Consequence Study of CO_2 Release from Carbon Capture and Storage (CCS) Using FLUENT-CFD Modeling

by

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Dissertation submitted in partial fulfillment of

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CERTIFICATION OF APPROVAL

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Approved by,

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TRONOH, PERAK

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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 the original work contained herein have not been undertaken or done by unspecified sources or persons.

(NURUL IZATI BINTI MAT YUSOFF)

ABSTRACT

Consequence study of accidental CO_2 released from Carbon Capture and Storage (CCS) pipelines is carried out due to the possibility of pipelines failure and the hazard imposed from the accidents to human and environment. A two dimensional (2D) CO_2 dispersion model is developed using FLUENT-CFD to be compared or validated against Kit Fox Field Experiment data and Fluidyn-PANACHE CFD tool. The validated model is then used to study the release of CO_2 from CCS. FLUENT is chosen since it has been widely used as tool to simulate atmospheric toxic dispersion in several previous studies. Geometry used for the model is the one used in Kit Fox Experiment with presence of obstacles. This study basically involves comparison of results obtained from FLUENT model against real experimental data and other CFD tool. Also by using the model, a case study is carried out on CO_2 accidental release from CCS facilities to observe its consequence towards surrounding population. From comparison, CO_2 concentration obtained by FLUENT exhibits under-prediction by 8% against field experiment, but it is closer to experimental data compared to the one obtained by PANACHE. FLUENT demonstrates average under prediction concentration due to average wind parameter used in the model, and it has been identified as one of characteristics for most of CFD models. From case study of CO_2 release from CCS pipelines, concentration given by FLUENT deviates significantly from theoretical calculation but the variation is due to simplification of using simple dispersion coefficients in theoretical calculation. Accumulation of high CO_2 concentration in region with obstacles imposes very high risks of adverse effects, including death towards human. Concentration prediction through FLUENT-CFD modeling can be utilized as tool to predict CO_2 dispersion and its impacts towards people.

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ABBREVIATIONS AND NOMENCLATURES

CCS	Carbon Capture and Storage
GHG	Green House Gases
CO_2	Carbon dioxide
IPCC	Intergovernmental Panel on Climate Change
AR4	Fourth Assessment Report
EOR	Enhanced oil recovery
2D	Two dimensional
CFD	Computational fluid dynamic
OSHA	Occupational Safety and Health Administration
TWA	Time weighted average
NIOSH	National Institute of Occupational Safety and Health
REL	Reference exposure value
STEL	Short term exposure limit
Y	Probit variable
k_1, k_2	Probit parameters
V	Dose (ppm)
<C>	Concentration (kg/m^3)
Q_m	Mass flow rate (kg/s)
x	Distance downwind (m)
y	Distance crosswind (m)
σ_y, σ_z	Pasquill-Gifford dispersion coefficients in y and z direction
TKE	Turbulence Kinetic Energy
WRI	Western Research Institute

PERF	Petroleum Environmental Research Forum
US DOE	United States Department of Energy
DRI	Desert Research Institute
URA	Uniform Roughness Array
ERP	Equivalent Roughness Pattern

CHAPTER 1: INTRODUCTION

1.1 BACKGROUND OF STUDY

1.1.1 Carbon Capture and Storage (CCS)

Escalating carbon dioxide (CO_2) concentration in atmosphere nowadays has becomes one of the main environmental issues discussed worldwide. In fact, it is highlighted in Kyoto Protocol as one of the main green house gases (GHG) that requires reduction in emission. CO_2 concentration has increased up to 388 ppm in 2010, which is at its highest level in the past 650,000 years (Rackley, 2010). This serious condition of escalating CO_2 concentration lead to more global issues, mainly global warming since it affect the balance of incoming and outgoing energy in earth atmosphere system. Intergovernmental Panel on Climate Change (IPCC) stated in Fourth Assessment Report (AR4) that increase in global average temperature in mid of 20th century is likely to happen (at 90% probability) since increase in CO_2 concentration is observed over the years (Rackley, 2010).

Many alternatives are executed to overcome this huge environmental issue of increasing CO_2 concentration. One of them is through carbon capture and storage (CCS). CCS is a new technology which is still under research and development in most of the countries, but some place already has it in deployment stage. CCS has a huge potential to succeed in reducing CO_2 emission. Basically in CCS, CO_2 produced from industrial and power plants is captured and being transported to storage site where it is sequestrated in deep geologic storage (Wilson & Gerard, 2007). Nowadays, enhanced oil recovery (EOR) is practiced as part of CO_2 injection into geological formation, which in this case oil reservoirs. It is the only available option that has been applied so far on commercial scale (Rackley, 2010).

Deployment of CCS technology demands transportation infrastructure, whereby pipeline networks seems to be the most reasonable transportation can be used for this large scale transportation of CO_2. Texas Gulf Coast CO_2 network currently in operation in United States estimated about 6200 km, and anticipated to be extended by an additional 17,500 to 37,000 km between 2010 and 2050. The pipeline networks have been developed progressively as result of high CO_2 demand in EOR projects in Permian Basin (Rackley, 2010). Thus it is important for us to look into the need of safe transportation of CO_2 in this developing field of CCS (Mazzoldi et al., 2009).

With increasing and developing CO_2 pipeline networks all over the world, there is a higher possibility of pipeline failure to occur. It might be due to corrosion, fractures or leaks. In the case of accidental CO_2 release like this, human exposure to elevated levels of CO_2 is hazardous through direct carbon toxicity. Exposure to high concentration of CO_2 will cause adverse effect, including death. CO_2 levels above 3% would give exponential increase in minute volume, the average volume breathed during 1 minute (Hepple, 2005). Increasing complexity of the system, which in this case the complex pipelines network is identified as one of critical challenges in implementing safety programs in the industry (Qi et al., 2011).

Lesson needs to be learnt from released of high concentration of CO_2 release from Lake Nyos (natural reservoir) event in 1986 which had caused fatality to 1746 people and many livestock near the lake, and up to 14 km distance from the area (Hepple, 2005). CO_2 leakage cases from natural reservoirs serves as analogues for potential CO_2 release from geologic storage in CCS projects (Lewicki et al, 2006). It is crucial for us to always consider past incidents in the industry in order to improvise today's industrial process safety (Qi et al., 2011).

Most of CO_2 pipelines in North American are located in less populated and remote areas. There are more plans of constructing CO_2 pipelines for CCS projects in Western Europe and these pipelines are going through populated areas. In fact, on shore CO_2 pipelines already built in Netherland and it passes very close to the residential areas (Molag & Dam, 2011). Risk is likely to emerge here due to increasing population density close to the vicinities of the facilities (Qi et al., 2011).

With the advancement in CCS technology, more CO_2 pipelines are anticipated to be built, giving higher risk of pipelines failure. Thus it is very important to carry out a consequence study of CO_2 accidental release due to pipelines failure to see how it would affect the surrounding population.

1.2 PROBLEM STATEMENT

Due to developing CCS technology today, more CO_2 pipeline networks are anticipated to be built all across the countries and might go through dense population areas. This condition contributes to more chance of CO_2 pipeline leakage. Release of high concentration of CO_2 from this pipeline gives significant adverse effects towards human health, and also to the environment.

Toxic release is a type of chemical plant accidents with probability of occurrence is the least compared to fire and explosion, but its potential for fatalities is the greatest. The past 26 years Bhopal disaster toxic gas release in 1984 killed 3000 lives and while other 300,000 sustain irreversible health injuries. The tragedy is a type of toxic release and still quoted as example of world worst industrial incident (Qi et al., 2011). The obvious risks of toxic release and its critical consequences are very serious. Hence, it is important to carry out a study on consequence of toxic CO_2 release to human and also environment (Crowl & Louvar, 2002). With growing CCS technology and pipelines facility, the risk imposed to the surrounding population will definitely be higher.

Buncefield Major Incident Investigation Board stated that in Buncefield incident, modeling of resulting overpressure from vapor cloud explosion, heat radiation and domino effects were not considered. One of the causes of insufficient attention to leading indicators (which is one of challenges of process safety implementation in process industries) occur due to insufficient consequence modeling tools for the prediction of process upsets (Qi et al., 2011). Availability of FLUENT modeling tool might assist in consequence study of CO_2 leakage form CCS pipelines network.

Therefore, it is seen to be very significant to carry out a consequence study of high concentration of CO_2 release from CCS. It is crucial to observe how the release would affect differently, in terms of concentration in different area in geometry, with presence of obstruction. There are conventional tools available to estimate toxic dispersion, such as PHAST 2D, SAFETI and EFEFCT but FLUENT has been proven to provide good results in estimating toxic dispersion (Sabatino et al., 2007).

This study chooses FLUENT model of computational fluid dynamics (CFD) to give a better estimation of toxic CO_2 dispersion. The model is available and thus can be used to develop the 2D model for the consequence study. Qi et al (2011) stated that modeling is a way to understand consequences as part of dedicating high quality scientific research to overcome problem of increasing complexity in process industries.

1.3 OBJECTIVES

1. To develop a model for CO_2 release simulation using FLUENT.
2. To compare CO_2 dispersion from FLUENT model against real experimental data and other CFD tool.
3. To study the consequence of CO_2 release from CCS pipelines towards surrounding human.

1.4 SCOPE OF STUDY

This study mainly focuses on developing a 2D simulation of high concentration CO_2 release by using geometry same as the one used in Kit Fox Field Experiment. The result obtained from FLUENT model will be compared to field experimental data and Fluidyn-PANACHE CFD. The model is then used later for consequence study of high CO_2 release from CCS pipelines.

In developing the FLUENT model, a suitable dispersion model needs to be identified in order to run the simulation. A number of turbulence models are provided in FLUENT (Tang et al, 2006). To develop the model itself, basic physical geometry needs to be defined. The geometry does not need to be too complicated. Simple geometry consists of release point and some obstruction (i.e buildings and large equipments) would suffice, since the objective is to develop a model which able to predict different concentration of toxic CO_2 at different points or area in the model.

Other criteria need to be determined is the boundary profile of the geometry. This includes height of source release, Schmidt number (Sc), atmospheric stability, wind speed and ambient temperature (Tang et al, 2006). Physical properties of CO_2 are also required, for instance density of the gas and phase of the released $CO_{2.}$ Mass flow rate, concentration and duration of released CO_2 are also important input data to simulate the model.

A good model should be able to simulate result or data until it converges or comparable to Kit Fox experimental data. The model is validated and can be used as an established model for further consequence study, which is high pressure release of high concentration CO_2 which the effects definitely would be more harmful and deadly.

CHAPTER 2: LITERATURE REVIEW

2.1 HAZARDS OF CO_2 TOWARDS HUMAN HEALTH

Intergovernmental Panel on Climate Change (IPCC) in its special report on CCS stated acute exposure to CO_2 at or above 3% would give effect to human health (Wilson & Gerard, 2007). Table 1 listed the adverse effects of exposure to CO_2 at different concentration together with existing recommendation and regulations.

Table 1: Adverse effects of CO_2 at different concentration (Wilson & Gerard, 2007)

CO_2 CONC.	ADVERSE EFFECTS	EXISTING RECOMMENDATION AND REGULATIONS
0.5%		OSHA Regualtions 8-hr TWA, NIOSH Guidelines, REL 10-hr TWA
3%	Local and cerebral vasolidator, breathing laboured and double normal rate, impaired hearing and vision, headache, high blood pressure and pulse, weak narcotic effect, mental confusion, acute exposure affects health	Vacated OSHA regulations, STEL, NIOSH guidelines STEL 15-minute TWA
4-5%	Breathing rate four times normal rate, feelings of intoxication, slight choking, headache, dizziness, increased blood pressure	4% NIOSH Guidelines: Immediate dangerous to life and health
>30%	Death within minutes	

The nature of gaseous CO_2 being 1.5 times denser and less viscous than air at ambient temperature has caused it to remain at the ground level once released and increase more risk imposed to humans (Mazzoldi et al, 2008).

2.2 CO_2 ASPHYXIATION

CO_2 is a type of asphyxiant. Asphyxiant gases usually are heavier than air and tend to accumulate in low areas. In 1986 Lake Nyos incident demonstrates lethal consequence when CO_2 displaced oxygen. It kills 1700 people who lived below or near the lake but spare the lives of the people living uphill, since CO_2 is denser than air (Holland, 2011).

Asphyxiant induces hypoxic injury by displacing oxygen from ambient air and causing asphyxiation or suffocation. Entry to high concentration CO_2 area would require self contained breathing apparatus (SCBA) or other supplied air respirators. Victim who collapses on floor is subjected to a higher concentration of the asphyxiant (Holland, 2011).

Knowledge on dangers of breathing high concentrations of CO_2 is generally low. With CCS technologies embarking fast nowadays, CCS pipelines are likely to have inventories of dense phase CO_2 in very large amount up to hundreds of thousands of metric tons. Definitely the potential of population exposure to high concentration CO_2 from this facility exist (Eldevik, 2008).

Inhalation of high concentration CO_2 will increase acidity of blood and would trigger adverse effects on respiratory, cardiovascular and central nervous systems. Breathing air with CO_2 concentration above 5% will pose significant hazard to people due to its toxicological effects. As explained by Wilson & Gerard (2007), inhalation of CO_2 at or above 30% can cause death within minutes, and this happens well before CO_2 asphyxiation impairment could even occur (Eldevik, 2008).

2.3 POINT SOURCE OF TOXIC RELEASE IN CCS

CCS technology is developing and would demand extensive CO_2 transportation facilities. It increases possibility of pipeline failure and would cause leakage and endangering lives (Mazzoldi et al, 2008). Toxic release usually would cause small damage to equipments, but contribute significantly to personal injuries, fatalities, legal compensation and cleanup liabilities. Mechanical failure is recognized to be the common cause of chemical plant accidents with 44% accidents, followed by operator error with 22% and process upsets with 11% (Crowl & Louvar, 2002).

Mechanical failure relates much to maintenance problem of equipments or hardware. In Figure 1, according to 'A Thirty-Year Review of One Hundred of the Largest Property Damage Losses in the Hydrocarbon-Chemical Industries', it shows 29% of largest losses are associated with piping systems (Crowl & Louvar, 2002).

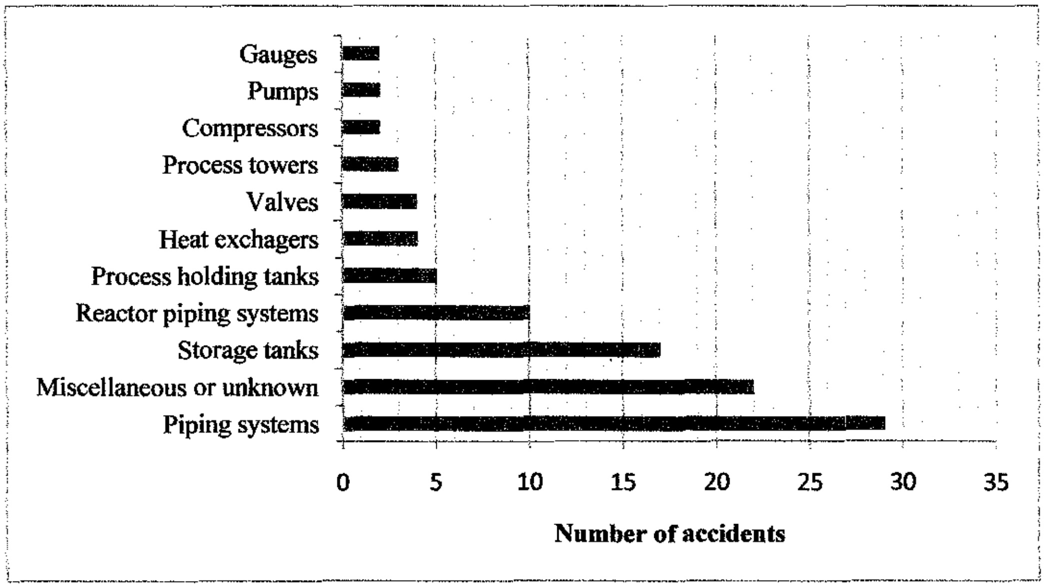

Figure 1: A Thirty-Year Review of One Hundred of the Largest Property Damage Losses in the Hydrocarbon-Chemical Industries (Crowl & Louvar, 2002)

Therefore, piping systems failure can be considered to be a critical CO_2 point of release due accidental leakage.

2.3 TOXICOLOGY

2.3.1 Probit Correlation for Toxic Release Damage

Toxic hazard is defined as likelihood of damage to biological organisms based on exposure resulting from transport and other physical factors of usage Human tend to react differently to the same dose of toxicant. Responds might vary from weak or low response to high response, which can be represented by a normal or Gaussian distribution with higher percentage of individuals affected will be in average response. For computational purpose, probit (probability unit) method is a convenient method can be used rather than response versus dose curve. Equation 2-1 shows the relation of probit variable (Y) to probability (P) (Crowl & Louvar, 2002).

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

Causative factor is represents the dose (V). Probit variable (Y) is calculated from Equation 2-2 (Crowl & Louvar, 2002).

$$Y = k_1 + k_2 \ln V \qquad (2\text{-}2)$$

where k_1 and k_2 are the probit parameters.

2.3.3 Source and Dispersion Model

Atmospheric dispersion of toxic materials is affected by several factors such as wind speed and direction, atmospheric stability, ground condition, height of release above ground level and also momentum and buoyancy of material released.

CO_2 is a heavy gas and denser than air. Hence, once released, the gas tends to sag towards the ground. Then, the gas will travel downwind and mixed with fresh air to a point where the gas is sufficiently diluted and considered to be neutrally buoyant. Plume type of neutrally buoyant vapor cloud dispersion model is used whereby continuous release of the toxic gas is assumed and occurs at steady state.

Concentration of the released CO_2 can be determined by using Equation 2-3 (Crowl & Louvar, 2002) which is the case for plume with continuous steady state source at ground level and wind moving in x direction at constant velocity.

$$\langle C \rangle(x, y, z) = \frac{Q_m}{\pi \sigma_y \sigma_z u} exp\left[-\frac{1}{2}\left(\frac{y^2}{\sigma^2{}_y} + \frac{z^2}{\sigma^2{}_z}\right)\right] \tag{2-3}$$

where Qm is constant mass release rate, σ_y and σ_z are the Pasquill-Gifford dispersion coefficients for plume dispersion in meter. Ground level concentration can be obtained by setting $z = 0$. While for ground level centerline concentration, y and z both should be set to zero.

Dispersion coefficients are obtained by using Equation 2-4 until 2-7 (Crowl & Louvar, 2002) for rural and urban conditions, respectively. Both coefficients represent standard deviations of concentration in the downwind, crosswind and vertical (x, y, z) directions. Equation 2-4 until 2-7 are used for dispersion model with atmospheric stability class A with wind speed less than 2 m/s, since wind speed used is case study is only 1 m/s to depicts worst case scenario where wind speed is very low during the time of CO_2 release.

Rural conditions:

$$\sigma_y(m) = 0.22x(1 + 0.0001x)^{-1/2} \tag{2-4}$$

$$\sigma_z(m) = 0.20x \tag{2-5}$$

Urban conditions:

$$\sigma_y(m) = 0.32x(1 + 0.0004x)^{-1/2} \tag{2-6}$$

$$\sigma_z(m) = 0.24x(1 + 0.0001x)^{1/2} \tag{2-7}$$

2.4 SIGNIFICANCE OF USING FLUENT-CFD FOR THE CONSEQUENCE STUDY

Consequence study can be carried out by using many tools. Conventional tools available such as PHAST, SAFETI and EFFECT only focus on two dimensional (2D) releases which areas affected are only depicted in contours. This does not take into account presence of obstacles in the geometry and therefore yields less accurate results.

Tauseef et al, 2011 stated that Computational Fluid Dynamics (CFD) is recognized as a potential tool can be used for realistic accidental loss of contaminants consequence since it takes into account the effects of obstacles and complexity of geometry. Heavy gas dispersion is assessed in the presence of obstacles. The data is compared to experiment conducted by Health and Safety Executive (HSE) UK at Thorney Island. From the results, closest prediction of concentration profile is obtained by using realizable k-ε model. It also capture phenomenon of gravity slumping associated with dense gas dispersion.

CFD also capable of simulating atmospheric transport of contaminants and the population exposure which allows proper emergency planning to respond to potential accidents in toxic industrial chemicals (Costa et al, 2007). Due to its reliability and accurate results, CFD has been used widely in LNG spills and urban environment studies. It is used to develop 3D model to simulate dispersion of contaminants Sulphur Mustard HD Agent in Lisbon city center.

There are varieties of CFD models available today, such as PHAST, QUIC-CFD, FLACS, VADIS and FLUENT. For this study, FLUENT model is used to simulate the dispersion of toxic release. The reasons are due to the availability of the software and also the fact that FLUENT is the most widely used CFD model for wide range of industrial applications and has an extensive use all over Europe due to its capability of simulating boundary layer (Sabatino et al, 2007).

Tang et al, 2006 used FLUENT-CFD to simulate atmospheric toxic dispersion within arrays of buildings (obstacles) and the result is validated against results from AERMOD database (model developed by US EPA in 2005). Turbulence model used is standard k-ε turbulence model. Concentration given by FLUENT matches the results from AERMOD at constant wind direction. Best agreement achieved at Schmidt number (Sc) equal to 1. FLUENT also manage to capture variation caused by variation in wind direction. FLUENT also provides good agreement with turbulence kinetic energy (TKE) profile developed based on similarity theory.

Sabatino et al, 2007 studied dispersion of pollutant in street canyons and validated it against ADMS-Urban (environmental software) and wind tunnel data (CEDVAL). FLUENT code is used where standard k-ε turbulence model is used. Standard k-ε model is the most optimum choice as compared to other models. Value of 0.013 is suggested to be used for coefficient used to define eddy viscosity, $C\mu$ in k-ε model. This is to prevent overestimating near ground turbulence levels, which is always happen by CFD codes. It is concluded results obtained from FLEUNT are in good agreement with ADMS-Urban predictions. In fact FLUENT gives more information on the pollutant (CO) distribution.

Kiša & Jelemenský (2008) used FLUENT-CFD to simulate dispersion of pressure liquefied ammonia. Two phase flow occurs at the release point of the toxic, forming a dense toxic cloud in near the point of release. The boundary condition used is identical to FLADIS experiment. In FLUENT, instantaneous position of plume is identified and plume statistics is calculated. This gave more accurate results since it neglects sudden changes in wind direction. From the data validation, it is concluded that by application of k-ε model is sufficient to simulate toxic plume dispersion. The results can be improved if Sc is assumed not constant throughout the atmospheric boundary layer.

Mazzoldi et al (2008) explains the importance of carrying out CO_2 dispersion modeling due to leakages from transportation facilities (pipelines) before deploying large scale CCS projects. The study utilize CFD tool Fluidyn-PANACHE and the results is validated against Prairie Grass and Kit Fox field experiments. Pollutant released in

Prairie Grass experiments is SO_2. On the other hand, Kit Fox experiments used pure CO_2. Due to that, comparison of results between PANACHE and Kit Fox will be discussed here, since the pollutant concerned for this study is CO_2. Constant mean wind speed and ambient temperature is assumed for boundary conditions. Two turbulence models are used, which are *k-ε* model and *k-l* model. Duration for release is 2 to 5 minutes (for continuous plume). *k-l* model performed better due to the latter tendency of underestimating gas concentration. Under prediction of concentration occurs due to simplicity of utilizing constant average wind speed and direction. But then, the tool able to give accurate average gas concentration in naturally occurring short term concentration peaks. Result of constant concentration prediction is obtained fairly to constant wind parameters used in the model. Nevertheless, the result is still well in the range of model acceptability. (Holland, 2011) (Placeholder1)

Witlox et al (2009) explains there is a significant impact in concentration prediction if presence of solid CO_2 and mixing of it with air is considered. In this study of atmospheric dispersion from CO_2 release, CFD model PHAST is used. Originally PHAST only predict release of toxic in liquid and vapor phase. The model is extended to include occurrence of solid transition. Neglecting solid phase in CO_2 dispersion results in under estimation in concentration in near field and over estimation in far field.

Molag & Dam (2011) provides basis assumption need to be considered in modeling of released high pressure CO_2 modeling. Some of the findings are:

- Solid effect inside the pipelines does not need to be taken into account.
- CO_2 will only be in vapor and solid phase after flashing since CO_2 cannot exist in liquid phase at ambient pressure.
- Using k-ε model for turbulence effect.
- Take into account stability of air, wind velocity, density of cloud (since dense gas is tested) and topology of geometry.
- Setting the right turbulent properties for atmospheric flow in each different stability class.

CHAPTER 3: METHODOLOGY

3.1 RESEARCH METHODOLOGY AND ACTIVITIES

Study and identify the most suitable dispersion model. **Realizable k-ε turbulence** model is chosen since it has shown successful applications in dense gas dispersion over complex geometry (Tauseef et al., 2011) and recommended for high pressure CO_2 modeling (Molag & Dam, 2011).

Analyze and develop the physical geometry as the one used in **Kit Fox Field Experiment** (Mazzoldi et al, 2008) since the experiment tested dispersion of pure CO_2.

Identify **input for boundary profile** of the FLUENT model (i.e wind direction, wind velocity, ambient temperature and etc) from Hanna & Chang, (2001) and Kashi et al., (2010).

Run FLUENT model simulation until the **solution converges.**

Compare FLUENT result against Kit Fox experiment and Fluidyn-PANACHE CFD (Mazzoldi et al, 2008). The FLUENT model having good agreement with experimental data is further used for case study.

CASE STUDY: Proceed to consequence study of CO_2 release from CCS pipelines at higher release pressure. Concentration given by FLUENT is compared against theoretical concentration calculation from Crowl & Louvar, 2002.

To develop the physical geometry of the region of study, topology in Kit Fox experiment is used since it was conducted to test dispersion of pure CO_2 to the atmosphere with presence of obstacles as part of Petroleum Environmental Research Forum (PERF) 93-16 project carried out in late summer 1995 at the US Department of Energy (DOE) Nevada Test Site (Hanna & Chang, 2001; Hanna & Steinberg, 2001). The topology not only been used by Mazzoldi (Mazzoldi et al, 2008) but also in many other CFD modeling of CO_2 dispersion by FLUENT or any other CFD model (Hanna et al., 2004; Hanna & Chang, 2001).

3.2 KIT FOX FIELD EXPERIMENT DESIGN AND SETUP

Field operation was carried out by Desert Research Institute (DRI) and Western Research Institute (WRI). In the experiment, pure CO_2 gas was released from ground level area source of 1.5m x 1.5m. Entire experiment in term of size was built to represent 1/10 of actual chemical plant or oil refinery (Hanna & Chang, 2001). In order to do that, thousands of plywood was installed in 120m x 314 whole field size to increase the surface roughness of the experiment area.

The plywood obstacles are installed in two different arrays of Equivalent Roughness Pattern (ERP) and Uniform Roughness Array (URA). URA covers the whole field size while ERP cover on the smaller field contained in the whole field with area of 39m x 85m (Hanna & Chang, 2001). Below is the simplified drawing of the experiment setup and other details of the experiment (Hanna & Chang, 2001; Hanna & Steinberg, 2001; Hanna et al., 2004; Mazzoldi et al., 2008; Kashi et al., 2010):

1. URA obstacles:
   Size: 0.2m high x 0.8m wide plywood billboards
   Spacing: 2.4 m (both lateral and longitudinal)

2. ERP obstacles:

   Size: 2.4m square plywood billboards

   Spacing: 6.1 m (lateral) and 8.1m along-wind

3. Representation of experiment field:

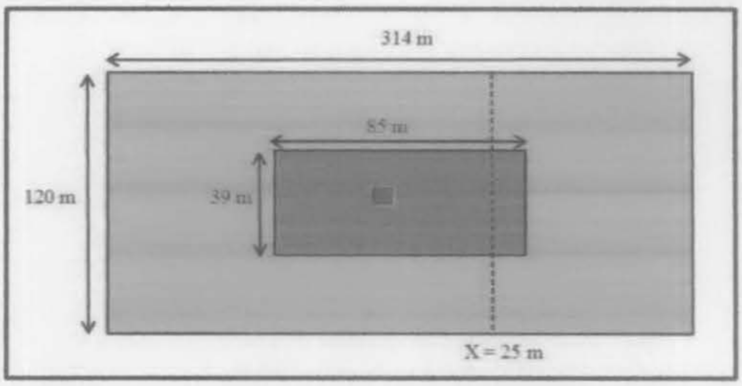

Figure 2: Kit Fox Experiment Setup

Yellow region represents URA array and green region represents ERP array. Source of release on ground level is represented by red box in the middle. The release point is set at coordinate of point of origin (0,0) of the whole geometry. This is to ease coordinate calculation for drawing geometry in Design Modeler. Note at x at 25 m is where the concentration obtained is used in Mazzoldi et al., 2008 and will be used in this modeling validation.

Below is the actual image of Kit Fox Experiment setup in Nevada Test Site:

Figure 3: Actual Kit Fox Experiment Setup in Nevada Test Site

It is important to consider presence of obstacles in dispersion modeling. Previously before Kit Fox Experiment was carried out, dense gas dispersion usually involves idealized experiments which underlying surface was relatively smooth. This contradict to actual accidental release likely to involve rough surface obstacles such as buildings, tanks, pipes and any other industrial facility (Hanna & Chang, 2001). This shows relevant industrial concern of CO_2 dense gas dispersion in rapidly developing CCS pipeline network.

3.2.1 Chosen Trial From Kit Fox Experiment Used in Fluent Modeling

Kit fox experiment consists of 52 trials. For this modeling project, validation is decided to be made against Mazzoldi et al, (2008) using trial 4-4. Detail of the trial is obtained from Hanna & Chang (2001) and described as follows:

Release category : plume / continuous release

Mass rate : 3.89 kg/s

Duration of release : 450 s (7.5 minutes)

Wind Speed : 2 m/s (average)

Temperature of gas : 29 °C (equal to surface ground temperature) (Kashi et al., 2010)

Constant value of wind velocity within the dense gas cloud is assumed since it is sufficient to know the wind velocity in the ambient air (Hanna & Chang, 2001). For this trial, concentration of CO_2 is provided downwind at x= 25 m for experimental data (Kit Fox) and Fluidyn-PANACHE CFD (Mazzoldi et al., (2008). These data will be compared against concentration value at x= 25 m obtained by FLUENT.

3.3 WORKFLOW BY STAGES IN USING ANSYS FLUENT

3.3.1 Drawing Two Dimensional (2D) Geometry Using Design Modeler

Analysis type of geometry is set to 2D. The geometry concerns only on ERP array of obstacles and does not include URA array and shown in Figure 4. Also, the length of the field considered is only up to x = 110 m from point of origin (total length of 200 m) for simplification purpose since bigger geometry needs more calculation and takes a longer time to converge. Original dimension is 314 m where x = 224 m.

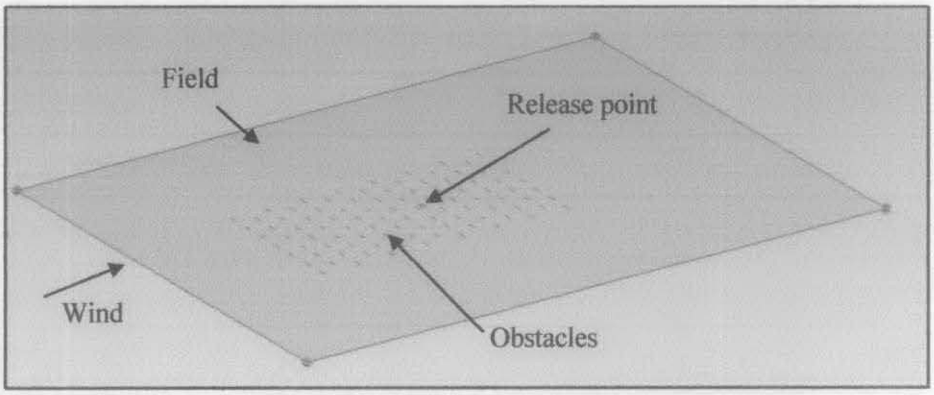

Figure 4: Simplified 2D Geometry With Presence of Only ERP Obstacles

Pattern or array function is used in DM to create the ERP obstacles. Method used to create surface of field, point of release and obstacles is done using surface from sketch function. To ensure obstacles are not meshed together with field surface, Boolean function subtract operation is used where field surface is set as Target Body and surface obstacles set as Tool Body.

3.3.2 Meshing Geometry Using Meshing Application

Edge sizing also been assigned for all edges of field as part of mesh control method. Number of division at each edge is set to 200 at all vertical and horizontal boundaries in order to have smaller grid along each edges as shown in Figure 5.

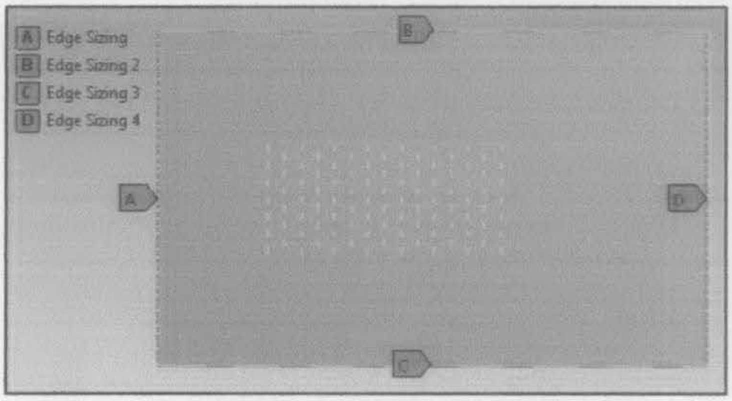

Figure 5: Edge Sizing at All Edges of the Region

Here in meshing is where boundary layers are set using Named Selections. They are inlet of air, inlet of CO_2 and outlets. Figure 6 shows the boundaries set for the geometry accordingly.

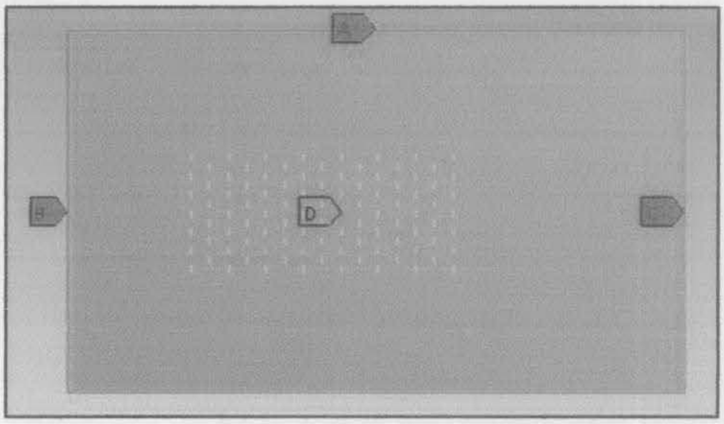

Figure 6: Boundary Layer (Named Selections) Set for the Geometry

where A = outlet for both vertical boundaries
B = inlet of air
C = vertical outlet
D = inlet of pure CO_2 gas

Below is the meshed geometry. Note at higher grid refinement is achieved at edges with edge sizing. Mapped face meshing setting is applied to get a more ideal meshing, more uniform, having less distorted elements and triangles, and also less nodes.

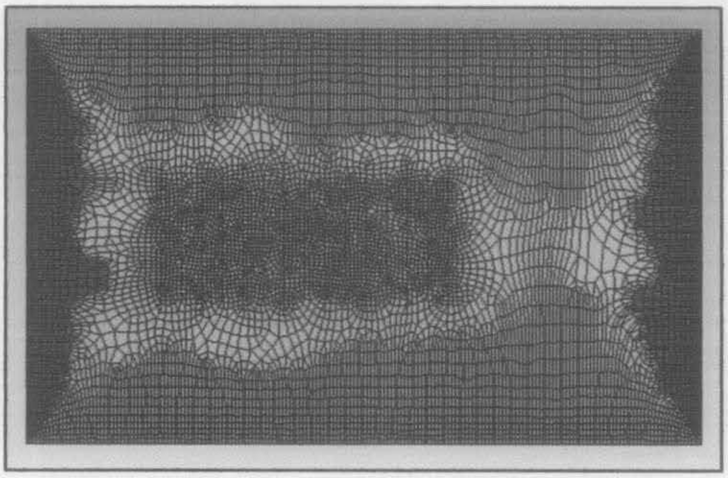

Figure 7: Meshed 2D Geometry in ANSYS Meshing Application

3.3.3 Setting-up FLUENT Boundary Conditions and other Calculation Parameters

Problem Setup

Meshed geometry is uploaded from Meshing application into FLUENT. Energy equation and viscous is set for the model. Viscous is changed from laminar to realizable k-ε model. Near wall treatment is set to standard wall function. Species transport is set since this study involves dispersion and transport of species. This model involves mixture of air into the system since air is coming from x direction at 2 m/s speed and sweep away the dispersion of CO_2 from the along the geometry (0,0).

Boundary conditions settings are shown in Table 2. For the purpose of comparing the model result against experimental data and PANACHE, initial gauge pressure from release source (inlet CO_2) is set to 4 bar. Other input required is listed in section 3.2.1.

Table 2: Type for Each Boundary or Zone

Inlet of air	Velocity inlet
Inlet of CO_2	Mass flow
Outlets	outflow
Interior surface body	Interior
Wall	Wall
Wall surface body	Wall

Solution

Pressure-velocity coupling scheme used is SIMPLE. For spatial discretization, gradient used is least square cell based and pressure is standard. Other properties are set to First Order Upwind except for momentum, which is set to Second Order Upwind. Default setting is used for solution control. As for residual, convergence absolute criteria are set to 1E-06 for energy and all species, while the rest is set to 1E-04. Solution is initialized from all zones and converges at 12642th iteration.

CHAPTER 4: RESULT AND DISCUSSION

4.1 COMPARISON OF FLUENT RESULT AGAINST KIT FOX FIELD EXPERIMENT AND PANACHE CFD.

3.89 kg/s pure CO_2 gas is released from release point with wind coming from x direction at 2 m/s. It is observed that toxic cloud dispersed in x direction and gets wider as distance increases from the release point, as shown in Figure 8. Concentration of CO_2 is higher inside the plume. Fraction of CO_2 is big at the region close to the release point, indicating very high toxic concentration at that area.

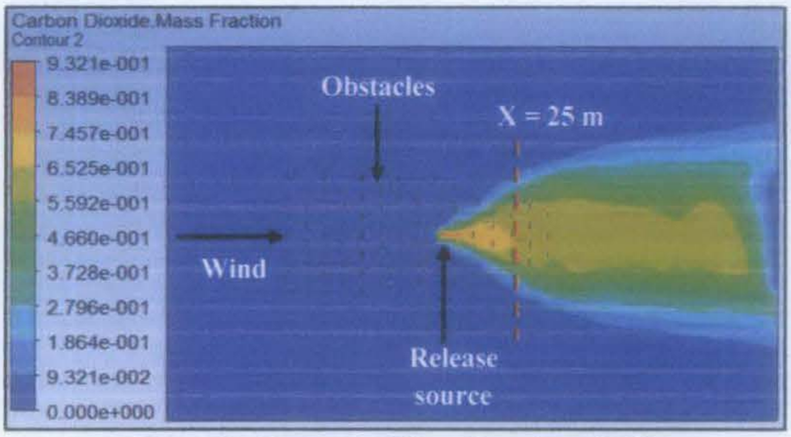

Figure 8: Contour of Mass Fraction of CO_2

From velocity contour in Figure 9, it is shown that velocity increases from 2 m/s from inlet as the wind moves outside of the obstacles region. Wind speed increases as it moves along the outer part of obstacles region and CO_2 toxic cloud. Presence of obstacles has reduces wind speed to near zero across the obstacles region. Area covered by toxic cloud as shown in Figure 8 is having low velocity in the cloud area as shown in Figure 9.

The toxic cloud is not dispersing well due to very low wind velocity in obstacles region. Condition of low wind velocity here promotes accumulation of high concentration CO_2 in that region. Nature of CO_2 which is denser and less viscous than air also cause it to remain close to ground, imposing major risks to humans especially in the condition of complex geometry and low wind speed. These characteristics also keeps CO_2 from mixing with air and creating a non-homogenous wind in dispersion area, leading to non-uniform concentration pattern within the toxic cloud where CO_2 is accumulating randomly inside the plume (Mazzoldi et al., 2008).

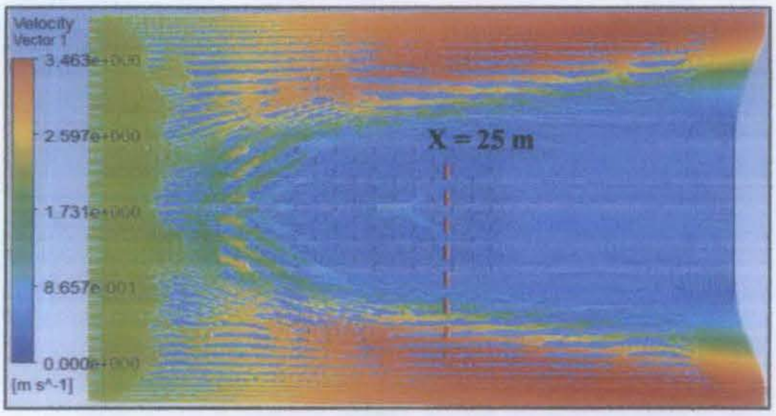

Figure 9: Contour of Velocity Vector (m/s)

Figure 10 shows wind profile crosswind at x = 25 m concentration arc. It is obvious reduction in wind velocity as the wind pass through area with obstacles. Here at x = 25 m is where the comparison of CO_2 concentration will be made against experimental data and PANACHE. The graph clearly shows reduce in velocity across obstacles region. This has caused the accumulation of toxic gas in the region.

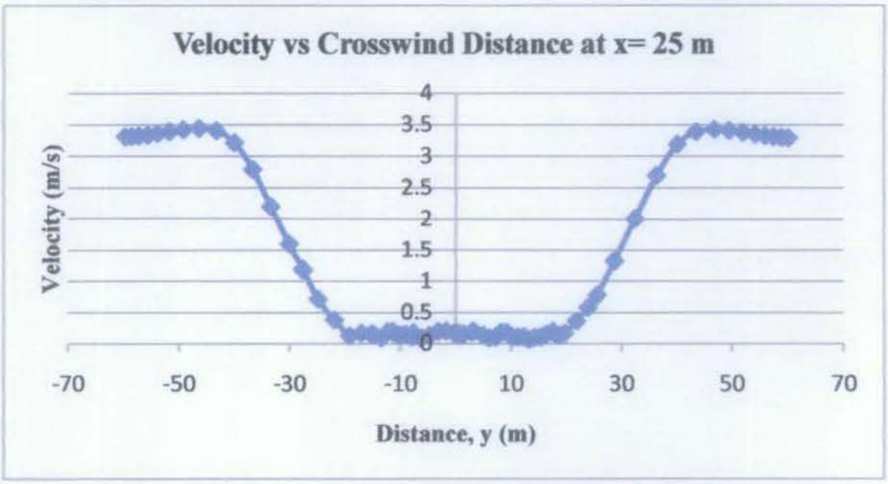

Figure 10: Graph of Velocity (m/s) vs. Crosswind Distance at x = 25 m

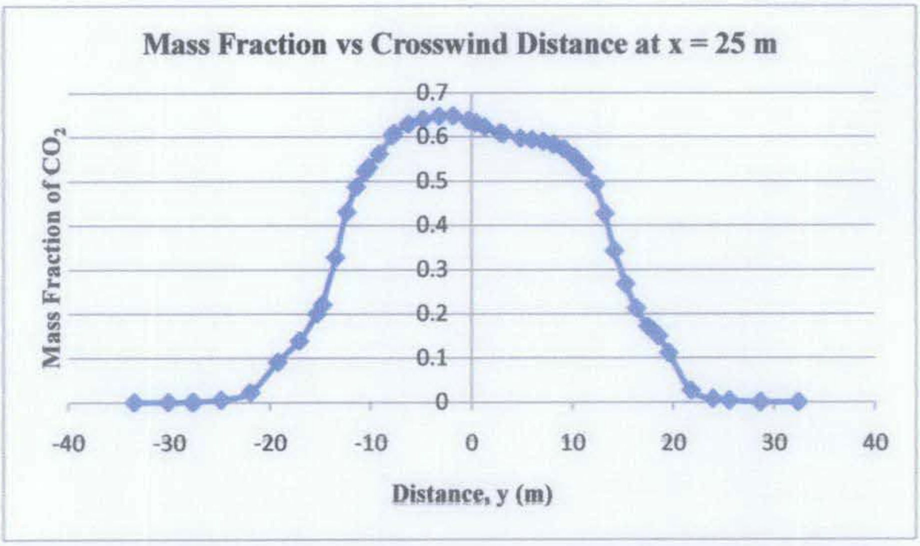

Figure 11: Graph of Mass Fraction vs. Crosswind Distance at x = 25 m

Figure 11 shows mass fraction of CO_2 along x = 25 m. The average CO_2 mass fraction obtained is 0.032 or 32124 ppm. The average value of CO_2 concentration from trial 4-4 of Kit Fox Experiment and PANACHE at monitor point (x = 25 m) is obtained from Mazzoldi et al., (2008) and is listed below. Experimental data shows fluctuation in concentration peaks but PANACHE result tends to give constant average concentration due to using constant value for wind speed and direction. The average concentration values are as below:

- Kit Fox Field Experiment : 34588 ppm
- PANACHE : 26470 ppm
- FLUENT : 32124 ppm

PANACHE gives **23%** difference from its under predicted value against Kit Fox Field Experiment. While FLUENT gives smaller under prediction by **8%** against experimental data. Therefore, FLUENT average concentration prediction is better compared to prediction by PANACHE.

Experimental data recorded maximum concentration of 100,000 ppm, which occur naturally but diverging from the mean CO_2 concentration. The difference from this maximum value recorded against average concentration obtained by PANACHE (26470 ppm) is almost **73%**, and it is a strong under-prediction. However, result by PANACHE is still well within the range of model acceptability (Mazzoldi et al., 2008).

Comparing the maximum concentration against FLUENT average CO_2 concentration of 32124 ppm, the difference is **68%**. Thus, FLUENT gives a smaller under prediction compared to PANACHE and therefore also within the range of model acceptability. The observed average under predictions of CO_2 concentration obtained by both CFD tools (PANACHE and FLUENT) is due to simplification of using average wind speed and direction. Constant value used for these parameters in modeling will fairly gives fairly constant concentration prediction. In fact, it is a characteristic of all CFD models (Mazzoldi et al, 2008). The actual experimental condition experienced changes of wind speed and direction significantly up to 5 m/s and 20°.

From the average concentration given by FLUENT (32124 ppm) and PANACHE (26470 ppm), the difference between these two values is 18%. Although both are CFD models but FLUENT model used *k-ε* turbulence model while PANACHE used *k-l* turbulence model. *k-ε* turbulence model has been widely used from previous studies and also realizable k-ε turbulence model is recommended for concentration profile prediction of heavy gas dispersion in presence of obstacles (Tauseef et al., 2011).

After comparison have been made against Kit Fox Field Experiment, FLUENT model can be used for concentration prediction of CO_2 atmospheric release with significant under prediction due to not accounting variation in wind speed and direction in the actual release condition (Mazzoldi et al, 2008). This established model will be further used for case study purpose of high pressure CO_2 from CCS.

4.2 CASE STUDY: CONSEQUENCE STUDY OF CO_2 RELEASE FROM CCS

In CCS pipelines, CO_2 is transported at a very high pressure, between 10 MPa to 20 MPa (Molag & Dam, 2011). Since this FLUENT model does not account for multiphase flow, we can only consider high pressure release of CO_2 in gas phase. Pressure used for the release is 70 bar (≈ 7 MPa). At 7 MPa and 300 K ambient temperature, CO_2 still exist in the gas phase. Wind speed is reduced to 1 m/s for this case study. Figure 12 shows contour of molar concentration of CO_2 across the geometry. The high concentration CO_2 cloud region (indicated by yellow to red colours) expanded and the whole plume dispersed more widely as compared to release at experimental scale as shown in previous Figure 8.

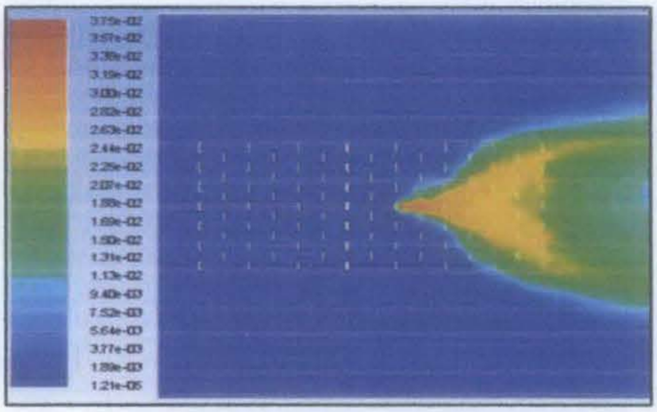

Figure 12: Contour of Molar Concentration of CO_2

The concentration profile of CO_2 released obtained from FLUENT is measured along downwind from release point until x = 80 m. and is shown in Figure 13. The concentration at x = 80 m from simulation is compared against concentration values obtained by using theoretical estimation in Equation 2-3 until 2-7 at the same downwind location.

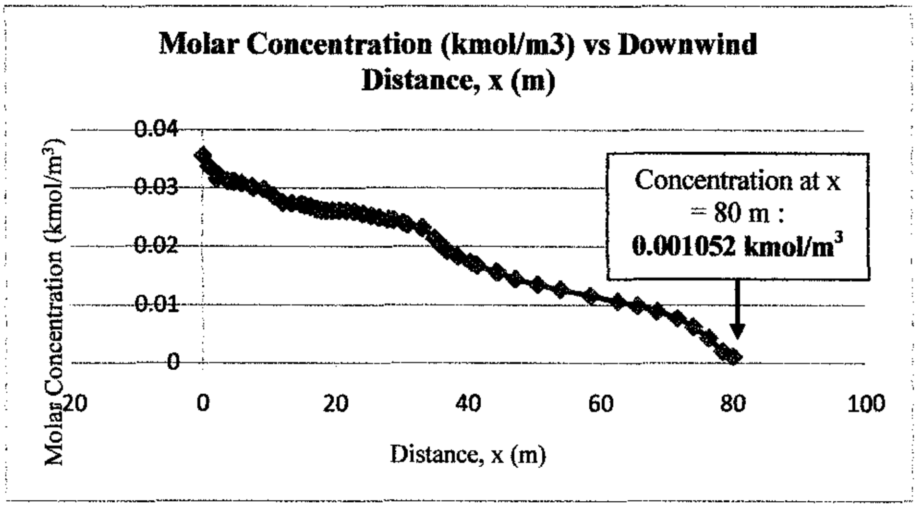

Figure 13: Concentration Profile of CO_2 Molar Concentration (kmol/m^3) vs. Downwind Distance (m)

From FLUENT result, concentration of CO_2 at x = 80 m is 0.001052 kmol/m^3. By using Equation 2-3 for both rural and urban condition at x = 80 m, the concentration obtained is shown below:

- Rural area : 0.001600 kmol/m^3 (59,930 ppm)
- Urban area : 0.000918 kmol/m^3 (34,400 ppm)
- FLUENT : 0.001052 kmol/m^3 (39,400 ppm)

Here at far field 80 m from release point, theoretical estimation of rural area gives higher concentration estimation because presence of obstacles is not considered for this case. Less obstacles will cause lower accumulation of CO_2 occur in near field, causing CO_2 to be swept away very well and has higher concentration at far field. With urban area case, definitely consideration of obstacles presence would accumulate more CO_2 at area close to the release point. Then, concentration of CO_2 at far field (i.e 80 m from release point) would be smaller since more CO_2 is accumulating at region with obstacles closer to the release point rather than being dispersed away.

The predicted theoretical concentrations for rural and urban area are compared against 0.001052 kmol/m^3 concentration from FLUENT. Rural area concentration is higher than FLUENT concentration by **34%** and urban area concentration is lower by **15%**. The difference is smaller when urban concentration is compared against modeling value. This is because the model for urban area might suits the problem more since the geometry itself involves arrays of obstacles and release source is located in the middle of the obstacles.

Difference in concentration between theoretical calculation and modeling might occur due to simplification used in theoretical model. The dispersion coefficients used are general and not specifically for CO_2. Use of simple Pasquill-Gifford (PG) model might lead to error in estimation since the correct dispersion coefficients for short term distance from the release source are usually unknown. A modified and more realistic dispersion coefficients obtained from experimental data has able to predict downwind concentration of toxic gas more accurately (Rege & Tock, 1996). Thus, the theoretical model used here does not consider difference in geometry and properties of the dispersed toxic. The usage of these uniform dispersion coefficients for all types of geometry and all types of toxic in both urban and rural area concentration estimation would definitely induce error in estimation.

At predicted CO_2 concentration downwind at x = 80 m of 39,400 ppm or 4%, personnel being on centerline 80 m away from release source will experience breathing rate four times normal rate, feelings of intoxication, slight choking, headache, dizziness and increased blood pressure. NIOSH guidelines stated concentration of CO_2 at 4% is immediate dangerous to life and health (Wilson & Gerard, 2007). This will endanger the working personnel near the release area especially during pipelines maintenance where this kind of transient operation will involve more human intervention compared to routine operation. Therefore during operation like this, more lives is exposed to the variety of adverse effects from CO_2 toxic release from the facilities.

CHAPTER 5: CONCLUSION AND RECOMMENDATIONS

In conclusion, FLUENT-CFD can be used as tool for CO_2 concentration prediction in atmospheric release with certain under prediction. The under prediction criteria has been explained as an identified characteristics for most of CFD models by Mazzoldi et al., 2008.

As for recommendations for this project, a transient solution of the model is proposed to be done in order to get concentration profile over time. By having this, a better comparison can be done on FLUENT transient data against real experimental data where variation of concentration obtained from both FLUENT and experiment can be observed in a more details manner instead of averaging out the concentration observed experimentally and compare it against average concentration predicted by FLUENT.

Due to simplification in CFD model by using mean wind parameters has caused average under prediction of CO_2 concentration obtained by FLUENT and other CFD models, it is recommended for future study on CO_2 dispersion to apply wind parameters as closely as possible to the used in actual field experiment. This is to overcome the overall simplification which causing FLUET to produce average concentration prediction.

In the future, modeling of CO_2 release in multiphase flow should be carried out to simulate the actual release of CO_2 from CCS pipelines. Leaks from pipelines will cause CO_2 to be dispersed out and experience gas to solid transition and might involve turbulent jet release. It is proven that presence of solid from the dispersion will definitely affect the predicted concentration given by CFD models. By taking pure CO_2 gas release and does not account for solid formation will cause under prediction for the region close to release point and over prediction in far field (Witlox et al., 2009).

A three dimensional model is recommended to be used in order to observe CO_2 toxic dispersion from pipelines in the area with obstacles. Developing geometry as closely to the one in actual CCS facilities inside or outside the plant will provide a better perspective for the consequence study of high concentration CO_2 release. By doing this, a specific safe distance from CCS pipelines can be established in order to enhance protection layer between facilities and working personnel and also the surrounding population.

For case study comparison purpose, modified Pasquill-Gifford dispersion coefficients is recommended to give a better and more realistic theoretical concentration estimation. Use of simple dispersion coefficients will induce error in estimation.

CHAPTER 6: APPENDIX

6.1 GANTT CHART AND KEY MILESTONES

Gantt charts for activities planned along for this final year projects first and second semester are shown in Table 2 and Table 3.

Table 3: Gantt chart for final year project first semester (FYP I)

No	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14
									Mid-Semester Break							
1	Selection of Project Topic	▨	▨													
2	Preliminary Research Work		▨	▨	▨	▨										
3	Submission of Extended Proposal						●									
4	Oral Proposal Defence									▨	●					
5	Project Work Continues											▨	▨	▨		
6	Submission of Interim Draft Report														●	
7	Submission of Finalized Interim Report															●

Table 4: Gantt chart for final year project second semester (FYP II)

No	Detail/ Week	1	2	3	4	5	6	7		8	9	10	11	12	13	14	15
									Mid-Semester Break								
1	Project Work Continues	▨	▨	▨	▨	▨	▨	▨									
	(ANSYS FLUENT modelling)																
2	Submission of Progress Report									●							
3	Project Work Continues									▨	▨	▨	▨	▨			
	(ANSYS FLUENT modelling and data validation)																
4	Pre-EDX												●				
5	Submission of Draft Report													●			
6	Submission of Dissertation (soft bound)														●		
7	Submission of Technical Paper														●		
8	Oral Presentation															●	
9	Submission of Project Dissertation (hard bound)																●

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