INVESTIGATION ON BIOGAS DISPERSION USING COMPUTATIONAL FLUID DYNAMICS MODELING

By

LAURA TIONG SIEW ZIN

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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A project dissertation submitted to the
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Approved by,

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TRONOH, PERAK
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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LAURA TIONG SIEW ZIN

ABSTRACT

Biogas technology is developing rapidly in the recent year due to increment of dependency in human on the renewable energy. Process safety of biogas plant is one of the current issues which is very critical for the process operations. Several cases of fire and explosion related to biofuel plant have alarmed the industries on the potential hazard from current running biogas plant. Limited failure data is available for consequence risk analysis to understand scenario of biogas dispersion. Thus, a study is carried out on the dispersion model of biogas to show the behavior of biogas from pressurized release into the environment by using Computational Fluid Dynamics (CFD) modeling. CFD is a branch of fluid mechanics that uses numerical method and algorithm to solve the problem which involves fluid flow. The code used is CFD-FLUENT by ANSYS Company. CFD dispersion model developed is validated against IP Model Code and PHAST which shows close agreement with deviation at 18% and is acceptable. Gas dispersion study is based on influence of wind speed and the presence of obstacle. Lower wind speed will pose higher risk of fire and explosion due to stable atmospheric turbulence. Presence of obstacle will cause the gas to be easily trapped and create flammable region. Biogas shows shorter hazardous distance as compared to that of methane gas. It can be explained as the lower composition of methane in biogas. Thus, biogas is less flammable than pure methane gas.

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This Final Year Project on Biogas dispersion would not be possible without the support of many individuals and organizations. First and foremost, I would like to acknowledge and extend my gratitude especially to my supervisor, Dr Risza binti Rusli for her abundant and invaluable assistance, encouragement and support all the time. Her guidance enlightens and inspires me to have constant great enthusiasm in my work. My thanks and appreciation also goes to Miss Diana and Miss Azurah for their guidance and valuable advices on the modeling problems that I met in the project. Last but not least, I would like to take this opportunity to thanks my family and friends for their support and encouragement throughout my project.

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CHAPTER 1: PROJECT BACKGROUND

1.1 Introduction

With the development of countries following by economies and population increment, human has becoming more and more dependent on the energy resources. “In the *IEO2011* Reference case, which does not incorporate prospective legislation or policies that might affect energy markets, world marketed energy consumption grows by 53 percent from 2008 to 2035.” (International Energy Outlook 2011). Primarily, the focus is put non-renewable resources like crude oil, natural gas, coal and the others. The consumption rate of non-renewable energy is increasing year by year. According to the data from Escapers (2010), the total world oil reserve by the date of 1st Jan 2010 was 1,175,686,472,626 barrels. It is estimated that the date of exhaustion will be in year 2047 with world usage per second of 986 barrels. Non-renewable energy is infinite and could not be replaced in a short time. Thus, research direction is pointed toward the finding of energy from renewable resources in order to meet the ever increasing need for power.

Recently, the renewable energy industry is being developed due to the awareness of environmental issue. It has become an important energy resource for the people. It is believed that when more and more technologies on renewable energy emerge, world dependant on the non-renewable energy will start to shift to renewable energy like hydroelectricity, biomass energy, wind power and solar power. The share of renewable power in global energy consumption reached 1.3% in 2010 as compared to only 0.6% in 2000 (Renewable power, retrieved 2012).

Biofuels industry is one of the renewable energy plants which have drastic rises in the recent year. Biofuel is fuel or energy source which is derived from biomass or biowaste. Biofuel production can be in the form of solid, liquid or gas. Some of the commonly produced biofuels are biogas, bioethanol and biodiesel. Statistics from BP Global as shown in Figure 1.1 shows that the world biofuels production grew by 13.8% in 2010 and it accounted for 0.5% of global primary energy consumption. Referring to

Figure 1.2, production of biofuels is increasing over recent year with more consumption from various parties and this trend is expected to continue with years.

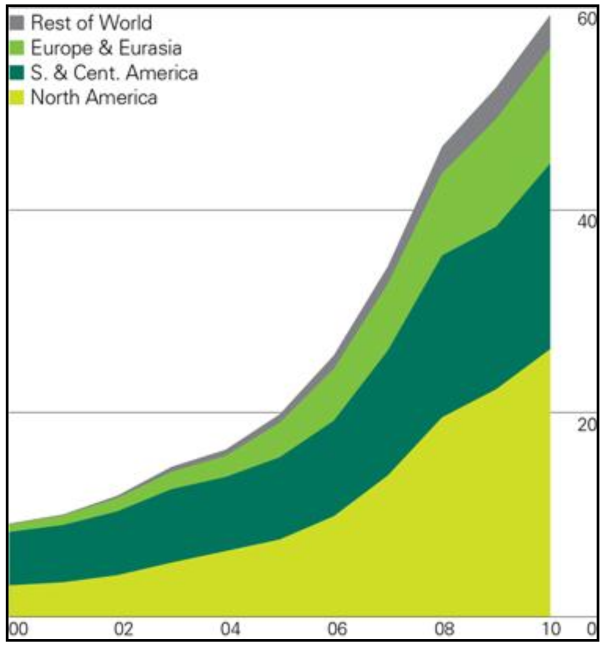

Figure 1.1: World Biofuels Production (Million tones oil equivalent versus year).

Source from BP Global.

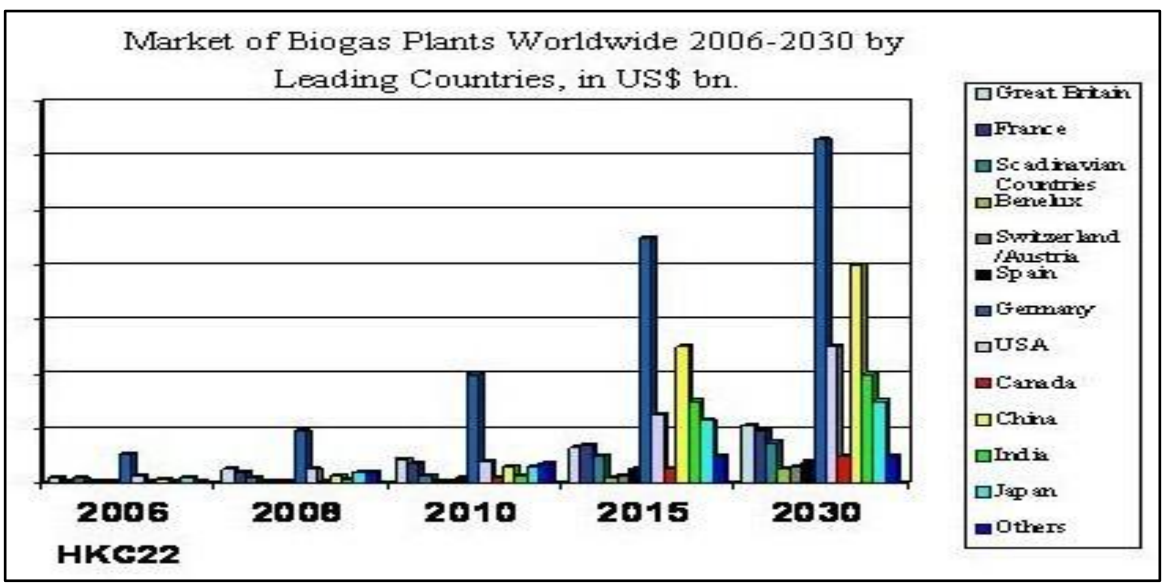

Figure 1.2: Market of Biogas Plants from year 2006-2030 in US bn. (Helmut Kaiser Consultancy, 2012)

Biomethane is a type of biogas which is produced from anaerobic digestion, the breakdown of organic matter in the absence of oxygen. Biomethane consists of 95-97% of methane. It is renewable and sustainable type of energy. Biomethane is upgraded from biogas and it can be injected into natural gas grid as transport fuel. Biomethane forms explosive mixture in air. It has high risk of ignition and explosion and the flammability range is 5% to 15% concentration (Airliquide, 2009).

The increasing in the plant capacity and complexity of biogas plants will lead to larger inventory of hazardous chemicals that can result in higher risk in the plant and this raised the awareness of operators on the process safety during the production. According to Saraf (2009), within the period of 3 years (2006-2009), there were 8 fires and 6 explosions in biodiesel facilities in U.S. which means there were average 5 incidents per year. "Based on the statistics, the biodiesel industry in the US is experiencing and accident every two-and-a-half months, i.e. approximately 10 weeks" (Saraf, 2009). This shows that many plants operators are not aware of the risk and process hazard associated with the production of biofuel.

Process safety of the operation in industries is emphasized since the deadly incident of Bhopal in 1984 for sustainability of the industry. The main idea is to balance up between optimal performance of the process operations and the process safety in order to prevent the recurrence of similar chemical incidents. Hazards and risk management in biogas industries is still very lacking as compared to other industries. Challenges like engineering unknown, limited failure rate data which is reliable, lacking of stringent safety rules and regulations, as well as the entry of unconventional operators who have minimal operator experience in biogas industries.

In this project, biogas which is made up of mainly methane and carbon dioxide is chosen to be studied on its process safety. The understanding of biogas dispersion phenomena and its fire or explosion characteristic is of utmost importance for the development of safety measures in order to prevent any potential accident.

1.2 Problem Statement:

Although every party is putting effort in improvement of process safety, accidents are still occurring at a rate which could not be ignored. This could be due to the rapid increasing complexity of the plant at which the research of process safety could not follow up. To tackle the problem of increasing complexity of process operations, high quality scientific research is needed to understand the reaction kinetics, properties of chemicals, consequences by way of modeling and renewed training of employees (Qi et.al., 2012).

In 2003, there are several explosions occurred in Canadian swine farms. The main reason to cause these explosions is due to the explosion of methane in biogas (Choinière, 2004). Another similar case is from Buncefield incident during December 2005. The overflowing of unleaded petrol leaded to dispersion of the vapour cloud in the atmosphere where the vapour cloud was then ignited producing severe explosion and fire (Gant & Atkinson, 2011). According to the authorities, the investigation on this incident adopted Computational Fluid Dynamic (CFD) tools to study the dispersion of the flammable vapour from the overfilling of the storage tank. Consequence modeling using CFD is adopted as it is capable of well describing fluid physics and allowing for the representation of complex geometry and its effects on vapor dispersion (Qi et. Al., 2012).

The various cases of explosion in others industries has alarmed the industries on the potential hazard from the current running biogas industry. However, there are very limited failure data available that could be used for the risk analysis to understand the process of biogas dispersion. The consequence modeling of accidental release of biogas is definitely necessary in order to determine the potential hazard affected area to prepare for the emergency response programme. Besides, consequence modeling of the pipeline leaking could also provide more proactive measures to improve the pipeline or plant design in order to make it inherently safer. The dispersion modeling could provide better insight on the possibility of various scenarios to happen due to high pressure gas leaking.

For consequence modeling of biogas dispersion, CFD could be adopted for the studies. But, the current existing biogas dispersion consequence model is insufficient for the effective examine of dispersion consequence. Thus, CFD is adopted in this study to examine the consequence model of biogas dispersion.

1.3 Objectives:

To study on the consequence model of biogas dispersion, this project is carried out in order to achieve the following objectives:

I. To study on dispersion of biogas from pressurized release by using Computational Fluid Dynamics (CFD) software.
II. To assess on hazard distance from methane and biogas release.

1.4 Scope of Study:

This project is mainly focusing on developing a 2D dispersion model of biogas leaking using CFD-FLUENT modeling. The model will be validated prior to the study of gas dispersion. The validated model will be further used to study on the potential hazard area under the effect of wind speed as well as the presence of obstacles.

As biogas is a developing new technology, it is important to study on the composition of biogas as compared to pure methane due to the similarities on their physical and chemical properties. In addition, biogas gas composition should be compared between several sources to ensure its validity.

The complexity of a biogas plant requires certain reasonable period of time to assess the hazards posed by every equipment. In order to ensure that the project can be done in the designated time, pipeline leaking is chosen to be studied on. The pipeline leaking scenario will be treated as a release of gas through a small hole. From Figure 1.3, pipeline accidents encountered for 25% of plant accidents which is the leading factor of industries accidents. Furthermore, Figure 1.4 shows the high number of pipeline fatalities throughout 10 years from 1992 to 2011 which make it significant to study on pipeline leaking.

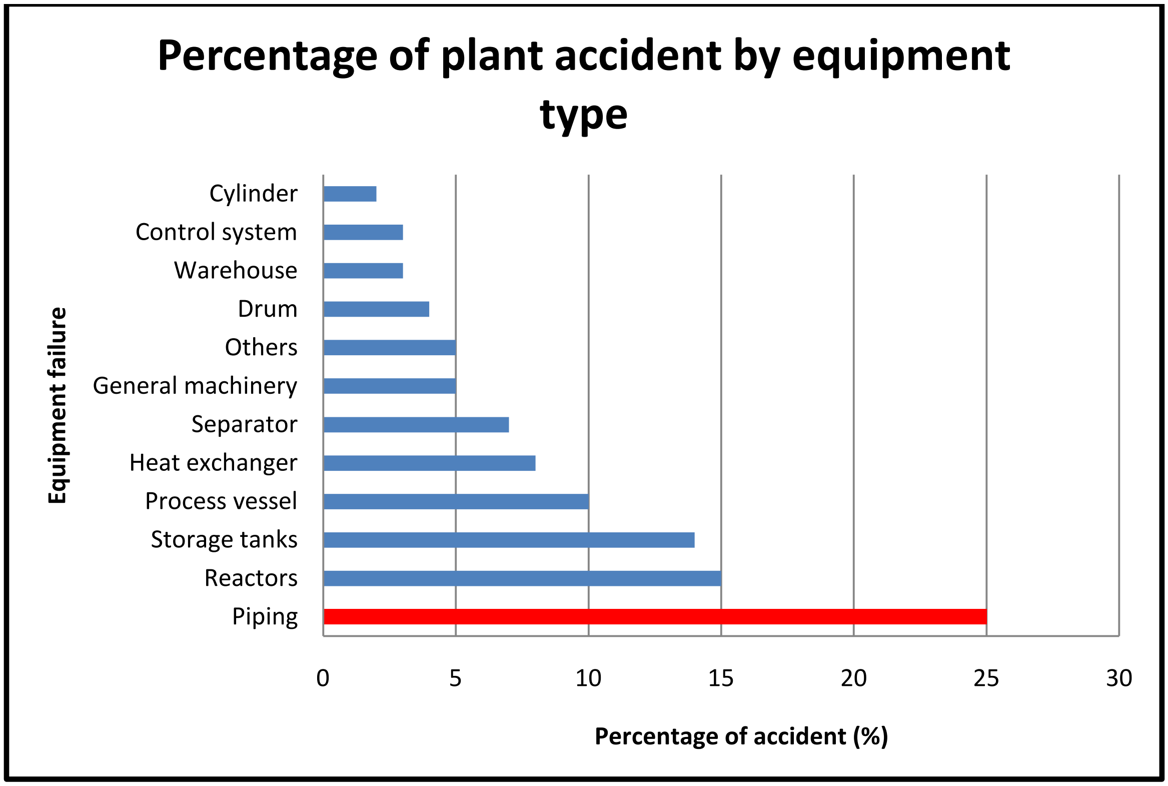

Figure 1.3: Percentage of plant accident by equipment type (Kidam et.al., 2010).

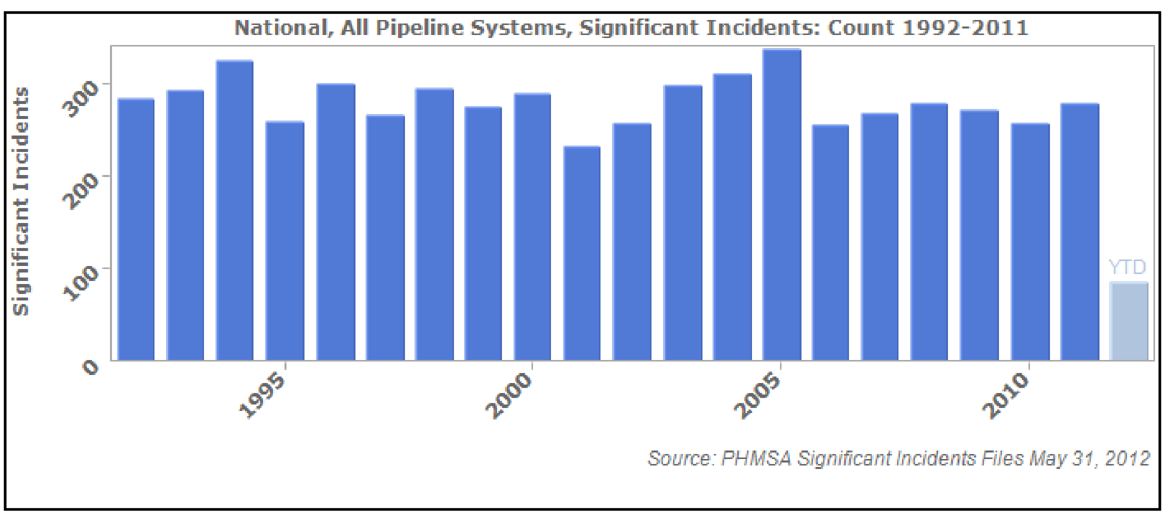

Figure 1.4: Pipeline accident property damage and fatalities statistic. Sources: US department of transportation.

CHAPTER 2: LITERATURE REVIEW

2.1 Hazard of Biogas

Biogas is a form of biofuel, which is produced from fermentation process of organic matter such as crop residues, agricultural waste, manure and sewage in the absence of oxygen which is also known as anaerobic digestion. Biogas can be produced in other environment such as landfills and waste water treatment plants too. It is usually defined based on its chemical composition and the physical characteristic which result from it.

Biogas component is mainly made up of methane and carbon dioxide with a small amount of hydrogen sulfide, ammonia and other gases depending on the source. Biogas mainly comprised of primarily methane and carbon dioxide with some inert gas like nitrogen and carbon dioxide.

Table 2.1: Makeup of biogas by major constituents (Mcdonald, 2009)

Constituent	Concentration(%)
Methane (CH_4)	55-65
Carbon dioxide (CO_2)	35-45
Nitrogen(N_2)	0.4-1.2
Oxygen(O_2)	0.0-0.4
Hydrogen Sulfide(H_2S)	0.02-0.4

However, different sources of biomass will lead to different composition of biogas produced. . Table 2.2 shows the composition of biogas produced from different sources of production, for example household waste, wastewater treatment plants sludge, agricultural wastes and waste of agrifood industry.

Table 2.2: Biogas Chemical Composition. (Biogas composition, 2009)

Components	Household waste	Wastewater treatment plants sludge	Agricultural wastes	Waste of agrifood industry
Methane (CH_4) (% vol)	50-60	60-75	60-75	68
Carbon dioxide (CO_2) (% vol)	38-34	33-19	33-19	26
Nitrogen(N_2) (% vol)	5-0	1-0	1-0	-
Oxygen(O_2) (% vol)	1-0	< 0,5	< 0,5	-
Water(H_2O) (% vol)	6 (40 ° C)	6 (40 ° C)	6 (40 ° C)	6 (40 ° C)
Total (% vol)	100	100	100	100
Hydrogen Sulfide(H_2S) mg/m3)	100 - 900	1000 - 4000	3000 – 10 000	400
Ammonia(NH_3) (mg/m3)	-	-	50 - 100	-
Aromatic (mg/m3)	0 - 200	-	-	-
Organochlorinated or organofluorated (mg/m3)	100-800	-	-	

The major hazard that methane will have if leaking happen is fire and explosion due to high pressure. Methane is non-toxic gas below 50000ppm (lower explosive limit of 5%). But if according to ACGIH (2000), methane can cause simple asphyxiant if present in high concentration in atmosphere. Methane can displace oxygen and place the people in a condition of oxygen deficiency. Oxygen level below 18% will be considered dangerous to human health (CCOHS, 2006).

Flammability limit of methane is as shown in Figure 2.1. When methane is mixed with air in STP condition at concentration of 5% to 15%, the mixture could be explosive. In high concentration, methane can be deadly if ignited. It is considered as flammable gas under DOT Hazard class of USA. The density of methane gas at +25 degrees Celsius is 0.656 kg/m^3 which is slightly lighter than the air. Thus, during the study of dispersion model using simulation, the buoyant force of methane should be considered. Methane has a critical temperature at -82.7 °C and a critical pressure at 45.96 bar (Methane, 2009). Methane is a highly flammable gas which need risk assessment for the safety of the process. Methane is also considered as buoyant gas because of its lower molecular weight as compared to the air.

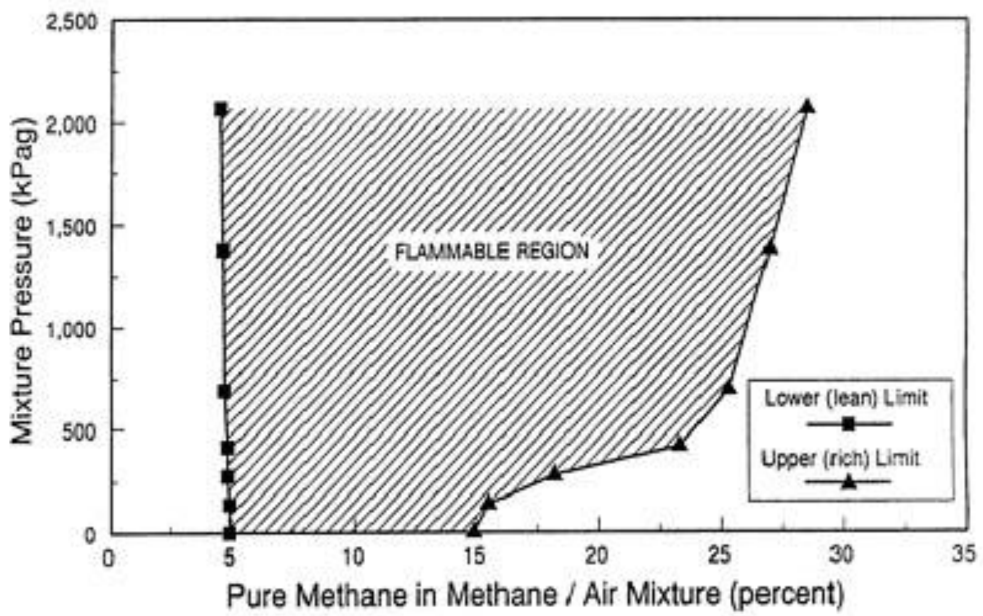

Figure 2.1: Flammability limit of methane.

2.2 Biogas VS Biomethane

There are differences between biogas and biomethane on its composition. Biogas is produced from gasification of organic waste and when it is further processed into pipeline-quality natural gas through catalytic synthesis, it will be known as biomethane. The composition of biogas and biomethane is compared as below:

Table 2.3: Comparison of biogas and biomethane composition (Gas Data Ltd)

Constituent	Biogas (%)	Biomethane (%)
Methane (CH_4)	50-75	95-97
Carbon dioxide (CO_2)	25-50	1-2
Nitrogen(N_2)	0-10	0
Oxygen(O_2)	0-0	0-1
Hydrogen Sulfide(H_2S)	0-3ppm	0-5ppm
Hydrogen(H_2)	0-1ppm	0-100ppm
Water(H_2O)	0-5ppm	0-500ppm

"Synthetic biomethane from gasification will be almost pure methane" (NGVA Europe, 2009). The statement above clearly shows that pure biomethane will have same composition as pure methane. The potential hazards of biogas and biomethane should be similar. However, whether similar behavior of dispersion model applies to biogas, biomethane and methane is not known yet. The High Flammability Limit (HFL) and Low Flammability Limit (LFL) of the three materials are unknown due to the different composition of methane and carbon dioxide content.

2.3 Experiment VS Simulation in Risk Analysis

"Fluid (gas and liquid) are governed by partial differential equation which represent conservation laws for the mass, momentum and energy. Computational Fluid Dynamics (CFD) is the art of replacing such PDE systems by a set of algebraic equations which can be solved using digital computer." (Kuzmin, 2012). CFD uses numerical method and algorithms to model fluid flow and other related physical phenomena. It provides the qualitative prediction of fluid flow by using mathematical modeling, numerical methods or software tools. It is a type of method which enables people to perform "numerical experiments" in a "virtual flow laboratory" without carrying out the actual experiment in lab scale which is time consuming and expensive. The table below shows the difference between experiment and simulation.

Table 2.4: Comparison of method between experiment and simulation (Kuzmin, 2012)

Factor	Experiment	Simulation
Concept	Quantitative description of flow phenomena by using measurements.	Quantitative prediction of flow phenomena by using CFD software.
Model	Laboratory scale	Actual flow domain
Cost	Expensive	Cheaper
Time taken	More	Less
Project flow	Sequential (One at a time)	Parallel
Project condition	Limited range of problems and operating conditions	Virtually every problem and realistic operating conditions
Error sources	Measurement errors, flow disturbance by the probes	Modeling, discretization, iteration, implementation

Due to the various benefits that simulations can offer more than experimental techniques, CFD method is adopted for the study of flow patterns that are difficult and expensive to be studied using experimental way. However, results from CFD simulation do not provide 100% reliability due to a few reasons. According to Kuzmin(2012), the three main problems of CFD simulation are the possibility of imprecise input data, inadequate mathematical model of the problem and insufficient computing power for high accuracy of the results. Thus, it is of utmost important to compare between the results from CFD simulation and experimental data in order to verify the validation of the CFD model chosen.

2.4 Biogas Dispersion

Biogas is in liquid from during the pipeline transportation. Biogas is a buoyant gas which can diffuse easily in air. When leaking happens, biogas will be released from high pressure pipeline into lower pressure atmosphere in vapor or droplet form. Two phase release might happen during the leaking. Dispersion of gas into atmosphere is normally guided by three mechanisms which are: general mean air motion, turbulent velocity fluctuations and diffusion due to concentration gradient.

Biogas is a light gas which will rise in air. It is a type of buoyant gas which is different from the dense gas behavior that tends to accumulate near to the ground level. The rising motion of the gas will dilute its concentration which makes the gas cloud neutral to the air. If the gas cloud loses its buoyancy, the ambient condition might become dominant which influence the direction of the motion. So, it is essential to study the effects of gas buoyancy to the dispersion behavior. During transportation, if methane is liquefied at very low temperature, leaking may produce cold gas cloud which the density will be higher than that of air. Thus, correct data should be obtained for the simulation running in order to simulate a more realistic dispersion model for specific condition.

When gas 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.

Biogas is normally being transported and stored in liquefied form in order to reduce the area need and ease the transportation process. When pressurized liquid leaked, there will be two phases as the pressure in the pipeline is higher than that of the atmospheric condition. According to Taiao (2004), there are two phases after releasing pressurized liquid. The liquid evaporates immediately then pulls energy from itself and surrounding to cool itself down, thus producing aerosol. If the leakage is large enough, it will accumulate and evaporate to produce a gas release which will act like a dense gas. The cooling of pressurized liquid will condense ambient humidity which then produces vapour cloud.

2.5 Conventional Dispersion Model

Generally, dispersion model for accidental leaking will require the below information for the simulation: gas leaking rate, characteristic of the release source, local topography, meteorology of the area and also the ambient and background concentration of the gas studied (Taiao, 2004). There are many conventional dispersion models available for the study.

Box model is the simplest air dispersion type among all. Box model assumes that the dispersion happens in an atmosphere which the volume is defined as a box. The concentration of the gas released is also assumed to be same at any point in the boundary condition defined. In addition, it does not provide the local concentration of the dispersion (Holmes, 2006). This model is very lacking in its accuracy of dispersion modeling due to its assumption on the homogenous distribution for the gas concentration.

Gaussian model is another modeling technology which is most commonly used in atmospheric dispersion modeling. Gaussian model is based on Gaussian distribution of gas in vertical and horizontal direction (Holmes, 2006). It is a type of steady state dispersion model. Gaussian model has it limitation in term of causality effects, wind speed and meteorological condition (Taiao, 2004). Gaussian model assumes that the dispersion is instantly targeted to the receptor regardless of the time taken in real scenario which the gas taken to reach the receptor. Hazards might occur in this time range which is not considered. Besides, Gaussian model does not work well in low wind speed condition due to the inverse wind speed dependence of the steady-state plume equation (Taiao, 2004). Gaussian model also treats the computational domain as in uniform atmosphere which makes it not so recommended for the use of developing a flammable gas dispersion model.

Thirdly, Lagrangian model is another model which can describe gas dispersion. Similar to box model, this model define the air region as a box but concentration follows the box trajectory as it moves downwind (Holmes, 2006). The model incorporate changes in concentration which is affected by the fluid velocity, wind turbulence as well as the molecular diffusion which is not confined by the stability classes like Gaussian model.

PHAST risk software is based on the Universal Dispersion Model (UDM) for gas dispersion modeling. UDM enable dispersion modeling from vapour, two-phase or liquid release at ground level. The material releases could be in continuous, instantaneous, constant finite-duration and general time-varying release (UDM, 2012). Besides, UDM also considers wind velocity and different atmospheric condition which provides more realistic gas dispersion model without under predicting or over predicting the situation. According to Colin (2011), the UDM has been accepted by Pipelines and Hazardous Materials Safety Administration (PHSMA) to be used on the LNG siting applications. However, a study done by Vianello et al (2011) on chlorine gas releases stated that gas cloud simulated from PHAST was not affected by the presence of the building that acted as the obstacles. There is a limitation for PHAST to consider the presence of obstacles which is existing in the real life situation.

2.6 Computational Fluid Dynamics (CFD) in Risk Analysis

With the increasing attention given in the industries' process safety, it is very useful to study the accidental release or leaking of biogas from pipelines. Since the comparison of simulation method and experiment method in the previous session shows that numerical simulation tools such as CFD is more feasible to use when considering the high costs that will be spent.

Computational Fluid Dynamic (CFD) is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problem that involve fluid flow. It is capable of well describe fluid physics. Besides, it is able to investigate the effects of different properties, for example density, diffusivity, viscosity and flammability limits of gas on the dispersion process (Qi et.al, 2011). By using CFD, it is possible to study how different release scenarios, geometrical configurations and atmospheric conditions can influence the gas dispersion process (Wilkening and Baraldi, 2007). CFD is reliable and it provides realistic simulation which has been validated with experimental data. According to a study done of LNG release and dispersion behaviour, the developed model showed less than 25% of error with test data (Karbaschi & Rashtachian, 2008). Furthermore, with the LNG spill field tests carried out in parallel to obtained data for model validation, the result was compared with CFX modeling for performance assessment. It is found out that CFX simulation of dense gas behavior of LNG vapor cloud is a success and its results of downwind gas concentration has close agreement when compared to the spill field tests data (Qi et. Al., 2011).

ANSYS FLUENT is a type of CFD software which has broad physical modeling capabilities needed to model flow, turbulence, heat transfer, and reactions for industrial application (Fluid Dynamics Solution, 2012). FLUENT is control volume-based for high accuracy and rely heavily on a pressure-based solution (Galphin, 2008). ANSYS FLUENT solver uses finite volumes (cell centered numeric) and offers several solution approaches (density-, segregated- and coupled-pressure-based methods) (Galphin, 2008). FLUENT provides turbulence models which include the physical phenomena such as buoyancy which is extremely crucial for the study of biogas as it is a gas which is lighter than air in atmospheric pressure.

According to Qi et.al. (2010), Mary Kay O'Connor Process Safety Center (MKOPSC) has conducted an experimental research to study on the LNG vapor dispersion parameter for CFD modeling. The dispersion parameter is essential for the development of effective safety measures and the emergency response program. In the LNG vapor dispersion study program too, ANSYS-CFX is used to simulate the scenarios of how the presence of obstacles influence the dispersion. According to Qi et. al., LNG's CFD simulation showed that obstacles in the form of vapor fences is not capable in holding the cloud within the source are but they induce further circulation and mixing of LNG and air. This is very dangerous as fire and explosion could be resulted from the mixing of flammable gas and air if the flammable limit is met. But looking from the point of view of Gant and Atkinson (2011) on their Buncefield incident CFD study, the presence of obstacles like hedges has its effect on the spreading of the vapor cloud where the gas can disperse more in the condition of unobstructed release. It is said that obstacles can increase the turbulence-combustion interaction which produce significant acceleration of flame (Hjertager, 1984).

Next, Vianello et.al. (2011) used CFD-Fluent for the simulation to study on the relationship between the complexity of a city's geometry and the distribution of a cloud of toxic substance. There is another conventional code of risk analysis which is PHAST. CFD-Fluent was chosen instead of PHAST is due to the reason that CFD takes into the consideration of the ground roughness which characterizes the atmospheric turbulence and dispersion. Ground roughness which means the number and size of roughness element in an area should be considered as in real scenario, because the area affected is not in homogenous. The presence of buildings and the geometry arrangement of the area might influence the dispersion of gas (Vianello et.al, 2011). However, in Buncefielf incident CFD study, when two different ground roughness height of h=0.1mm and h=1.0mm were used, it was found out that the results were identical (Gant and Atkinson, 2011).

Besides, gas dispersion can be influence by the wind condition too. Taking the case of methane release, methane has a narrow flammability limit; However, CFD simulation shows that the configuration with wind is more dangerous as flammable mixture may accumulate in large circulation zone formed by the wind. If the circulation zone is stable and flammable area is larger, ignition causing fire and explosion is very much possible in cases with wind than without wind (Wilkening and Baraldi, 2007). In addition, buoyancy of the gas plays an important role too. This is because if the gas accumulate closer to the ground, ignition is more likely to happen. Thus, wind condition is very influential when studying about gas dispersion in the atmosphere.

In most of the current available research paper, the study of CFD on the hazardous material dispersion is mostly involving only dense gas dispersion (Gant & Atkinson, 2011; Labovsky & Jelemensky, 2011; Chiara et.al. 2011). Different CFD package like FLUENT, CFX, FLACS and others are used but most of them adopt the Navier –stokes equation and k-epsilon model as their turbulence model. The suitability of these turbulence models in the CFD study of positive buoyant gas like biogas is yet to be verified. Turbulent viscosity is needed to simulate the modeling process. In this study, k-ε (k-epsilon) model is used due to the other researchers' works which achieved good agreement with experimental data by using this model.

As there is no universal turbulence model that can account for the entire situation that might occur, FLUENT provides a number of turbulence model for the user to choose based on the need of the situation to be modeled. Standard k-ε model is applied in the simulation of biogas dispersion model. Standard k-ε model is a semi-empirical model based on model transport equation for the turbulence kinetic energy (k) and its dissipation rate (ε). The model assumes a fully turbulent environment which neglects the molecular viscosity. In addition, the standard k-ε model considered the buoyancy for the generation of k value when non-zero gravity field and temperature gradient present in the same time.

Although standard k-ε model is widely used in the gas dispersion study, it has the limitation being a high Reynolds-number model. Realizable k-ε model is improved from the traditional model. By being realizable, this model can predict the spreading rate on planar and round jets more accurately beside provide better performance for flow involving rotation, boundary later under strong adverse pressure gradients, separation and recirculation (ANSYS-FLUENT 12.0 Theory Guide, 2009). The new features can predict gas dispersion model in geometry which involves obstacles more accurately.

In conclusion, CFD is an economical tool for process safety analysis due to its broad physical modeling capabilities that is able to take into account the complexity of fluid flow. CFD is capable of simulating both ideal and realistic condition which enables the prediction of gas concentration at any time and point within the computational domain (Zhang & Chen, 2010). However, related metrological and geometry factors should be considered during the CFD simulation in order to make sure that real case scenario is taken care of for the validity of the result obtained.

2.7 PHAST: Universal Dispersion Model

Process Hazard Analysis Software Tool or PHAST is comprehensive risk analysis software which could be utilized to carry out consequence analysis. It is normally used to identify situation which poses potential hazards to life, property or environment. PHAST is able to examine the process of incident from initial release to far field dispersion besides simulating various release scenarios such as leaks, long pipelines releases or pressurized pipes (Pandya et al, 2008). It could be utilized to calculate concentration, fire radiation, toxicity and explosion overpressure. PHAST is reliable and it has outstanding technical superiority.

PHAST is based on Universal Dispersion Model (UDM) which is an integral model to calculate dispersion following a two-phase pressurized released. As biogas is transported in high pressure through pipeline, a rupture is pipeline will cause two-phase release of the gas into the atmosphere. Droplets of biomethane might be formed due to the lower atmospheric pressure as compared to higher pipeline pressure. Besides, PHAST also consider the vertical variation in meteorology condition such as wind speed, temperature and pressure which suits the objectives of the project to develop realistic dispersion model of biogas leaking.

In the case study, an approximate area of biogas plant will be chosen to represent the possible accident location for the pipeline leaking. The same input information will be applied for the simulation to ensure that the situation controlled is the same for the development of the dispersion model by using CFD-FLUENT. Wind condition is applied with obstacles included in the computational domain. The results will be analyzed on the difference between CFD and UDM modeling.

Through comparison between dispersion model of CFD and UDM, it is possible to see the benefits or limitation of CFD modeling when compared to the standard code of risk analysis. Modification could be done to the dispersion model to make it a realistic one.

CHAPTER 3: METHODOLOGY

3.1 Research Methodology

3.1.1 Computational Fluid Dynamics (CFD)

In Buncefield incident, the CFD model simulation produced good agreement with the real dispersion behavior which is observed in the CCTV footage (Gant and Atkinson, 2011). Thus, CFD is chosen as the methodology for this project. The CFD software is generally used in the studies in following sequence.

PRE-PROCESSING
• Geometry/CAD/Solid model definition of domain • Surface cleanup/preparation • Volume mesh preparation • Definition of boundaries and conditions • Physical property settings • Numerical controls

SOLVING
• Performing computation using suitable turbulence model

POST PROCESSING
• CFD results analysis • Export result • Improve analysis

Figure 3.1: CFD simulation process.

FLUENT simulation is based on the 3-D Reynolds-averaged Navier Stokes equations. However, the knowledge of atmospheric dispersion is required in order to describe the turbulence condition applied to simulate the dispersion model. According to Ivings et.al. (2007), FLUENT has the advantages of:

- Flexible which is applicable to wide range of scenarios
- Capable of handling complex geometries and terrain
- Widely accepted as commercial CFD package
- Up-to-date
- Wide variety of output is available

Through FLUENT, it will allow the simulation of the dispersion of biogas from pipeline leaking over time. Concentration could be estimated to determine the area which is under high risk of fire and explosion hazard.

3.1.2 Project flow

Simulation is used to study the dispersion model of biogas by using ANSYS-FLUENT of CFD method. The project flow is as shown in Figure 3.2:

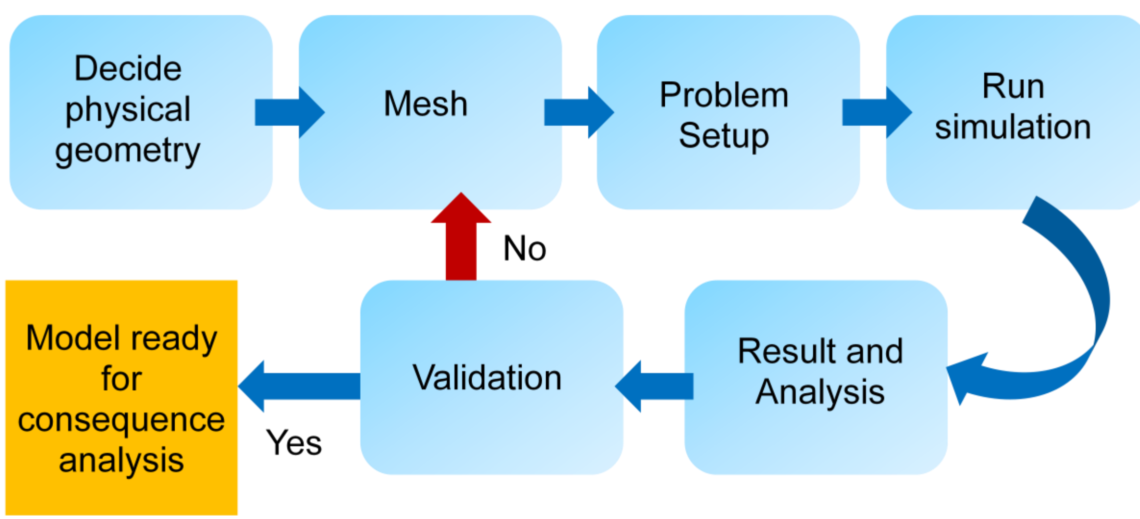

Figure 3.2: Project flow.

The project flow is generally described as below:

I. Decide the composition of biogas and pure methane gas.
II. Decide physical geometry as computational domain.
III. Decide the suitable mesh with consideration of computational time and accuracy of calculation.
IV. Problem setup.
V. Run simulation.
VI. Results and analysis.
VII. Model validation with IP model code and PHAST.
VIII. Gas dispersion case study: Assessment of hazardous distance from gas released.
IX. Case study by using PHAST.

3.2 Simulation: ANSYS-FLUENT

3.2.1 Model Physical Geometry

The model is developed starting from the definition of computational domain. The physical geometry is drawn using Design Modeler. The analysis type is done in 2D on XY plane in order to shorten the computational time. The geometry is an environment area of 10m wide and 5m high as shown in Figure 3.3.

Pipe leaking size is influenced by many factors including failure mechanism, pipe material properties, stress levels and others which make the size variable (US EPA). Majority oil and gas pipelines diameter is in the range of 8-12 inches (200-300mm) (Rademaekers et al, 2011). The conservative worst case will allow for assuming the pipeline diameter as the leaking size. However, 10 mm leaking size is to be set in this project case with a reference based on IP Model Code (2005). The gas leaking will happen at ground level. Gas released will be dispersed into the atmosphere which is also the environment area. The name selection for each boundary is shown in Figure 3.4.

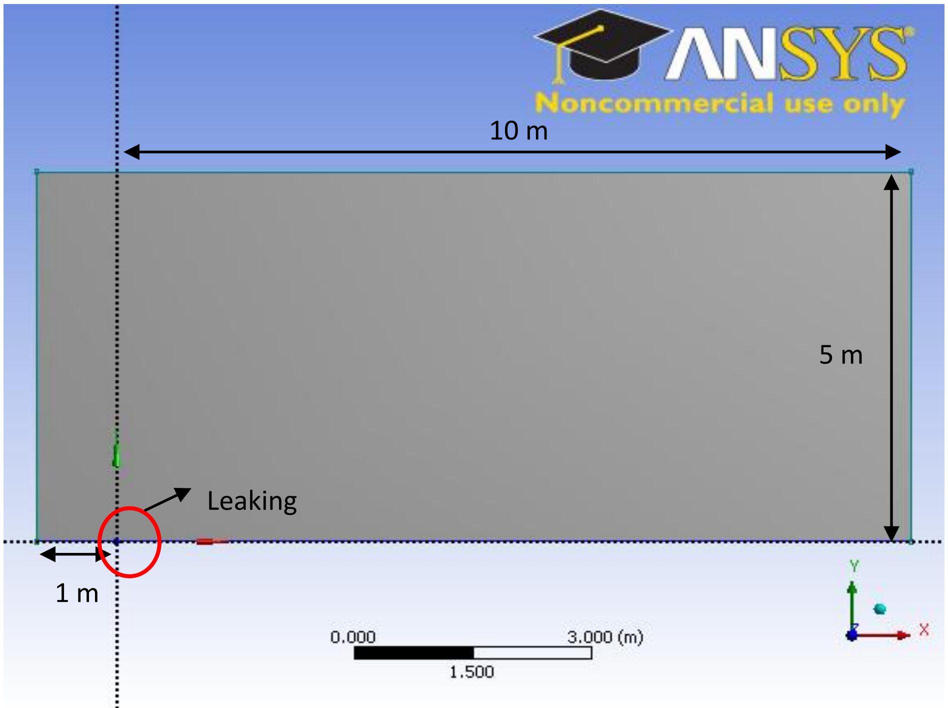

Figure 3.3: Physical geometry for release without obstacle.

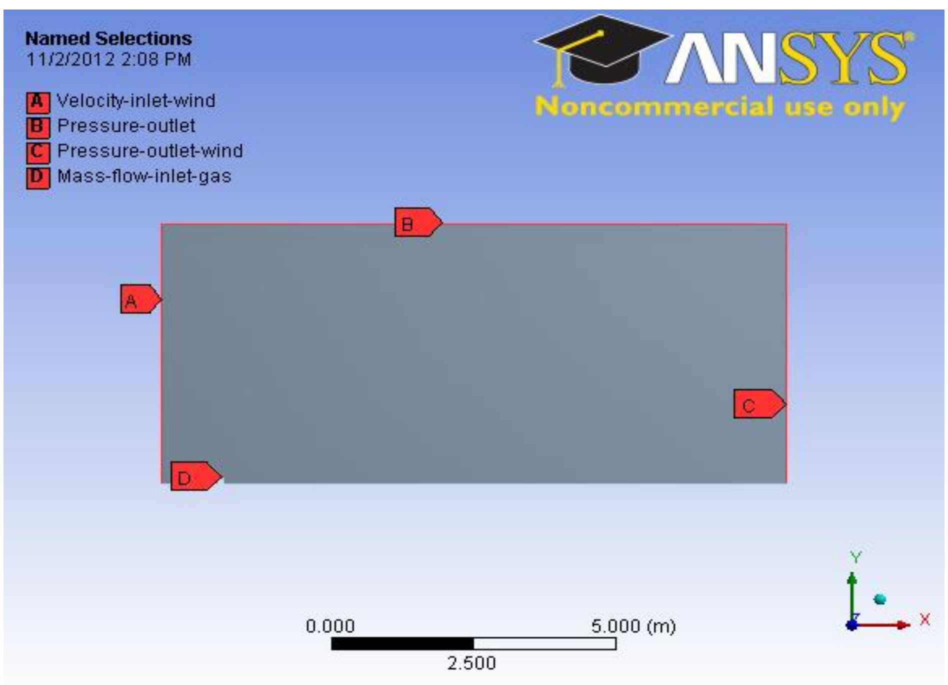

Figure 3.4: Name selection of boundaries.

3.2.2 Meshing

A good mesh will give better precision. The aim of meshing is to balance up between the quality of the mesh and the computational time. Simulation is run comparing two meshing quality which includes default meshing and finer meshing. Mesh 1 is shown in Figure 3.5:

Table 3.1: Information of Mesh 1

MESH 1	
Relevance center	Coarse
Smoothing	Low
Span angle center	Fine
Curvature Normal Angle	18 degree
Refinement	Off
Inflation	Off

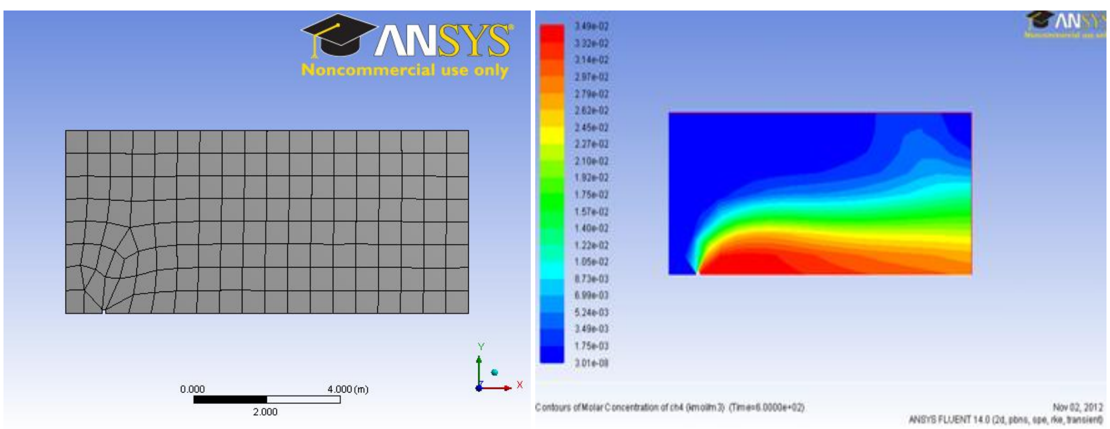

Figure 3.5: Mesh 1

Higher grid refinement should be achieved for more accurate and smoother flow of the gas simulated. The biogas leaking is expected to be at high velocity as it is highly pressurized in the transmission pipeline. The large pressure drop will create high velocity outlet flow from the leaking hole. So, the mesh is highly refined at the pipeline leaking area. Besides, the wind is entering from the left side of the computational domain which smaller element size is defined as well. It is found out that the Mesh 2 can simulate smoother flow of the gas with higher accuracy as compared to Mesh 1. Mesh 2 is done with specification as shown in Table 3.2:

Table 3.2: Information of Mesh 2

MESH 2	
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

To ensure the accuracy of Mesh 2, Mesh 3 is created using edge sizing. Edges sizing is another way of having high quality mesh instead of refinement. Finer grid is defined at the leaking inlet for 0.01 m, ground area for 0.03 m and the atmosphere for 0.05m. Inflation is activated. Mesh 3 used is as shown in Figure 3.7.

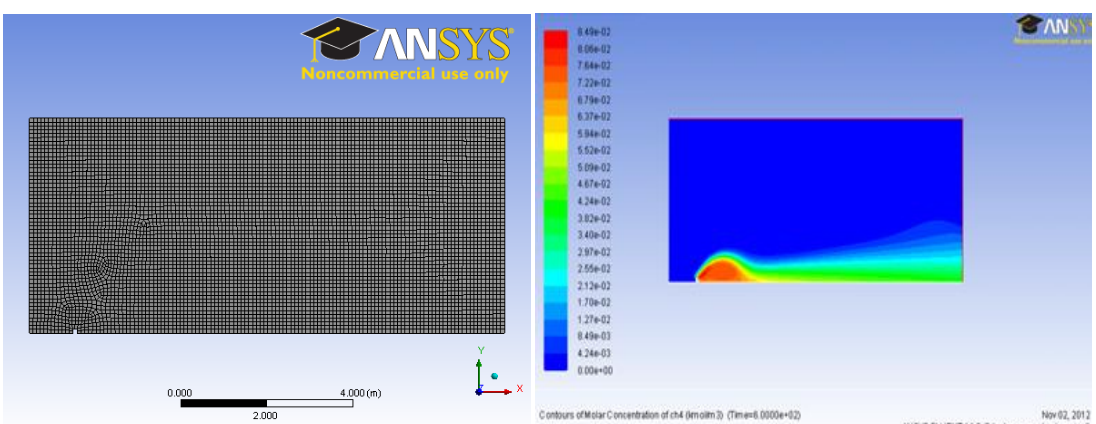

Figure 3.6: Mesh 2

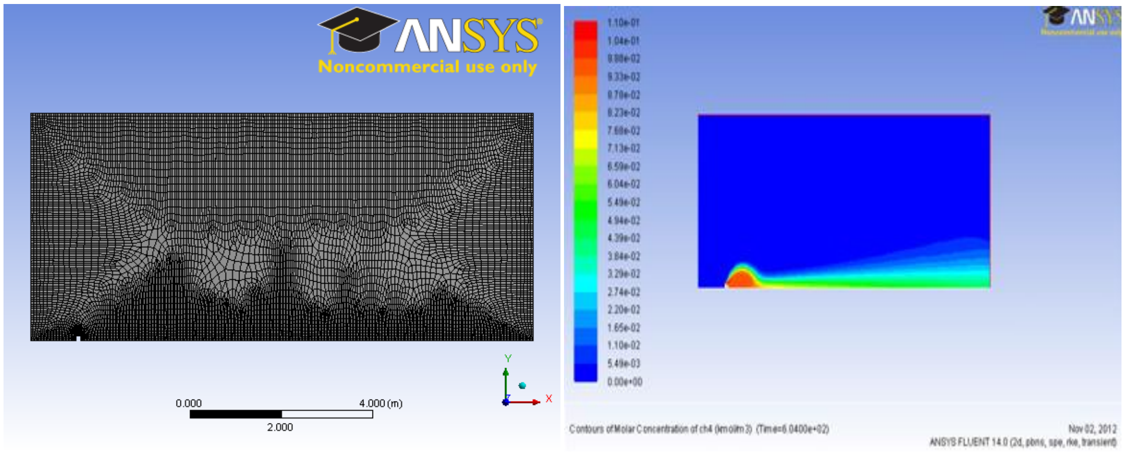

Figure 3.7: Mesh 3

Mesh 2 and 3 can clearly show the mixing of methane gas and air after release. The concentration is getting diluted with upward flowing. Methane gas that is just released will stay on the ground area as it is denser than the air under cold temperature and high pressure. However, when time goes by, the gas is warmed by the atmosphere air which makes it lighter and become positively buoyant. Thus, the gas floats upward. From Figure 3.8, Mesh 2 and 3 has similar concentration obtained from same input of data. However, Mesh 3 requires a longer computational time as compared to Mesh 2 for convergence. Thus, in order to save computational time, Mesh 2 is chosen for the model validation and consequence study.

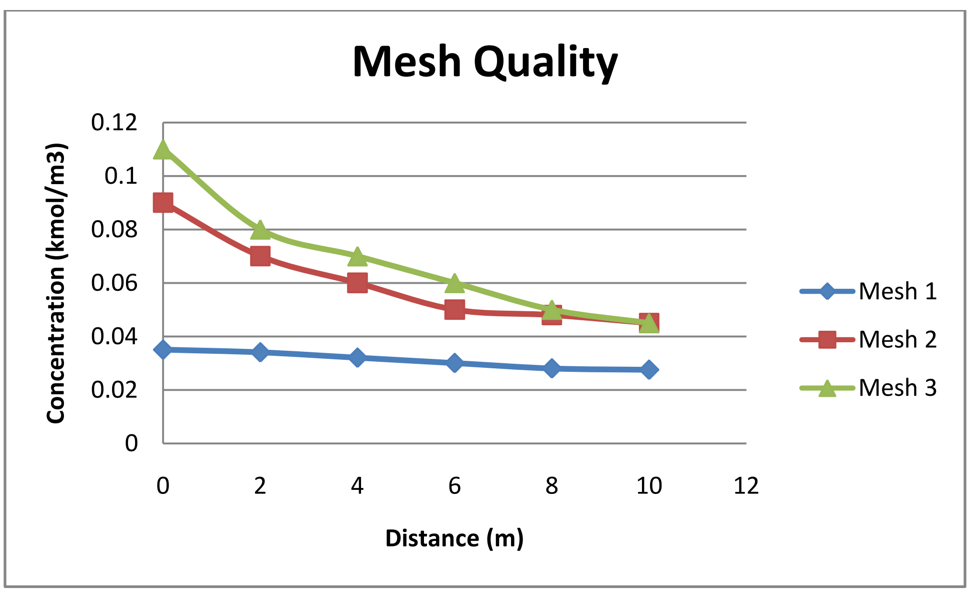

Figure 3.8: Mesh quality comparison.

3.2.3 Turbulence Model

Before the computational domain is solved, meshing quality is checked to make sure that the volume statistics is in positive value to ensure the validity of the mesh. Pressure-based solver is used with absolute velocity formulation. Gravity acceleration is defined at -9.81m/s^2 with regard to Y-axis.

Turbulence model is one of the factors that will influence the gas dispersion. Laminar model is not suitable in this case as there will be mixing of air and unstable turbulence in the atmosphere due to meteorological condition. Realizable k-epsilon model is used as it is the most common turbulence model for gas dispersion that is recognized. The realizable k-epsilon model provides good performance for flows that involve rotation, boundary layers under strong adverse pressure gradients, separation and recirculation (ANSYS, 2009). This model is suitable for the intention to simulate the gas dispersion that is related to release into the environment. Full buoyancy effect is activated as the methane density is a function of temperature. The density reference is set as 1.225 kg/m^3.

3.2.4 Species Transport Model

In order to simulate the dispersion of methane gas, the concentration of the gas released and its movement will indicate the hazardous distance. Species Transport model is chosen with the mixture material as methane-air as this model is capable of simulating the transport of species in the computational domain without involving any chemical reaction. The mixing and transport of chemical species can be modeled by solving conservation equations describing convection, diffusion, and reaction sources for each component species (ANSYS, 2009). This model allows the study of concentration resulted from individual component as well. The mixture will be defined further in the boundary condition to specify the composition of carbon dioxide for biogas. Energy equation will be activated automatically following the species model. As the species transport is without reaction, volumetric reaction is remained inactive.

3.2.5 Boundary Condition

The problem setup is defined to suit the dispersion condition to be simulated. As the atmospheric flow is being predicted by the model, the boundary conditions of the geometry and computational domain are being specified before the simulation. The boundary conditions are defined as Table 3.3:

Table 3.3: Boundary condition for the physical geometry designed.

Boundary	Types	Remarks
Wind inlet boundary	Velocity inlet	Mass flow, temperature and turbulence values for wind inlet flux
Wind outlet boundary	Pressure outlet	Constant pressure outlet surface
Gas inlet boundary	Mass flow inlet	Mass flow, temperature and turbulence values for gas inlet flux
Top boundary	Pressure outlet	Constant pressure outlet surface
Ground boundary, Building wall	Wall	No slip condition, roughness, fixed temperature

3.3 Model Validation

The gas dispersion model developed must undergo validation in order to ensure the reliability of the model. Two standards adopted are IP model code and PHAST software. PHAST as mentioned is based on the Universal Dispersion model and is commonly used for risk analysis. Model Code of Safe Practice Part 15 or IP model code on the other hand is a standard reference data generally used for area classification for installations handling flammable fluids. It is a well-established and internationally accepted code that provides guidance for specifying hazard radii during the selection and installations of equipment. It applies dispersion modeling to the calculation of hazard radii and also taking account variables like composition of material released, release pressure, release temperature, atmospheric condition and the other necessary information. To validate the model developed, the problem setup of the dispersion is used as stated in

Table 3.4 (IP model code, 2005). The same condition is used in the simulation for both CFD and PHAST software to create the similar release scenario.

Table 3.4: Physical parameters used in model validation.

IP Model Code Dispersion Modeling Physical Parameters	
Fluid category	G(i)
Methane composition	0.88
Hole diameter	10 mm
Ambient temperature	20°C
Relative humidity	70%
Wind speed	2 m/s
Stability class	D
Surface roughness	0.03 m
Sample time	18.75 s
Release height	1 m
Reservoir temperature	20°C
Release orientation	0° in relation to wind direction

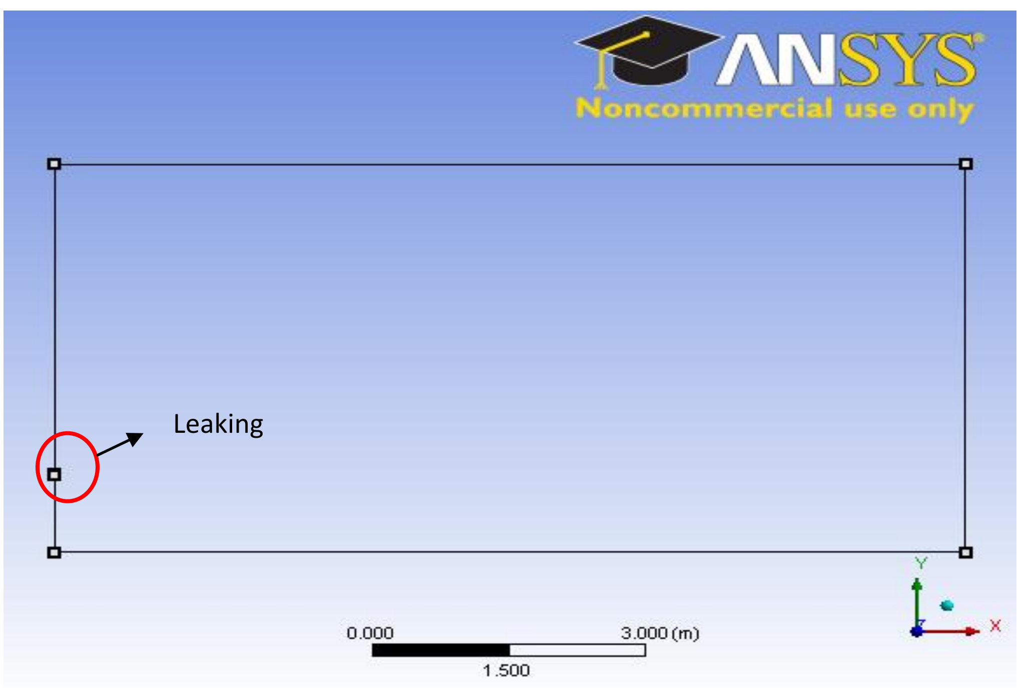

Figure 3.9: Physical geometry for model validation.

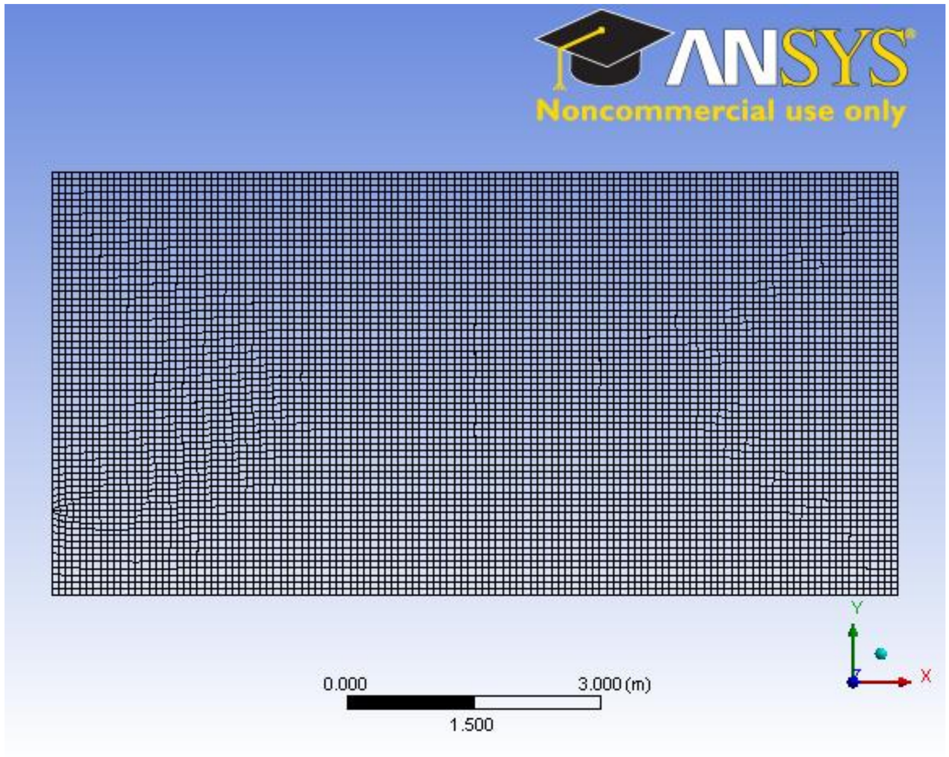

Figure 3.10: Meshing for model validation.

3.4 Model Dispersion Study

Model validation is done with a satisfactory reliability. Thus, the model is now used for dispersion study from pure methane and biogas release. The gas released is entering in flow rate of 0.1 kg/s with a gauge pressure of 1,000,000 Pascal. LNG gas which contains more than 90% methane composition has a boiling point of 111k at atmospheric condition (Qi et.al., 2010). However, the gas will be set to enter at its reservoir temperature, 20°C referring to IP Model Code (2005). The dispersion of LNG vapor cloud goes through three stages which include negative buoyant, neutrally buoyant and positive buoyant (Qi at.al, 2010). When LNG is first released into the atmosphere, it is a dense gas due to the cold temperature which makes it negative buoyant. When mixing is happening between the LNG gas and the air, the gas temperature will slowly increases and become positive buoyant. Full buoyancy effect is activated for the consideration of density changes with temperature. Thermal diffusion and diffusion energy source is also used.

3.4.1 Type of gas

Two types of gas are being studied in the simulation which involves biogas and pure methane gas. Assumption is made where the biogas and pure methane gas will be in gas phase instead of multiphase for simplification. Pure methane gas is similar to the LNG due to its high methane composition and thus the behavior of methane can be assumed to be the same as LNG. For biogas, it is made up of 60% methane and 40% carbon dioxide composition. Carbon dioxide is commonly used in fire extinguishers to put off fire. Its ability to inhibit ignition is an important issue that cannot be overlooked during the study. The composition of carbon dioxide should be considered.

3.4.2 Wind speed

For the simulation of the influence of wind speed on the gas dispersion, Wind direction will be coming in from left and the flow is parallel to x-axis. Unstable atmosphere condition often raises the atmospheric turbulence which increases the dilution of the released gas and reduces the hazard risk probability.

The intensity of the atmospheric turbulence has great effect on the gas dispersion due to the ability of turbulence to increase the entrainment and mixing of the gas with ambient atmosphere. Concentration may be reduced if mixing happens. The atmospheric stability is classified using Pasquill atmospheric stability classes which categorize the amount of atmospheric turbulence into six classes as shown in Table 3.5.

Pasquill-Gifford considers the horizontal wind speed, cloud cover, ceiling height and also the time of observation. The meteorological condition is planned according to the Pasquill-Gifford stability classes as atmospheric stability condition other than wind speed might influence the process of gas dispersion. In order to be precise, results will be analyzed with the consideration of atmospheric stability too.

Thus, the wind profile is simulated at wind speed of 1.5 m/s and 5 m/s which represent the stability class D that is the most common atmospheric stability (CPQRA, 2000). The atmospheric pressure is at 101325 Pascal and the atmospheric temperature is staying at 20℃.

Table 3.5: Pasquill-Gifford stability categories.

Stability class	**Definition**	**Stability class**	**Definition**
A	Very unstable	D	Neutral
B	Unstable	E	Slightly stable
C	Slightly unstable	F	Stable

Surface Wind Speed (at 10 m), m/s	Day			Night	
	Incoming Solar radiation				
	Strong	Moderat e	Slight	Thinly overcast or ≥ 4/8 cloud	Clear or ≤ 3/8 cloud
0 – 2	A	A – B	B	–	–
2 – 3	A – B	B	C	E	F
3 – 5	B	B – C	D	D	E
5 – 6	C	C – D	D	D	D
≥ 6	C	D	D	D	D

Figure 3.11: Pasquill-Gifford stability classes according to meteorological condition.

3.4.3 Presence of obstacles

The leaking origin at is set at origin with x-coordinate = 0m which is 1m away from the wind inlet boundary. The hole leaking size is set at a diameter of 10 mm. The release scenario without the presence of the obstacle is shown in Figure 3.3. Obstacle is believed to cause turbulence interaction between the gas released and atmosphere. For the release scenario with the presence of obstacle, an obstacle is introduced into the computational domain which has a dimension of 1m x 1m. The obstcles is placed at a distance of 3 meters from the point of release. The geometry with presence of obstacles is shown in Figure 3.11.

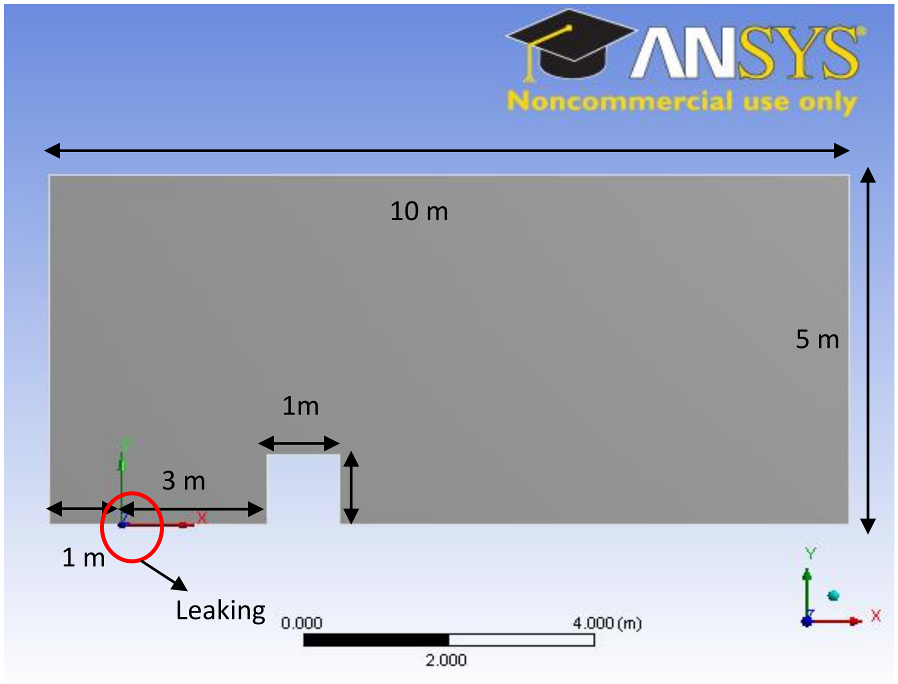

Figure 3.12: Physical geometry for release with presence of obstacle.

3.4.4 Release Duration

The initial steady simulation without any release has been performed to evaluate the wind flow behavior as the initial condition. Later, pure methane gas or biogas is released for 20 seconds and 10 minutes continuously. The leaking time is set as standard duration of 10 minutes which allocates time for detection and mitigation (CPQRA, 2000). Comparison of gas released after 20 seconds and 10 minutes will allow further details of changes of potential flammability region with time.

3.5 Key Milestone

Table 3.6: Key milestone of FYP I

No	Action Item	Remarks
1	Regular meeting with supervisor to discuss the project and prepare project proposal	Ongoing
2	FYP Briefing	Week 1
3	Literature Search & LFSU Briefing	Week 3
4	Submission of Extended Proposal	Week 6
5	Mid- Semester Break	Week 7
6	Proposal Defense (Oral Presentation)	Week 7-8
7	Submission of Interim Draft Report	Week 13
8	Submission of Interim Report	Week 14

Table 3.7: Key milestone of FYP II

No	Action Item	Remarks
1	Project work continues	Ongoing
2	CFD modeling	Week 1
3	Submission of Progress Report	Week 7
4	PHAST modeling	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

3.6 Gantt Chart

No.	Detail/Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	Preliminary Research Work - Project background - Objectives - Scope of study								Mid semester break							
2	Literature Review - Potential hazard of biogas - Biogas composition & properties - CFD in risk analysis															
3	Methodology - Research method - Project activities - Milestones and gantt chart															
4	Submission of Extended Proposal Defense						●									
5	Learn FLUENT															
6	Proposal Defense Oral Presentation										●					
7	Project work continues															
8	Submission of Interim Draft Report														●	
9	Submission of Interim Report															●

Table 3.8: Gantt chart of FYP I.

● Key milestone

No.	Detail/Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1	CFD Project work - Physical geometry - Meshing - Problem setup - Develop dispersion model from FLUENT - Result analysis								Mid semester break							
2	Submission of Progress Report							●								
3	CFD Dispersion Model validation - LNG dispersion model															
4	PHAST Project work - Learning UDM - Develop dispersion model from UDM															
5	Result Analysis on CFD and UDM dispersion model differences															
6	Oral Presentation													●		
7	Submission of Technical Paper														●	
8	Submission of Dissertation														●	
9	Submission of hard bound Project Dissertation															●

Table 3.9: Gantt chart of FYP II.

● Key milestone

CHAPTER 4: RESULT AND ANALYSIS

4.1 Model Validation

For post-processing process, the results obtained are evaluated to determine whether the FLUENT model is performing well. If the model shows large deviation with the other two standards, then modification has to be done to the model. The target percentage of error should be less than 25% (Karbaschi & Rashtachian, 2008). Figure 4.1 shows the CFD simulation for model validation for natural gas (88% methane composition) with different gas release flow rate ranged from 0.06 kg/s, 0.1 kg/s, 0.7 kg/s and 1.5 kg/s. The pressure of the gas released varied with the release rate. The colour scale shows that concentration of the natural gas released.

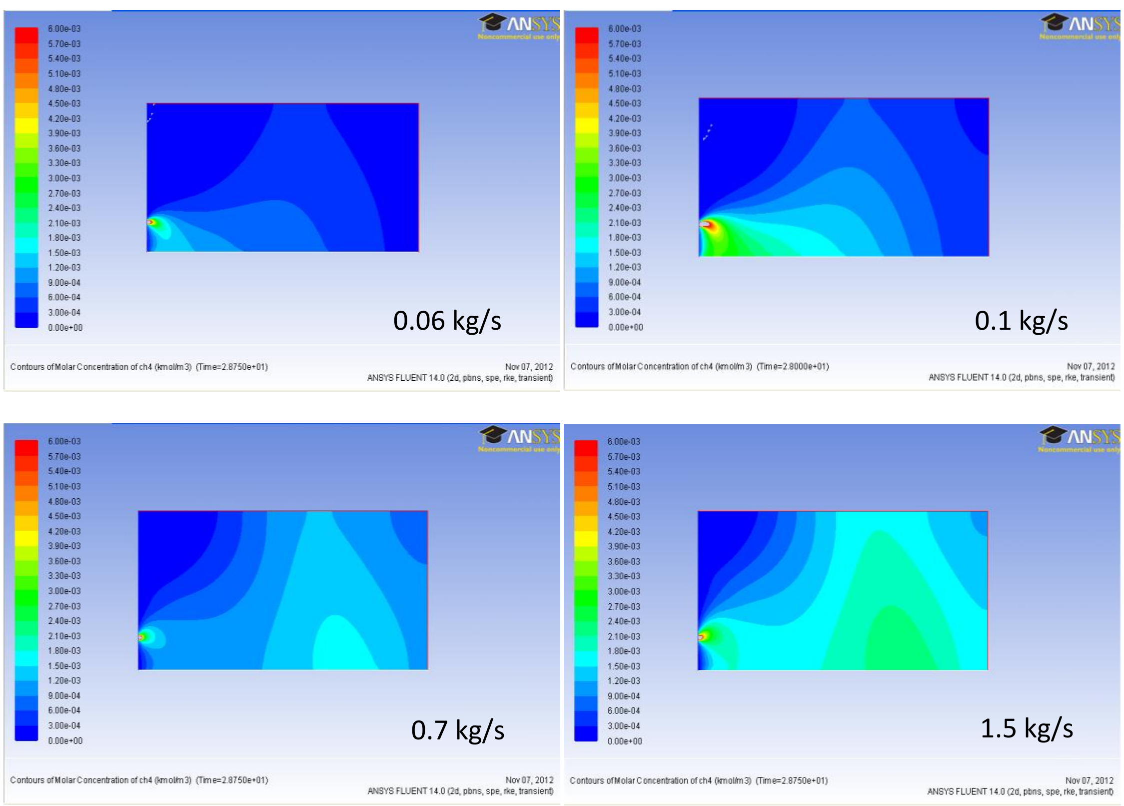

Figure 4.1: CFD simulation for natural gas (88% methane) with different release rates.

The colour scale of the simulation is being ranged between 5 %(0.002 kmol/m^3) and 15 %(0.006 kmol/m^3) in order to fit the flammability limit of methane. The vapor cloud in the figure indicates the flammability region that is caused by the gas released. With wind velocity of 2 m/s, the gas released is transported downstream following the direction of the wind.

From Figure 4.1, the methane gas released is observed to flow along the ground level. The gas is released at 20°C and 10 bar which makes it a dense gas at release. However, after mixing with the air, the vapor cloud starts to flow upward. Full buoyancy effect is activated during the problem setup. Thus, when the mixing happen, the gas will become lighter in density and float upward. The vapor cloud size is more significant in larger release rate due to higher concentration. In addition, it is clearly shown that the flammability region is wider spread when the release rate is larger.

The model is validated against IP Model Code and PHAST. From Figure 4.2, FLUENT model shows close agreement with IP model code and PHAST. The highest deviation occurs at higher release rate is calculated to be at 18%. Possible reason for the deviation is due to the different functionality of the risk analysis software. The error is less than 25 % and thus the validation is accepted. This model will be used for further biogas dispersion study.

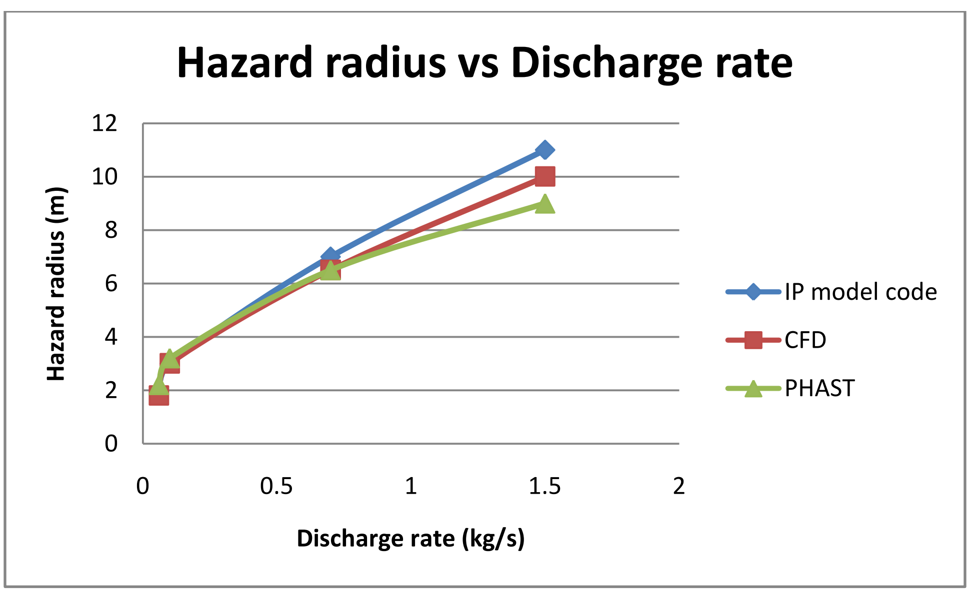

Figure 4.2: CFD model validation.

4.2 Gas Dispersion Study

Biogas consists of 60% methane and 40% carbon dioxide is specified in the simulation. Biogas with this composition has a flammability limit of 9-17% (Ekelen & Wolters, 2011). Although the flammability range is quite small, a leakage of biogas from pipeline may cause fire and explosion as biogas is normally transmitted through pipeline in high pressure. The release of gas is through a 10mm hole under a pressure of 10 bar.

As gas pipelines such as transmission pipelines are normally fixed on ground, the leaking or release point is set at ground level instead of 1m height which is done in the model validation. The hazard radius is evaluated with reference height on ground level. The hazard radius is defined as the hazard downwind distance that it takes for the gas to reach its lower flammability region. Beyond the distance, the gas concentration is assumed to drop out of the flammability limit and will not cause severe harm to the safety. The safety measure should be focusing within the hazard radius.

For the gas dispersion study, the effect of the wind speed and the presence of the obstacle will be included for both biogas and pure methane gas release. Besides, the evaluation of the hazard downwind distance will be carried out in each scenario to evaluate the potential flammability region resulted from the gas release.

4.2.1 The effect of wind speed on biogas dispersion

Wind speed can influence on the size and direction of the vapor cloud. To understand the effect of the wind speed on biogas dispersion, the wind condition is varied at 1.5 m/s and 5 m/s. Figure 4.3 and Figure 4.4 show the concentration of biogas and methane.

Firstly, for the size of vapor cloud, the height of the cloud is not considered in the case as the simulation is only done in 2D. The height might be an overestimation as 2-D simulation reduce the friction of the gas jet and the surrounding, thus making the height higher (Wilkening & Baraldi, 2007). Thus, the vapor cloud is studied from the side view in order to obtain the potential hazard distance.

The vapor cloud is wider spread in lower wind speed. The atmosphere is stable and experience lower turbulence. Thus, buoyancy effect plays an important role during low wind speed. The vapor cloud is carried upward as the biogas' density is getting lighter after mixing with the air. On the other hand, the vapor cloud in higher wind speed scenario is smaller as compared to that of the lower wind speed. The flow of the gas in higher wind speed is driven by the wind force. A large amount of gas is transported downstream to the right following the wind direction. Buoyancy force in this case does not play much role as the wind force restricts the movement of the gas upward.

Secondly, as pure methane gas contains high composition of methane as compared to biogas, the flammability region of the dispersion is more significant as shown in Figure 4.4. The gas is more concentrated on the ground level near to the point of release. The dispersion of methane and biogas are of the same behavior. But, the size of the vapor cloud varied with the concentration of respective gas. Higher concentration of methane composition will produce larger speeded flammable vapor cloud.

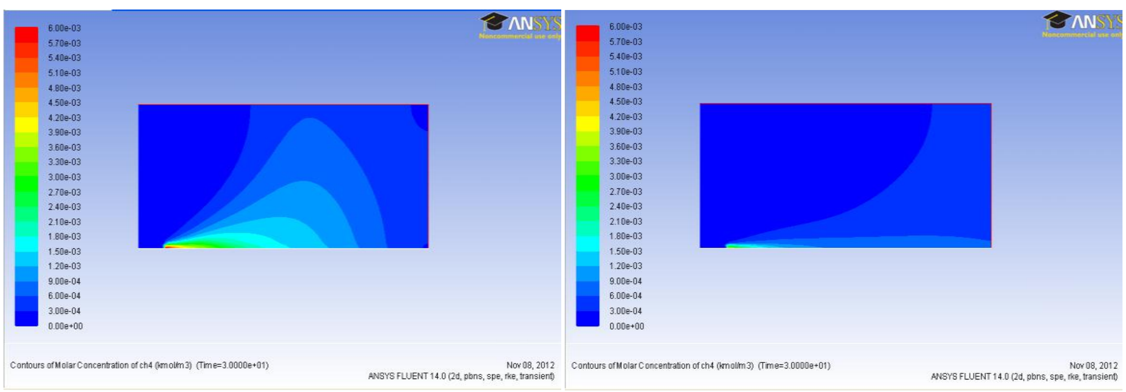

Figure 4.3: Biogas leaking under wind condition 1.5m/s(left) and 5m/s(right).

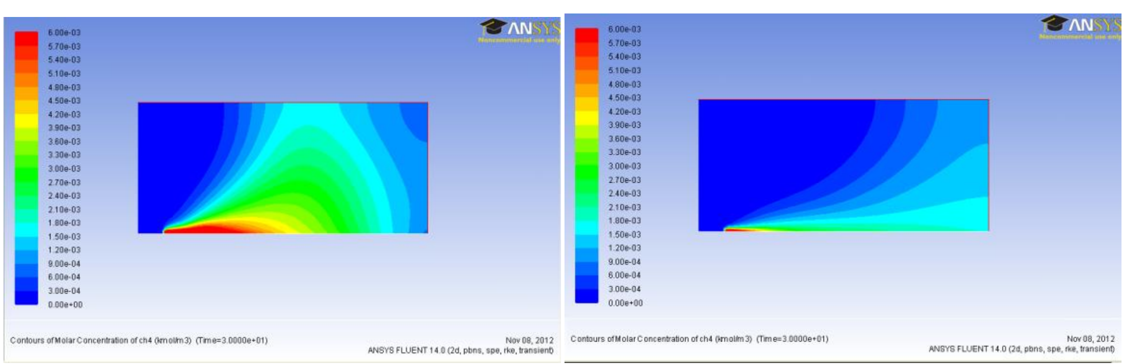

Figure 4.4: Methane leaking under wind condition 1.5m/s(left) and 5m/s(right).

Figure 4.5 shows the comparison in concentration changes between two wind speeds for both gases. The concentration reaches upper flammability limit in lower wind speed for biogas. Thus, it can be concluded that the release of biogas in lower wind speed will pose a higher risk for fire and explosion because dilution occurs more drastically when there is higher wind speed.

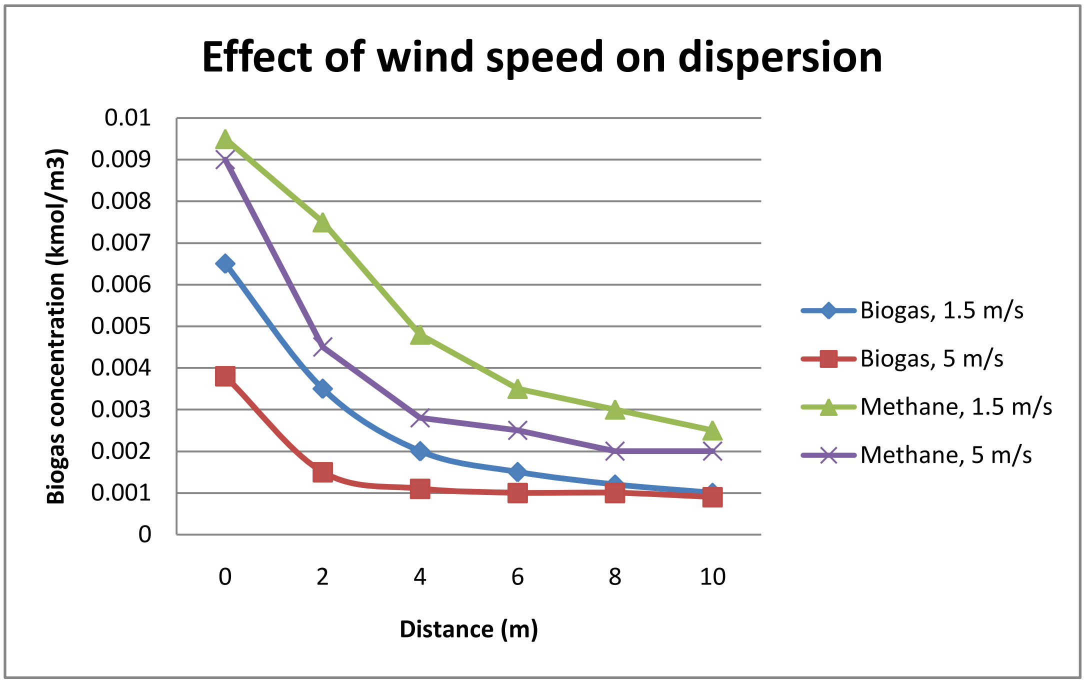

Figure 4.5: Effect of wind speed on biogas dispersion.

4.2.2 The effect of obstacles on biogas dispersion

In a biogas plant, there will be many types of equipment like anaerobic digesters, storage tanks, pipelines and the others placed in the same area. It will be not practical to assume the release of biogas in an open area without any obstruction. The presence of obstacle is believed to increase the turbulence-combustion interaction and producing significant acceleration of flame (Wilkening & Baraldi, 2007). Thus, it is essential to study on the effect of obstacles to the gas dispersion behavior.

An obstacle with the dimension of 1m x 1m is placed at a distance of 3 meters from the point of release which is still within the flammability region. The purpose of the obstacle is to introduce turbulence distraction to the leaking gas flowing direction in order to observe the gas behavior when the gas flow is being obstructed. Figure 4.6 and Figure 4.7 show the behavior of biogas and methane dispersion in contour when meeting with obstacles with different wind speed respectively.

From Figure 4.6 and 4.7, the gas is trapped around the obstacle and creating the flammability region which is indicated by the vapor cloud. The gas trapped in front of the obstacle will induce fire and explosion easily. The obstacle inhibits the dilution of the gas mixture with air. The contour of the gas concentration around the obstacle shows that there will be high probability for ignition especially at low wind speed when the atmosphere is stable. On the other hand, when there is higher wind speed, the vapor cloud is carried downstream easily instead of accumulating in front of the obstacle. Higher wind speed enables faster rate of dilution between the gas and air producing lower concentration of gas mixture. The vapor cloud creating the flammability region is smaller.

The obstacle is placed at 3m distance from the release point. Figure 4.8 shows the two gases concentration with the presence of obstacles under different wind speed. It is observed that for biogas, the gas concentration fall out of the flammability limit of 5% which is equal to concentration of 0.002 $kmol/m^3$ at 4m distance. Thus, the region in front of the obstacle is categorized as the flammability region and the region behind the obstacle is safe from the risk. The same case goes to methane gas during the release that the gas accumulates in front of the obstacle creating flammability region. However, in methane case, the obstruction of the obstacle provides momentum and impulse for the vapor cloud to move upward covering the obstacle. Possible explanation is due to the higher concentration of methane. The region behind the obstacle is still within the flammable zone. The amount of biogas close to the ground behind of the obstacle is rather small as compared to that of methane's.

Thus, presence of obstacles will restrict the movement of the gas for further dilution which creates higher risk of fire and explosion. Higher concentration of gas will contribute to the flammable risk too.

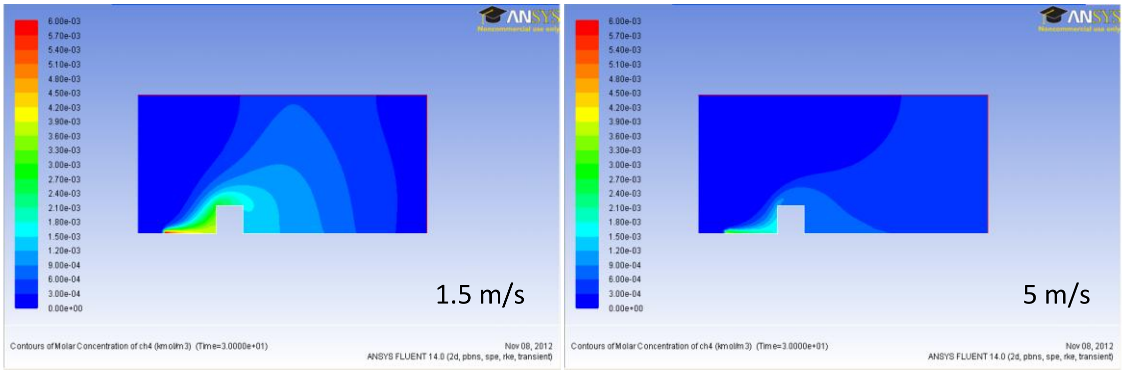

Figure 4.6: Biogas leaking with presence of obstacle under different wind speed.

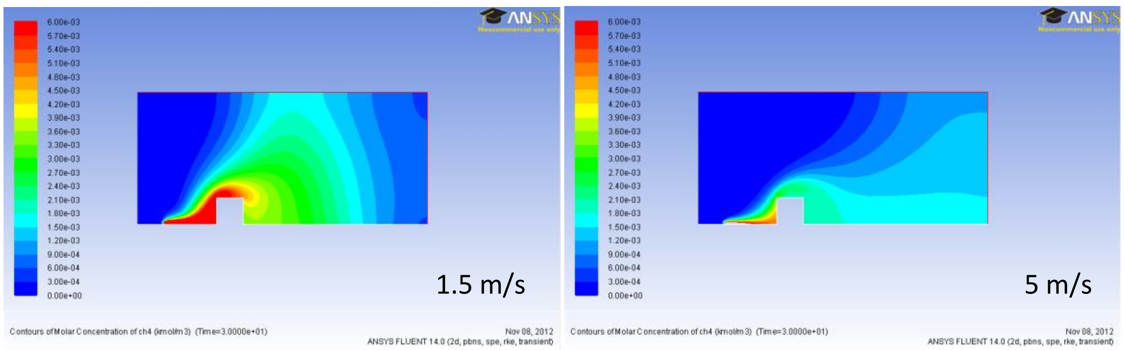

Figure 4.7: Methane leaking with presence of obstacle under different wind speed.

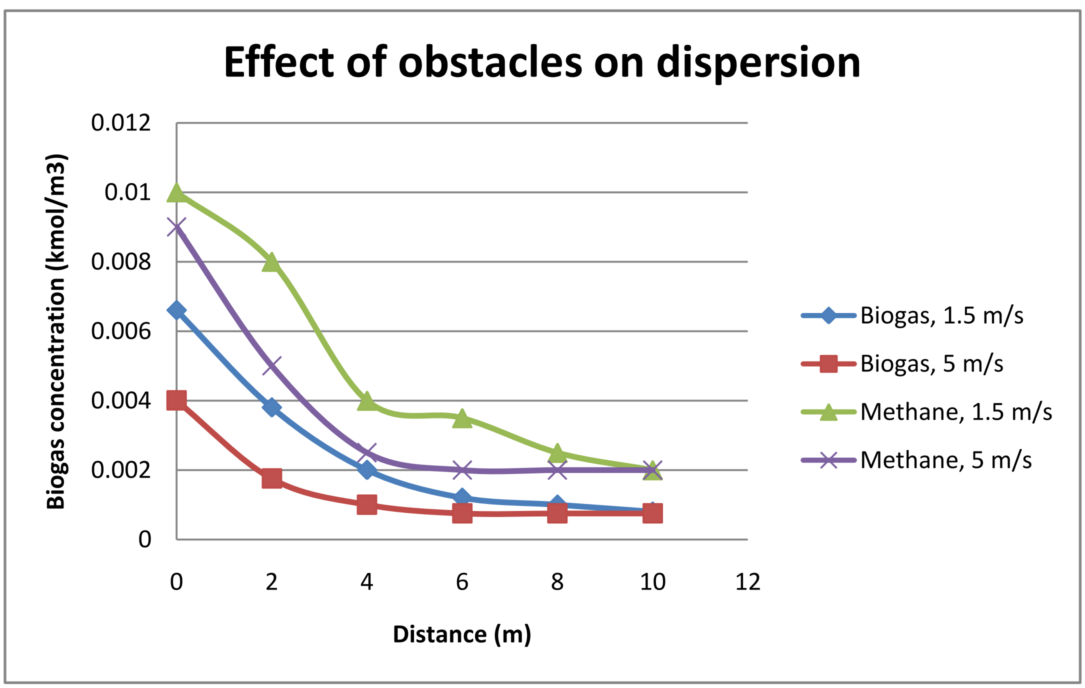

Figure 4.8: Effect of obstacle on biogas and methane dispersion.

4.2.3 Assessment of hazardous distance

A further understanding on the hazardous distances resulted from biogas and methane released is needed in order to implement suitable and effective safety measures. For the location of safety measures like gas detectors, it is advisable to place the detectors within the flammable region to ensure the effectiveness.

The assessment is done through simulation for the two gases considering the wind speed and presence of obstacle. Hazard downwind distance is compared between pure methane gas and biogas. Figure 4.9 shows the hazardous distance comparison. In overall, pure methane gas has longer hazard distance as compared to biogas. This is due to its higher composition of methane component. For obstructed scenario where there is the presence of obstacle, the hazardous distance is affected. For biogas, the flammable region stops at the location of the obstacle. Beyond the obstacle, although the vapor cloud still exists, the region is not within flammability limit.

On the other hand, methane gas dispersion is not affected much by the obstacle. The hazardous distance in lower wind speed has insignificant changes. However, for higher wind speed, the hazardous distance decreases. The larger wind force contacting with the obstacle where the concentration of methane gas accumulation is large carries the gas upward into the atmosphere. The gas flows upward instead of staying on the ground level. This is different with biogas as biogas has lower methane composition where the gas concentration is diluted easily to drop outside of the flammability limit.

In order to further ensure the validity of the hazardous distance, the changes of hazard downwind distance with release time is also evaluated. Figure 4.9 and Figure 4.10 are constructed from the data obtained from simulation done from gas release after 20 seconds and 10 minutes respectively. Same behavior of the hazardous distance is observed from the result. The results show that there is not much deviation of the hazard distance. So, time influence is negligible. However, the longer hazardous distance should be considered when placing the gas detectors.

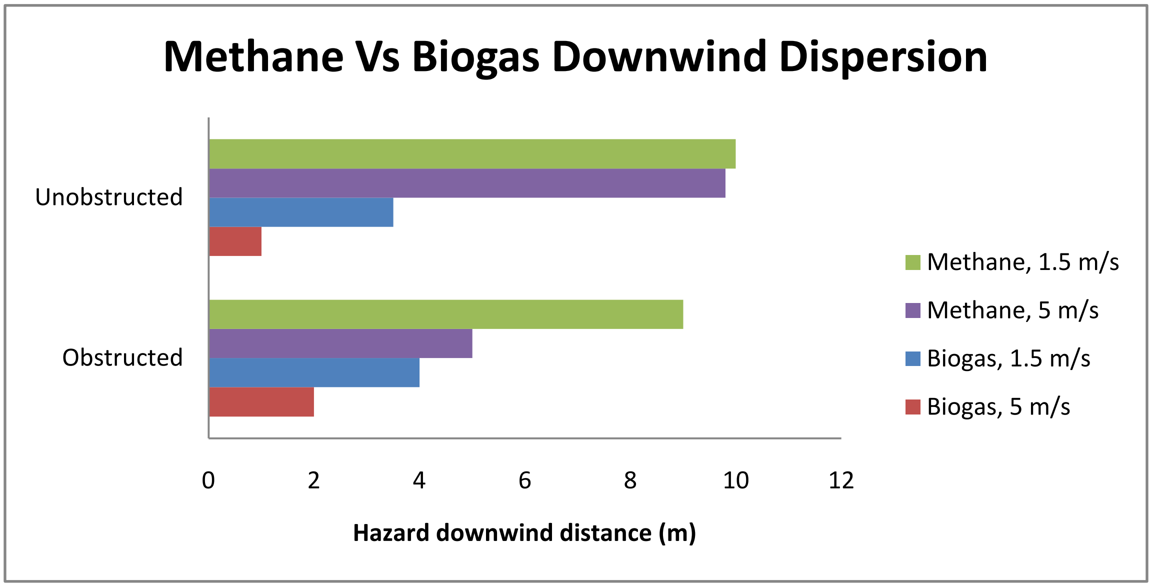

Figure 4.9: Hazard downwind distance for biogas dispersion after 20 seconds.

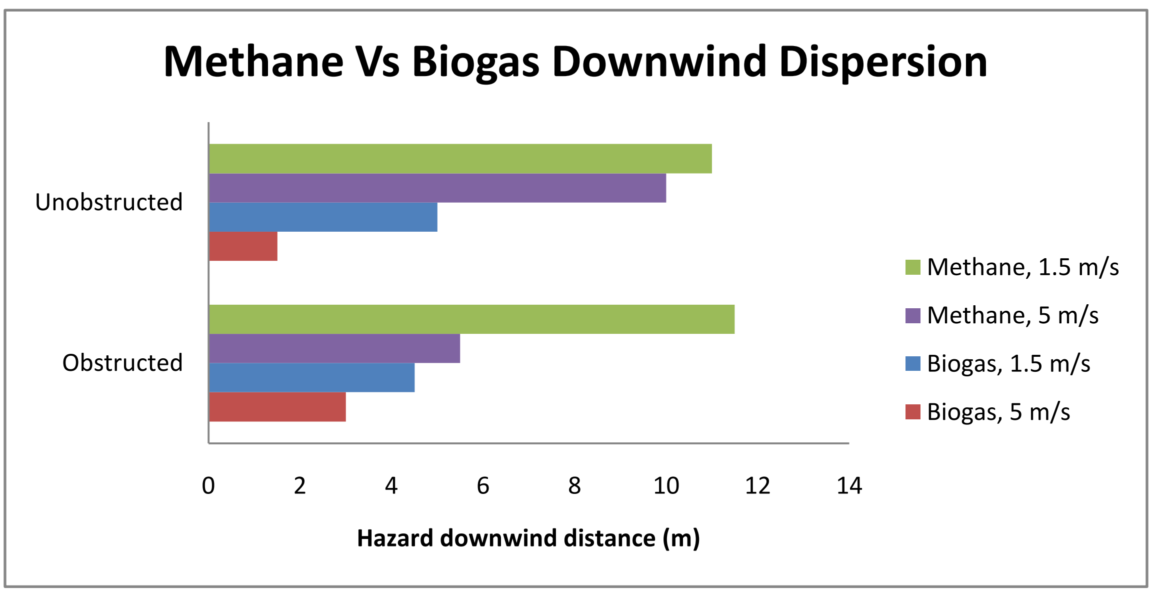

Figure 4.10: Hazard downwind distance for biogas dispersion after 10 minutes.

4.3 Case Study:PHAST

PHAST is a standard code of risk analysis that is often used for quantitative risk assessment. The case study is done by using PHAST to evaluate the hazardous distance for biogas released. PHAST generally does not consider the influence of complex geometry (Wilkening & Baraldi, 2007). The result from PHAST is compared to the unobstructed scenario generated by FLUENT as shown in Figure 4.11.

The result shows that there is some deviation of the hazardous distance generated by PHAST and FLUENT although the input of the inventory, the release scenario and the atmospheric condition are the same. For pure methane gas, the two softwares show close agreement for the hazardous distance with some allowance of error. However, for biogas, the results are not in agreement as expected.

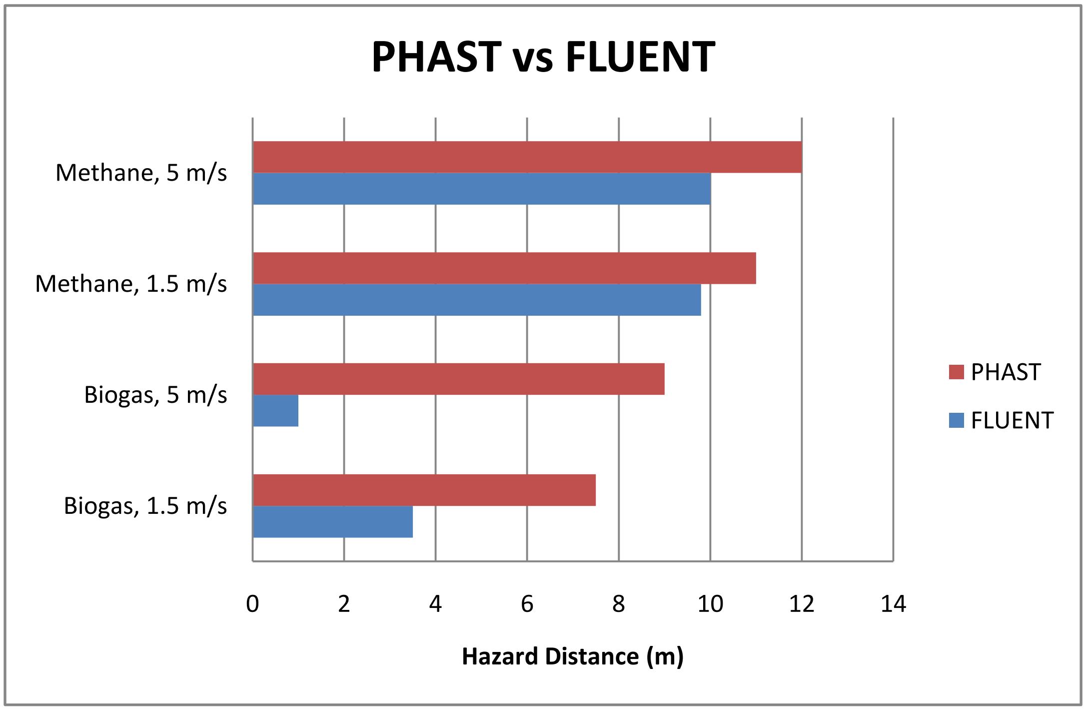

Figure 4.11: Hazard downwind distance comparison between PHAST and FLUENT.

To understand about the large difference between the PHAST and FLUENT's hazardous distance, the difference in the gas composition is the main factor that should be discussed. PHAST and FLUENT present close agreement in hazardous distance for pure methane gas which reflects that the two codes are reliable and suitable for simulation involving pure chemical only. Biogas is a combination of two chemical species which are methane and carbon dioxide. As the assessment stressed on the flammable region, the difference in the hazardous distance for biogas release show that the influence of carbon dioxide to the hazardous distance is significant. However, among PHAST and FLUENT, there is no justification yet to indicate which software can point out the influence of carbon dioxide to the flammable region efficiently. It is suggested to have future study on the release of gas mixture simulated by both softwares.

4.4 Recommendation

The hazardous distance which is mentioned in this study only involve the flammability region resulted from methane gas dispersion. However, biogas contains 40% of carbon dioxide which should be considered critically. Carbon dioxide has been recognized as one of the crucial workplace hazard due to its toxicity. Carbon dioxide has a higher density than air at approximately 1.98 kg/m^3 which makes it a dense gas that will likely accumulate on the ground level instead of being positively buoyant like methane. The toxicity of carbon dioxide is related to its concentration and time of exposure. Besides, carbon dioxide poses a health threat as inhalation of this gas can cause asphyxiation which replaces the oxygen in human body down to dangerous low level. Acidity of blood might happen and bring adverse effect on respiratory, cardiovascular and central nerve systems. Thus, the hazardous distance from dispersion of biogas should be evaluated in term of toxicity of carbon dioxide as well.

Secondly, with regard to the problem of disagreement that is mentioned in Section 4.3 on hazardous distance of biogas dispersion, another alternative model is suggested to be studied which is Multiphase Model. Multiphase model is capable of simulating matters with different chemical substances but with the same phase which describe the composition of the biogas. There are three different types of Multiphase model which are Volume of Fluid (VOF), Mixture and Eulerian. However, the main goal will be to identify the validity of the dispersion model to simulate biogas dispersion that considers the effect of carbon dioxide in the mixture.

Thirdly, in this project, there is only one particular hole leaking size and one release rate is studied. In reality, there are many leaking and release condition that can happen anytime. Thus, different leaking size and release rate should be studied as a reference database.

CHAPTER 5: CONCLUSION

Process safety is a crucial issue in biogas industry. Biogas has different composition as compared to pure methane gas. Biogas consists of 60% methane and 40% carbon dioxide. The CFD gas dispersion model developed using FLUENT has been validated against IP Model Code and PHAST with an error less than 25% which is acceptable. The dispersion model is used for biogas release consequence analysis.

Influence of wind speed and the presence of obstacle on gas dispersion are studied. Lower wind speed will pose higher risk of fire and explosion due to stable atmospheric turbulence. Higher wind speed will enable the dilution of gas concentration at faster rate. For the presence of obstacle, the gas is easily trapped in front of the obstacle which creates flammable region. The hazardous distance from pure methane gas and biogas dispersion is assessed. From the simulation results, biogas shows shorter hazardous distance as compared to that of methane gas. It can be explained as the lower composition of methane in biogas. Biogas is less flammable than pure methane gas. In conclusion, the objectives of the project are met where the biogas dispersion is studied and the hazardous distance is assessed.

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