# STUDY ON TRANSIENT FUEL GASES DISPERSION AND FLAMMABILITY IN AIR FOR THE APPLICATION OF LEAKAGE IN OFFSHORE SAFETY MANAGEMENT

 $\mathbf{B}\mathbf{Y}$ 

YONG JENN

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

SEPTEMBER 2012

Univeristi Teknologi PETRONAS Bandar Seri Iskandar 31750 Tronoh Perak Darul Ridzuan

### CERTIFICATION OF APPROVAL

# STUDY ON TRANSIENT FUEL GASES DISPERSION AND FLAMMABILITY IN AIR FOR THE APPLICATION OF LEAKAGE IN OFFSHORE SAFETY MANAGEMENT

BY

YONG JENN

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

Approved by,

(DR. RAJASHEKHAR PENDYALA)

# UNIVERSITI TEKNOLOGI PETRONAS TRONOH, PERAK, MALAYSIA 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.

YONG JENN

## ABSTRACT

To meet world's insatiable gas demand, offshore production of natural gas must be carried out efficiently, effectively and most importantly safely. The lack of fundamental understanding of how these offshore fuel gases behaves and interacts with air after leakage occurrence has prompted this study into action which is essential in offshore safety management. Gaseous fuels are being labeled the "silent killer" as the biggest hazard of a gas leak is fatal explosion. Undetected gas leak is due to poor understanding and prediction of fluid dynamics interaction between the fuel gases and air as well as the flammability envelope at different times. Using ANSYS Fluent 14.0, 2D simulation is carried out to study the transient mixing behavior of selected fuel gases which are natural gas (primarily methane), carbon monoxide, ethane, propane, butane and lastly acetylene. Shravan and Umit, 2009 studied on transient hydrogen mixing with air are used as a benchmark for our study. A simple geometry of 1m by 0.5m is used alongside different scenario settings. 3 scenarios analyzed are fuel gas release near the bottom enclosed geometry, comparison between a smaller leak volume and a bigger leak volume, and lastly fuel gas release at the top enclosed geometry. Navier Stokes equations describe the fluid dynamics of their hydrogen diffusion model alongside using laminar model. The major steps in the CFD simulation are Geometry Construction, Meshing, Model Setup, Solution and Display of results. The results have shown that the transient dispersion of fuel gases and flammability in air is affected by the mixing buoyancy effects, diffusivity differences and density differences between the fuel gas and air. Hydrogen and natural gas leak (less dense gases compared to air) has high risk; they form flammable vapor cloud at short times that could ultimately lead to fatal explosion in presence of ignition sources. Compared to heavier fuel gases such as propane and butane, vapor cloud formation is rather unlikely in cases when the leak is at bottom. Aside from potentially high risk gas explosion, carbon monoxide hazardous leak into open environment brings fatality to the platform workers even at ppm level. Closed geometry outlines the importance of proper ventilation whereas open geometry outlines the estimation of evacuation period after leakages occurrence. All in all, this thesis has delivered a comprehensive understanding and comparison between different transient gaseous fuels mixing with air based on different geometry settings as well as how the formation and decay of flammable zones changes.

## ACKNOWLEDGEMENT

The author would like to acknowledge the opportunity and support given by Chemical Engineering Department of Universiti Teknologi PETRONAS in providing the Blok 5 Simulation Lab as the venue for my project simulation for 2 semesters. My sincerest gratitude is extended to my supervisor namely Dr Rajashekhar Pendyala for his assistance in my final year project entitled "Study on Transient Fuel Gases Dispersion and Flammability in Air for the Application of Leakage in Offshore Safety Management". Dr Raja had also guided me the usage of the ANSYS Fluent 14.0 software to simulate simple fluid dynamics problems. His consistent attention from week to week never fails to motivate me to perform in this project. With the guidance, advice and support of everyone which includes FYP Coordinators (Dr. Anis Suhaila binti Shuib and Norhayati binti Mellon) and all FYP Examiners, this thesis has turned out to be a successful and meaningful paper for fundamental research understanding of transient fuel gases dispersion and flammability in air in the case of leakages.

# **TABLE OF CONTENTS**

i.	Certification of Approval		2
ii.	Certification of Originality		3
iii.	Abstrac	t	4-5
iv.	Acknow	ledgements	6
v.	Table of	Contents	7
vi.	List of F	ïgures	8-9
vii.	List of <b>T</b>	ables	9
Chap	oter 1: Intr	oduction	
	• 1	.1 Project Background	10-11
	• 1	.2 Problem Statement	11
	• 1	.3 Objective of study	12
	• 1	.4 Relevancy & Scope of project	12
Chap	oter 2: Lite	erature Review/or Theory	13-19
Chap	oter 3: Res	earch Methodology	20-33
	• 3	.1 Work process flow	20
		<ul> <li>3.1(a) Pre-analysis &amp; Geometry Modeling</li> <li>3.1(b) Meshing</li> <li>3.1(c) Setup physics</li> <li>3.1(d) Solution</li> <li>3.1(e) Results</li> <li>3.1(f) Verification &amp; Validation</li> </ul>	21 22-23 23-27 28-29 29-30 31
	• 3	.2 Software tools	31
	• 3	.4 Gantt Chart	32-33
Chap	oter 4: Res	ults & Discussion	34-41
Chap	oter 5: Con	clusion & Recommendations	42-43
Refe	rences		44

# 4.0 LIST OF FIGURES

Figure 1.2	Gas Explosion in Piper Alpha, 1988
Figure 1.3	Geometry Setting
Figure 2.1	Geometry Setting (Shravan K. Vudumu & Umit O. Koylu, 2009)
Figure 2.2	Hydrogen mole fraction contours for open top cylinder
Figure 2.3	Hydrogen mole fraction contours for partially open top cylinder
Figure 2.4	Hydrogen mole fraction contours for closed top cylinder
Figure 2.5	Flammability envelope at t=3s for open, partially open and closed
	cylinder respectively
Figure 3.1(a)	Geometry Modeling Using Design Modeler, GAMBIT
Figure 3.1.1(b)	Comparison between uniform meshing and non-uniform meshing
Figure 3.1.2(b)	Geometry meshing
Figure 3.1.1(c)	General setup
Figure 3.1.2(c)	Energy equation model setup
Figure 3.1.3(c)	Laminar setup
Figure 3.1.4(c)	Species model setup
Figure 3.1.5(c)	Boundary conditions specifications
Figure 3.1.6(c)	Solution initialization
Figure 3.1.7(c)	Patching
Figure 3.1.8(c)	Desired outcome after solution initialization and patching
Figure 3.1.1(d)	Solution methods
Figure 3.1.2(d)	Residual convergence
Figure 3.1.1(e)	Initial Setup
Figure 3.1.2(e)	Desired outcomes
Figure 3.1.3(e)	Graphics and animation display
Figure 3.3	Gantt chart
Figure 4.1(a)	Initial setting of fuel gas release near the container bottom

Figure 4.1(b)	Comparison of mixing behavior among fuel gases at different times	
Figure 4.1(c)	Snapshot of <i>methane</i> mol fraction distribution along vertical cylinder	
	of Y-axis direction (Bottom leak)	
Figure 4.1(d)	Snapshot of <i>acetylene</i> mol fraction distribution along vertical cylinder	
	of Y-axis direction (Bottom leak)	
Figure 4.3(a)	Snapshot of <i>butane</i> mol fraction distribution along vertical cylinder	
	of Y-axis direction (Top leak)	

# 5.0 LIST OF TABLES

Table 2.1	Density comparison between fuel gases with Air
Table 2.2	Range of flammability limits for different fuels by volume %
Table 4.1(a)	Time taken for fuel gas to reach to the top (Enclosed geometry)
Table 4.3(a)	Time taken for fuel gas to reach to the bottom (Enclosed geometry)

## **CHAPTER 1: PROJECT BACKGROUND**

#### **1.1 INTRODUCTION**

To meet world's gas demand, offshore production of natural gas must be carried out efficiently, effectively and most importantly safely. Safety challenges which involve upstream production, transportation and finally processing of natural gas need to be fully addressed by developing standards and comprehensive understanding of dynamic properties of natural gas and other fuel gases. Offshore gas leakage is indeed naked to our eyes, odorless and certainly poses the biggest threat of all hazards; sudden fatal explosion when expose to ignition sources such as flames (e.g. flaring) or sparks. A gas *leak* refers to a leak of natural gas, from a pipe or other containment, into a living area or any other area where the gas should not be. For instance, the Piper Alpha 1988 incident took 167 lives due to offshore gas disaster leakage certainly dampen the safety image of offshore industry. And recently in Daily Mail Online News (2012), "One spark and we'll have another Piper Alpha on our hands; naked flame that threatens repeat of Britain's deadliest rig disaster is still alight" referring to Eglin Gas Field located near Aberdeen. According to another source Wall Street Journal (2012), "TOTAL leak underlines offshore gas risks". These transient mixing of the gas with air is yet to be comprehensively understood and studied. With the application of Computational Fluid Dynamics (CFD) and ANSYS Fluent software, the numerical simulation displays the spatial and temporal distributions (concentrations) of natural gas for all configurations studied. Running a simulation on software is certainly easier, cheaper and advantageous compared to performing experimental work since the accurate predictions of formation and decay of flammable zones are difficult with experiments and theoretical hand calculations (Zhang J, 2009). As the natural gas concentration decays in surrounding air during an unintended release, there is an envelope (approximately 4-14% by volume) beyond which the natural gas-air mixture can no longer be ignited. These lowest and highest concentrations below and above which flame propagation cannot be sustained are called lower and higher flammability limits (Shravan K. Vudumu & Umit O. Koylu, 2009). Natural gas is technically lighter than air as natural gas mainly comprises of methane. Thus, natural gas can disperse and dissipate high above the air quickly should a leak occur. Comparing to other fuel gases, propane and butane which are technically heavier gases than air, they will settle in lower areas if a leak occur. This explains *why heavier hydrocarbon gases would not lead to vapor cloud explosions when compared to light gases such as methane and hydrogen.* The study allows us to predict gas cloud movement and formation according to time, thus observing the flammability envelopes for these unintended releases of gases. The present case study pin points on the fundamental features of natural gas dispersion for different cases in simple geometries that can be used as a benchmark in simulating a more complicated natural gas release scenario and complex geometries. Simple geometries which include closed environment, partially-open environment and open environment. The results obtained in this paper are expected to be utilized for developing necessary fire safety codes, minimizing risks and mitigation plan in case of gas leak out in offshore platform.

### **1.2 PROBLEM STATEMENT**

Natural gas and most gaseous fuels such as propane, butane, hydrogen and carbon monoxide are *all colorless and odorless*. These properties are indeed "**silent killer**" as the biggest hazard of a gas leak will lead to fatal explosion. A distinct disaster would be the Piper Alpha as shown below. There are not many simulation studies on transient dispersion of natural gas or other types of fuel gases mixing with air in the case of unintended release.



Figure 1.2: Gas Explosion in Piper Alpha, 1988

Undetected gas leak is due to poor fundamental understanding and prediction of fluid dynamics interaction between the fuel gases and air as well as flammability envelope at different times.

### **1.3 OBJECTIVE OF STUDY**

This paper discusses on the development of a comprehensive understanding of the transient dispersion behavior of fuel gases and its associated flammability limits in air. The geometry orientations are as shown in Figure 1.3 whereby fuel gas is initialized 10% at bottom and air is initialized 90% at top and vice versa:



**Figure 1.3 Geometry Setting** 

### **Selected Fuel Gases**

- 1. Natural Gas (90% Methane)
- 2. Hydrogen
- 3. Carbon monoxide
- 4. Ethane
- 5. Propane
- 6. Butane
- 7. Acetylene

Using ANSYS Fluent 14.0, our end objective is to come up with a transient dispersion display of results of different fuel gases mixing with air and its associated flammability limits are analyzed in 2D simulation modeling.

### 1.4 REVELANCY & SCOPE OF PROJECT

This paper will be a significant study for the fundamentals for in case of leakage mitigation plan in *offshore safety management*. As our world is moving towards gas era as the clean and "sustainable" fuel, the offshore gas exploration and production has stepped up exponentially to meet up the insatiable gas demand. However, recent gas leakage incidents resulted from offshore mishap has highlighted the *need to improve the process safety and loss prevention*. The first step is to understand the behavior of these gases interacting with air by running on 2D simulation. On top of that, this research

project is expected to come up with a *video motion* which shows the transient behavior of different fuel gases mixing with air.

# **CHAPTER 2: LITERATURE REVIEW/THEORY**

In this research project, we are studying the behavior and predictions of various fuel gases mixing with air over a period of time and how do the flammability zone forms and decays. Fuel gas such as *hydrogen*; which has been previously studied in the referred journal Shravan K. Vudumu & Umit O. Koylu (2009) will be significantly used as a benchmark for studying other various gaseous fuels mixing behavior with air. Below selected fuel gases are studied for our case and density comparison with air is made to roughly predict the mixing behavior:

Substances	Density(kg/m3)	Comparison with Air density
Natural Gas (90% Methane)	0.668	Less Dense
Hydrogen	0.0899	Less Dense
Acetylene	1.092	Slightly Less Dense
Carbon monoxide	1.165	Slightly Less Dense
Ethane	1.264	Slightly More Dense
Propane	1.882	More Dense
Butane	2.489	More Dense

#### Table 2.1: Density comparison between fuel gases with air

### Adapted from Engineering Toolbox.com

Each density fuel gases are compared with air density of **1.205kg/m3** at standard conditions. Quick dispersion between each selected fuel gases and air is predicted when there are high density differences between those two. From the table shown, it can be predicted that Natural Gas, Hydrogen and Carbon monoxide will pose the highest risk among other heavier fuel gases such as propane and butane. This is simply due to these light gases will quickly disperse to the top of the air and explosive vapor cloud will be formed. Whereas, heavier gases will settle at the bottom of the air thus, explosive vapor

cloud formed is rather unlikely. Gases which have similar density with air will not portray much mixing behavior over time.

To study these mixing behavior and transient prediction, running a simulation on CFD tools is certainly easier, cheaper and advantageous compared to performing experimental work since the accurate predictions of formation and decay of flammable zones are difficult with experiments and theoretical hand calculations (Zhang J, 2009).

When leakage occurs within a building, the gas or vapor will undergo some mixing before emerging from any openings. The degree of mixing will depend upon the building geometry and the nature of the ventilation, which in turn may be modified by the leak (D.M. Deaves, S. Gilham, H. Spencer, 2000). Thus, *Geometry & Release Scenario* must depict the model of our case study which is natural gas leakage in offshore. Gas leakage could happen across the transportation pipelines, from gas well production, and throughout offshore platform.



Figure 2.1: Geometry Setting (Shravan K. Vudumu & Umit O. Koylu, 2009)

According to Shravan K. Vudumu & Umit O. Koylu (2009), they present their case using hydrogen as the selected fuel mixing with air in a simple 2D geometry of vertical cylinder of 1 m height and 0.5 m diameter with gravitational force acting downwards. They run with 3 different configurations with open top, partially open top and lastly closed top. According to Mumby Christopher (2010), the author concentrated on modifying existing models that had been developed to predict confined vented and unconfined vapor cloud explosions involving natural gas. Three geometries were studied: a confined vented enclosure, an unconfined cubical region of congestion and an unconfined high aspect ratio region of congestion.

To express the behavior of this fluid movement, *Navier Stokes equation* is used as together with supplemental equations (for example, conservation of mass) and well formulated boundary conditions, the Navier–Stokes equations seem to model fluid motion accurately; even turbulent flows seem (on average) to agree with real world observations.



Navier-Stokes General Equation

The Navier–Stokes equations assume that the fluid being studied is a continuum (it is infinitely divisible and not composed of particles such as atoms or molecules), and is not moving at relativistic velocities (Fluid Mechanics McGraw-Hill, 2008). Specifically, the complete set of transient equations for the conservation of mass, momentum and energy as well as the non-reacting transport equations/mass diffusion are considered (Shravan K. Vudumu & Umit O. Koylu, 2009). The governing equations used are as shown below:

$$\frac{\partial \rho}{\partial t} + \nabla \bullet (\rho \vec{V}) = 0$$

Mass Conservation

$$\frac{\partial}{\partial t}(\rho \vec{V}) + \nabla \bullet (\rho \vec{V} \vec{V}) = -\nabla \rho + \nabla \bullet (\vec{\tau}) + \rho \vec{g}$$
  
$$\vec{\tau} = \mu [(\nabla \vec{V} + \nabla \vec{V}^{T} - (2/3)\nabla \bullet \vec{VI})]$$
 Is the stress tensor

Momentum Equation

$$\frac{\partial}{\partial t}(\rho E) + \nabla \bullet (\vec{V}(\rho E + p)) = \nabla \bullet (k\nabla T - \sum_{j} h_{j} \vec{J}_{j} + (\vec{\tau} \bullet \vec{V})) + \rho(\vec{V} \bullet \vec{g})$$
$$E = h - (p / \rho) + (V^{2} / 2) \qquad h = \sum_{j} Y_{j} h_{j}$$

Energy Conservation

$$\vec{J}_i = -\rho D_i \nabla Y_i$$
*Mass diffusion*

A laminar flow analysis is used in most journals' study of transient mixing during leakage. Earlier studies have clearly shown that turbulence models tend to over predict mixing of gas released from slow leaks and laminar analysis is more suitable for the purpose of safety engineering (Barley CD, Gawlik K, Ohi J, Heweet R., 2007). Shravan K. Vudumu & Umit O. Koylu, (2009) said that Reynolds numbers at the leak exits were always low enough to be in laminar regime whereas Rayleigh numbers which indicates the type of buoyant flow due to temperature difference was also in the laminar region. Assumption is made on variables such as wind direction and weather conditions.

According to Shravan K. Vudumu & Umit O. Koylu, (2009), to accommodate the highly diffusive nature of hydrogen in air, a fine mesh size (minimum size=0.1mm) and a small time-step (0.001s) are used. About 50 iterations are performed at each time step for achieving convergence at every time step. Stationary, no- slip and adiabatic wall boundary conditions are applied on the walls of the cylinder unless at open atmosphere, pressure outlet is applied at the top boundary. In our research study, we can simulate

natural gas using the similar boundary conditions as natural gas is light as well as having a high diffusive nature in air. For other heavy hydrocarbon gases, mesh sizing, number of iterations and other solutions will be slightly different.

Snapshots of the simulated results for hydrogen mole fraction contours and flammability envelope at different times are shown (Shravan K. Vudumu & Umit O. Koylu, 2009).



Figure 2.2: Open Top Cylinder



Figure 2.3: Partially-Open Top Cylinder



Figure 2.4: Closed Top Cylinder



Figure 2.5: Flammability envelope at t=3s for open, partially open and closed cylinder respectively

It is found out that when the mixing is buoyancy controlled, hydrogen rapidly moves up. For the closed top container, *hydrogen moves twice as fast* near the axis compared to the open top case due to a decrease in pressure along the axis when the cylinder is completely closed. This observation suggests installation of a safety alarm near the symmetry axis that triggers not only the sound but also the ventilation opening instead of continuous ventilation at the top of an enclosure (e.g. offshore platform rooms).

From the computed hydrogen concentration distributions for all three top conditions, important information related to fire detection and prevention can be obtained. For example, 1% hydrogen concentration by volume is usually sufficient to trigger many safety alarms in transportation and stationary applications, while a range of 4–75% hydrogen by volume potentially creates a flammable mixture with a fire safety risk (Shravan K. Vudumu & Umit O. Koylu, 2009). In our case study, a range of UFL and LFL for different fuels by volume potentially creates a flammable mixture as shown below.

Substances	LEL or LFL(%)	UEL or UFL(%)
Natural Gas (90% Methane)	4.4-5	15-17
Hydrogen	4	75
Carbon monoxide	12	75
Ethane	3	12.4
Propane	2.1	10.1
Butane	1.86	8.41
Acetylene	2.5	81

### Table 2.2: Range of flammability limits for different fuels by volume %

### Adapted from Engineering Toolbox.com

With the comprehensive understanding and comparison of how these fuel gases behaves in mixing with air and the formation of flammability cloud and decay over period of time is certainly crucial and timely. The computational modeling will be run on ANSYS Fluent 14.0 to predict each calculated point of meshing as it is accurate and precise in its proven prediction.

# **CHAPTER 3: RESEARCH METHODOLOGY**

## 3.1 WORK PROCESS FLOW



### 3.1 (a) Pre-analysis & Geometry Modeling

▼	A		
1	🔇 Fluid Flow (FLUENT)		
2	随 Geometry	<	
3	🥩 Mesh	2	
4	🍓 Setup	? 🖌	
5	🗑 Solution	2 🖌	
6	🥪 Results	? 🖌	

The first step is to construct a geometry that depicts the case study model. In the study of transient fuel gas mixing with air, a cylindrical geometry suits best. The simple geometry can be drawn using Autocad, Design Modeler, or other drawing software whether in 2D or 3D.



Figure 3.1(a) Geometry Modeling Using Design Modeler, previously known GAMBIT

Before a construction of geometry, pre-analysis must be carried out to accurately determine the point of interest. In our case, we need to find out where is the boundary wall, outlet pressure and axis symmetry. The constructed geometry then can be transported into ANSYS Fluent for further meshing and subsequent solving steps.

### 3.1 (b) Meshing

▼	A		
1	🔄 Fluid Flow (FLUENT)		
2	随 Geometry	<ul> <li>_</li> </ul>	
3	🧼 Mesh	× .	
4	🍓 Setup	2	
5	🕼 Solution	? 🖌	
6	🥩 Results	? 🖌	

Mesh is any of the open spaces in a net or network; an interstice. Meshing is required after the geometry is completed. It is important to define the right meshing condition so as to yield a more accurate display of results. Meshing tells the software to perform calculations on the open spaces network. Non-uniform meshing has more coverage points compared to uniform meshing as shown below.



Figure 3.1.1(b): Uniform meshing Non-Uniform meshing

Uniform meshing is preferred near boundary wall whereas non-uniform meshing is preferred near our point of interest which is the axis symmetry where the dispersion behavior of gas mixing with air is predicted. Advanced size function is curvature whereas automatic inflation used in meshing is programmed-controlled. Minimum mesh size used is 0.1mm in the hydrogen study due to highly diffusive nature of itself. A lower diffusivity gases such as ethane and acetylene will use a slightly larger mesh size to decrease computing time. A trial and error is conducted to yield the best mesh size for each selected fuel gases. The meshing details are found in *Appendix A*.

and they then been a	the second s	
the two data take re	A CONTRACTOR OF AC	N day - Constanting - 14
*	1	· 代 图 Q Q 苹 // a □-
	Prestan - Ondats - Ethern	
and the second	and the second second	A A A M AND THE REPORT OF A DESCRIPTION
Decisi oblacile . BA wannesses	weak canad . V. V. V	N.N.N. M.H. Management Streeter Streeter Street
h juxine Streak - 1	B. Medi Contral - Aronnovill	
Project Project(ACO) Profile Connetry Profile		
March New York		
Defeate		
Phones Proference	070	
Solary Parlimence	field	
Releases		
Side		
The Advanced Stat Function	for Oresten	
Releases Center	fine .	
Added Non York	Artist Assessed	
Transform .	1940	
Statute Carter	Ena .	
Cariature North Ende	Defait (18.0.1)	
Ne Sau	Defa.4 (1.6322e-004 m)	
Mer Fare Ste	Default (1.6322a-002 m)	
Mar Stre	Tela # (3,2143+002 m)	
Growth-Rate	(tellad (1.20))	
Minimum Ellips Length	0.50 m	
Inflation		
Line Automatic Sylletion	Drogram Centrolled	
3-Fater Option	Smooth Transition	
Transition Robo	0.272	
Maximum Loopes	2	
Goodt-Rate	1.2	
2/54an Agethn	ine .	
View Advanced Options	No	
Assentity Heating		
Philad	Scena .	
Patch Conforming Options		•
Triangle Sulface Moder	Program Caribolied	1 M 1 M 1 M 1
Advanced		1.00 0.000
Traps Cherking	010	0.00
Clement Platede Nodes	Draced	
Shape Checking Element Platele Nodes Humbury of Putrasis	Orb Drapped	0.00 0.00

Figure 3.1.2(b): Geometry Meshing

## 3.1 (c) Setup physics

After meshing is complete, the geometry model is checked and run in ANSYS Fluent 14.0. The subsequent steps are to specify the general setup and model setup as shown below. For the general setup, the solver is pressure based, absolute velocity formulation, transient, 2D planar and with gravitational force acting.

General			
Mesh			
Scale Check Report Quality			
Display			
Solver			
Type Velocity Formulation			
Opensity-Based Relative			
Time 2D Space Steady Steady			
Transient     Axisymmetric			
Axisymmetric Swiri			
Gravity Units			
Gravitational Acceleration			
× (m/s2) 0 P			
Y (m/s2) -9.81			
Z (m/s2)			

Figure 3.1.1(c): General setup

Model setup in our fundamental research is mainly Navier Stokes-related equations which comprise of energy equation; laminar flow model and species transport model.

Models	1: Mesh 🔹
Models Multiphase - Off Energy - On Viscous - Laminar Radiation - Off Heat Exchanger - Off Species - Species Transport Discrete Phase - Off Solidification & Melting - Off Acoustics - Off	Energy Energy Energy Equation OK Cancel Help
Edt	

Figure 3.1.2 (c):Energy Equation Model Setup

Viscous Model
Model
<ul> <li>Inviscid</li> <li>Laminar</li> </ul>
Spalart-Allmaras (1 eqn)
k-omega (2 eqn)
<ul> <li>Transition k-kl-omega (3 eqn)</li> <li>Transition SST (4 eqn)</li> </ul>
<ul> <li>Reynolds Stress (5 eqn)</li> <li>Scale-Adaptive Simulation (SAS)</li> </ul>
Options
Viscous Heating
OK Cancel Help

Figure 3.1.3 (c):Laminar Model Setup

Species Model	<b>X</b>
Model Off Species Transport Non-Premixed Combustion Premixed Combustion Partially Premixed Combustion Composition PDF Transport	Mixture Properties Mixture Material hydrogen-air Number of Volumetric Species
Reactions	
Options Inlet Diffusion Diffusion Energy Source Full Multicomponent Diffusion Thermal Diffusion	
ОК	Apply Cancel Help

Figure 3.1.4 (c):Species Model Setup

The mixture material for example; hydrogen-air is specified in the species transport model.

After completing the general setup and model setup, the boundary conditions are specified. In our model, the wall boundary is stationary and non-slip condition as shown below.

Wall Wall	×
Zone Name	
wall-surface_body	
Adjacent Cell Zone	
surface_body	
Momentum Thermai Radiation Species DPM Multiphase UDS Wall Film	
Wall Motion Motion	
Stationary Wall     ✓ Relative to Adjacent Cell Zone     Moving Wall	
Shear Condition	
No Slip	
Specified Shear     Specularity Coefficient	
Marangoni Stress	
Wall Roughness	
Roughness Height (m) 0 constant v	
Roughness Constant 0.5 constant v	
OK Cancel Help	

Figure 3.1.5(c): Boundary conditions specification

After specifying the boundary conditions, solution initialization is performed. In our case study model, air composition (21%  $O_2$ , 79%  $N_2$ ) is initialized above the fuel gases (depending on the case study model). The air covers 90% of the geometry whereas the selected fuel gas covers the bottom remaining 10% of the simple geometry.



**Figure 3.1.6 (c):Solution Initialization** 

The solution initialization performed is as shown in the figure above. 0.21 initial values is assigned to  $O_2$  whereas the remaining 0.79 is assigned to  $N_2$ . The entire geometry is now initially filled with air. To assign fuel gas at the bottom of the geometry, a method called " patching" is done.

To patch the fuel gas, for example hydrogen that comprise of total 10% of the geometry model, region adaption is carried out by inputing coordinates of X and Y axis as shown in the figure. After coordinates input, click "Mark". Then go to the solution initialization page, click " patch" and assign value "1" for hydrogen for that particular patched region.

Region Ada	ption	×	Y	Patch		X
Options <ul> <li>Inside</li> <li>Outside</li> </ul> Shapes <ul> <li>Quad</li> <li>Circle</li> <li>Cylinder</li> </ul> Manage Controls	Input Coordinates X Min (m) 0 Y Min (m) 2 Min (m) 0 Z Min (m) 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0 0	X Max (m) 0.5 Y Max (m) 0.1 Z Max (m) 0		Reference Frame          Relative to Cell Zone         Absolute         Variable         Pressure         X Velocity         Y Velocity         Temperature         h2         o2         h20	Value 1 Use Field Funct Field Function	Zones to Patch  🗐 🗐 Surface_body ion Registers to Patch 🗐 🚍 hexahedron-r0
	Select Poin	ts with Mouse				
Adapt	t Mark Close	e Help		Patch	Close Help	

Figure 3.1.7 (c):Patching

9.05e-01	
8.60e-01	
8.14e-01	
7.69e-01	
7.24e-01	
6.79e-01	
6.33e-01	
5.88e-01	
5.43e-01	
4.98e-01	
4.52e-01	
4.07e-01	
3.82e-01	
3.17e-01	
2.71e-01	
2.28e-01	
1.81e-01	
1.38e-01	
9.05e-02	
4.52e-02	
0.00e+00	

Figure 3.1.8 (c):Desired outcome after solution initialization and patching

#### 3.1 (d) Solution

After setup physics is ready, solution can be performed. Solution method used in our case would be SIMPLE Algorithm. In CFD, SIMPLE algorithm is a widely used numerical procedure to solve the Navier-Stokes equation. SIMPLE is the acronym for Semi-Implicit Method for Pressure Linked Equations.

	Solution Methods
	Pressure-Velocity Coupling
	Scheme
1	SIMPLE
	Spatial Discretization
	Gradient
	Least Squares Cell Based
	Pressure
	Second Order
	Momentum
	Second Order Upwind 🛛 💙
	Species
	Second Order Upwind 🗸 🗸
	Energy
	Second Order Upwind
	Iransferit Formulation
1	Second Order Implicit
	Non-Iterative Time Advancement
	Frozen Flux Formulation
	Options
	Set All Species Discretizations Together
	Default

**Figure 3.1.1(d): Solution methods** 

Second order implicit scheme is used for unsteady flow equations in order to obtain better accuracy(Shravan K. Vudumu & Umit O. Koylu, 2009). Time Step used is 0.01s whereby the simulation is captured/auto-save every 1 second. The number of iterations varies for each case study as long the solution accurately converges. For a start, the no. of iterations used is 50 for the solution to converge. For further improved analysis of the transient mixing behavior of these fuel gases, no. of time steps will be decreased and no. of iterations will be increased.

Residual Monitors					×		
Options	Equations						
Print to Console	Residual	Monitor Check C	onvergence	Absolute Criteria	<u> </u>		
V Plot	continuity	▼ [	1	0.00001			
	x-velocity		<b>v</b>	0.00001			
Iterations to Plot	y-velocity	<b>V</b> [	<b>v</b>	0.00001			
	energy		<b>v</b>	1e-06	•		
	Residual Values			Convergence Cr	iterion		
Iterations to Store	Normalize	Iterati	ons	absolute	-		
	Scale						
	Compute Loca	l Scale					
OK Plot Renormalize Cancel Help							

Figure 3.1.2(d): Residual Convergence

To increase accuracy of results, absolute convergence criteria of each residual equation is at 10 E-5.

# 3.1 (e) Results



Figure 3.1.1(e): Initial Setup



Figure 3.1.2(e): Desired Outcome

Graphics display chosen is *contours*. Contours of concentration, mol fraction, flammability are selected for our case study analysis. Scene animation is recorded to observe the transient mixing between fuel gas and air.

Graphics and Animations	1: Mesh	<b>*</b>	
Graphics	Contours		
Vectors Pathlines Particle Tracks	Options	Contours of Pressure Static Pressure Min Max	<b>~</b>
Set Up	Clip to Range Draw Profiles Draw Mesh	0 0 Surfaces	
Animations Sweep Surface Scene Animation Solution Animation Playback	Levels Setup	interior-air interior-hydrogen mixing_point pressure_outlet symmetry-air symmetry-hydrogen	
Set Up Options Scene Views	Surface Name Pattern	New Surface  Surface Types axis clip-surf exhaust-fan fan	
Lights Colormap Annotate	Display (	Compute Close Help	

Figure 3.1.3(e): Graphics and animation display

### 3.1 (f) Verification & Validation

Initial prediction based on density differences and buoyancy effects, hydrogen will move up fastest to the top compared to natural gas whereas heavy hydrocarbon such as propane and butane will remain at the bottom of the air. From the results of our case study simulation, comprehensive analysis is carried out to verify our hypothesis. The fundamentals study will then be used in a more complicated geometry in offshore safety management.

### 3.2 SOFTWARE TOOLS



ANSYS FLUENT 14.0 is a computational fluid dynamics (CFD) software package to simulate fluid flow problems. It uses the finite-volume method to solve the governing equations for a fluid. It provides the capability to use different physical models such as incompressible or compressible, in viscid or viscous, laminar or turbulent, etc. Geometry and grid generation is done using GAMBIT which is the preprocessor bundled with FLUENT under ANSYS.

# 3.3 GANTT CHART

Details/Week	<b>S1</b>	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
Developing a fundamental understanding of transient dispersion and its flammability of different fuel gases with air based on different sets of geometry a) Reading various literature sources b) Meeting with supervisor																
Basic exposure on Simulation Tool: ANSYS Fluent 14.0																
<b>Developing ANSYS Fluent methodology</b> for our fundamental case study of different fuel gases dispersion behavior and its flammability changes																
<ul> <li>Carry out simulation results</li> <li>a) 2D Closed &amp; Open Geometry with 1m X 0.5m</li> <li>b) Fuel gases: H<sub>2</sub>, Natural Gas, C<sub>2</sub>H<sub>6</sub>, C<sub>3</sub>H<sub>8</sub>, C<sub>4</sub>H<sub>10</sub>, C<sub>2</sub>H<sub>2</sub>, CO</li> <li>c) Obtainment of help from supervisor to help with understanding</li> </ul>					M1											
<ul> <li>Analysis and improvement of generated simulated results</li> <li>a) Improve meshing size</li> <li>b) Analysis of heavier/lighter fuel gases and air mixing</li> <li>c) Improve time steps and no. of iterations for different fuel gases</li> <li>d) Obtainment of advice from supervisor to help with understanding</li> <li>e) Study on buoyancy effects on dispersion behavior of fuel gases</li> <li>f) Study on transient dispersion and its flammability connection</li> </ul>							M2									

Progress Repo	ort					M3				
a) b)	Preparation and submission of progress report Discussion of generated results with supervisor									
Further analy	sis							M4		
a) c) d)	Simulate video motion on its dispersion behaviour and flammability Reading of more specific literature to verify and enhance results Finalize findings and conclusion									
Final Report									M5	
a) b)	Preparation and submission of draft report Submission of final report									
VIVA										

## Figure 3.3: Gantt chart

### Legend

**S1** – Semester 1 / FYP 1

- M1 Milestone 1 Successful development of results for different fuel gases at different sets of geometry
- M2 Milestone 2 Successful analysis run on different fuel gases
- M3 Milestone 3 Submission of progress report

M4 – Milestone 4 – Successful fundamental understanding of transient fuel gases dispersion and its flammability in air in application of offshore safety management

M5 – Milestone 5 – Submission of Final Report

### 4.0 **RESULTS & DISCUSSION**

The fundamentals knowledge on how these dispersion of gases and its flammability in air need to be addressed and understood properly as we need to curb on gas leak incident especially the oil and gas industry is heading towards "gas era". What is the impact of each density differences between the selected fuel gas and the air can affect the mixing behavior in air? How the deduced mixing behavior between air and fuel gas is related to its formation of flammable vapor cloud that could lead to fatal explosion? The burning questions are verified in our comprehensive findings. 3 scenarios are analyzed which are fuel gas release near the bottom enclosed geometry, comparison between a smaller leak volume and a bigger leak volume, and lastly fuel gas release at the top enclosed geometry.

#### 4.1 Fuel gas release near bottom container (Enclosed Region)

In our paper study, simple geometry 1m by 0.5m is used to investigate the behavior of these fuel gases dispersing in air due to buoyancy and diffusion effects. Initially the lower 10 cm of cylinder is filled with pure selected fuel gas (mol fraction 1), which is suddenly released at time, t=0s and starts mixing with the overlying air that occupies 90% by volume cylinder. The higher the density differences between the fuel gas and the air, the greater the mixing behavior is observed. Thus, faster formation of flammable vapor cloud will take place. Shravan K. Vudumu & Umit O. Koylu (2009) states that the formation of flammable mixtures depends on axial and radial locations at a certain time.

There are 2 main analyses. Technically, hydrogen, natural gas, acetylene and carbon monoxide are deemed light fuel gases compared to air. On the other hand, the heavier fuel gases such as ethane, propane and butane are categorized and anaylzed among each other. Compared with air, hydrogen is the least dense fuel gas among other fuel gases selected; butane is the most dense fuel gas selected.



Figure 4.1(a):Initial setting of fuel gas release near the container bottom



Figure 4.1(b): Results display of different mixing behavior among fuel gases at different time

Fuel Gas (From Bottom)	Comparison with air	<b>Density Ratio (Fuel</b>	Time taken to reach
	density	Gas/Air)	top (s)
Hydrogen	Less Dense	0.075	3-4
Natural gas (Methane)	Less Dense	0.554	4-5
Acetylene	Slightly Less Dense	0.906	20
Carbon Monoxide	Slightly Less Dense	0.967	25
Butane	More Dense	2.066	-

Table 4.1(a): Time taken for fuel gas to reach to the top (Enclosed geometry)

In the enclosed geometry of 1m height by 0.5m width, the hydrogen and natural gas (primarily methane) is observed to reach to the top fastest respectively at 3-4s and 4-5s compared to ethylene and carbon monoxide at 20s and 25s respectively to reach at the top. Heavy fuel gases such as ethane, propane and butane never made to the top as they remain settling at the bottom.

In Figure 4.1(b), hydrogen and natural gas had shown similar mixing behaviour pattern as both fuel gases have small density ratio of 0.075 for hydrogen/air and 0.554 for natural gas/air respectively. The dispersion across the geometry is supported by the *bouyancy effects* as this fundamental study dose not involve variables such as pressure, temperature neither wind direction nor velocity leak. It should be emphasized that our simulations match almost exactly with the recently published journal; Shravan K. Vudumu & Umit O. Koylu, 2009 for hydrogen case. Such quick dispersion of fuel gas especially hydrogen or natural gas in air will create dangerous flammable mixtures at a frightening pace. For hydrogen, 4-75% by volume is a flammable region which signifies that at t = 3-4s onwards poses the risks of flammability in air are always high. As for natural gas, 5-17% by volume which gives way for formations of flammable mixtures will only occur at t = 4-5s onwards. This is supported by the fact when at 7s and 9s respectively; the hydrogen and natural gas already covers all the cylinder volume which deduces a well mixture.



White dot- Interior surface body; Red dot- Top wall; Green dot- Wall surface body

Figure 4.1(c): Snapshot of *natural gas (methane)* mol fraction distribution along vertical cylinder of Y-axis direction at t = 0s, t = 1s, t = 6s, t = 10s respectively

Figure 4.1(c) further illustrates the mol fraction distribution pattern of natural gas (methane) across the vertical cylinder geometry that could lead to flammable region predictions. At 10s, the mol fraction methane is at 8 -10% distribution which falls onto the flammability region of natural gas.

In Figure 4.1(b), the mixing behaviour of  $C_2H_2$  and CO hardly change for the first 4s. This is due to density ratio close to unity which means the density between the fuel gas and air is very similar. At 5s,  $C_2H_2$  starts to rapidly disperse in air and occupies the top at 20s. Whereas at 10s, CO starts to rapidly mix and disperse and occupies the top at 25 s. The validity and accuracy of the simulation is proven as  $C_2H_2$  density ratio of 0.906 is smaller than CO density ratio of 0.967 at which  $C_2H_2$  reaches the top slightly faster than CO.

White dot- Interior surface body; Red dot- Top wall; Green dot- Wall surface body



Figure 4.1(d): Snapshot of *acetylene* mol fraction distribution along vertical cylinder of Y-axis direction at t = 1s, t = 5s, t = 15s, t = 30s respectively

Theoretically, the UFL/LFL limit of CO is 12-75% by volume whereas the UFL/LFL limit of  $C_2H_2$  is 2.5-81% by volume. For example in Figure 4.1(d), at 30s, the acetylene reaches the top and deduces a well mixture at 10% mol fraction volume across the vertical cylinder geometry which falls in the flammbility limit thus leading to formation of flammable cloud.

In safety terms, CO is highly toxic when exist in ppm level in air. Thus, even if CO does not form flammable mixture upon release, it will endangers the occupants after dispersing into the air. Our fundamental study clearly shows that in 1m by 0.5m area, we have 20s response time before CO starts to disperse rapidly.

The driving force behind the bouyancy diffusion effects is mainly the density ratio differences and diffusivity differences between the fuel gas and the overlying air. Fuel gas which has higher density than air is technically unable to reach the top of the container if the fuel gas is released at the bottom of the overlying air. Figure 4.1(b) had clearly shown that ethane, propane and butane are too heavy to disperse and move along the axis direction towards the top. This confirms bouyancy effects does not play a role in the mixing of heavier gases in air when released at the bottom. The mixing process is driven mostly by molecular diffusion differences. Ethane which has very similar density and similar molecular weight with air shows no behavorial changes in mixing even after 60s from the start of the release. This applies to other heavier fuel gases such as propane and butane. They portrays non-obvious mixing until certain time. At t=30s, both propane and butane show some mixing behaviour along the radial direction. This is due to higher density ratio differences. The release of heavy fuel gas from bottom is very unlikely to generate a flammable mixture at the top. In offshore platforms, the presence of sparks is the common catalyst to a vapor cloud explosion in a presence of flammable cloud mixtures. Ethane, propane and butane are all highly unlikely to disperse to the top of the flaring point which are few hundred metres high above whereby the presence of sparks exists. Yet the UFL/LFL limits of these heavy fuel gases are very small in range and its volume percentages. In most cases of offshore platforms, the concentration of these heavy gas leakages are small when compared to methane gas leakage.

Another interesting analysis from Figure 4.1(b) is the distinct mixing behaviour that is much obvious in the axial geometry compared to the geometry wall due to decrease pressure along the axis symmetry. Thus, a well deduced mixture signifies formation of flammable fuel

vapor cloud. The initial stages of fuel gas mixing in air shown symmetrical behaviour. Realistically, a gas detector would be best fit in the middle of the axial distance of source leak and the flaring point. Carbon monoxide is deemed as a lethal gas to offshore workers. Thus, the location of CO detector should be located at the bottom and CO removal system should be installed in an enclosed room/cabin platforms. Of course, the safety reponse time will be decreased in the presence of wind and the velocity of the leak.



### 4.2 Comparison between 10% volume and 20% volume leak at bottom (Natural Gas)

Time taken to reach the top for both scenario is the same. Mixing behavior is similar in am eclosed region. The analysis has shown us that we can deduce a *more concentrated dispersion* in 20% natural gas as shown in the comparison at t= 9s when both mixture well-mixed is formed.

#### 4.3 Fuel gas over air



Initially the upper 10 cm of cylinder is filled with pure selected fuel gas, which is suddenly released at time, t=0s and starts mixing with the bottom air that occupies 90% by volume cylinder.

Fuel Gas (From Top)	Time taken to reach bottom (s)	Density Ratio (Fuel Gas/Air)
Butane	5	2.066
Propane	7-8	1.562

Table 4.3(a): Time taken for fuel gas to reach to the bottom (Enclosed geometry)

To evaluate the relative effects of buoyancy and diffusion on the mixing of the fuel gas and air, another configuration in which fuel gas is initially above the air in the closed cylinder is considered. Compared to the previous scenario, this case configuration is being viewed upside down. For heavier fuel gases overlying the air, buoyancy driven diffusion will take place as butane and propane respectively took 6s and 9s to reach the bottom and covers the entire cylinder geometry. However, for lighter fuel gas such as hydrogen and natural gas, the problem is viewed vice-versa. There are no mixing behavioral changes when these light fuel gases leak at the top.



Figure 4.3(a): Snapshot of *butane* mol fraction distribution along vertical cylinder of Y-axis direction at t = 0.2s, t = 3.5s, t = 8s, t = 10s respectively (Left to right)

#### **CHAPTER 5: CONCLUSION & RECOMMENDATION**

In a nutshell, this work discussed on the fundamentals of transient dispersion display of different fuel gases mixing with air and its associated flammability limits are simulated and analyzed in 2D cylindrical geometry of 1m by 0.5m in ANSYS Fluent 14.0. Fuel gases selected in this fundamental research are hydrogen, natural gas, carbon monoxide, ethane, propane, butane as well as acetylene. The rate of diffusion and mixing is influenced by density ratio differences, molecular weight differences and its buoyancy effects. When the leak is at the bottom, the simulated results clearly show that the hydrogen reaches the top fastest at 3s compared to natural gas at 4s whereas heavier fuel gases will settle at the bottom. The dispersion of methane is considerably as fast as hydrogen leak. This indicates that buoyancy driven diffusion is a controlling parameter for light fuel gases when the leak is at the bottom whereas negligible in cases for heavier fuel gases. When the leak is at the top, the problem is viewed as vice-versa. This indicates that buoyancy driven diffusion is then a controlling parameter for heavier fuel gases when the leak is at the top whereas negligible in cases for lighter fuel gases. Ethane, Propane and Butane leakage is unlikely to create flammable cloud mixture based on the simulation itself when the source leak is at bottom. To sum it up, proper ventilation is crucially needed in an enclosed region whereby detector is best placed at the axis symmetry of the geometry setting as distinct mixing behavior is observed. The dispersion concentration is uniform in the enclosed geometry thus it is very predictable of its mixing behavior. If it is an open pressure configuration, the dispersion of methane will be harder to predict. Flammability envelope increases in a well-mixed enclosed region. A more concentrated dispersion in initial 20% volume of natural gas at the bottom in the comparison with initial 10% natural gas at the bottom portrays similar mixing behaviour, however 20% natural gas portrays a more concentration dispersion after well-mixed. Closed geometry outlines the importance of proper ventilation. Open geometry outlines the estimation of evacuation period after leakages.

From the analysis results of our case study simulation, comprehensive analysis has successfully verified our fundamental objectives. Currently, time steps used is 0.01s whereas no. of iterations is 50 to decrease computing time. In later stages, more improved simulated results can be generated with better meshing size and better time steps at 0.001s. More accurate pattern

of fuel gas dispersion in air and its flammability changes can be analyzed thoroughly. A video of the simulation of each fuel gas dispersing in air can be captured. The understanding of this transient pattern dispersion of gaseous fuels in air can be further investigated for incident of explosion after leakages which will take in the account of important parameters such as temperature and pressure. The fundamental study enables numerical prediction of more complicated leakage geometry.

•

#### REFERENCES

- Shravan K. Vudumu & Umit O. Koylu. March 2009. Detailed simulations of the transient hydrogen mixing, leakage and flammability in air in simple geometries. International Journal of Hydrogen Energy. Volume 34, Issue 6, P 2824-2833.
- Zhang J, Hereid J, Hagen M, Bakirtzis D, Delichatsios MA, Venetsanos AG. September 2007. Numerical studies of dispersion and flammable volume of hydrogen enclosures. HYSAFE International Conference on Hydrogen Safety, Spain: 11-3.
- 3. James Herron, Alexis Flynn & Sarah Kent. March 30, 2012. *Total Leak Underlines Offshore Gas Risks*. The Wall Street Journal.
- 4. Mumby Christopher. 2010. Predictions of explosions and fires of natural gas/hydrogen mixtures for hazard assessment.
- 5. M. Potter & D.C. Wiggert. 2008. *Fluid Mechanics (Schaum's Series)*. McGraw-Hill (USA).
- C.D. Barely, K. Gawlik, J. Ohi, R. Hewett. September 2007. *Analysis of buoyancy-driven ventilation of hydrogen from buildings*. HYSAFE International Conference on Hydrogen Safety, Spain. P 11–13.
- D.M. Deaves, S. Gilham, H. Spencer. January 7, 2000. *Mitigation of dense gas releases in buildings: use of simple models*. Journal of Hazardous Materials. Volume 71, Issues 1–3, P 129–157.
- Wilkening H, Baraldi D. 2007. CFD modeling of accidental hydrogen release from pipelines. Int J Hydrogen Energy 2007. 32:2206-15.
- 9. Houf W, Schefer R. 2008. Analytical and experimental investigation of small-scale unintended releases of hydrogen. Int J Hydrogen Energy 2008. 33:1435-44.
- 10. Versteeg HK, Malalasekera W. 1995. An introduction to computational fluid dynamicsthe finite volume method. New York: Longman Scientific and Technical.