence effect on the interaction between the gas release and atmosphere. For this project, the obstacle will be placed at the distance of 3m and 5m from the point of release (origin) with the size of 1m x 1m.

### 3.4 Key Milestone

NO	ACTION ITEM	REMARKS
1	Regular Meeting with Supervisor	Ongoing
2	FYP Briefing	Week 1
3	Journal Reading and Research	Week 3 - 5
4	Submission of Extended Proposal	Week 6
5	Mid-Semester Break	Week 7
6	Proposal Defense	Week 7 – 8
7	Submission of Interim Draft Report	Week 13
8	Submission of Interim report	Week 14

Figure 7: Key Milestone of FYP 1

NO	ACTION ITEM	REMARKS
1	Continue of the project	Ongoing
2	CFD Modeling	Week 1
3	Submission of Progress Report	Week 7
4	Validation Using PHAST	Week 8
5	Oral Presentation	Week 12
6	Submission of Technical Paper	Week 13
7	Submission of Dissertation	Week 13
8	Submission of Hard Bound Project Dissertation	Week 14

Figure 8: Key Milestone of FYP 2

### 3.5 Gantt Chart

DETAIL/ WEEK	1	2	3	4	5	6	7		8	9	10	11	12	13	14	
Research on: Project Background, Objectives, Scope of Study								S e m e s t e r B r e a k								
Review on Biogas process, Hazard, and composition																
Advance learning on CO2 Toxicity and properties																
Submission of Extended Proposal																
Learn Simulation Software: CFD, FLUENT, PHAST																
Proposal Defense Presentation																
Continue on Simulation Project																
Submission of Interim Draft Report																
Submission of Interim Report																

Figure 9: Gantt-Chart for FYP 1

DETAIL/WEEK	1	2	3	4	5	6	7		8	9	10	11	12	13	14	
CFD Simulation Work - Identify and creating the physical geometry - Generating the mesh - Setup the problem - Solve the simulation - Analyse the result	█	█	█	█				M I D - S E M  B R E A K								
Submission of Progress Report							█									
PAST Software Advance Learning					█	█	█									
Validate the Project Using PHAST							█			█						
Result Analysis and Data Gathering										█	█					
Oral Presentation														█		
Submission of Technical Paper															█	
Submission of Dissertation															█	
Submission oh Hard Bound																█

Figure 10: Gantt-Chart for FYP 2

## CHAPTER 4

### RESULT AND ANALYSIS

#### 4.1 Effect on Wind Speed.

To study on the effect of the wind speed variation towards the CO<sub>2</sub> gas dispersion behavior, several simulations were done by varying the value of the wind speed. The mass inlet for the biogas concentration is set to 1.5 kg/s for each case. The simulation results were display as shown in Figure 11, 12 13 and 14 below:

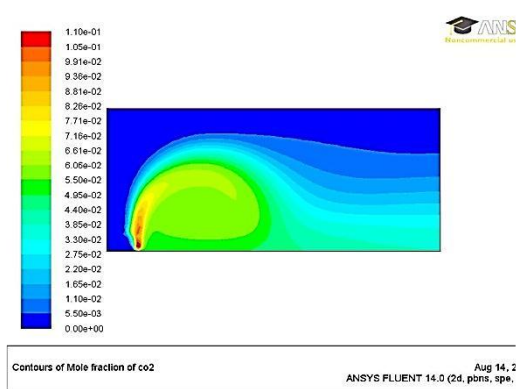


Figure 21: Wind Speed 3 m/s

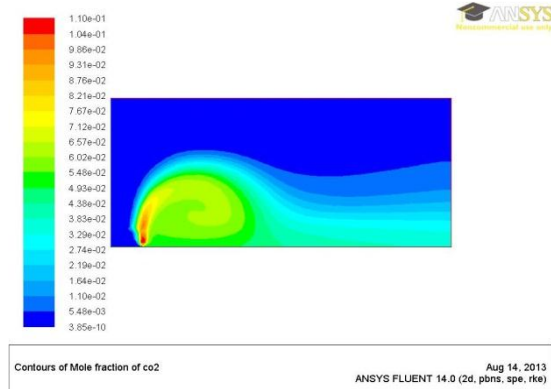


Figure 12: Wind Speed 4 m/s

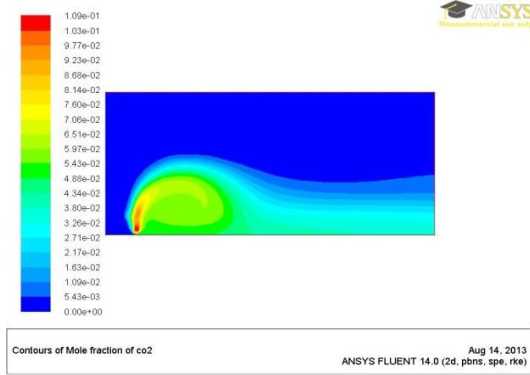


Figure 33: Wind Speed 5 m/s

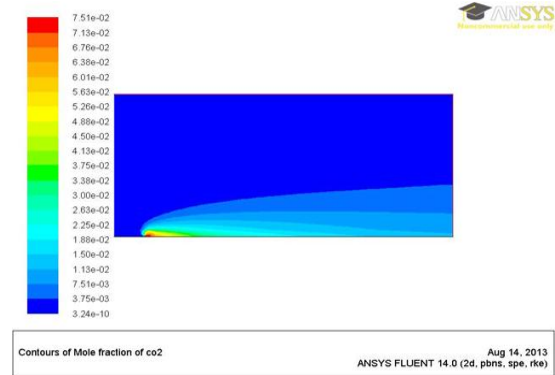


Figure 44: Wind Speed 6 m/s

Based on Figure 11, the simulation was done with wind speed condition of 3 m/s. The wind condition is slow and stable hence caused no much disturbance to the CO<sub>2</sub> gas dispersion during its released. This condition explained why at this wind speed condition, the CO<sub>2</sub> gas cloud is bigger than other wind speed condition.

Unlike Figure 14, the wind speed condition of 6 m/s starts to show the effect of high turbulence to the CO<sub>2</sub> gas concentration. The wind speed condition caused the CO<sub>2</sub> gas dispersion moves downstream to the right. During this condition, no formation of CO<sub>2</sub> gas cloud appears. However, the CO<sub>2</sub> gas concentration also gets diluted as it moves to the right.

In order to find the safe distance during the biogas incident leakage, the data was plot based on the CO<sub>2</sub> gas concentration from the biogas process. The graphs of each simulation for CO<sub>2</sub> gas concentration versus distance are shown in Appendix 1, 2, 3 and 4. From the data, the highest CO<sub>2</sub> gas concentration releases from leaking point for each condition and CO<sub>2</sub> gas concentration after 2 m distance from leaking point are extracted and tabulated as in Table 9 below:

Table 9: CO<sub>2</sub> gas concentration based on Wind Speed

WIND SPEED, m/s	CO <sub>2</sub> CONCENTRATION AT DISCHARGE POINT, ppm	CO <sub>2</sub> CONCENTRATION AFTER 2 m, ppm
3 m/s	110, 000	66, 800
4 m/s	110, 000	54, 800
5 m/s	109, 000	54, 300
6 m/s	75, 100	48, 800



From table 9, the highest CO<sub>2</sub> gas concentration at leaking point is 110, 000 ppm which is during the wind condition of 3 m/s and 4 m/s. However, the concentrations of CO<sub>2</sub> gas concentration reduce for all cases of wind condition. The highest CO<sub>2</sub> gas concentration after 2 m distance from release point is when the wind condition at 3 m/s. The concentration of 66, 800 ppm of CO<sub>2</sub> gas concentration at this concentration is the only concentration that will give hazard compare than other condition. Based on Table 3, the minimum concentration of CO<sub>2</sub> gas is 63, 000 ppm for every inhalation exposure time. Hence, the data for wind condition of 3 m/s is analyzed in order to find the safe distance for this condition and the result is tabulated in Table 10.

Table 10: CO<sub>2</sub> gas concentration based on distance for 3 m/s wind condition

Distance, m	3 m/s
	CO2 Concentration, ppm
0	110,000
0.5	99,700
1	82,700
1.5	77,800
2	71,800
2.5	66,800
3	49,800
3.5	44,800
4	38,800
4.5	33,800
5	27,500
5.5	22,000
6	16,500
6.5	11,000
7	5,500
7.5	3,700
8	2,900
8.5	1,080
9	700
9.5	600
10	500

Based on Table 10, the safe distance is after 3 m from the leaking source as the CO<sub>2</sub> gas concentration reduce to 49, 800 ppm and no more longer possess any threat to human beings. The comparison in term of CO<sub>2</sub> gas concentration and the distance for each wind condition can be seen in Figure 15 below.

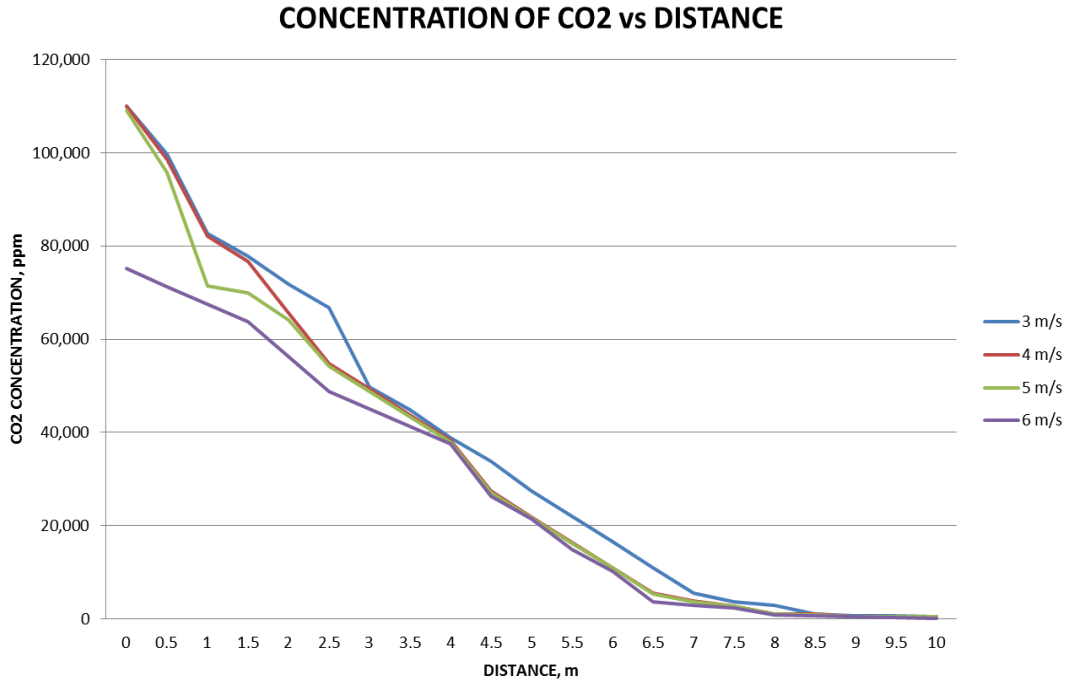


Figure 15: Graph of CO<sub>2</sub> gas concentration vs. Distance (Wind Speed)

The trending for all graph shows that the all concentration of CO<sub>2</sub> gas in biogas process is decreasing over the 10 m distance. The concentration becomes diluted because of the mixing between CO<sub>2</sub> gases with the surrounding air.

#### 4.2 Effect on Discharge Rate.

According to the IP Model Code (2005) that developed specifically for flammability test on biogas simulation study, the release rate for biogas is 0.1 kg/s. However, because of limited data on CO<sub>2</sub> gas toxicity study from biogas process, the release rate for biogas dispersion is vary from 0.06 kg/s up to 2 kg/s. The objective here is to study on the effect of release rate with the behavior of biogas dispersion. Besides, the value for the CO<sub>2</sub> gas concentration also recorded over the distance. For the wind speed, 2 m/s is set based on the data provided by the IP Model Code (2005). The simulation results are display as shown in Figure 16, 17, 18 and 19 below:

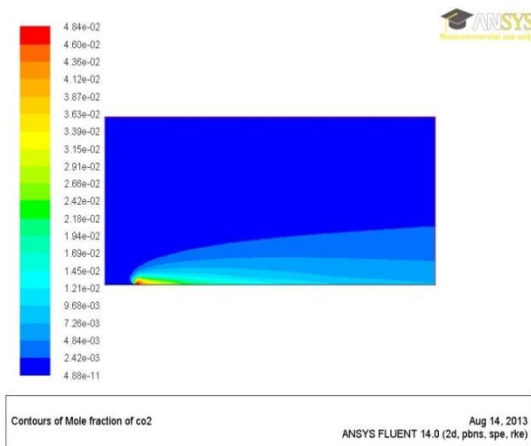


Figure 16: Discharge Rate 0.06 kg/s

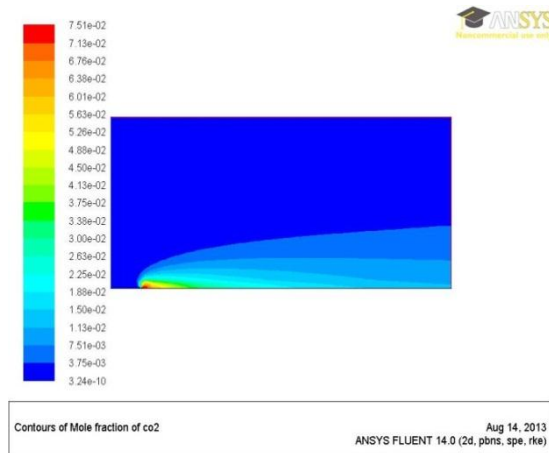


Figure 57: Discharge Rate 0.1 kg/s

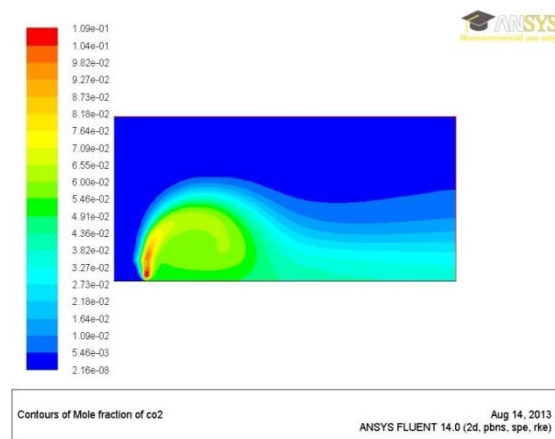


Figure 18: Discharge Rate 0.7 kg/s

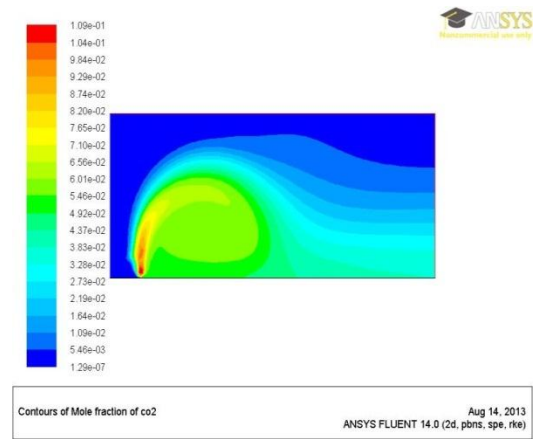


Figure 19: Discharge Rate 2 kg/s

According to Figure 16 and 17, the simulation result looks same for both discharge rates of 0.06 kg/s and 0.1 kg/s respectively. From here, the simulation indicates that the low discharge rate of the biogas in stable wind condition of 2 m/s will be result in dispersion of CO<sub>2</sub> gas that followed the downwind direction.

However, for higher discharge rate, it will show another result. Like Figure 18 and 19, the discharge rate is 0.7 kg/s and 2 kg/s respectively. Both of the result shows the large vapor cloud of CO<sub>2</sub> gas form during simulation. For discharge rate of 2 kg/s, the vapor cloud of CO<sub>2</sub> gas is much larger than 0.7 kg/s discharge rate.

Despite the size of the CO<sub>2</sub> gas cloud for each condition, the CO<sub>2</sub> gas concentration release for all cases is following the same trend which is reduce from left to right. The safe distance for each case is identified by plotting the graph of CO<sub>2</sub> gas concentration within 10 m distance. The raw data from the graph are shown in Appendix 5, 6, 7 and 8. However, the analyzed data from the graph that shows the highest CO<sub>2</sub> gas concentration at leaking point and also the CO<sub>2</sub> gas concentration after 2 m distance can be seen in Table 11 below:

Table 11: CO<sub>2</sub> gas concentration based on Discharge Rate

DISCHARGE RATE, kg/s	CO <sub>2</sub> CONCENTRATION AT DISCHARGE POINT, ppm	CO <sub>2</sub> CONCENTRATION AFTER 2 m, ppm
0.06	48, 400	24, 200
0.1	75, 100	33, 800
0.7	109, 000	70, 900
2	110, 000	82, 900

Based on Table 11, the highest CO<sub>2</sub> gas concentration at discharge point is 110, 000 ppm with the discharge rate of 2 kg/s. However, the concentration reduces to 82, 900 ppm after 2 m distance from leaking source. Based on standard used (Table 3), the minimum safe CO<sub>2</sub> gas concentration is 63, 000 ppm. By comparing the standard with the result from Table 9, after 2 m distance from release point discharge rate of 0.7 kg/s and 2 kg/s will give significance hazard based on its CO<sub>2</sub> gas concentration which is 70, 900 ppm and 82, 900 ppm respectively. So, in order to find the safe distance for this condition, the data is tabulated based on the CO<sub>2</sub> gas concentration and the distance as shown in Table 12. From the result, the safe distance can be known by looking at the CO<sub>2</sub> gas concentration that will reduce away from the leaking point.

Table 12: CO<sub>2</sub> gas concentration based on Discharge Rate of 0.7 kg/s and 2 kg/s

	0.7 kg/s	2 kg/s
Distance, m	Concentration of CO <sub>2</sub> , ppm	Concentration of CO <sub>2</sub> , ppm
0	109,000	110,000
0.5	98,200	104,000
1	92,700	98,400
1.5	87,300	92,900
2	76,400	87,400
2.5	70,900	82,900
3	65,500	76,500
3.5	60,000	71,000
4	54,600	65,600
4.5	49,100	60,100
5	43,600	54,600
5.5	38,200	49,200
6	32,700	43,700
6.5	27,300	38,300
7	21,800	32,800
7.5	16,400	27,300
8	10,900	21,900
8.5	5,460	16,400
9	4,167	10,900
9.5	2,255	5,460
10	1,099	3,290

For 0.7 kg/s discharge rate, the safe distance is after 3.5 m distance from leaking point. The CO<sub>2</sub> gas concentration drop to 60, 000 ppm and smaller than standard value which is 63, 000 ppm. The distance is much shorter if compare with the discharge rate condition of 2 kg/s. The safe distance for 2 kg/s discharge rate is after 4.5 m distance from leaking point. The CO<sub>2</sub> gas concentration drop to 60, 100 ppm which can be consider as standard safe CO<sub>2</sub> gas concentration.

The trend for CO<sub>2</sub> gas concentration within 10 m distance from release point for each discharge rate can be observe based on graph in Figure 20.

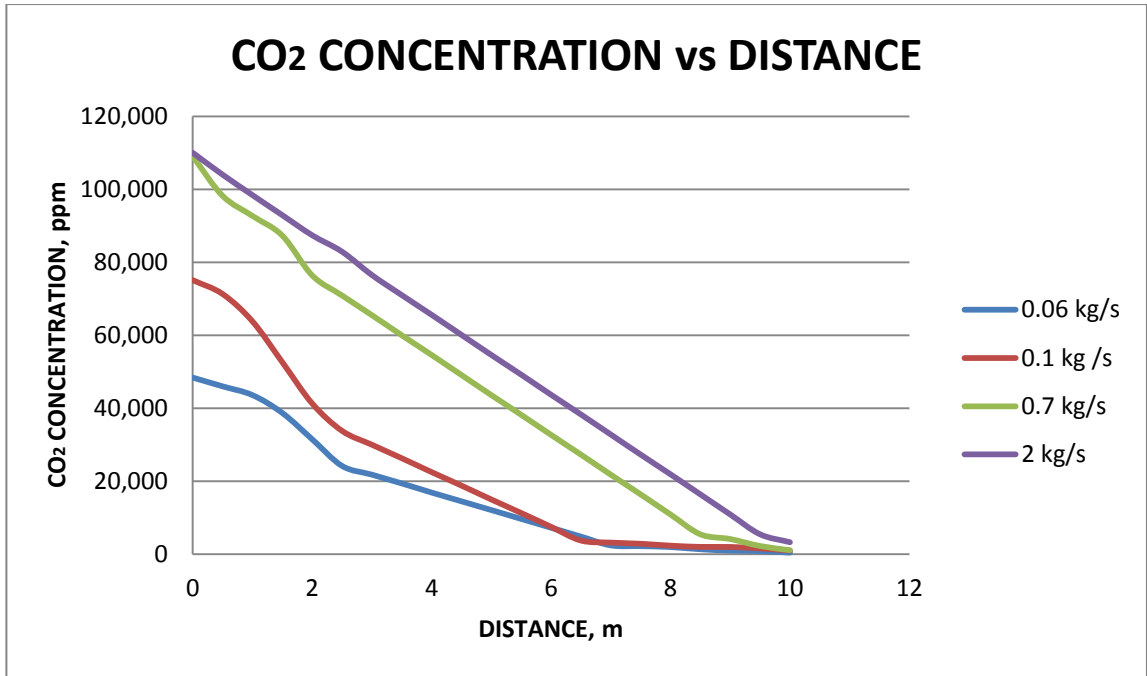


Figure 20: Graph of CO<sub>2</sub> gas concentration vs. distance (Discharge Rate)

## **CHAPTER 5**

### **CONCLUSION AND RECOMMENDATION**

#### **5.1 Recommendation**

As for the result, more case studies will be varying in order to collect as much data for this study. The point of biogas discharge from certain place will change from ground level to 1 meter height.

Other than that, there will be a presence of obstacle place inside the geometry area to investigate the behavior of the gas dispersed when hit the specific obstacle. Besides, the time release for the biogas will also different from one case to another case.

Besides, this simulation will best visualized in 3-D in order to locate the precise safe distance during biogas leakage incident. 2-D view only give one side view without asses what happen to the biogas dispersion from another view.

#### **5.2 Conclusion.**

As a conclusion, the result shown above indicates the behavior of CO<sub>2</sub> gas in biogas process during the discharge. The higher wind speed will cause the great turbulence surrounding hence will dilute the concentration of CO<sub>2</sub> gas. Besides, the higher discharge rate of biogas will give higher CO<sub>2</sub> gas concentration release. The vapor cloud formation of CO<sub>2</sub> gas also affected by the discharge rate of biogas.

## REFERENCE:

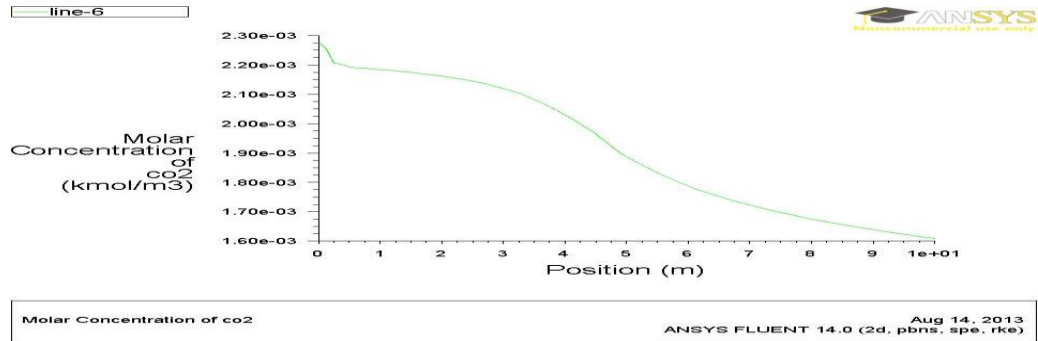
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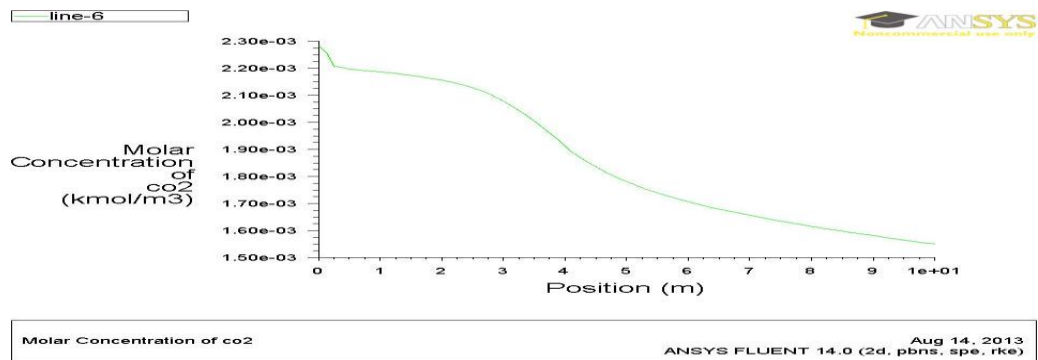
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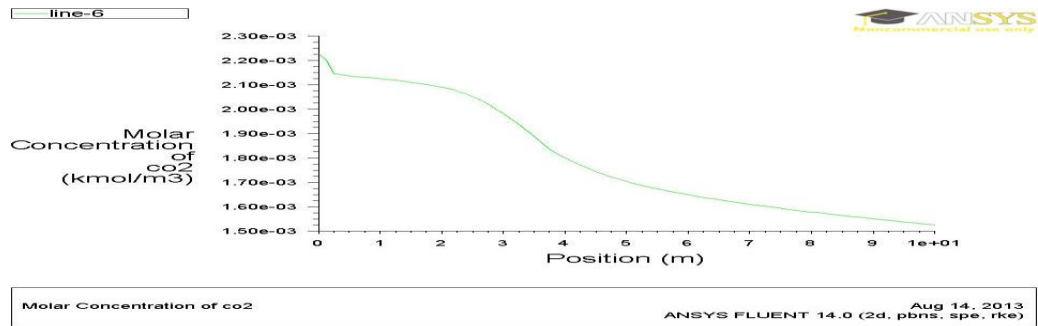
## APPENDIX:



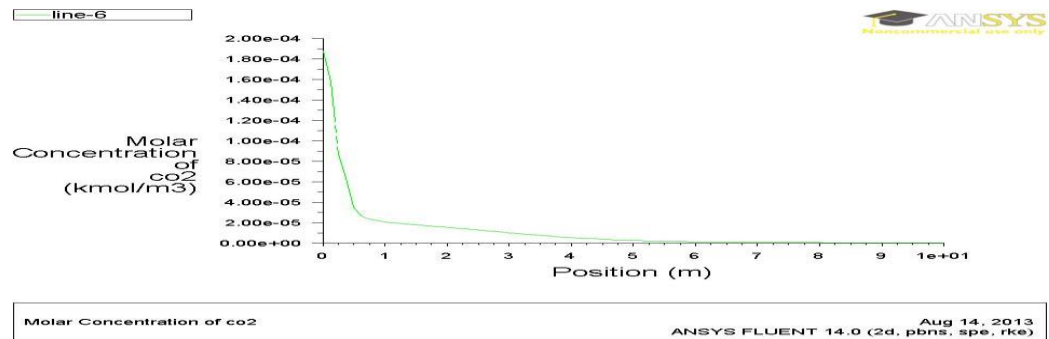
APPENDIX 1: Graph of CO<sub>2</sub> gas concentration versus distance (3 m/s)



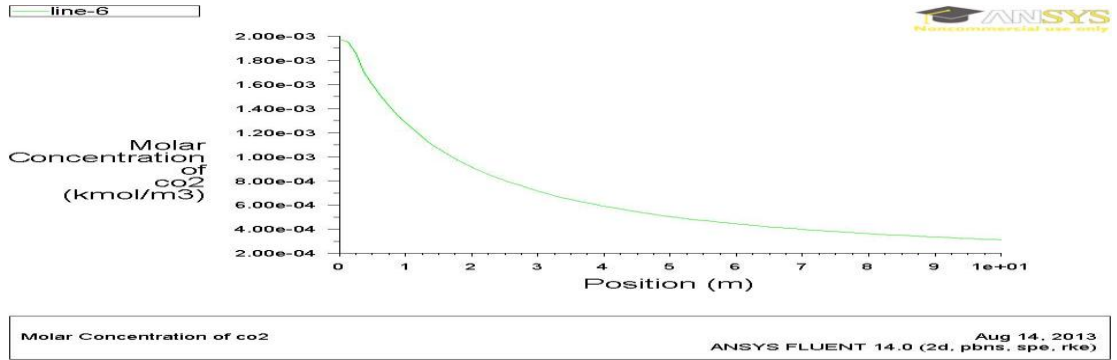
APPENDIX 2: Graph of CO<sub>2</sub> gas concentration versus distance (4m/s)



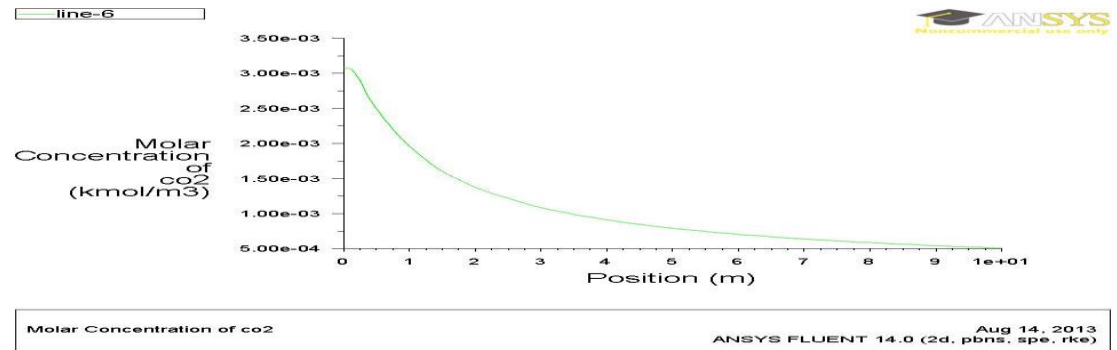
APPENDIX 3: Graph of CO<sub>2</sub> gas concentration versus distance (5m/s)



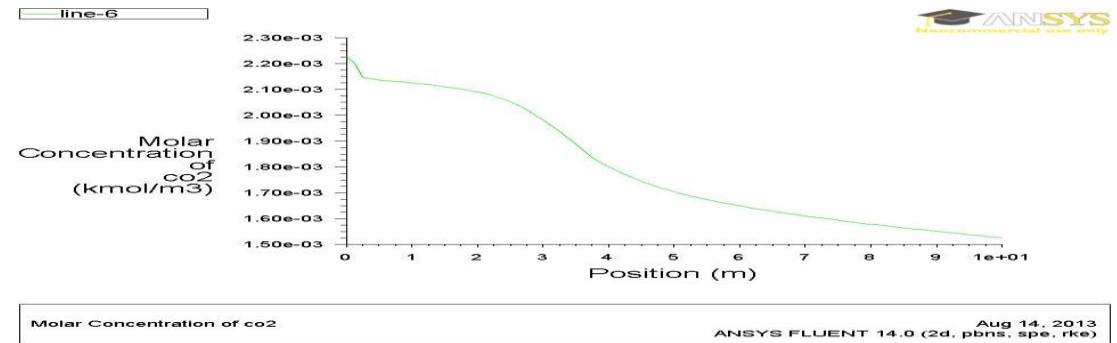
APPENDIX 4: Graph of CO<sub>2</sub> gas concentration versus distance (6m/s)



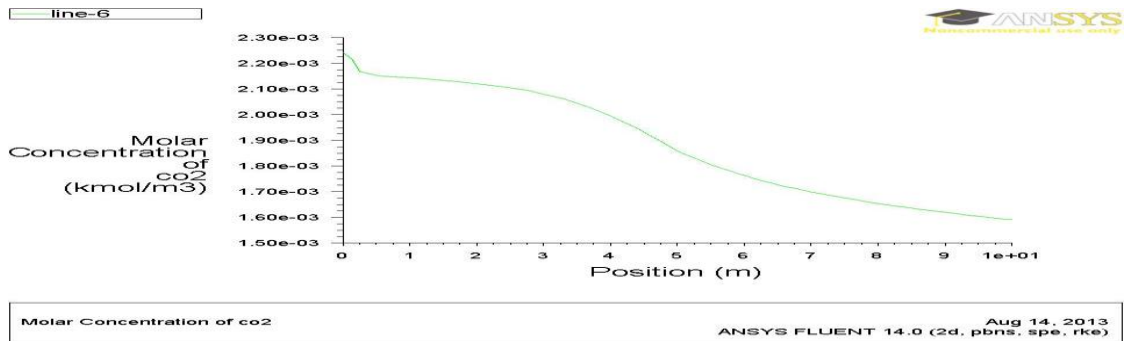
**APPENDIX 5:** Graph of CO<sub>2</sub> gas concentration versus distance (0.06 kg/s)



**APPENDIX 6:** Graph of CO<sub>2</sub> gas concentration versus distance (0.1 kg/s)



**APPENDIX 7:** Graph of CO<sub>2</sub> gas concentration versus distance (0.7 kg/s)



**APPENDIX 8:** Graph of CO<sub>2</sub> gas concentration versus distance (2 kg/s)