

**DISPERSION STUDY OF HYDROGEN GAS RELEASE VIA  
PIPELINE NETWORK USING COMPUTATIONAL FLUID  
DYNAMIC APPROACH**

By

**Wan Muhammad Aizat Bin Wan Abdullah**

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

MAY 2012

Universiti Teknologi PETRONAS  
Bandar Seri Iskandar  
31750 Tronoh  
Perak Darul Ridzuan

**CERTIFICATION OF APPROVAL**

**DISPERSION STUDY OF HYDROGEN GAS RELEASE VIA  
PIPELINE NETWORK USING COMPUTATIONAL FLUID  
DYNAMIC APPROACH**

By

Wan Muhammad Aizat Bin Wan Abdullah

A project dissertation submitted to the  
Chemical Engineering Programme  
Universiti Teknologi PETRONAS  
in partial fulfilment of the requirement for the  
BACHELOR OF ENGINEERING (Hons)  
(CHEMICAL ENGINEERING)

Approved by,



(Dr. Risza Bte. Rusli)

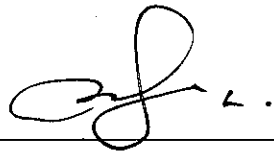
UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

MAY 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.



---

**WAN MUHAMMAD AIZAT BIN WAN ABDULLAH**

## **ABSTRACT**

Use of hydrogen is continually growing and there will be widespread of plants installation with high capacity storage. For the next few years, use of hydrogen will be demanding in the context of hydrogen economy. For economical reason, huge amount of hydrogen will be produced in large scale facilities and most likely distributed via pipeline network. Hydrogen has the widest explosive or ignition mix range in air where a in certain critical condition it may lead to an explosion. Hence, a high-momentum release likely to produce huge amount of thermal energy to be released into the environment. Thus, it is crucial to study the resulted consequences of high-momentum of hydrogen accidental release via pipeline. By using a FLUENT-CFD tool, it considers various kind of turbulence and dissipation model of hydrogen on the dispersion process. In this paper, realizable k-epsilon model will be used as it ability to provide superior performance for flows involving rotation, boundary layers under strong adverse pressure gradients, separation, and recirculation. The aim of this paper is to study the hazard region from release of hydrogen by encountering two parameters that affect the dispersion process which refers to wind velocity and obstacle. From the result, wind speed affects the flammability limit region of hydrogen-air mixture at certain extent. The result of the simulated model will be compared with the experimental data conducted by Hydrogen Pipe Break Test (HPBT) as a validation of hydrogen dispersion model.

## **ACKNOWLEDGEMENT**

Alhamdulillah praises to The Almighty Allah for blessing me with the strength and health towards completing this project. It is a pleasure to thank the many people who made this thesis possible. First and foremost, I would like to say a million of thankfulness to my supervisor, Dr. Risza Bte Rusli who has been very supportive from the beginning to the end of the project. Her patience and support rendered to me is greatly appreciated and is contributory to the success of the research. Much appreciation is also accorded to Dr Anis Suhaila, FYP coordinator who has given much needed guidance and advice on the Final Year Project (FYP).

My utmost appreciation goes to my family and friends who inspired, encouraged with never ending prayers and fully supported me for every trial that come in my way. Their advices will always be remembered and become the motivation in continuing the journey of my life. The love, support and precious time together has made this journey more meaningful.

# TABLE OF CONTENTS

<b>ABSTRACT</b> .....	<b>iv</b>
<b>ACKNOWLEDGEMENT</b> .....	<b>v</b>
<b>CHAPTER 1 INTRODUCTION</b> .....	<b>1</b>
1.1 Background of Study .....	1
1.2 Problem Statement .....	2
1.3 Objective .....	2
1.4 Scope of Study .....	3
<b>CHAPTER 2 LITERATURE REVIEW</b> .....	<b>4</b>
2.1 Hydrogen safety .....	4
2.2 Code description of FLUENT CFD tool .....	6
2.3 Turbulence model.....	7
2.3.1 Transport Equation for Realizable k-epsilon model.....	7
2.4 Validation of CFD-model for hydrogen dispersion .....	8
<b>CHAPTER 3 METHODOLOGY</b> .....	<b>10</b>
3.1 Research Methodology .....	10
3.1.1 Identify and study the experimental activity.....	11
3.1.2 Model geometry development .....	12
3.1.3 Model meshing.....	13
3.1.4 Identify boundary profile condition .....	14
3.1.5 Model validation .....	16
3.1.6 Model dispersion study.....	17
<b>CHAPTER 4 RESULT AND DISCUSSION</b> .....	<b>18</b>
3.2 Model meshing.....	18
3.3 FLUENT Analysis Results .....	20
3.3.1 Model validation .....	20

3.4	Dispersion study .....	23
3.4.1	Influence of wind speed.....	24
3.4.2	Influence of obstacle.....	24
<b>CHAPTER 5 CONCLUSION AND RECOMMENDATION .....</b>		<b>27</b>
<b>REFERENCES .....</b>		<b>29</b>
<b>APPENDICES .....</b>		<b>30</b>
APPENDIX 1-1: VISCOUS MODEL .....		31
APPENDIX 1-1: SPECIES MODEL.....		32
APPENDIX 2-1: FUEL INLET .....		33
APPENDIX 2-2: WIND INLET .....		34
APPENDIX 2-3: PRESSURE OUTLET .....		35
APPENDIX 3-1: SOLUTION METHOD.....		36
APPENDIX 3-1: SOLUTION CONTROL .....		37

## LIST OF TABLE

Table 1: Properties comparison between hydrogen and natural gas .....	4
Table 2: Geometry dimension .....	13
Table 3: Boundary condition properties .....	16
Table 4: Mesh properties .....	20
Table 5: Percentage of error for model validation .....	22



## LIST OF FIGURES

Figure 1: Ignition energy and flammability limits of hydrogen, gasoline and natural gas by vol% .....	5
Figure 2: HPBT pilot plant.....	11
Figure 3: 2-D Model geometry.....	13
Figure 4: Model meshing .....	14
Figure 5: Boundary naming .....	15
Figure 6: Geometry for consequence study .....	18
Figure 7: Grid display (a) model validation (b) with obstacle .....	19
Figure 8: Contour of molar concentration of H <sub>2</sub> .....	21
Figure 9: Graph molar concentration vs distance for model validation .....	22
Figure 10: Contour for flammability limit .....	23
Figure 11: Graph of molar concentration H <sub>2</sub> (LFL) vs distance .....	24
Figure 12: Contour of molar concentration H <sub>2</sub> within flammability limit (a) with wind (b) no wind .....	25

# CHAPTER 1

## INTRODUCTION

### 1.1 Background of Study

There is a large interest in the possibility of using hydrogen as an energy carrier, especially growth in global concern about the impact of greenhouse gases and the finite nature of fossil fuel reserves (O.R. Hansen, 2010). By concerning the potential of hydrogen as energy carrier, a lot of safety investigation involved hydrogen application has been developed in oil and gas industry. There are many hydrogen generation plants that are design to continuously produce hydrogen at certain capacity.

Faulty of equipments or human error are the major concern that contributes to incidents. Hence, the consequences of the hydrogen gas release may affect property damage and for serious cases leads to fatality. In 2007 a chemical plant that produces sodium chlorate for bleaching pulp and paper are explode within the hydrogen processing system where hydrogen is produced as secondary product (O.R. Hansen, 2009). After operating with the increased oxygen level and the hydrogen concentration below the UFL for several hours, the hydrogen ignited and an explosion occurred in the system. The explosion caused extensive damage to piping, process vessels and the containment building (O.R. Hansen, 2009).

Prior to the incident, risk and safety studies can be conducted to evaluate the significance of potential hazard or incident incurred of a hydrogen plant. Furthermore, potential hazard posses by hydrogen gas release are well-known and it is expected to demonstrate the consequence.

With the increasingly hydrogen production and application in oil and gas industry, it is important to conduct a consequence study of hydrogen gas release and to observe the effect of subsequent release towards environment and surrounding area.

## **1.2 Problem Statement**

Currently, there are a lot of studies have been conducted to evaluate the potential risk and impact of hydrogen release. For example, hydrogen release for automotive scenarios, hydrogen release in hydrogen energy station, hydrogen release in a private garage, and release of hydrogen in pressurized vessel.

However, the use of hydrogen is increasing in the context of the so-called hydrogen economy. For economical reasons large amounts of hydrogen will be produced in large-scale facilities and distributed most likely via pipeline networks. There are no large field experimental site conducted for hydrogen release such as Kit Fox model (carbon dioxide) and Prarie Grass model (propylene), only laboratory experimental study had been done. Since the experimental approach is not feasible because of unaffordable costs (H. Wilkening, 2007).

Furthermore, smaller quantities of hydrogen are produced on-site or delivered by road tanker. With the potential of hydrogen as energy carrier, it may require a pipeline network like natural gas pipelines to transport the gas. Hence, new technology requires responsible care approach asking industry and public authorities to protect people, environment and property.

Therefore, it is very significant to carry out a study of hydrogen release in a pipeline networks using a numerical simulation tool such as Computational Fluid Dynamics (CFD). Also it is important to observe how the release would affect differently and studying the details of the release jet.

## **1.3 Objective**

1. To develop a simulation of the accidental hydrogen release from a pipeline using FLUENT CFD tool.
2. To compare the result using FLUENT model against the experimental data.
3. To study the trend of dispersion of released gas and flammability limit region in the effect of wind velocity and presence of obstacle.

#### **1.4 Scope of Study**

Generally, the aim of this work is to be able to investigate the trend of gas dispersion from numerical point of view by developing a 2D simulation of hydrogen release via a pipeline network using FLUENT CFD tool. The result obtained from FLUENT CFD tool will be compared against an experimental activity as purpose of model validation.

Prior to the experiment, several simulations to predict the outcome of the experiment were modelled using FLUENT. To conduct the simulation of the experiment, a simple physical geometry needs to be defined. The model will be consisting of a horizontal release point, obstacle, wind inlet and pressure outlet.

A comprehensive model might be able to simulate the result obtained by using FLUENT. The validated model will be further use to study the hazard region in the effect of wind speed and obstacle for hydrogen release via a pipeline network.

## CHAPTER 2

### LITERATURE REVIEW

#### 2.1 Hydrogen safety

The growing use of hydrogen in our society requires a scientific and suitable basis for the evaluation of credible safety issues. This aspect will become progressively very important because of the widespread installation of plants with high capacity storages in several towns as automotive refuelling stations (M.N. Carcassi, 2010). Moreover as we all know, hydrogen is a highly flammable substance and in case of fire or explosion the consequences can become serious under certain conditions. Plus, hydrogen has the widest explosive or ignition mix range with air of all the gases. With the mix proportion between air and hydrogen, a hydrogen leak will likely to lead to an explosion.

With the conjunction of hydrogen economy capability, a high pressure of gas compression is likely to be considered during transporting the hydrogen gas thus increasing gas pressure would improve the energy density. Thus in comparing the hydrogen as the energy carrier for the future to replace natural gas, more safety attention needs to be focused on the consequences or the impact that may resulted. This can be verified by looking at the properties of hydrogen as tabulated below.

**Table 1: Properties comparison between hydrogen and natural gas (B.B Borner, 2008)**

No.	Properties	Hydrogen	Natural Gas
1.	Colour	None	None
3.	Impact – Fuel	None	CO <sub>2</sub> /NO <sub>x</sub>
4.	Diffusion Coefficient (cm <sup>3</sup> /s)	0.61	0.15
5.	Flame Temperature (°C)	2318	2148
6.	Flammability Range (% in air)	4% - 75%	5.3% - 15%

With such properties, hydrogen can be classified as a fuel that is that is capable to massive impact to environment if fire or explosion incident occur. Besides having a high flammability range, hydrogen also has high detonable range which is about 18.3% - 59% by volume in air. Furthermore, hydrogen has two times heating value compared to natural gas. Higher heating value will be very hot and carry high energy compared to same amount of mass that release in air. With low ignition energy value at 0.02mJ, it has a tendency to ignite before large energy accumulation. Figure below shows the ignition energy of hydrogen, gasoline and natural gas with air. It can be conclude that flammability limits of hydrogen are seven times wider than natural gas.

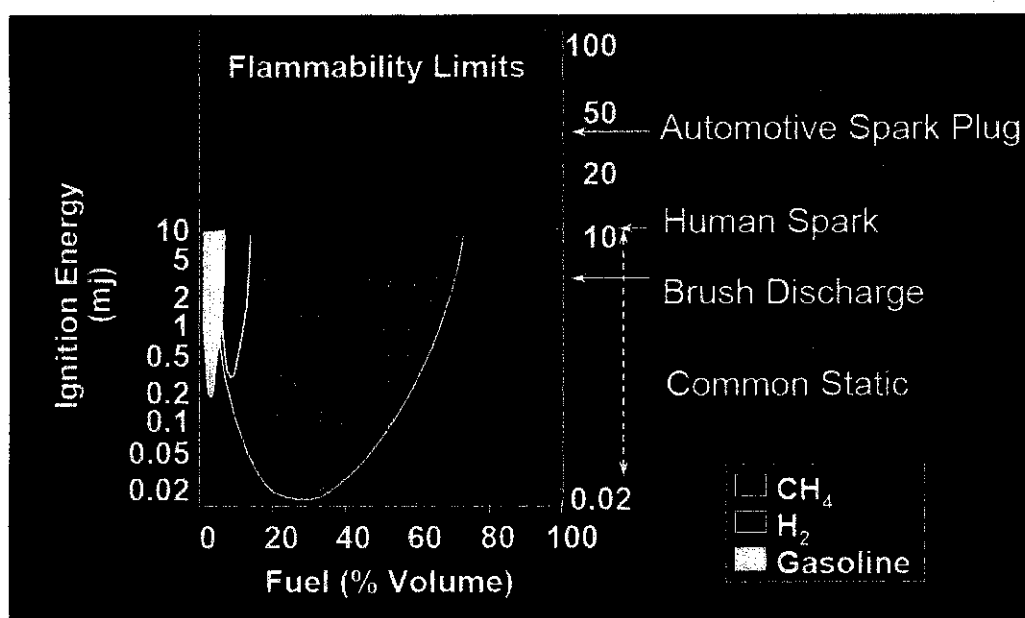


Figure 1: Ignition energy and flammability limits of hydrogen, gasoline and natural gas by vol% (B.B Bonner, 2008)

By judging the use of hydrogen as an alternative source of energy, some countries had successfully converted existing natural gas pipeline to hydrogen pipeline (B.B Bonner, 2008). Hence, several standards and regulation on pipelines had been imposed. Several environmental impact studies have been conducted to designate additional design condition. This is to ensure pipeline application to transport the hydrogen gas will not be an issue towards the health and environment.

## 2.2 Code description of FLUENT CFD tool

Computational Fluid Dynamics (CFD) tools have increasingly begun to play an important role in risk assessments for the process industry. While CFD-based consequence analyses have largely been limited to the oil and gas industry in the past, it is expected that these kinds of calculations will be used more and more for safety investigations for hydrogen applications (P. Middha 2007). There is a huge significant in application of CFD tools in risk and safety studies. The ability to consider various kinds of boundary conditions, turbulence kinetic model, dissipation rates, physical geometry etc make the consequence predicted from CFD tool is comparable with the realistic cases that might be occurred.

A computer models for calculating gas dispersion within the atmosphere have been available for many years and are generally applicable over scales of up to about 50 km of release (A. Riddle et al, 2004). One such model, Atmospheric Dispersion Modelling System (ADMS) uses current understanding of the structure of the atmospheric boundary layer (Carruthers, 1994). However, ADMS only can simulate on the movement and dispersion of gas. It is not able to assess the local effects on the flow field and turbulence of the gas.

Commercial CFD software such as FLUENT offers a method of modelling flow and dispersion around groups of building. Like other CFD code, its offers the flexibility to represent complex geometries and predict the air flow with varying resolution. In addition, FLUENT offers various grid resolutions which maximize the simulation flow of the importance region. It also provides detailed output of flow fields, turbulence levels and concentration fields generated around the model.

FLUENT CFD code particularly follows a general deterministic procedure to approximate the problem; it considers the fundamental governing equations for mass, momentum, and heat transfer processes, in conjunction with other partial differential equations for describing further processes such as turbulence (J.W. Hwang, 2007). This described the ability of FLUENT code in simulating the dispersion and turbulence model.

## 2.3 Turbulence model

One of the main factors influence the dispersion of the gas release is turbulence model. A correct choice of turbulence model is crucial to a successful implementation of CFD in the modelling. Few turbulence models have been widely used such as k-epsilon (standard), k- $\omega$  (standard), shear stress transport, SSG-Reynolds stress, and realizable k-epsilon (S.A. Abassi, 2010). There are numerous attempts was made to determine the effective turbulent viscosity in simulating the dispersion of a negatively buoyant gas in the presence of obstacle. For example, Sklavounos and Rigas (2004) compared the simulation results by employed four different turbulence models: k-epsilon (standard), k-omega (standard), shear stress transport (SST), and SSG-Reynolds stress (SSG-RSM). They concluded that SSG-RSM provided the best fit while the k-epsilon model were slightly less than the experimental data and had the advantage requiring less-computational time than SSG-RSM (S.A. Abassi, 2010).

### 2.3.1 Transport Equation for Realizable k-epsilon model

The transport equation for k and epsilon in realizable k-epsilon model are

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_j}(\rho k u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_k} \right) \frac{\partial k}{\partial x_j} \right] + G_k + G_b - \rho \epsilon - Y_M + S_k$$

$$\frac{\partial}{\partial t}(\rho \epsilon) + \frac{\partial}{\partial x_j}(\rho \epsilon u_j) = \frac{\partial}{\partial x_j} \left[ \left( \mu + \frac{\mu_t}{\sigma_\epsilon} \right) \frac{\partial \epsilon}{\partial x_j} \right] + \rho C_1 S \epsilon - \rho C_2 \frac{\epsilon^2}{k + \sqrt{\nu \epsilon}} + C_{1\epsilon} \frac{\epsilon}{k} C_{3\epsilon} G_b + S_\epsilon$$

$$C_1 = \max \left[ 0.43, \frac{\eta}{\eta + 5} \right], \quad \eta = S \frac{k}{\epsilon}, \quad S = \sqrt{2 S_{ij} S_{ij}}$$

In these equations,  $G_k$  represents the generation of turbulence kinetic energy due to the mean velocity gradients,  $G_b$  is the generation of turbulence kinetic energy due to buoyancy.  $Y_M$  represents the contribution of the fluctuating dilatation in



compressible turbulence to the overall dissipation rate.  $\sigma_k$  and  $\sigma_{\epsilon}$  are the turbulent Prandtl numbers for  $k$  and  $\epsilon$  where it is defined as constant with value of  $\sigma_k = 1.0$  and  $\sigma_{\epsilon} = 1.2$ . The  $C_1$  and  $C_2$  are held constant with value of 1.44 and 1.9.

In another study, Gavelli, bullister, and Kytomaa (2008) simulated the test in the “Falcon” series of LNG spill tests using CFD. Turbulence was modelled using the standard  $k$ - $\epsilon$  model inline with Reynold stress model (RSM). Again, standard  $k$ - $\epsilon$  model give the best solution of the turbulence. However compared to the above mentioned turbulence models used by different authors, the realizable  $k$ - $\epsilon$  model was introduced but hasn’t surprisingly been explored till recently (S.A. Abassi, 2010). This model differs from the standard  $k$ - $\epsilon$  model in two important ways:

- i. Realizable  $k$ - $\epsilon$  model contains a new formulation for turbulence viscosity.
- ii. A new transport equation for the dissipation rate has been derived from an exact equation for the transport of the mean square vorticity fluctuation.

The realizable  $k$ - $\epsilon$  model is one of the prominent turbulence prediction tools implemented in many general purpose CFD codes. The realizable  $k$ - $\epsilon$  model is also likely to provide superior performance for flows involving rotation, boundary layers under strong adverse pressure gradients, separation, and recirculation (ANSYS, 2009). With such properties or elements countered, numerous validations on gas dispersion by using CFD has been encountered by applying the realizable  $k$ - $\epsilon$  model. Thus, used of realizable  $k$ - $\epsilon$  model provide better accuracy and precision in the CFD based simulation of turbulence.

#### **2.4 Validation of CFD-model for hydrogen dispersion**

Hydrogen is being considered to form the first sustainable energy system. Hydrogen infrastructure consisting of generation, storage tanks, transportation facilities and dispensing facilities is already continually developing. Nowadays hydrogen is mainly distributed by trailers, mobile fueler, gas tube trailer and liquid tank trailer. In concern of hydrogen as an alternative source of energy, the

distribution of hydrogen is likely by means of pipelines. This is more suitable for larger amounts of hydrogen are produced on industrial scale.

There are ranges of experiments conducted by parties concerned to study the consequence of hydrogen gas release. All these experiments are well-validated with CFD simulations including low-momentum releases in a garage, subsonic jets in a garage with stratification effects and subsequent slow diffusion, low momentum and subsonic horizontal jets influenced by buoyancy, free jets from high-pressure vessels and liquid hydrogen releases are also considered (O.R. Hansen, 2009). All of these validated experiments were conducted to demonstrate only for small scale use of hydrogen.

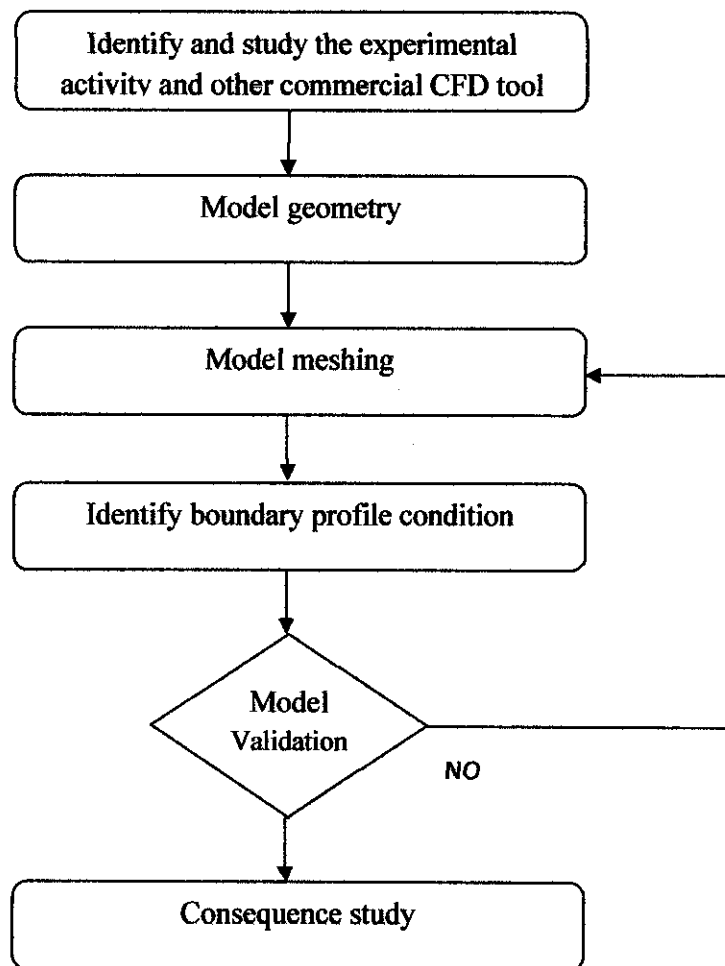
Therefore from safety point of view it is essential to conduct a simulation model resulted from pipeline release where use of hydrogen pipelines is well establish today. Prior to this issue, an experimental activity conducted by the Department of Energetics of Politecnico of Torino with the collaboration of the University of Pisa study the hydrogen release and atmospheric dispersion via pipeline (M.N. Carcassi, 2010).

Some of the experiments are validated by using simplified tools for dispersion and explosion predictions. It is normally not very useful in order to get the best estimation or prediction of dispersion as they lack the ability to model the physical well for performing proper consequences modelling.

## CHAPTER 3 METHODOLOGY

### 3.1 Research Methodology

Basically the research methodology can be divided into three processes which are pre-processing, solving and post-processing. Pre-processing process consist of model geometry development, model meshing and boundary set-up condition. All equations use for the computation process will be considered in solving process. Finally, post-processing process concern more on the analysis work on the result generated. It is important to analyse the result in order for us to retrieve more accurate result by do checking and repair on the model meshing or boundary identification.



### 3.1.1 Identify and study the experimental activity

Generally several simulation models, whether or not concerned with fluid dynamics, used in safety and risk studies are validated in the past for hydrogen use. Since this paper is to study the accidental hydrogen release from pipeline, it is required to look for an experimental activity that investigates the behaviour of hydrogen leakage from pipeline. Once an experimental activity has been decided, all experiment set-up need to be understand thoroughly. Normally, there are some tests run conducted during the experiment and the most stable and uniform result will be taken as reference to compare with the simulation results. Next, the experiment configuration and properties encountered during the experiment need to be identified clearly. This is to ensure the model is meshed accordingly and the condition considered during the experiment in taken into account. For example, the variation discharge orifices diameter and discharge pressure values during the experimental activity are noted.

A pilot plant called Hydrogen Pipe Break Test (HPBT) was built to study the release. The apparatus consisted of a 12m<sup>3</sup> tank which was fed by high pressure cylinders. The maximum internal pressure was 1 MPa. A 50m long pipe moved from the tank to an open space and the far end of the pipe had an automatic release system that could be operated by remote control (M.N. Carcassi, 2010). The layout of the HPBT apparatus can be divided into four parts.

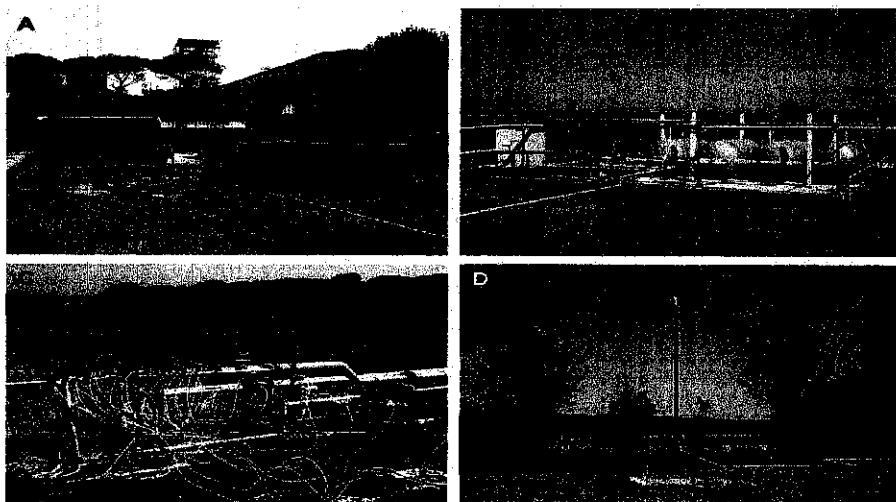


Figure 2: HPBT pilot plant

**a) Hydrogen and nitrogen storage:** There were two gas boxes the first housing the hydrogen banks; the second containing the nitrogen banks. Each bank consisted of 25 cylinders with an initial pressure of 20 MPa.

**b) Gas reservoir (test pressure):** Composed of four storage tanks  $3\text{m}^3$  each with a maximum working pressure of 1 MPa making it possible to store up to  $130\text{ Nm}^3$  of hydrogen. The reservoir was connected to the banks by a pipe of 2 in. (0.0508 m) internal diameter. The reservoir delivered hydrogen to the pipeline system by a discharge manifold.

**c) Pipeline system:** A pipe of 4 in. (0.102m) internal diameter and 50m long leading from the gas reservoir to an automatic release system (ARS) where the hydrogen leakage took place in an open field.

**d) Vent line:** 6 m high pipe of 2 in. (0.0508 m) internal diameter that was able to vent the gas when necessary.

### **3.1.2 Model geometry development**

Once the experimental set-up have been studied, it is important to study the geometry or condition encountered during the experimental activity. This is to ensure the simulation model are conducted as the real case scenario as the experiment. Hence, the simulation model geometry was constructed by using Design Modeller (DM). There are two important elements that need to be focused in constructing the model geometry which are fluid domain and release point domain.

The fluid domain are considered as the atmospheric area which has a fixed dimension while the release point domain refers to the leakage or hole diameter from a pipeline. The model geometry was constructed in 2-D as below. This model was constructed in 2-D in order to reduce the computational time in CFD analysis.

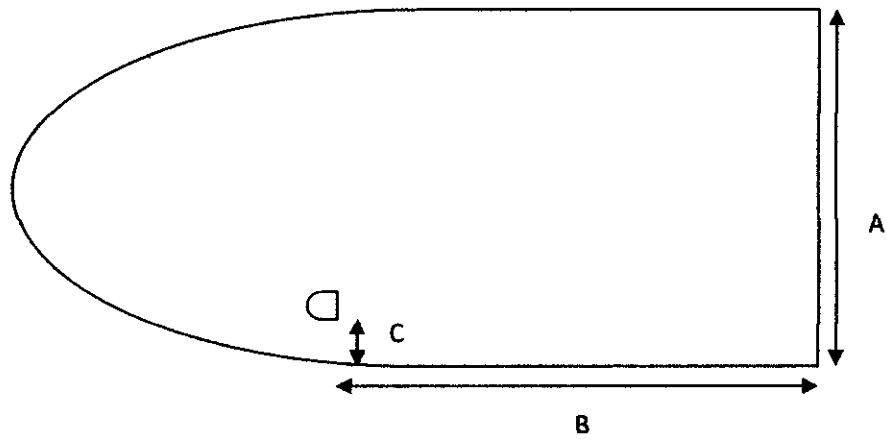


Figure 3: 2-D Model geometry

### 3.1.2.1 Geometry dimension

Table 2 described the dimension of model geometry as in metre. In addition, the case encountered in HPBT experiment is a horizontal release from a pipeline. However, the direction point of release is approximately horizontal because of slightly upward inclination which is about  $4^\circ$  due to erroneous installation during the experiment.

Table 2: Geometry dimension

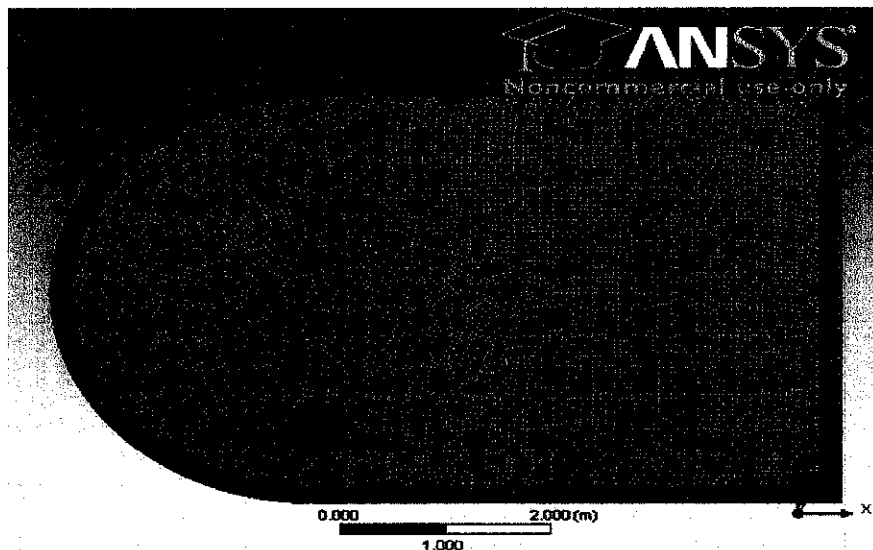
	Dimension (m)
Domain height (A)	5
Domain width (B)	10
Distance of release from ground (C)	0.9
Leakage diameter	0.011

### 3.1.3 Model meshing

Next is to mesh the model once the model geometry is finalized. The domain was carefully meshed in a manner which maximized the detailing of the importance region. Fine mesh and huge number of cell elements was applied near to the leak or release hole. As this is the point of interest to observe the molar concentration of  $H_2$  at 0.14m from the release point. Refinement command was used at the edge of

release hole, wind inlet, pressure outlet and wall as this command will automatically refine the importance region.

Meshing process in ANSYS basically consist of several meshing methods for 2-D geometry. Quadrilateral meshing methods was used as the interested methods. It is noted that the gas dispersed horizontally along x-axis, thus a very fine mesh was considered at every geometry boundary. By applying quadrilateral mesh type, four intersection points will be the calculation point to calculate the transport equation in FLUENT analysis. Figure 4 shows the final meshing for the model geometry by using ANSYS Mesh with total 5567 elements and 5387 nodes.



**Figure 4: Model meshing**

#### **3.1.4 Identify boundary profile condition**

After the meshing works completed, next process is solving process. Solving process plays an important role in CFD simulation where all the boundary condition considered during the experimental activity will be applied. At this point, realizable k-epsilon model was used instead of other turbulence model listed in FLUENT FD tool such as k-omega, or RSM model. For better convergence, the k and epsilon value was determined by manual calculation instead of default value set by

FLUENT. Basically, there are four boundaries condition prompted in FLUENT which are wind inlet properties, fuel inlet properties, pressure outlet properties and wall properties.

Figure 5 shows the location and named selection for the geometry boundary. As the wind flows from left to right of the geometry, wind inlet was specified at left-hand-side of the geometry. Pressure outlet was defined at the upper and far end of geometry. Release point was represented by the fuel inlet and wall represents the ground surface. Table 3 summarized the boundary condition properties considered in FLUENT analysis. The fuel inlet properties was considered as likely during the HPBT experimental activity where the initial release condition data was simulated exactly the same.

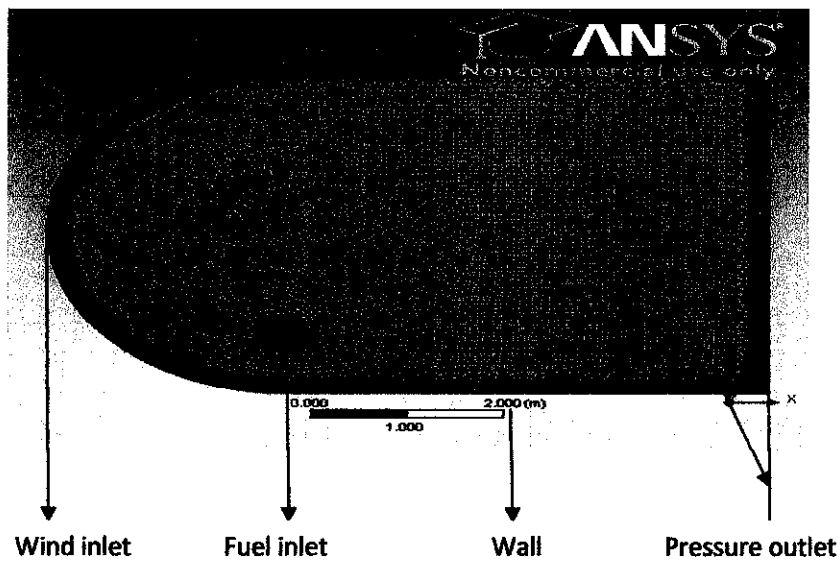


Figure 5: Boundary naming



**Table 3: Boundary condition properties**

	Wind inlet	Fuel inlet	Wall	Pressure Outlet
Velocity (m/s)	1	769.14	-	-
Initial gauge pressure (Pascal)	0	1000000	-	0
Temperature (K)	298	300	298	298
Mass fraction	0.0998 (Oxygen)	1 (Hydrogen)	-	0.0998 (Oxygen)
Turbulence kinetic energy ( $m^2/s^2$ )	1	1	-	1
Turbulence dissipation rate ( $m^2/s^3$ )	1	1	-	1
Velocity specification method	Magnitude, normal to boundary	Magnitude, normal to boundary	-	-
Reference frame	Absolute	Absolute	-	-

### 3.1.5 Model validation

For post-processing process, executed results will be evaluated. In order to determine whether the FLUENT simulation model is performing well, the concentration value from experimental work was compared against FLUENT model. If the value from simulated model is not close enough with the experimental data, hence some changes or modification works need to be done. Enhancement process is essential for model validation and it can be start with the model meshing refinement followed by the boundary profile condition identification.

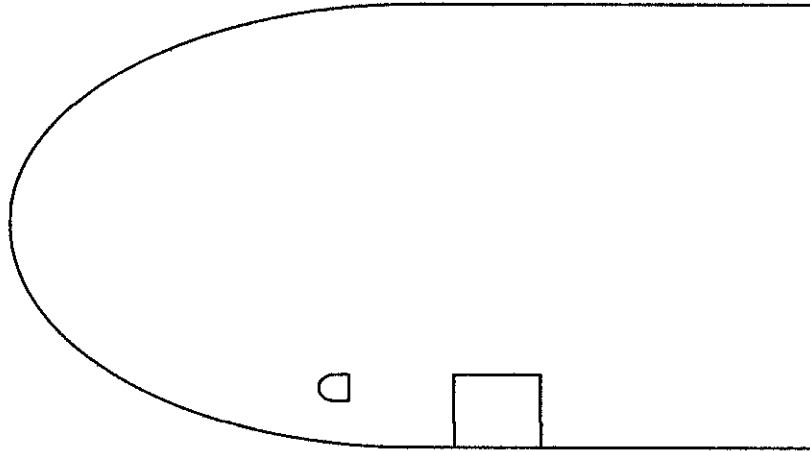
The target percentage of error for model validation is in a range between 10-20%. The molar concentration of  $H_2$  can be underestimated or overestimated from the experimental value. Thus once the result shows an error between 10-20% range, the simulated model will be used for the dispersion study.

### 3.1.6 Model dispersion study

After the FLUENT simulation model is validated, next is to conduct a dispersion and leakage study of hydrogen release through a pipeline. Before proceeding with the dispersion study, the lower flammability limit (LFL) and upper flammability limit (UFL) region of released hydrogen gas was evaluated. The flammability limit region was considered as the importance or hazard region of the simulated model. To determine the hazard region, the contour of molar concentration of H<sub>2</sub> generated by FLUENT was manually scale at 4-75% of hydrogen by volume in air yet this will execute the contour only without specifying at what distance does the flammability limit reach. Thus to determine the distance of flammability limit region, a graph molar concentration of H<sub>2</sub> vs distance downwind was plotted.

It is important to know the distance of flammability limit region to place the obstacle nearby to the region. An obstacle with 1m x 1m cuboid was located at furthest distance of the flammability region. The obstacle represents as any facilities such as storage tanks, pressure vessel and etc. to study the impact towards such facilities if the leakage of hydrogen via pipeline occurs. At this stage, new model geometry was constructed. Figure 6 shows the new geometry for consequence study with an obstacle located adjacent to release point.

In this study, there are two different parameters that are interested to be investigated; wind velocity effect and presence of obstacle. . On the other hand, wind velocity will affect the buoyancy and momentum on the release, thus it may affect the probability of ignition and the flame acceleration in case of ignition. Two wind speed condition was defined at 1m/s and 0m/s to study the trend of the dispersion of hydrogen cloud and concentration value around the cubical building. The presence of obstacle was expected to influence the flammability region, velocity magnitude and molar concentration value of H<sub>2</sub>.

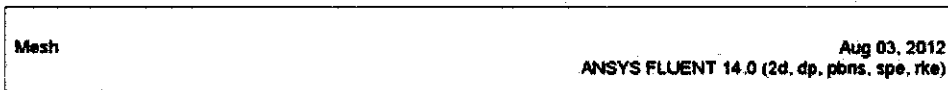
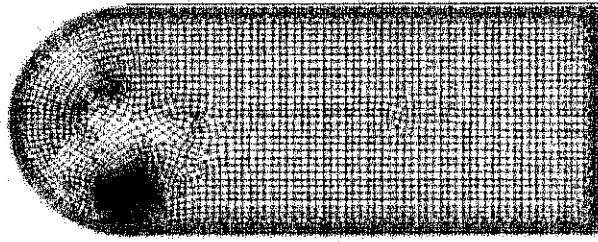


**Figure 6: Geometry for consequence study**

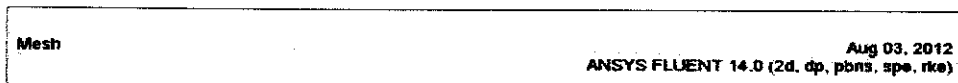
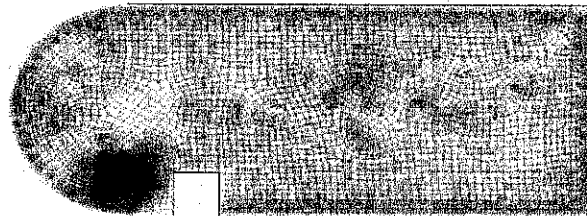
## **CHAPTER 4 RESULT AND DISCUSSION**

### **3.2 Model meshing**

Figure 7 shows the grid display of mesh generated using ANSYS Mesh total element number is 5148 and nodes number 5363 for (a) domain geometry. For (b) domain geometry the total element number is 5653 and nodes number is 5876. At point of release, a very fine mesh was applied to ensure the computational of energy and momentum calculation are done precisely. This is because the region around the release point was classified as the importance region to observe the molar concentration of  $H_2$  at this point.



(a)



(b)

**Figure 7: Grid display (a) model validation (b) with obstacle**

As the geometry was developed in 2-D, quadrilateral type of mesh was used. Quadrilateral mesh provided four intersection points as the calculation point for every transport equation that encountered in computational fluid dynamic tool. Thus, it will give the best result for this simulation model.

Table 4 shows the properties for both geometries are summarized as tabulated below. Based on the orthogonal quality, model mesh is in a good form as the element metrics value is close to 1.

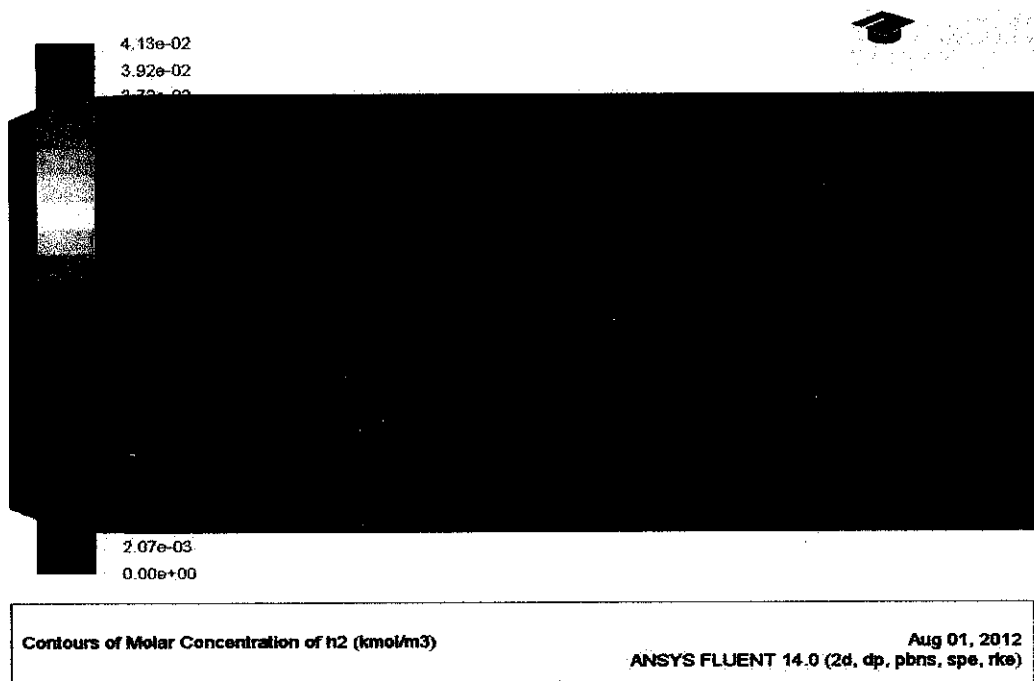
**Table 4: Mesh properties**

	<b>Geometry</b>	
	<b>(a)</b>	<b>(b)</b>
<b>Element metrics (min)</b>	0.56	0.62
<b>Element metrics (max)</b>	1	0.99
<b>Element metrics (average)</b>	0.98	0.98

### **3.3 FLUENT Analysis Results**

#### **3.3.1 Model validation**

Figure 8 shows the molar concentration of H<sub>2</sub> when hydrogen gas was discharged from the pipeline. With wind velocity 1m/s, the dispersion described the airborne transportation of plume gas along distance downwind. Highest molar concentration of H<sub>2</sub> recorded at the point of release with value of 931,169 ppm.



**Figure 8: Contour of molar concentration of H<sub>2</sub>**

The contour of the molar concentration of H<sub>2</sub> is critically observed to be along the ground. This might be because of the height of release point where it is only 0.9m above the ground level. Thus it is significantly affecting the ground-level concentration where the plume gas dispersed in a very short distance vertically. Since the simulation was done for a low-momentum release of hydrogen, the cloud formation was observed in a vertical motion after the plume gas travel at a short distance from the release point. This is because the dispersed gas does not acquire enough energy and low velocity to travel further downwind. Hence if the simulation was done for high-momentum release of hydrogen gas, the cloud formation is expected to be further away from the release point

This model was validated against experimental result from a pilot plant called Hydrogen Pipe Break Test (HPBT). Result generated by FLUENT are underestimated with molar concentration of H<sub>2</sub> value is 481260ppm at 0.14m distance the molar concentration value is 482160ppm. While the experimental data gives the molar concentration of H<sub>2</sub> value is 588000ppm. Table 5 shows the percentage of error which is about 18% differ from the experimental data. The error between the simulation model and experimental activity might be because of the

sensor located in the experimental activity is quite complicated and not parallel with the release point. In FLUENT, the molar concentration of H<sub>2</sub> was measured only above the ground and parallel with the point of release. However, since the percentage of error is within the acceptable limit (15-20%) the model was considered validated and used to conduct the dispersion study by encountering the influence of wind velocity and presence of obstacle.

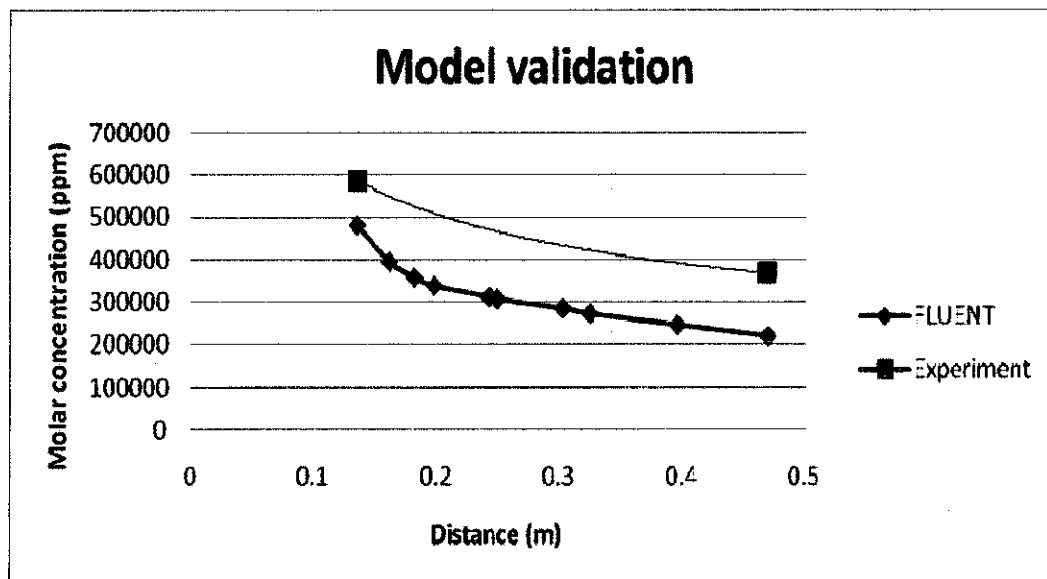


Figure 9: Graph molar concentration vs distance for model validation

Table 5: Percentage of error for model validation

Sampler position	FLUENT (ppm)	Experiment (ppm)	Error %
X4 (0.14m, 0m, 0m)	482160	588000	18

### 3.4 Dispersion study

Hydrogen has a very wide expansion of flammability limit which is at 4-75% by volume in air (Mao, 2005). Hence release of hydrogen through leakage from a pipeline may cause a very serious fire or explosion incident. For a worst case scenario, the explosive limit of hydrogen reported to be at 18.3-59% by volume. This may lead to a severe impairment towards properties installed nearby to the pipeline. Therefore the transportation distance (horizontal and vertical distance) of the flammability region was observed.

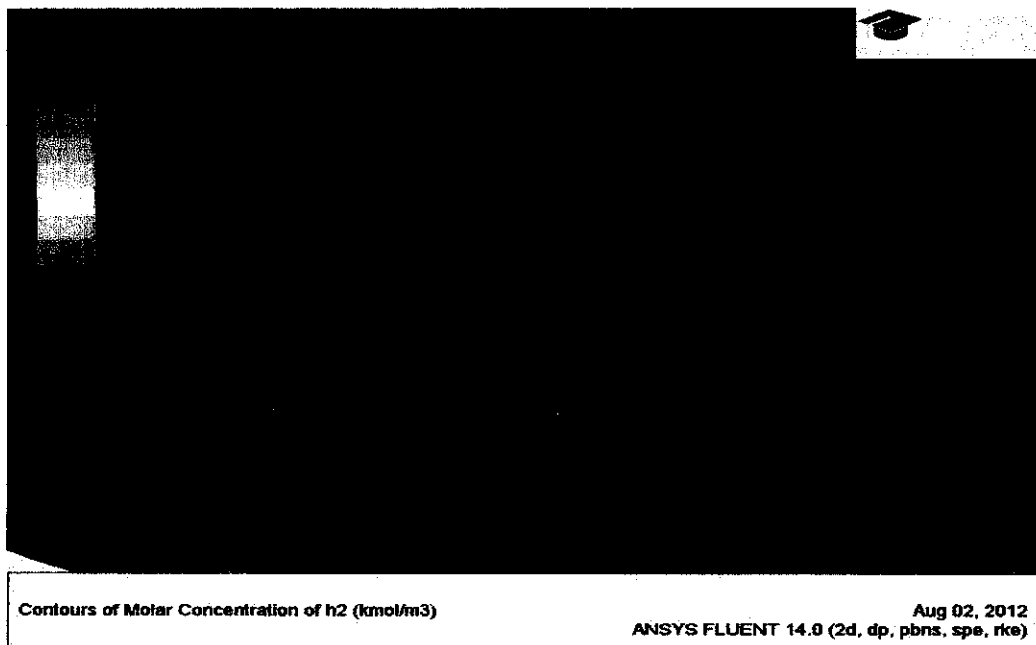


Figure 10: Contour for flammability limit

From figure above, it can be concluded that the experimental activity conducted by (F. Ganci, 2010) does not reach the upper flammability limit (UFL) which up to 75% volume by air. This is because the experiment was conducted only for small scale purpose where the mass of hydrogen release are likely low which is reported from HPBT experiment at 0.059 kg/s. However, released hydrogen gas did reach lower flammability limit (LFL) at 4%. Thus, the transportation distance of released gas towards atmosphere was observed. FLUENT executed the travel distance at LFL up to 0.9m along distance downwind. Therefore, this distance was classified as the hazard region and as a safety measure 0.9m radius from the point of release is the importance region thus safety attention are highly recommended to be focused on within this region.



### 3.4.1 Influence of wind speed

Figure 11 shows the molar concentration of  $H_2$  along downwind distance with the effect of wind speed. Basically the LFL region for both wind and no wind are same which is up to 0.9m. However, with the presence of wind the molar concentration of  $H_2$  tend to be decrease lower than no wind condition after the hydrogen gas travel 0.2m away from the release point. This can be described by the mixing of hydrogen-air mixture diluted faster by large quantity of air.

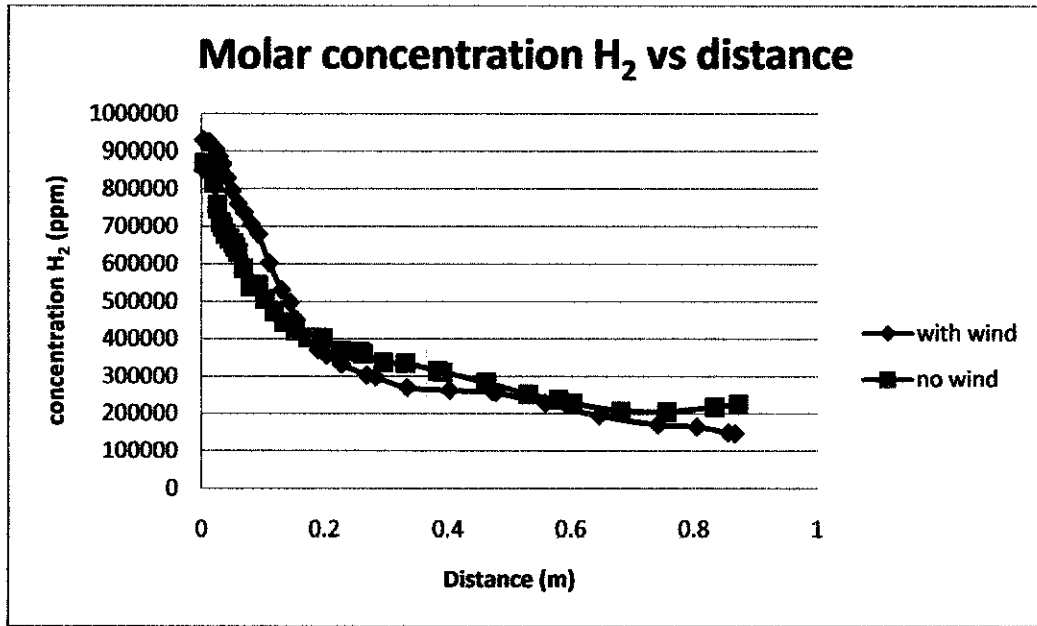
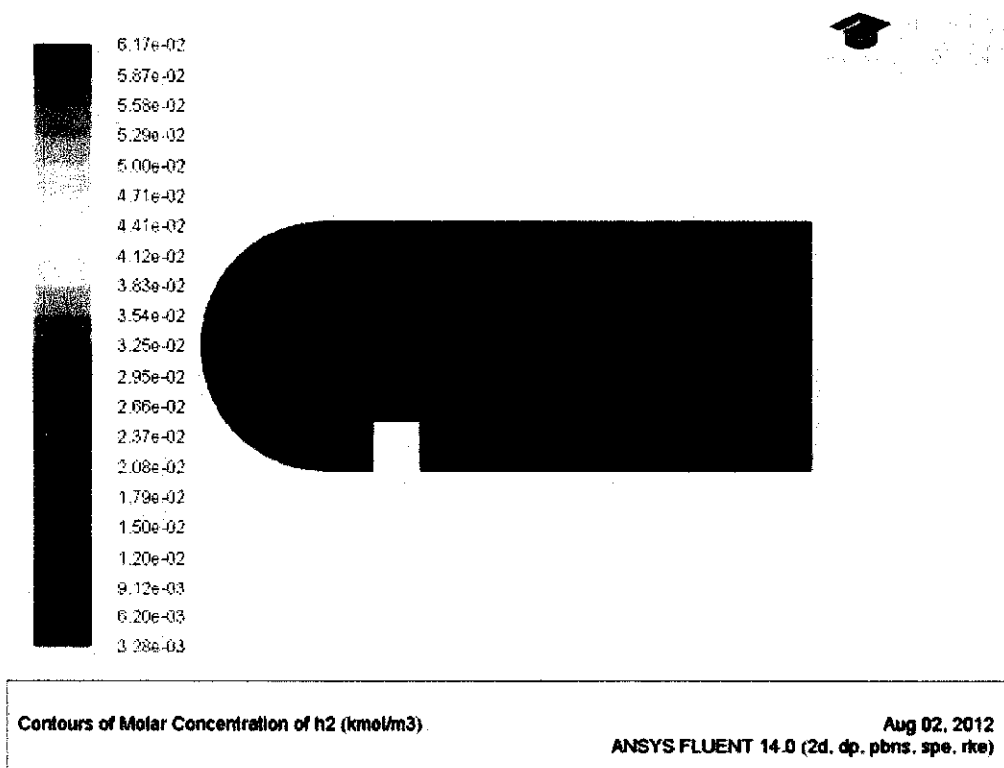


Figure 11: Graph of molar concentration  $H_2$  (LFL) vs distance

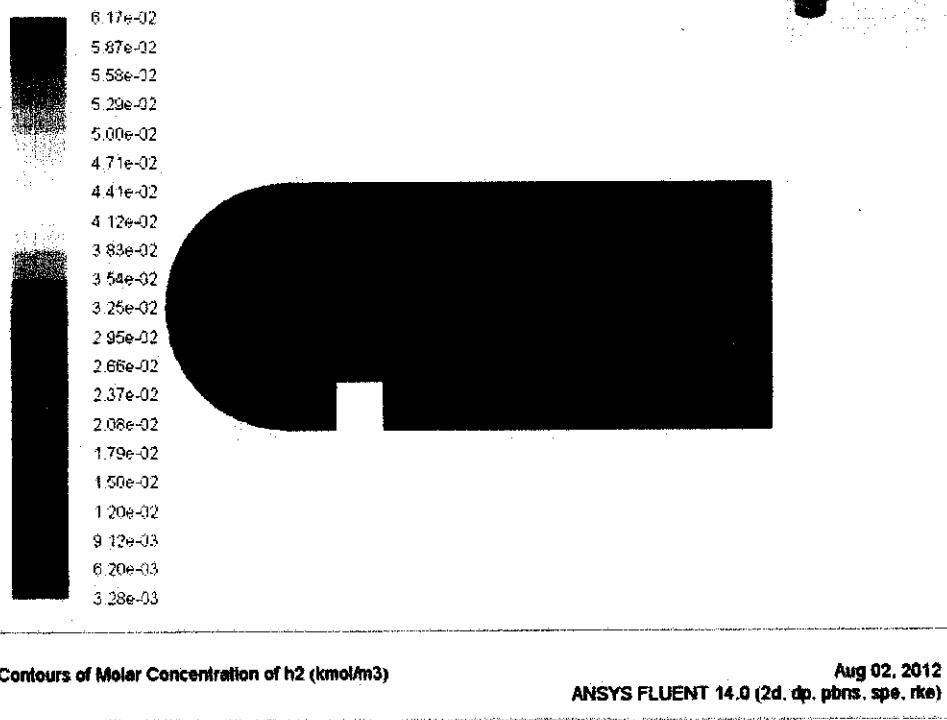
### 3.4.2 Influence of obstacle

In a real practice the surrounding area of the pipeline may consist of several equipment installations for an onshore plant. In case of leakage of the pipeline the released gas may impair the equipment or properties installed nearby. Previous studies conducted indicate that the presence of obstacle may increase the turbulence-combustion interaction also the transportation of the flammable mixture. Presence of obstacle may affect the turbulence kinetic energy of hydrogen-air mixture and dissipation rate of the released gas into atmosphere. Hence, the hydrogen gas is likely to accumulate at point of behind the obstacle where there will be an air entrapment and air recirculation. In this study, realizable k-epsilon model was chosen as the turbulence model encountered in FLUENT simulation.

A study on the influence of obstacle towards the dispersed gas was carried out where a  $1\text{m}^3$  cuboid act as an obstacle was placed within the flammability limit region at  $1\text{m}$  from release point. Figure 12 described the contour of molar concentration of  $\text{H}_2$  only reach the LFL and the released gas did not reach the UFL at 75%. Plus, obstacle may affect the trend of dispersed gas where dispersed gas is likely move in vertical motion once it hit the obstacle. Thus, the ground-level concentration behind the obstacle is likely low. Since the experimental activity was conducted for small scale purpose hence, the recirculation of dispersed gas behind the obstacle was unseen because it did not reach within the flammability limit either under wind condition and no wind. From figure 12 the flammability limit region or the hazard region under wind condition is wider compared to under no-wind scenario. Under wind condition the turbulence kinetic energy created in vertical motion as the gas dispersed from the leakage point. Hence the gas was transported further higher in vertical motion.



(a)



(b)

**Figure 12: Contour of molar concentration H<sub>2</sub> within flammability limit (a) with wind (b) no wind**

The influence of wind speed into the concentration of H<sub>2</sub> around the obstacle was observed and shown in figure 13. At point of release until 0.8m downwind distance, the molar concentration of H<sub>2</sub> is higher under no wind condition. But as the dispersed gas reaches closer to the obstacle the concentration value are reaching identical value which is approximately at 224782ppm. This is because under presence of wind the hydrogen-air mixture tends to diluted rapidly with air.

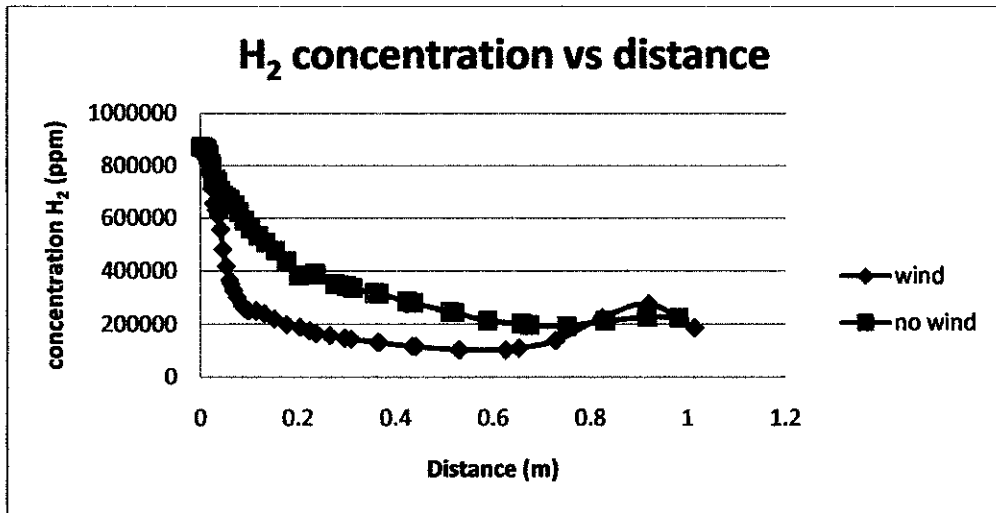


Figure 13: Comparison of H<sub>2</sub> concentration over distance at certain wind condition

## CHAPTER 5 CONCLUSION AND RECOMMENDATION

As a conclusion, the ability to develop a good simulation model on accidental hydrogen release from pipeline is expected. The simulation model was well validated with 18% underestimate compared to HPBT pilot plant result. Hence, the simulated model can be applied to analyse the trend of hydrogen gas dispersion from low pressure pipeline. The distribution region along downwind distance can be predicted at what certain extent.

Once the leakage of the pipeline occur, the dispersed gas reach the LFL limit at 4% by volume in air but did not reach the UFL limit at 75%. However the hazard region generated by the dispersed gas was observed up to 0.9m along the downwind distance.

Presence of wind and obstacle may affect the extent of flammability limit region. For under wind condition the hazard region around the obstacle is wider compared to no-wind condition. The region was observed to be in a vertical motion

once the dispersed gas hit the obstacle. This proves that wind can accelerate the transportation rate of flammability limit region.

For recommendations, a large-scale experimental activity on hydrogen release from a pipeline should be conducted to simulate the real consequence release from pipeline network. Other parameters affecting the trend of dispersion gas can be encounter in simulation model for example hole size diameter, obstacle height and ambient temperature.

## REFERENCES

- Francesco Ganci, Andrea Carpignano, Nicola Mattei, Marco Nicola Carcassi, 2010, Hydrogen release and atmospheric dispersion: Experimental studies and comparison with parametric simulations
- Héctor A. Olvera, Ahsan R. Choudhuri, 2006, Numerical simulation of hydrogen dispersion in the vicinity of a cubical building in stable stratified atmospheres
- Jin-Woo Hwang, Do-Young Yoon, Kil-Ho Choi, Younghun Kim and Lae Hyun Kim, 2007, 3D CFD analysis of the hydrogen releases and dispersion around storage facilities
- N. Matteia, M. Schiavettia, M.N. Carcassia, 2010, Experimental studies on wind influence on hydrogen release from low pressure pipelines
- N. Grassoa, F. Pilob, N. Ciannellic, M.N. Carcassid, N. Matteid, F. Ceccherinie, 2008, Fire prevention technical rule for gaseous hydrogen transport in pipelines
- Prankul Middha, Olav R. Hansen, Idar E. Storvik, 2007, Validation of CFD-model for hydrogen dispersion
- H. Wilkening, D. Baraldi, 2007, CFD modelling of accidental hydrogen release from pipelines
- Yan-Lei Liua, Jin-Yang Zhenga, Ping Xub, Yong-Zhi Zhaoa, Hai-Yan Biea, Hong-Gang Chena, Huston Dryverc, 2008, Numerical simulation on the diffusion of hydrogen due to high pressured storage tanks failure
- S.M. Tauseef, D. Rashtchian, S.A. Abbasi, 2010, CFD-based simulation of dense gas dispersion in presence of obstacles
- A. Sully, M. Heitsch, D. Baraldi, H. Wilkening, 2010, Numerical simulations of hydrogen and hydrogen chloride releases in a nuclear hydrogen production facility
- K. Ramamurthia, Karnam Bhadraiaha, S. Srinivasa Murthyb, 2009, Formation of flammable hydrogen-air clouds from hydrogen leakage
- Barbara Joan Lowesmith, , Geoffrey Hankinson, 2011, Large scale high pressure jet fires involving natural gas and natural gas/hydrogen mixtures
- A. Riddle, D. Carruthers, A. Shapre, 2004, Comparisons between FLUENT and ADMS for atmospheric dispersion modelling
- B.B. Bonner, 2008, Hydrogen delivery/safety
- M. Craig, 2009, Introduction to Using ANSYS FLUENT in ANSYS Workbench

# **APPENDICES**

## APPENDIX 1-1: VISCOUS MODEL

### Viscous model

- (i) Realizable k-epsilon model was selected
- (ii) Other parameters are held under default value

**Viscous Model**

**Model**

- Inviscid
- Laminar
- Spalart-Allmaras (1 eqn)
- k-epsilon (2 eqn)
- k-omega (2 eqn)
- Transition k-k-omega (3 eqn)
- Transition SST (4 eqn)
- Reynolds Stress (5 eqn)
- Scale-Adaptive Simulation (SAS)

**k-epsilon Model**

- Standard
- RNG
- Realizable

**Near-Wall Treatment**

- Standard Wall Functions
- Scalable Wall Functions
- Non-Equilibrium Wall Functions
- Enhanced Wall Treatment
- User-Defined Wall Functions

**Options**

- Viscous Heating
- Full Buoyancy Effects
- Curvature Correction

**Model Constants**

C2-Epsilon: 1.9

TKE Prandtl Number: 1

TDR Prandtl Number: 1.2

Energy Prandtl Number: 0.85

**User-Defined Functions**

Turbulent Viscosity: none

**Prandtl and Schmidt Numbers**

TKE Prandtl Number: none

TDR Prandtl Number: none

Energy Prandtl Number: none

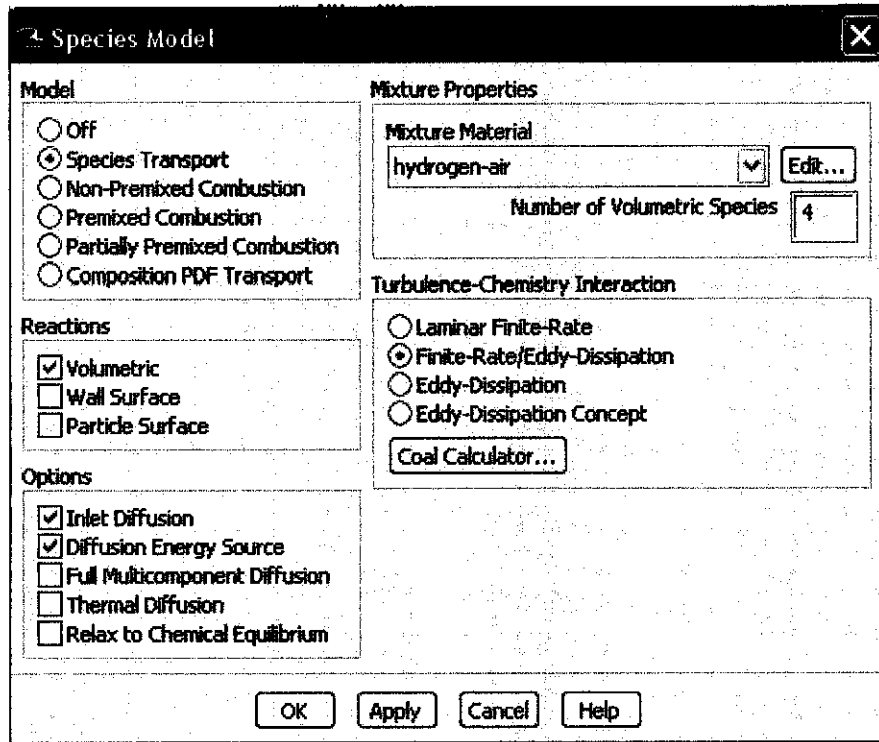
OK Cancel Help



## APPENDIX 1-1: SPECIES MODEL

### Species model

- (i) Species transport model was selected
- (ii) Hydrogen-air mixture was selected from drop down list under mixture properties.
- (iii) Enable the volumetric reaction under reactions column and Finite-rate/eddy-dissipation under turbulence-chemistry interaction



## APPENDIX 2-1: FUEL INLET

### Boundary Conditions (fuel inlet)

- (i) Enter 769.14 m/s for velocity magnitude
- (ii) Enter 10bar for Initial gauge pressure
- (iii) Under thermal tab enter the temperature at 300K
- (iv) Under species tab enter the mass fraction of H<sub>2</sub> equal to 1

Velocity Inlet

Zone Name  
fuel\_inlet

Momentum | Thermal | Radiation | Species | DPM | Multiphase | UDS

Velocity Specification Method: Magnitude, Normal to Boundary

Reference Frame: Absolute

Velocity Magnitude (m/s): 769.14 constant

Supersonic/Initial Gauge Pressure (pascal): 1000000 constant

Turbulence

Specification Method: K and Epsilon

Turbulent Kinetic Energy (m2/s2): 1 constant

Turbulent Dissipation Rate (m2/s3): 1 constant

OK Cancel Help

## APPENDIX 2-2: WIND INLET

### Boundary condition (wind inlet)

- (i) Enter the velocity magnitude at 1m/s
- (ii) Under thermal tab enter the temperature at 298K
- (iii) Under species tab enter the mass fraction of oxygen equal to 0.0998

**Velocity Inlet**

Zone Name  
wind\_inlet

Momentum | Thermal | Radiation | Species | DPM | Multiphase | UDS

Velocity Specification Method: Magnitude, Normal to Boundary

Reference Frame: Absolute

Velocity Magnitude (m/s): 1 constant

Supersonic/Initial Gauge Pressure (pascal): 0 constant

Turbulence

Specification Method: K and Epsilon

Turbulent Kinetic Energy (m2/s2): 1 constant

Turbulent Dissipation Rate (m2/s3): 1 constant

OK Cancel Help

## APPENDIX 2-3: PRESSURE OUTLET

### Boundary condition (pressure outlet)

- (i) Gauge pressure was remained at 0 pascal
- (ii) Under thermal tab enter the temperature at 298K
- (iii) Under species tab enter the mass fraction of oxygen equal to 0.0998

Pressure Outlet

Zone Name  
outlet

Momentum | Thermal | Radiation | Species | DPM | Multiphase | UDS

Gauge Pressure (pascal) 0 constant

Backflow Direction Specification Method Normal to Boundary

Average Pressure Specification  
 Target Mass Flow Rate

Turbulence

Specification Method K and Epsilon

Backflow Turbulent Kinetic Energy (m2/s2) 1 constant

Backflow Turbulent Dissipation Rate (m2/s3) 1 constant

OK Cancel Help

## APPENDIX 3-1: SOLUTION METHOD

### Solution Methods

- (i) Simple solver was selected.
- (ii) Under spatial discretization, all components was defined as first order upwind except gradient, pressure and momentum component.

**Solution Methods**

Pressure-Velocity Coupling

Scheme  
SIMPLE

Spatial Discretization

Gradient  
Least Squares Cell Based

Pressure  
Standard

Density  
First Order Upwind

Momentum  
Second Order Upwind

Turbulent Kinetic Energy  
First Order Upwind

Transient Formulation

Non-iterative Time Advancement

Frozen Flux Formulation

Pseudo-Transient

High Order Term Relaxation Options...

Set All Species Discretizations Together

Default

Help

## APPENDIX 3-1: SOLUTION CONTROL

### Solution Control

(i) Default setting was used for each components in under-relaxation factors

**Solution Controls**

Under-Relaxation Factors

Pressure  
0.3

Density  
1

Body Forces  
1

Momentum  
0.7

Turbulent Kinetic Energy  
0.8

Default

Equations... Limits... Advanced...

Set All Species URFs Together

Help