Modelling Of CO2 Leakage in Cement Plug in Abandoned Well

by

Muhammad Adib bin Mohamed Yousop

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

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CERTIFICATION OF APPROVAL

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Approved by,

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(Dr. Anis Suhaila bt Shuib)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

May 2012

CERTIFICATION OF ORIGINALITY

This is to certify that I am responsible for the work submitted in this project, that the original work is my own except as specified in the references and acknowledgements, and that the original work contained herein have not been undertaken or done by unspecified sources or persons.

MUHAMMAD ADIB BIN MOHAMED YOUSOP

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ABSTRACT

Greenhouse gasses emission is serious problem to the environment. Carbon capture and storage is one of the methods to control and reduce the number of gasses release. There is a significant amount of CO_2 stored in the well bore that suffered from leakage. The potential leakage paths of CO_2 can be identified thorough the cement plug in the abandoned wellbore due to the exposure of high CO_2 concentration after years of operation. The permeability and integrity of the cement will determine how effective it is in preventing leakage. This research is to discover the effects of permeability of the cement plug which is made by Portland cement' with the risk of CO_2 leakage from abandoned well in Carbon Capture and Storage projects.

A computational fluid dynamics tools, ANSYS FLUENT will be employed where the solution of K-epsilon Model and Eddy Dissipation model in the wellbore geometry is sought. However, the reaction of Portland cement has to be defined earlier before the permeability of cement plug can be determined using Darcy Law equation. The flow will be modelled and simulated in which the effect of permeability will be studied.

The results show the mass fraction of calcium bicarbonate has been increased after the iteration is completed and the value of the density at different cement length is obtained from the simulation. The density is found to be decreased by the increment of cement plug length, thus it given high value of permeability at face sizing of 200000μm and 2135 numbers of mesh elements is applied in the model.

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CHAPTER 1

INTRODUCTION

1.1 BACKGROUND

Greenhouse Gas (GHG) emissions become a serious threat to the environment presently. The primary greenhouse gases in the earth's atmosphere such as carbon dioxide, methane, nitrous oxide, and ozone are a major issue in the context of global climate change and it is already recognized by all experts, government and public opinions throughout the globe.

In 1997, an outline called Kyoto Protocol stated that all participated parties or countries must ensure that their total anthropogenic carbon dioxide equivalent emissions of the greenhouse gases do not exceed their assigned amounts, calculated pursuant to their quantified emission limitation and reduction commitments and in accordance with the provisions of this, with a view to reducing their overall emissions of such gases by at least 5 per cent below 1990 levels in the commitment period 2008 to 2012 (Nations, 1998).

Among the portfolio of measures to reduce GHG emission, carbon sequestration project or carbon capture and storage (CCS) projects may control and reduce the numbers of gaseous from being released to the atmosphere (Houdu, Poupard, & Meyer, (2008)). According to Beckwith (Beckwith, 2011), over 200 CCS projects were active or planned worldwide at the end of 2010, a net rise of 26 from 2009. Of these, 77 large-scale integrated projects at various stages development. North America, Europe and Australia are home to 87% of all projects. The amount of CO_2

Table 1 : Active Large-Scale Integrated Carbon Capture and Storage Projects

Name	Location	Capture	Storage
Operation Stage`			
Sleipner CO_2 Injection	Norway	Gas Processing	Deep Saline Formation
Snohvit CO_2 Injection	Norway	Gas Processing	Deep Saline Formation
In Salah CO_2 Injection	Algeria	Gas Processing	Deep Saline Formation
Weyburn-Midale CO_2 Monitoring and Storage Project	Canada / United States	Precombustion (synfuels)	EOR with measurement monitoring and verification (MMV)
Rangely Waber Sand Unit CO_2 Injection Project	United States	Gas Processing	EOR with MMV
Salt Creek EOR	United States	Gas Processing	EOR
Enid Ferillizer	United States	Precombustion	EOR
Sharon Ridge EOR	United States	Gas Processing	EOR
Execution Stage			
Southern Company IGCC Project	United States	Precombustion	EOR
Occidental Gas Processing Plant	United States	Gas Processing	EOR
Gorgon Carbon Dioxide Injection Project	Australia	Gas Processing	Deep Saline Formation

stored in the oil reservoirs was 2284 million tonnes for the 40 years injection period which is 31% of the total amount stored.

Risk assessment and management is a vital area of research and development since they were related to the impacts of health, safety and environment. At the same time, this assessment can measure the efficiency of the CCS project in terms of the emission reduction of GHG. Ergo, numerous mathematical models and numerical simulation tools have been developed as they play an important role in quantifying the risk of any possible environmental contamination. Wellbore integrity is a main challenge to prove the reliability and safety of the CO_2 storage within geological formations. It means that the well will not be a source of leakage pathway.

1.1.1 Computational Fluid Dynamic

Computational Fluid Dynamic will be applied in the present study to simulate the potential leakage pathways along with leakage distribution. This is the initial attempt to formulate concept of the fluid mechanics and develop an understanding of complex process.

Computational fluid dynamic (CFD) is a branch of fluid mechanics that uses numerical methods and algorithms to solve and analyze problems that involve fluid flows. The fundamental bases of almost all CFD problems are the Navier-Stokes equations which define any single-phase fluid flow. These equations can be simplified by removing terms describing viscosity to yield the Euler equations.

Basically, there are three main procedures when modelling using CFD which are pre-processing step, the simulation step and the post processing step. There are several reasons CFD is being widely used today. One of them is it can predicts performance before modifying or installing a new system. CFD cost also much less compared to experimental method. Furthermore, the time consumes to run a CFD modelling is also less compared to experimental method.

1.2 PROBLEM STATEMENT

CO_2 leakage within the wellbore environment became a serious concerned to the people nowadays as the emission of this gas may harm to the environment. Abandoned wells are typically sealed with cement plugs intended to block vertical migration of fluids. In addition, active wells are usually placed with steel casing, with cement filling the outer annulus in order to prevent leakage between the casing and formation rock.

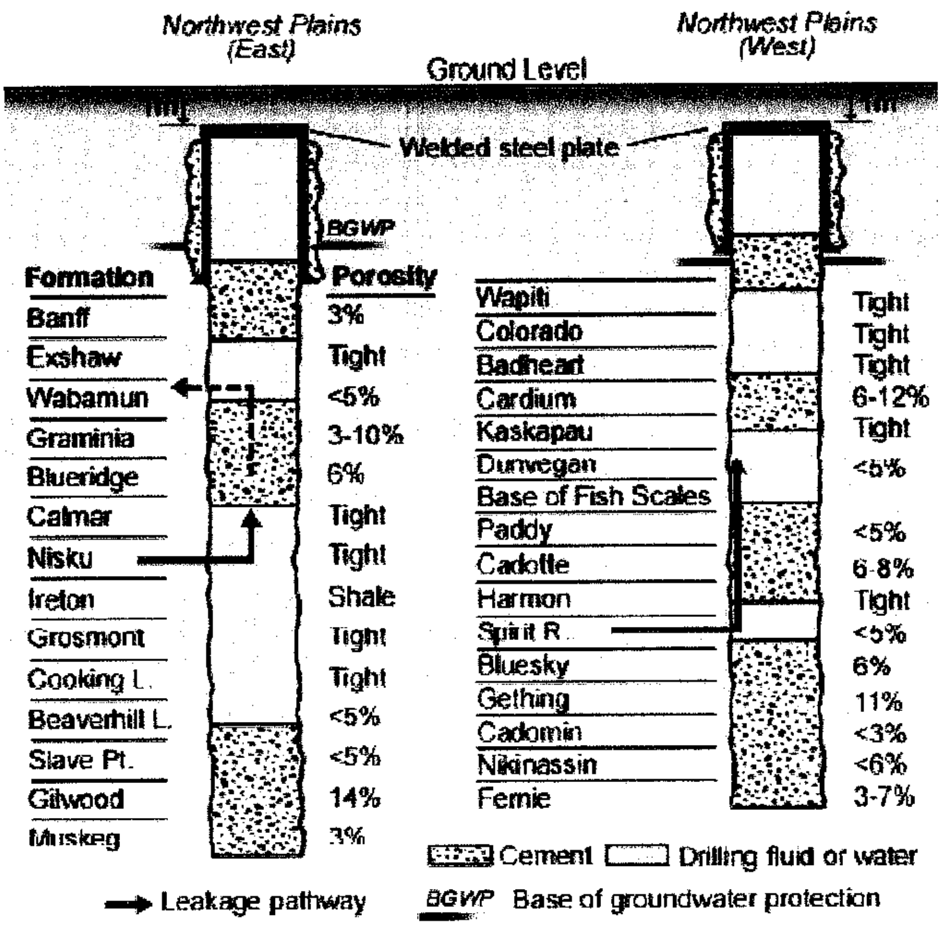

Figure 1a

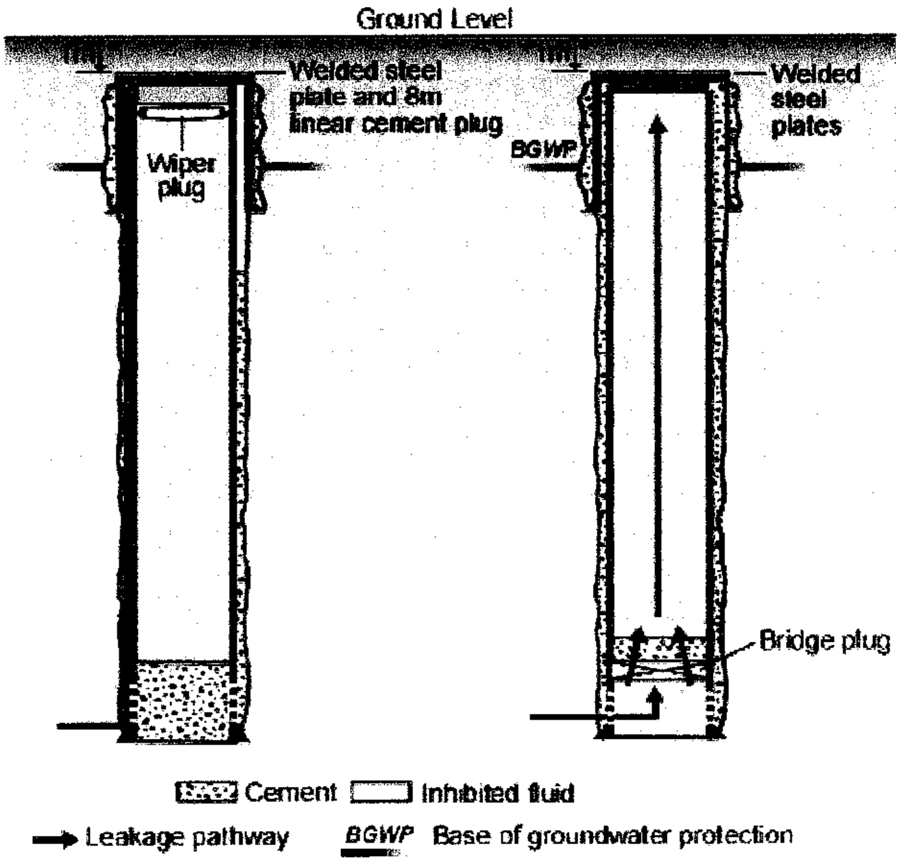

Figure 1b

Figure 1 : Typical well abandonment in Alberta Canada (a) Drilled and abandoned well (D&A) Open Hole; (b) Cased, completed and abandoned (Watson & Bachu, 2007)

The permeability and integrity of the cement plug cement in the abandoned wellbore will determine how effective the cement is in preventing fluid leakage. The cement must be able to maintain a low permeability over lengthy exposure to reservoir conditions in a CO_2 geological storage project (Djimurec, Pašić, & Simon, 2010). A common type of cement which is normally used in industry is Portland cement. However, due to degradation of the cement over time and bad cementation process, several potential leakage pathways are identified as the area where carbon dioxide can penetrate to the formation or the surface layer (Celia, Bachu, Nordbotten, Gasda, & Dahle, 2004). These include leakage between the cement and the outside of the casing (Figure 2a), between casing and cement well plug (Figure 2b); through the cement plug (Figure 2c); leakage through the casing (Figure 2d); through the fractures (Figure 2e) and finally between cement and formation (Figure 2f) as described on the figure below.

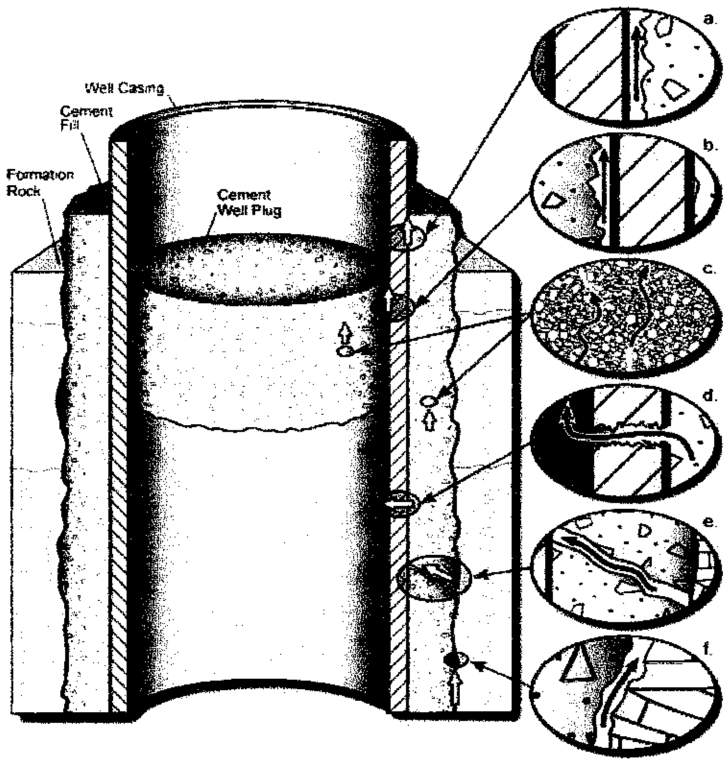

Figure 2 : Potential leakage pathway in the wellbore (Celia, Bachu, Nordbotten, Gasda, & Dahle, 2004)

High concentration of carbon dioxide may cause the acidic environment within the wellbore and it is identified as a critical factor in evaluating deeper leakage potential. Thus, it will effect the wellbore cement, casing and elastometer and reduce the integrity of one particular well (Watson & Bachu, 2008).

Numbers of researchers develops the fluid dynamic modelling in order to study the distribution of CO_2 leakage. This report will focus volume of CO_2 disperse from the well through the cement plug as shown in Figure 2c and how the reaction involved in the cement plug will affected the result. Various parameters such as relative permeability, capillary pressure, fluid saturation and wettability have been investigated by previous scholars to correlate the multiphase flow in the porous media with the risk of CO_2 leakage. However, this thesis work only considered permeability as the parameter.

The well of 4.5ft internal casing diameter is abandoned for the geological storage project purposes and the 200ft height of cement plug is located in the production line of the abandoned well. Conventionally, Portland cement plug is used to avoid the CO_2 migration to the surface layer through the wellbore. However, high composition of Calcium Hydroxide present in the Portland cement leads to increase in permeability within high CO_2 concentration environment. CO_2 and water reacted between one another to produce acid carbonic and flows within the wellbore with the velocity of 30m/s.

Typically, the well temperature increases about 3°C for each 100m depth (Sauki & Irawan, 2010), therefore the temperature of 316.653K used for total depth of 2040ft. For depleted gas reservoir, the upper limit storage pressure is related to the reservoir discovery pressure which is usually in the range of 0.43 to 0.52psi/ft of depth which is equal to 5.92Mpa at given depth.

1.3 OBJECTIVES

1. To study the chemical reaction involved in Portland cement using computational fluid dynamic (CFD) simulation.
2. To evaluate the effect of permeability of Portland cement (cement plug) with the risk of CO_2 leakage from the abandoned well.

1.4 SCOPE OF STUDY

The main focus in this research is on the effect of Portland cement's permeability with the volume of CO_2 leakage within the abandon wellbore in Carbon Storage Project. The form of data is shown in Computation Fluid Dynamic simulation since this kind of simulation is recognized as one of the effective practice to relate the mathematical equation with the case study when the boundary condition is given. In fact, many models can be used in order to complete the simulation. Density of the reaction is taken into account in order to determine the permeability of the cement plug of the reaction took place. This step is important in order to correlate the multiphase flow in the porous media with the risk of CO_2 leakage. From that, the feasibility to place to place the Portland cement as the plug in abandoned well is questioned.

1.4.1 Relevancy of project

This project aims to help in determining the feasibility of Computational Fluid Dynamic (CFD) modelling in monitoring the effect of permeability of Portland cement (cement plug) with the volume of CO_2 leakage. Further study of relating the effect of permeability of Portland cement and the volume of CO_2 leakage distribution in Carbon Capture and Storage Project can be performed if the CFD modelling approach is proven to be viable for the process.

1.4.2 Feasibility of project

The project will be supervised by modelling the computational fluid dynamic by using Ansys Fluent. The chemical reaction involved in Portland cement (cement plug) is simulated using the software and the permeability of the Portland cement is determined. Then the effect of permeability with the volume of CO_2 leakage is connected by Darcy Law. Thus, this equation becomes the most significant thing throughout the project span which is two (2) semesters of Final Year Project.

1.4.3 Limitation of the study

There are several limitations while this research is conducted. This has resulted in difficulty to find specific journal or article related to this study because of limited access to the information while some of them have to be paid for. In addition, most of the data were used in this thesis is from the secondary sources that obtain from the library, the accuracy and reliability were fully depends on the publish materials. Any error occurs in the published sources will give incorrect data for this thesis work.

CHAPTER 2

LITERATURE REVIEW

2.1 INTRODUCTION

This chapter describes the equation used in the simulation such as k-epsilon model and eddy dissipation model plus the relationship between the Darcy law in homogenous porous medium in determining the volume of CO_2 dispersed from the wellbore through cement plug based on several research which have done earlier by external researchers. Permeability of the cement plug is the main concern in this report.

2.2 EFFECT OF HIGH CO_2 CONCENTRATION ON CEMENT PLUG

CO_2 can react with the different materials used to construct a well. When it reacts with cement, the strength of the set cement is decreases (Djimurec, et al., 2010; Ide, Friedmann, & Herzog, 2006; Nygaard, 2010) Thus, its permeability and porosity increased and it may leads to loss of well isolation. Portland cement is thermodynamically unstable in CO_2-rich environments and can degrade rapidly upon exposure to CO_2 in the presence of water (Onan, 1984).

The reaction products are soluble and the carbon dioxide gas may migrate out of the cement sheath or plug. Four major crystalline compounds in Portland cement are tricalcium silicate ($Ca3SiO_5$), dicalcium silicate (Ca_2SiO_4), tricalcium aluminate ($Ca_3Al_2O_6$), and tetracalcium aluminoferrite ($Ca_4Al_2Fe2O_{10}$). The most plentiful phases in Portland cement are the silicates, containing over 80 wt % of the cement, mostly in the form of tricalcium silicate. When the compounds of Portland cement mixed with water, the main hydration products formed are C-S-H and calcium hydroxide $Ca(OH)_2$ (Kutchko, Strazisar, Dzombak, Lowry, & Thaulow, 2007)

Other scholar found that there is another way on how the permeability and porosity of the Portland cement can increase. For example, Santra et al (2009) found that there are mainly three different chemical reaction stages involved in Portland cement- CO_2 interaction which are formation of carbonic acid, carbonation of Portlandite and/or cement hydrates and dissolution of calcium carbonate ($CaCO_3$) (Santra, Reddy, Liang, & Fitzgerald, 2009)

At the beginning of the stage, carbon dioxide gas is reacted with water to form Carbonic Acid (H_2CO_3) as the product. The reaction may causes lowering in local pH but its depend on other parameters such as temperature involved in the reaction, partial pressure of CO_2, ion present in water and others.

The second stage which is carbonation of Portlandite and /or cement hydrates, the calcium hydroxide – $Ca(OH)_2$ is reacted with carbonic acid to produce calcium carbonate ($CaCO_3$) and water. The side reaction may produce silica (SiO_2) as the side reaction between crystalline phase and carbonic acid take place. Those reactions may result densification, leading to increased hardness and volume expansion of the Portland cement. In severe case, it may result to the development of cracks or fracture of the cement.

The last step is dissolution of carbonic acid where in this stage carbonic acid and calcium carbonate will react to form calcium bicarbonate – $Ca(HCO_3)_2$. Effects of this reaction are increase porosity and permeability of the Portland cement. At the same time, it may reduce the overall mechanical integrity of the well and potential loss of the wellbore in extreme cases. However this stage only can happen when the cement is surrounding by dissolved CO_2 in long period or end of well life cycle.

2.3 MATHEMATICAL EQUATIONS

In order to simulate the effect of permeability of Portland cement (cement plug) with the volume of CO_2 leakage from the wellbore, mathematical equation must be defined earlier so that the all the parameters can be linked simultaneously. All the equation related to the case study will be discussed in Chapter 2: Literature Review. Those equations are important in order to model the fluid dynamic of CO_2 leakage volume.

Apparently, numbers of researchers start to develop the correlation to correlated the effect of permeability with the volume of CO_2 disperse. In few examples, the data is represented just by showing the graph (Celia, et al., 2004; Chang, Minkoff, & Bryant, 2008; Geloni, Giorgis, & Battistelli, 2011; Viswanathan, et al., 2008.). However, not all modelling can be clearly seen if it is demonstrated in that kind of representation. As the improvement, this thesis work will discuss the effect of leakage within the wellbore environment by using Computational Fluid Dynamic (CFD) in order to represent the data effectively

2.3.1 Darcy Law

Darcy's law can be defined as proportional relationship between the instantaneous discharge rate throughout porous medium, the viscosity of the fluid and the pressure drop over a given distance (Ren & Wijshoff, 2008). This relation can be expressed in mathematical equation as below;

$$Q = \frac{-kA}{\mu}\frac{(P_b - P_a)}{L} \tag{1}$$

Where;

Q = Units of volume per time (m^3/s)

k	=	Permeability of the medium (m^2)
A	=	Unity of area (m^2)
Pi	=	Pressure of phase i (Pa) ~ Pb – Pa =Pressure drop
μ	=	Viscosity (Pa.s)
L	=	Length the pressure drop is taking place over (m)

The negative sign represents the direction of the fluid flows. Fluids flow from high pressure to low pressure. The flow will be in the positive 'x" direction if the change in pressure is negative (where Pa > Pb). Dividing both sides of the equation by the unit of area can be written in the form

$$q = \frac{-k}{\mu} \nabla P \qquad (2)$$

Where;

q	=	Flux – discharge per unit area, with unit of the length per time (m/s)
∇P	=	Pressure gradient vector (Pa/m)
k	=	Permeability of medium (m^2)
μ	=	Viscosity (Pa.s)

Permeability is part of the proportionality constant in Darcy's law which relates discharge (flowrate) and fluid physical properties (e.g. viscosity), to a pressure gradient applied to the porous media:

$$\kappa = \upsilon \frac{\mu \, \Delta x}{\Delta P} \qquad (3)$$

Where;

υ	=	Superficial fluid flow velocity through the medium (m/s),
κ	=	Permeability of a medium (m^2)

μ	=	Dynamic viscosity of the fluid (Pa·s)
ΔP	=	Pressure difference (Pa)
Δx	=	Thickness of the bed of the porous medium (m)

The proportionality constant specifically for the flow of specific fluid (i.e oil, air and water) through a porous media is called the hydraulic conductivity (Kumar & Jain, 2012). Permeability is a portion of this, and it is a property of the porous media only but not the fluid. Given the value of hydraulic conductivity for a subsurface system, κ, the permeability can be calculated as;

$$\kappa = K\frac{\mu}{\rho g} \qquad (4)$$

Where;

κ	=	permeability (m^3/s)
K	=	hydraulic conductivity, m/s medium (m^2)
ρ	=	density of the fluid (kg/m^3)
μ	=	dynamic viscosity (kg /m.s)
g	=	acceleration due to gravity, (m/s^2) = 9.81 m/s^2

2.3.2 K-Epsilon Model

K-epsilon model is a two equation model type of turbulence model. The equation is widely used for most of the CFD based problems and become the industry standard models lately. It used commonly for most types of engineering application since it allows a two equation model to account for history effects like convection and diffusion of turbulent energy (Subrahmanyam, 2008; Wilcox, 1998). However, it is known that k-epsilon model is less stable in comparison with other turbulence model such as SST model, thus it makes it a bit more complicated to use.

2.3.3 Eddy-Dissipation Model

The Eddy Dissipation model is best applied to turbulent flows when the chemical reaction rate is fast relative to the transport processes in the flow. The model is differs in especially relating the dissipation of eddies to the mean concentration of irregular quantities instead of concentration fluctuation (Yeoh & Yuen, 2009). Significantly the model does not call for a solution of equation for the entities; $\widetilde{Y_{fu}''^2}, \widetilde{Y_{fu}''Y_{ox}''}, \widetilde{Y_{fu}''^2}$ *and* $\widetilde{Y_{ox}''^2}$.

Nevertheless, the simplification of the eddy dissipation model should be viewed from the proposition whereby the mean quantities appear intermittent within the turbulent fluid. Strictly speaking, the eddy dissipation model should only be used for one step and two step reaction. To extend the eddy dissipation model to include detailed reaction mechanism, it is more preferable to adopt the generalized eddy dissipation concept model develop by Magnussen (Magnussen, 1981)

CHAPTER 3

METHODOLOGY

3.1 INTRODUCTION

Methodology is a set of procedure or methods used to conduct research. These research methods are important to gather information such as users' preferences, opinions and suggestions. This involves the data collection method and sample data used in this study as well as the development of the theoretical framework. The aim of this study is to show the effect of permeability of Portland cement (cement plug) with the volume of CO_2 leakage using Ansys Fluent.

3.2 RESEARCH METHODOLOGY

Essentially, there are three major steps in creating Computational Fluid Dynamic (CFD) simulation. The process comprises of pre-processing, solving, and post-processing steps (Eesa, 2009). In the pre-processing phase, it is required to model the geometry and the physical properties of the design, as well as the environment in the form of applied loads or constraints. The methodology includes building the geometry, generating a computational mesh, determining the equitation to be solved, specifying the boundary condition, and entering the data. After pre-processing, the CFD solver does the calculation and produces the results. Solving is the phase where the flow characteristic of the mesh is determined using some mathematical equation at every node of the mesh. Finally, post-processing process concern more on the analysis work on the result generated. It involves organization and interpretation of the data and images. It is important in order for users to retrieve more accurate result by do checking and repairing on the model itself.

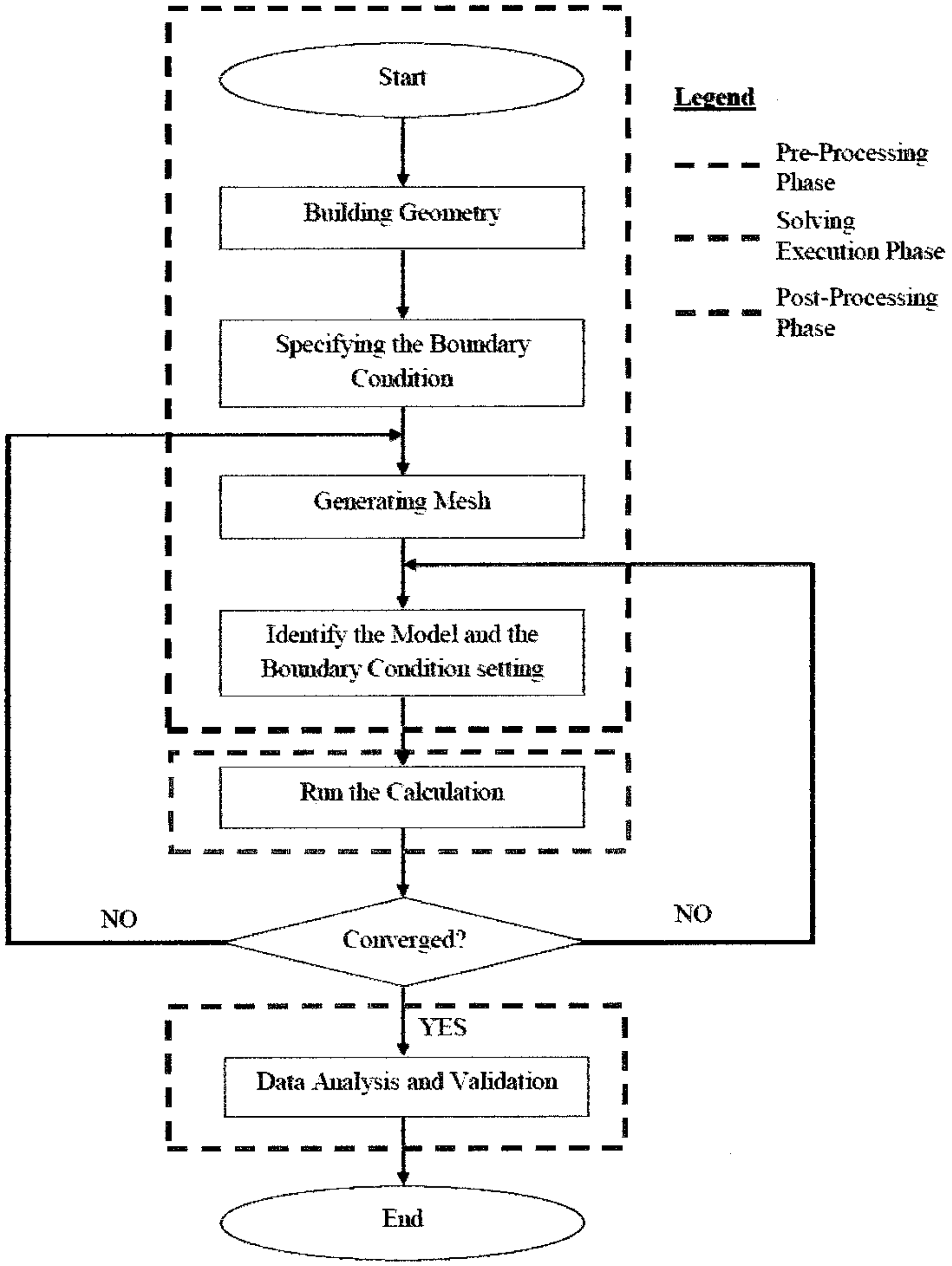

Figure 3 : Methodology Flow Chart

3.3 IDENTIFY THE CASE STUDY

Generally several simulation models, whether or not concerned with fluid dynamics, used in well integrity and well monitoring studies in the past few years. Since this thesis work is to study effect of high concentration of CO_2 to the volume leakage through cement plug during well abandonment, it is required to look for a cause that may lead to the leakage of CO_2 from abandoned well.

In order to analyse the effect and cause of the situation happened in Portland cement, a set of simulation was built throughout the research. This thesis will focus on the reaction involved in Portland cement particularly during dissolution of Calcium Carbonate ($CaCO_3$). Then, the data reported from the simulation is used and the permeability graph is plotted at different density value to increase the relevancy of the project. This method is important in order to study the effect of the density to the change on permeability of Portland cements.

To achieve the first objective, the reaction is assumed to happen inside an empty space instead of simulating the model directly in porous media. The generalized eddy-dissipation model has been used to analyze the chemical reaction involved in Portland cement. The reaction is modelled using a global multi-step reaction mechanism, assuming complete conversion of the CO_2 and H_2O to Calcium bicarbonate $Ca(HCO_3)_2$. The reaction equation is;

Reaction 1: Formation of Carbonic Acid

$$\mathbf{CO_2 + H_2O \rightarrow H_2CO_3}$$

Reaction 2: Carbonation of Portlandite and/or Cement Hydrates

$$\mathbf{Ca(OH)_2 \; + H_2CO_3 \rightarrow CaCO3 + H_2O}$$

Reaction 3: Dissolution of Calcium Carbonate (CaCO3)

$$CaCO_3 + H_2CO_3 \rightarrow Ca(HCO_3)_2$$

The mass fraction of 0.5 for both Carbon Dioxide and water is used to initiate the reaction. The second objective in this research is more to the validation of the result. This section will be discussed more in Chapter 4: Result and Discussion.

3.4 PRE-PROCESSING PHASE

Pre-processing phased provides a Graphical user interface (GUI) to define physical properties. In this phase, a goal is set and the problem is define .This is the part which decision on what results are actually is looking for. Once the problem is defined, conditions must be defined for the problem. These are known as initial conditions.

3.4.1 Model geometry development

It is important to study the geometry or condition encountered for the case that has been mentioned earlier in this chapter. This is to ensure the simulation model is conducted as in real condition. Therefore, the simulation model geometry was constructed by using Design Modeller (DM) in Ansys Fluent. In order to study the reaction involved on Portland cement, a rectangular shaped model is used to represent the cylindrical shaped cement plug in 2-Dimension in order to avoid complexity throughout this research. In fact, it becomes one of the promising solutions to represent the data clear and effective. 3-Dimensional diagram is not feasible to use since it may took longer time for the model to complete the calculation. Besides, the meshing process and specification of the boundary condition step becomes more challenging.

A rectangular is first drawn on XY-Plane with the dimension of 4.5ft × 200ft. Calcium Hydroxide is defined as fluid domain and the other chemical component is coming from the bottom side of the geometry (the wellbore inlet). All measurement is defined in feet.

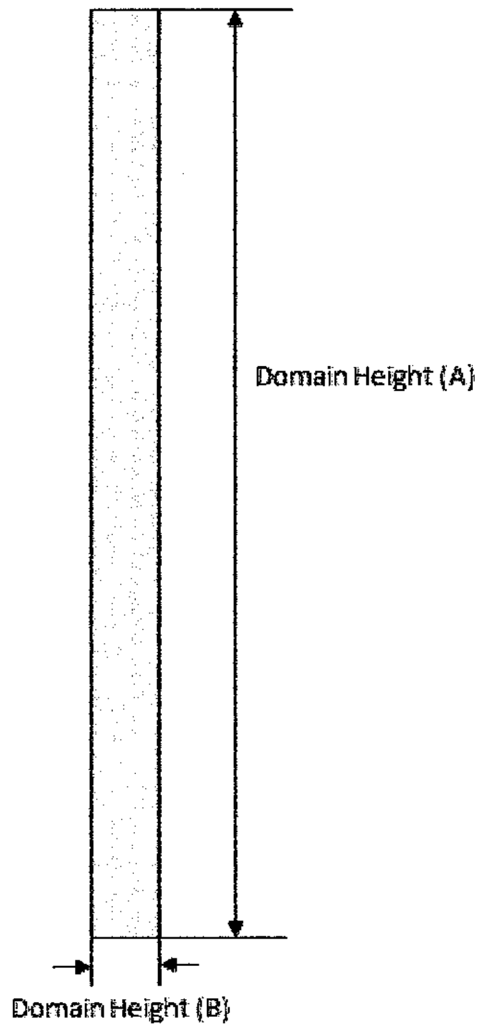

Figure 4: 2-D model geometry

Table 2: Geometry dimension

	Dimension (ft)
Domain height (A)	200
Domain width (B)	4.5

3.4.2 Specifying the Boundary Condition

The boundary conditions must be defined to act as boundaries for the problem. In this phase, the problem that will be studied is identified, such as what method of discretization, what numerical methods to use, and what programming language to use. This step is important since it ensures the model mesh accordingly and all condition is considered during the experiment in taken into account. For example, the variation discharge orifices diameter and discharge pressure values during the experimental activity are noted.

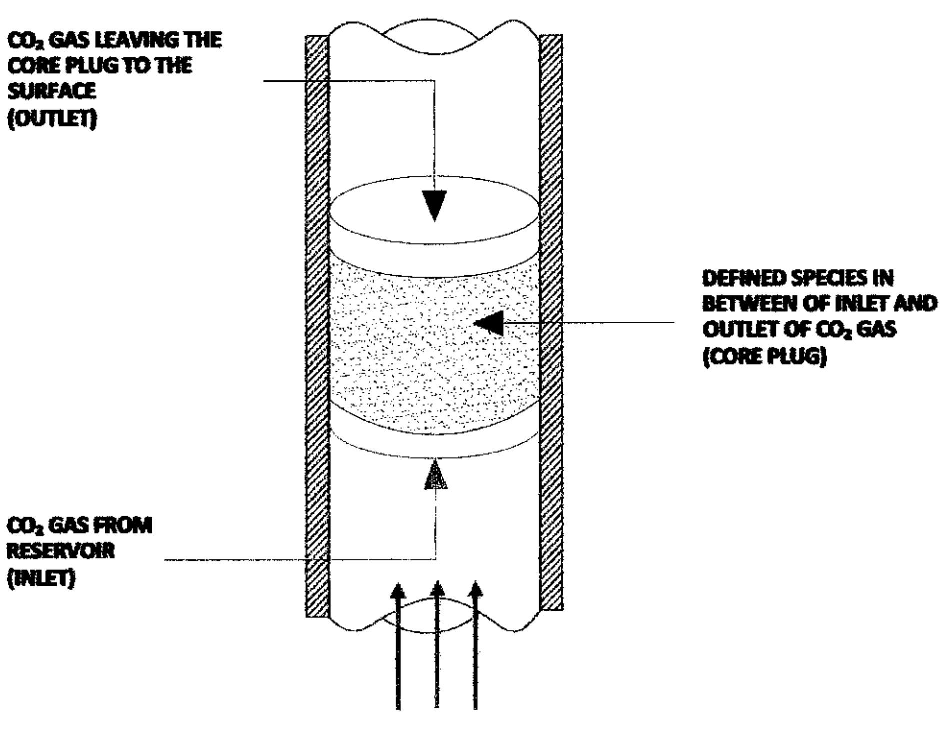

Figure 5 : General Boundary Condition Used

In this report, there are three different set of boundary condition has been identified. The first boundary condition is cement plug inlet. The Velocity Inlet sets the boundary conditions for a velocity inlet zone, the area where all the material except calcium hydroxide is added before they enter to the surface body. The inflow velocity can be defined by considering the velocity magnitude and direction, the velocity components, or the velocity magnitude normal to the boundary. Furthermore, the velocity is applied normal to the boundary in this case under consideration as velocity inlet.

The second boundary condition is cement plug outlet, the area where all the mixture is leaving the surface body. The boundary condition at the section parallel to the axis is specified as pressure outlet, which indicates that the pressure acts on the drop and the gauge pressure is set to zero and the hydraulic backward flow is set as 10% to the pressure outlet section.

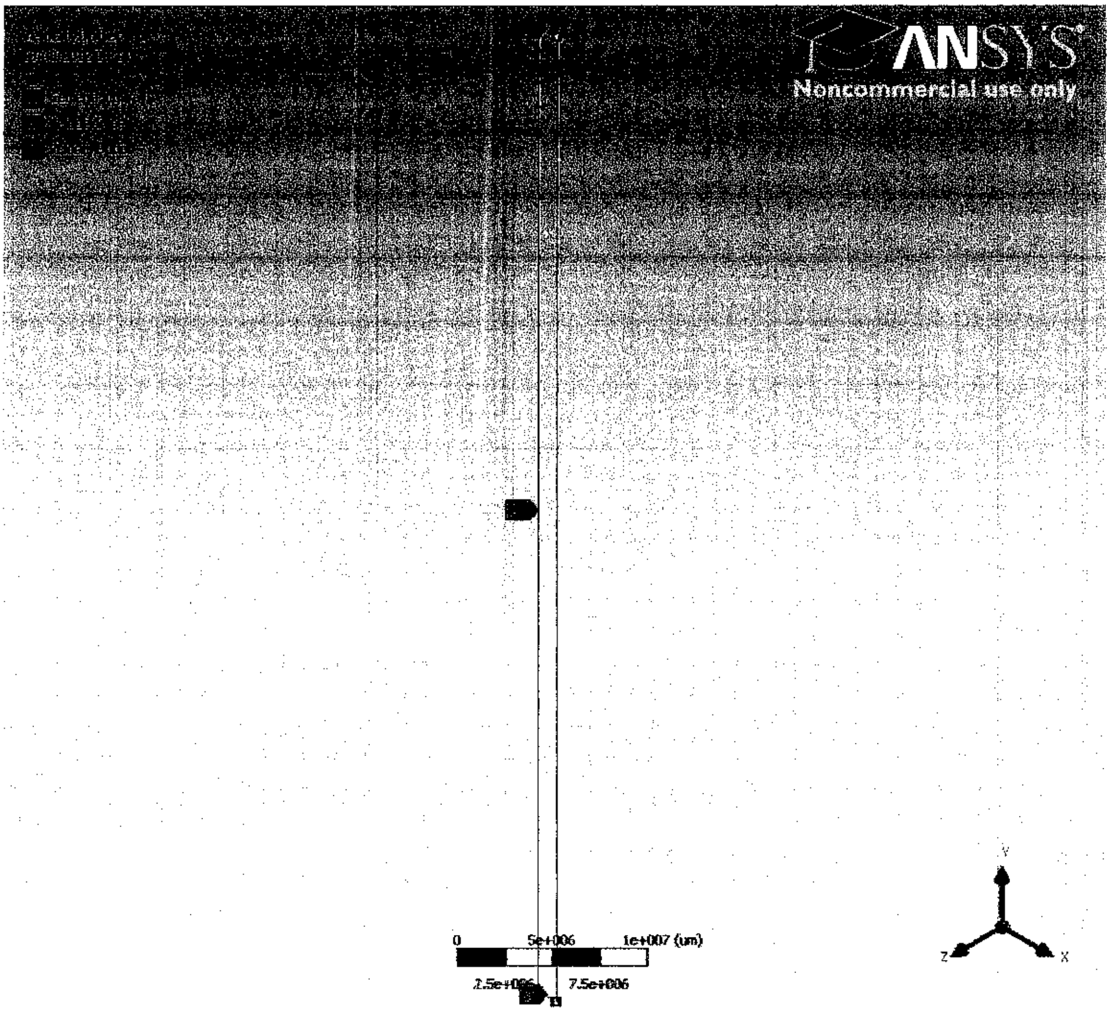

Figure 6: Boundary Condition Setup in Ansys Design Modular

The final boundary condition for the first part in this report is the surface body. This area represents the porous zone where all the reaction takes place. Initially, Calcium Hydroxide is defined as the domain fluid in the surface body since the major element of the Portland cement is known to be Calcium Hydroxide. For simplicity, in this art the reaction is assumed happened in empty space instead of simulating it in the porous zone. The boundary condition is summarized as shown in the Table 3 below.

Table 3: Summary of the boundary condition used

Boundary Condition	Description
Cement plug inlet	Velocity inlet where all the material except calcium hydroxide is added before they enter to the surface body
Cement plug outlet	area where all the mixture is leaving the surface body
Surface Body	Area represents the porous zone where all the reaction takes place.

3.4.3 Model Meshing

Next is to mesh the model when the geometry is finally dimensioned. In this stage the continuous space of the flow domain is divided into sufficiently small discrete cells, the distribution of which determines the positions where the flow variables are to be calculated and stored. Variable gradients are generally more accurately calculated on a fine mesh than on a coarse one. A fine mesh is therefore particularly important in regions where large differences in the flow variables are expected. A fine mesh, however, requires more computational power and time. The mesh size is optimised by conducting a mesh-independence test whereby, starting with a coarse mesh, the mesh size is refined until the simulation results are no longer affected by any further refinement.

The domain was carefully meshed in a manner which maximized the detailing of the importance region. In this thesis work, high number of cell elements was applied to the surface body. The value of mesh sizing at the surface body is used in order to increase or decrease the cell element. It is unnecessary to refine any specific area of the boundary condition since the observation and result depends only on the surface body. System geometry is represented by using front view.

Preliminary simulations were performed from a quadrangle mesh for the space discretization (Houdu, et al., (2008)). The maximum layer is increased up to 10 layers and fine relevance and span angle centre is applied. In addition, Curvature mode is implemented in this 2D axisymmetric flow geometry as an advanced size function in order to improve the orthogonal quality of the mesh. The model mesh was constructed as figure below with the total of 2135 elements and 2144 nodes.

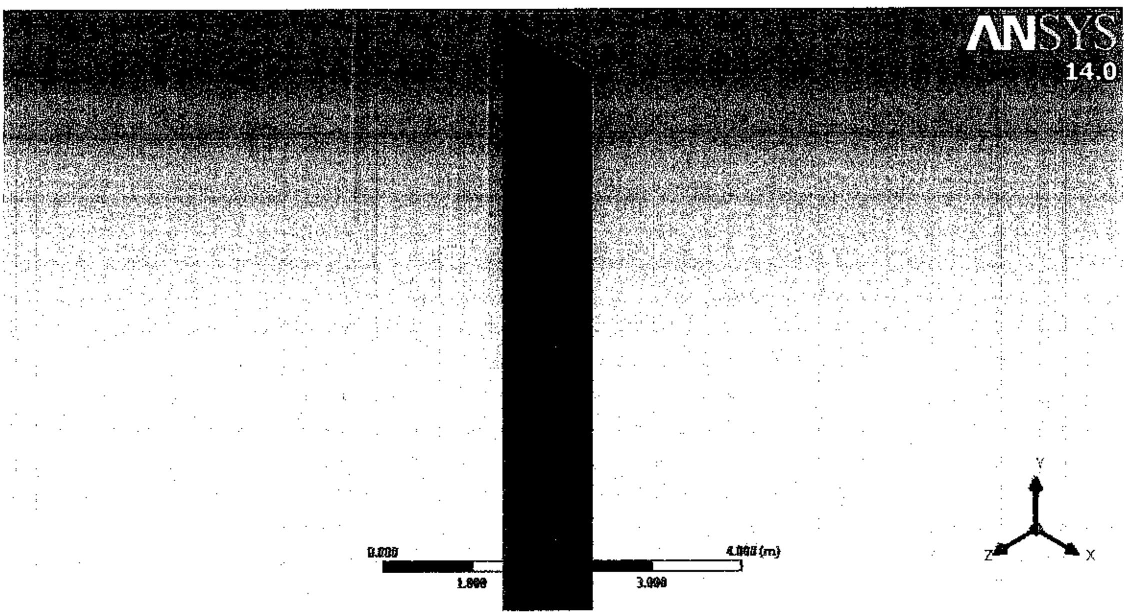

Figure 7: Model meshing

The different value of mesh sizing is also used in order to validate the data accurately. It is rather important in order to obtain the optimum number of mesh while the orthogonal quality of the mesh is still on top. This process called grid generation study.

Grid generation study is conducted in order to achieve the optimum number of element or mesh size, yet the value of orthogonal mesh quality must close to 1. The highest point at element metric is near to 1, the higher quality of mesh produced in a good form. This study is important to see the effect of different mesh sizing or the number of the element towards the accuracy of the result. Different set of mesh size is decided in order to obtain the best result with lowest number of mesh elements used in the model. Four different models with different mesh sizing and number of element are generated using Ansys Mesh prior to the solving process. The specifications of the grid generated are summarized as tabulated below.

Table 4: Mesh properties

Face Sizing (μm)	Number of element	Element Metric (min)	Element Metric (max)	Element Metric (average)	Standard Deviation
50000	32913	0.9991253208	1	0.999993758	2.45031E-05
100000	8540	0.9996279797	1	0.999995855	1.65349E-05
150000	3654	0.9997687306	1	0.999992882	2.03541E-05
200000	2135	0.9998550894	1	0.999998514	7.84335E-06

The orthogonal quality chart is shown in Figure 8 to Figure 11. The value of number of element may influence the orthogonal quality of the mesh.

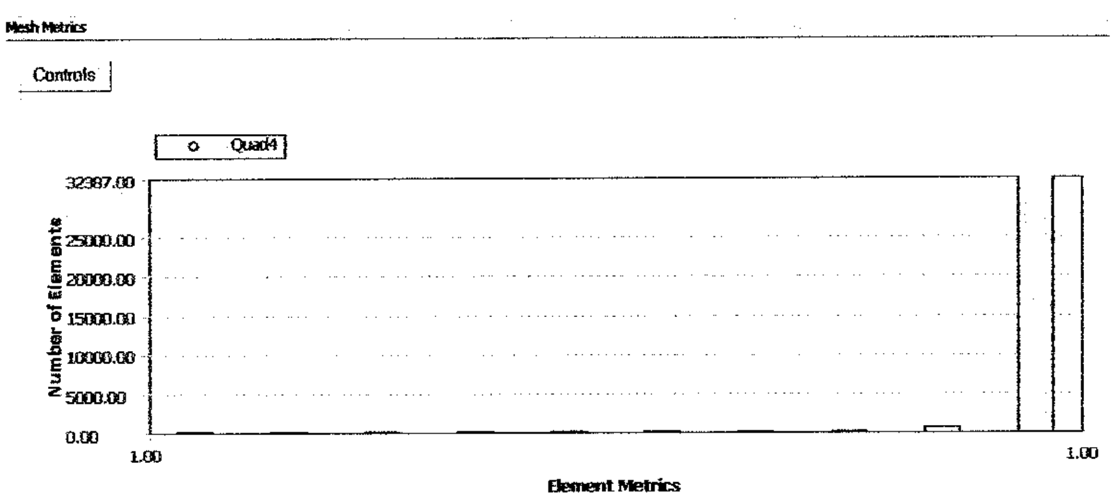

Figure 8: Orthogonal quality report at Mesh Sizing = 50000μm

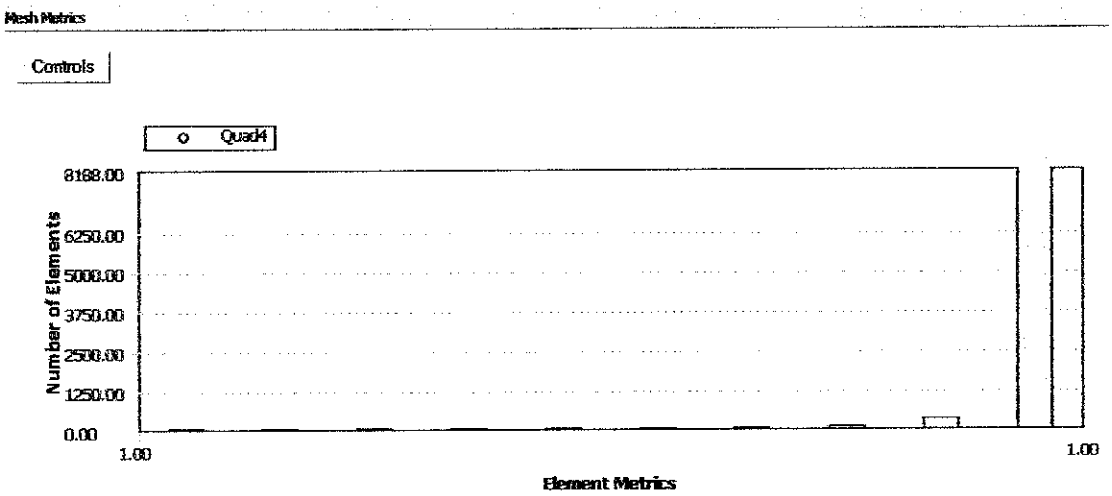

Figure 9: Orthogonal quality report at Mesh Sizing = 100000μm

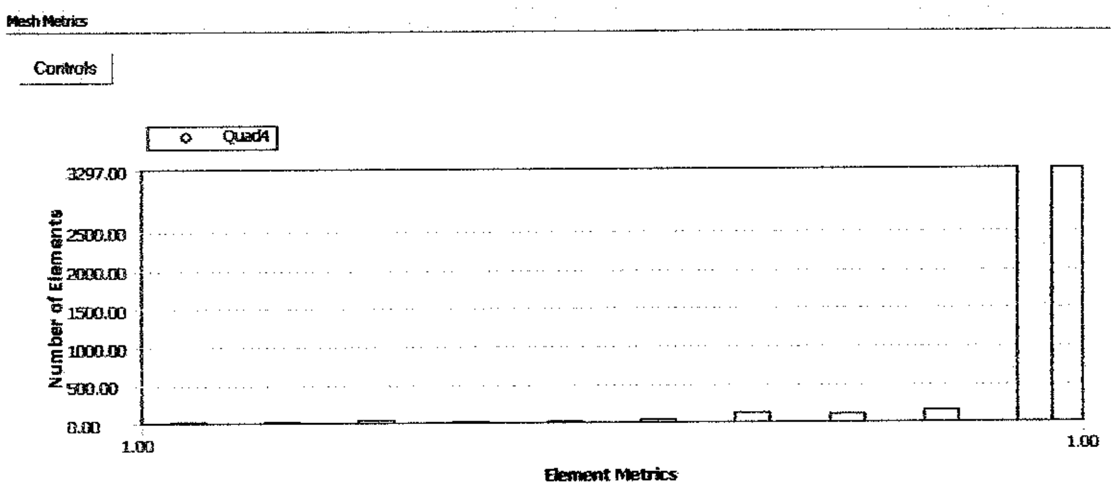

Figure 10: Orthogonal quality report at Mesh Sizing = 150000μm

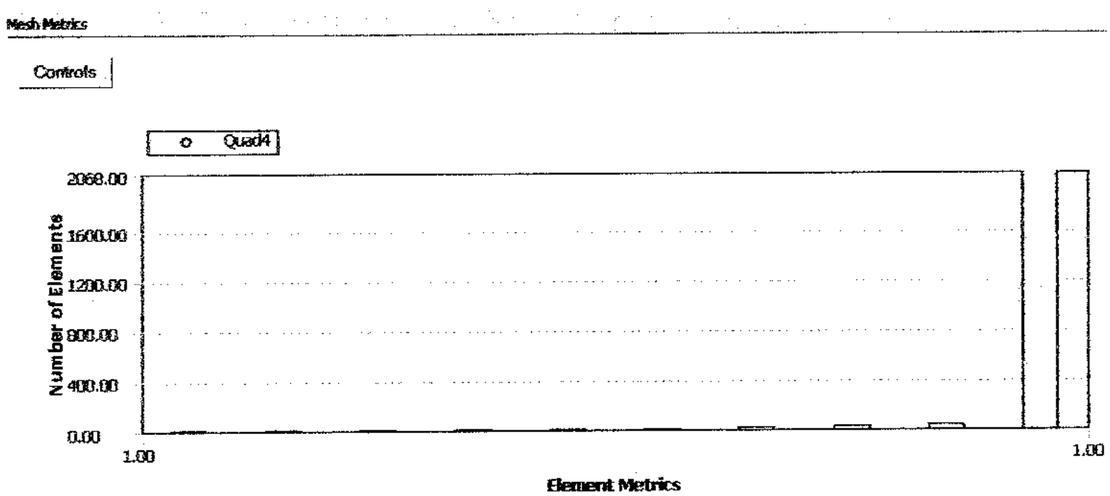

Figure 11: Orthogonal quality report at Mesh Sizing = 200000μm

From the result, it is observed that different size of mesh sizing generates different number of element thus it produced different result between one another. Smaller size of mesh requires more computation time and processor capability which is sometimes not favourable within the time constraint. Generally, all models produced the same value of mass fraction and density. The value does not really dependent with mesh sizing and number of element.

However, other specification must be analyzed before the mesh is chosen. First, the closes mesh quality to 1. Models with face sizing of 50000μm and 200000μm seem to have higher quality compare to the models 100000μm and 150000 of face sizing. Then, the element metric and standard deviation of the element metric must put into consideration. A model with higher minimum element metric and lower standard deviation is preferred since it shows the consistency of the mesh and has small error within the node; therefore the result is calculated smoothly. In addition, the model must has smaller mesh number since it may require less processing work and save more time to generate the model. It becomes more effective and feasible when there is time limitation to follow. After all of the criteria is taken into consideration and evaluated deeply, as a result model with mesh sizing of 200000μm is selected in this project.

3.4.4 Identify the models setting

Energy equation is applied to make sure the heat transfer model is able to use. Turbulence model is implemented since the value of the Reynolds number is greater than 2000. Thus, it leads the model to behave as fully turbulence and therefore the laminar flow regime in FLUENT viscous model tool becomes insignificant. In addition, the inviscid flow model also can be neglected since all the fluid involved in the reaction assumed to have the viscosity.

Realizable k-epsilon model was used instead of other turbulence model such as k-omega and Spalart-Allmaras model since the model is compatible for axis symmetry flow. For better convergence, the value for k and epsilon value is remained default by FLUENT. Standard wall treatment is implemented rather than choosing enhanced wall treatment. Enhanced wall treatment only gives better solution on highly refined wall mesh as while recovering the behaviour of Standard Wall Functions on coarse meshes. As the activity on the wall is not the main interest in this project, thus the default near-wall treatment model (Standard Wall Function) is highly recommended.

For species model, the Eddy-Dissipation model is applied in the Turbulence-Chemistry Interaction group box since the model computes the rate of reaction under the assumption that chemical kinetics are fast compared to the rate at which reactants are mixed by turbulent fluctuations (eddies).

Seven different materials and three simultaneous first order reactions are added in material setup. For every reaction, the default value for mixing rate of A is equal to 4 and B is equal to 0.5are used since the Arrhenius rate is inactive. The eddy-dissipation reaction model ignores chemical kinetics such as the Arrhenius rate. The values for Rate Exponent and Arrhenius Rate parameters are included in the database and are employed only when the alternate finite-rate/eddy dissipation model is used. The summary for the list of materials and the reaction involved is shown as Table 5 below.

Table 5: Summary of materials list and the reaction involved

Reaction 1					
Reactant			**Product**		
Species	**Stoich. Coefficient**	**Rate Exponent**	**Species**	**Stoich. Coefficient**	**Rate Exponent**
CO_2	1	1	H_2CO_3	1	0
H_2O	1	1			
Reaction 2					
Reactant			**Product**		
Species	**Stoich. Coefficient**	**Rate Exponent**	**Species**	**Stoich. Coefficient**	**Rate Exponent**
$Ca(OH)_2$	1	1	$CaCO_3$	1	0

H_2CO_3	1	1	H_2O	2	0
Reaction 3					
Species	**Stoich. Coefficient**	**Rate Exponent**	**Species**	**Stoich. Coefficient**	**Rate Exponent**
$CaCO_3$	1	1	$Ca(HCO_3)_2$	1	0
H_2CO_3	1	1			

The calculation will be performed assuming that all properties except density and specific heat are constant. The use of constant transport properties (viscosity, thermal conductivity, and mass diffusivity coefficients) is acceptable because the flow is fully turbulent. The molecular transport properties will play a minor role compared to turbulent transport. In solution method setup, Coupled Pseudo Transient solution method is applied and Pseudo Transient is enabled. The Pseudo Transient option enables the pseudo transient algorithm in the coupled pressure based solver. This algorithm effectively adds an unsteady term to the solution equations in order to improve stability and convergence behaviour. For general fluid flow problems this option is highly recommended.

3.5 PROCESSING AND SOLVER EXECUTION PHASE

After the pre-processing works are completed, next process is solving or processing process. In the processing phase, the computer code used to solve the problem at hand has been written and is compiled. This phase is mainly user-free because the computer is performing hundreds and thousands of calculations in order to simulate the problem at every step in time. Solving process plays an important role in CFD simulation where all setting and the formula involved in the boundary condition will be applied. The end result of this phase is a large collection of data.

3.6 POST PROCESSING PHASE

After the pre-processing works are completed, next process is solving or processing process. In the processing phase, the computer code used to solve the problem at hand has been written and is compiled. This phase is mainly user-free because the computer is performing hundreds and thousands of calculations in order to simulate the problem at every step in time. Solving process plays an important role in CFD simulation where all setting and the formula involved in the boundary condition will be applied. The end result of this phase is a large collection of data.

3.6.1 Model validation

For post-processing process, executed results will be evaluated. Validation of CFD models is often required to assess the accuracy of the computational model. This assessment can assist in the development of reliable CFD models. Validation is achieved by comparing CFD results with available experimental, theoretical, or analytical data. Validated models become established as reliable, while those which fail the validation test need to be modified and revalidated. Validated CFD models contribute the application of CFD in industry and research to grow for better result in the future. However, validation using experimental or theoretical data is not always possible, since such data are sometimes unavailable in the previous work. A review of the literature in CFD validation can be found in Oberkampf and Trucano (Eesa, 2009).

3.6.2 Permeability validation

Since the second objective in this dissertation is to determine the permeability of Portland cement with the volume of CO_2 leakage through the cement plug, different length of cement plug is selected to produce the XY-graph of permeability versus the density. For each reaction, the value of density and the viscosity is reported from the simulation and the value is then used to complete the Darcy Law equation. The density at different cement plug height is reported from the Ansys Fluent. The value of permeability is then calculated and the graph is produced.

CHAPTER 4

RESULT & DISCUSSION

4.1 REACTION MODEL

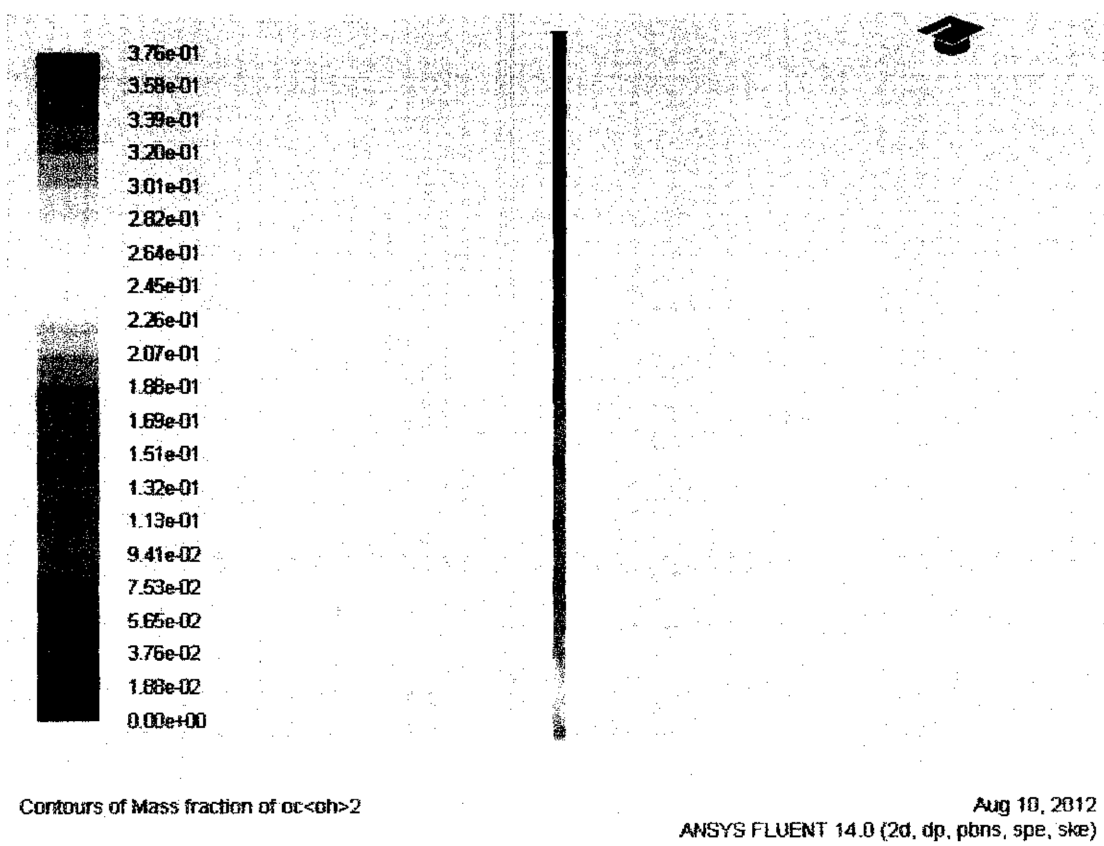

Figure 12: Contours of mass fraction of carbonic acid

High concentration of Carbon Dioxide is reacted with the water to produce acid carbonic. The volume of carbonic acid inside the surface body is higher at the initial phase of the reaction. In fact, the mass fraction of carbonic acid is increases over time since the reaction of acid carbonic formation keeps going over time. The mass fraction of carbonic acid is higher at the inlet area (bottom part of the surface body) is because the flowrate of 30m/s for both 0.5 mass fraction of Carbon Dioxide and 0.5 mass fraction of Water is supplied constantly until the iteration is completed. However, the mass fraction of carbon dioxide and water is reducing since the both of them are used as reactant for the reaction. Figure 12 show the mass fraction of carbonic acid after the iteration is completed.

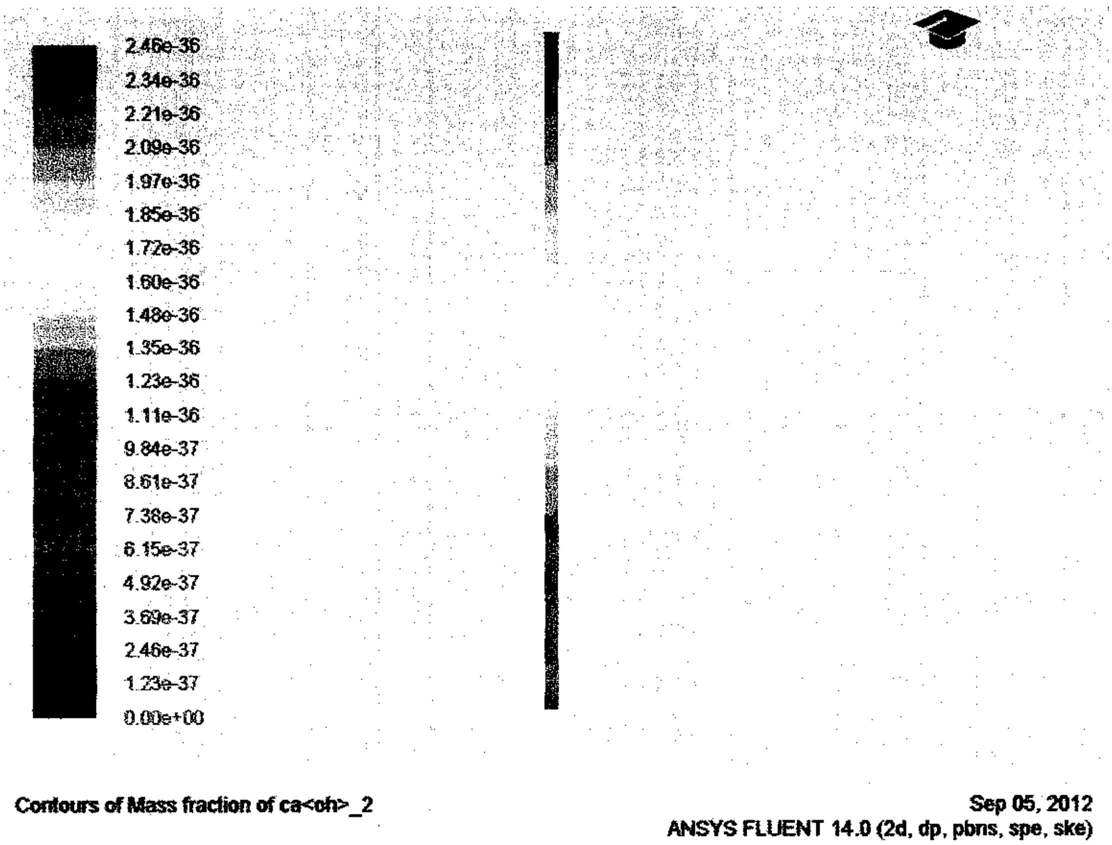

Figure 13: Contours of mass fraction of calcium hydroxide

Over the time, most of the carbonic acid that enters to the surface body is reacted with calcium hydroxide. Calcium hydroxide is the major hydration product of Portland cement when it mixes with water. It is also selected as the domain fluid in the surface body at the initial stage. The rate of acid carbonic attack the calcium hydroxide may differ relative to the temperature and pressure in the system. The hydration of Portland cement increase as the temperature and pressure increases. Thus, it may leads to the formation of calcium hydroxide at large scale and at the same time increases the value of mass fraction of calcium hydroxide (Sauki & Irawan, 2010). In addition, flowrate of carbonic acid also plays an important role in determining the rapidity of the Portlandite carbonation. Further explanation will not be discussed in this report since this dissertation only interested with the reaction involved at constant temperature and pressure. In addition, the flow rate of carbonic acid is also set as constant without regard to the flowrate reduction while the reaction is carried out. The process of Carbonation of Portlandite or Cement Hydrates formed calcium bicarbonate and high percentage of water. Simultaneously, the mass fraction of the Calcium hydroxide is declining at the bottom part of the surface body, leaving the high percentage at the outlet area as it shown in Figure 13.

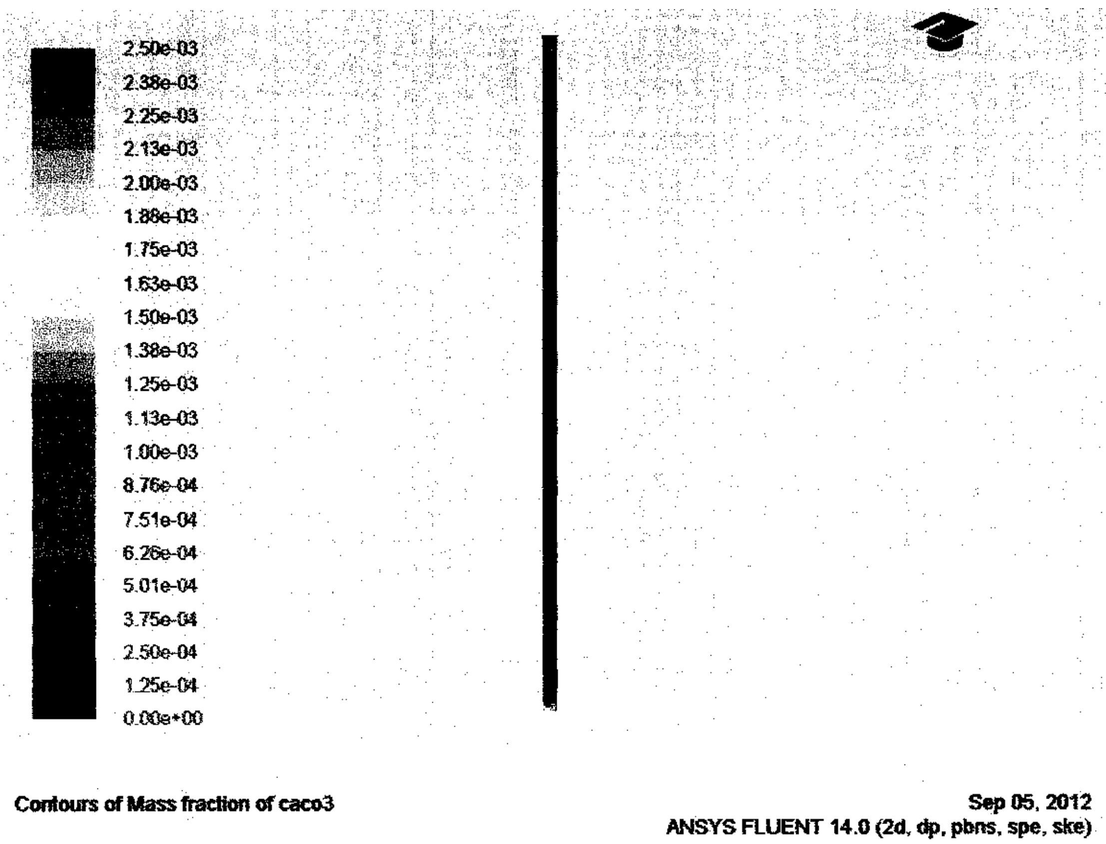

Figure 14: Contours of mass fraction of calcium carbonate

Figure 14 show the mass fraction of Calcium Carbonate after the iteration is completed. Only few percentage of calcium carbonate left in the system since most of them are used as one of the reactant to perform the following reaction which is the dissolution of calcium carbonate. At this stage, again acid carbonic is then reacted with the calcium carbonate to form the last product of all three reactions. It shows that, the remaining element left in the surface body is dominating by Calcium Bicarbonate as it shown In Figure 15.

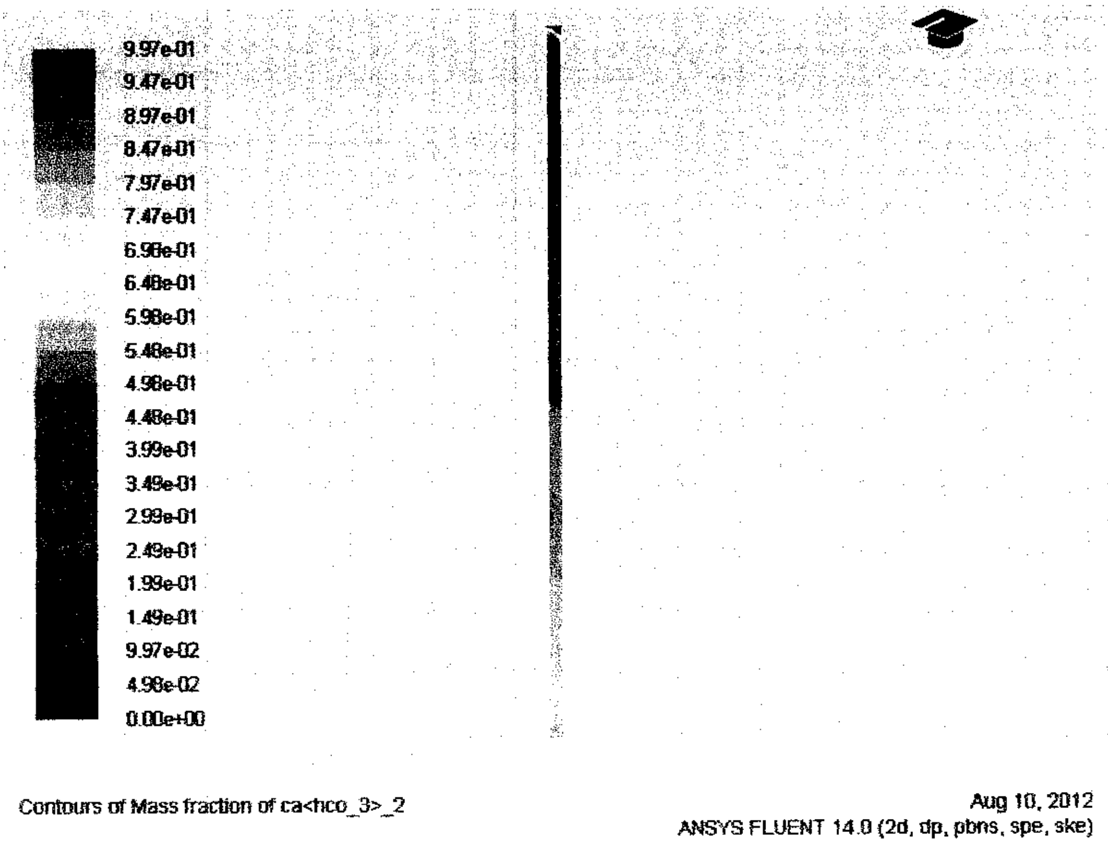

Figure 15: Contours of mass fraction of calcium bicarbonate

Therefore, the equation is proven since the mass fraction of calcium bicarbonate is increasing after the reaction is completed. In addition, the final mixture has lower density than the calcium hydroxide. The result is used in the next section to prove the relationship between the density with the value of permeability at given length of cement plug. However, some errors had occurs when conducting the simulation. It is due to several limitations such as unavailability of the parameters detail and the boundary condition setting led the simulation is not display in the appropriate manner.

4.2 EFFECT OF PERMEABILITY WITH THE VOLUME OF CO_2 LEAKAGE

Table 6: Summary of the dimension used

Cross section area of cement plug (m^2)	0.47032
Inlet Pressure (Pa)	5929491
Outlet Pressure (Pa)	5336592
Dynamic Viscosity (kg/ms)	0.0000172
Length the of cement plug (m)	60.96

Table above shows the entire dimension and the setting used for the simulation. This information is important in order to relate the correlation between permeability with the volume of liquid by using Darcy Law.

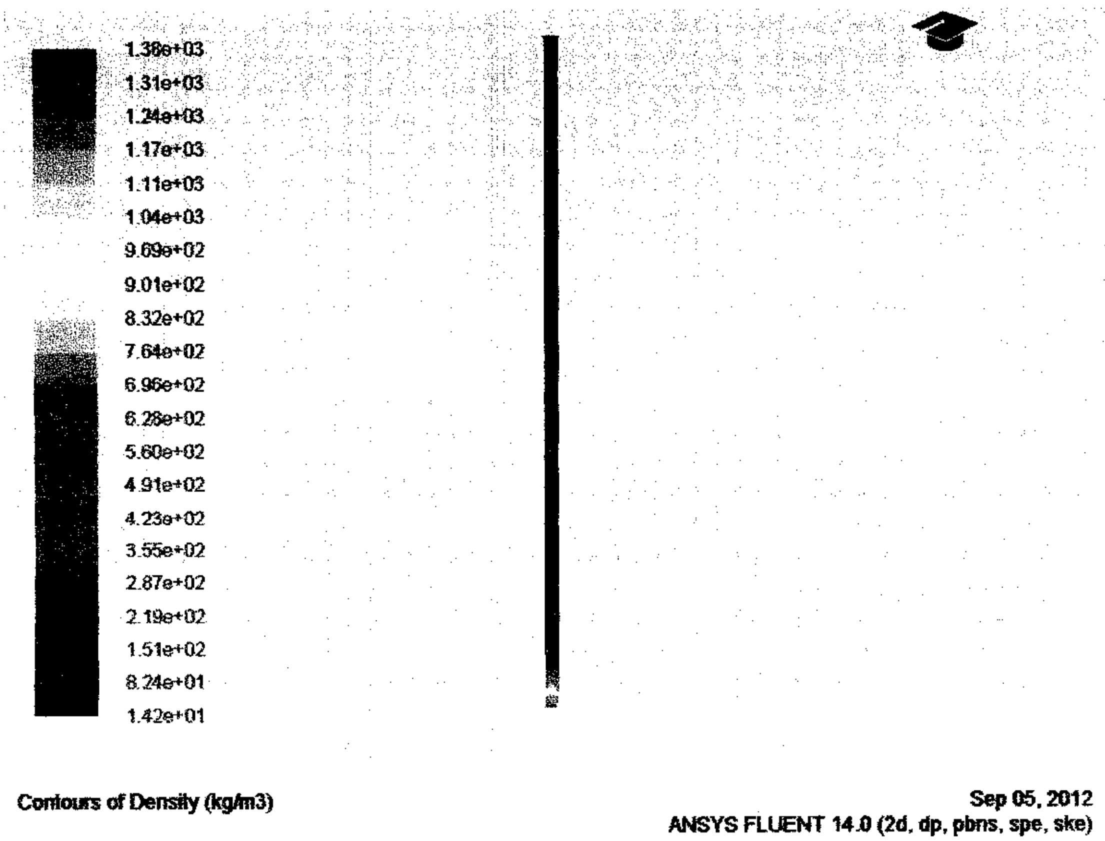

Figure 16: The contours of the density

Figure 16 show the value of the density inside the surface body (cement plug) after the reaction is completed. Bottom part of the model has higher density in comparison with the top part of the model due to high number of material in the bottom part. The value of the density at different length of cement plug is reported using Ansys Fluent using line / rake surface function. The data obtained is given in the table below.

Table 7: Value of the density at different length

Cement plug length (m)	**Density (kg/m^3)**
10.96	329.17731
20.96	190.06601
30.96	136.83118
40.96	108.45309
50.96	90.66333
60.96	78.38903

The graph is below is plotted to show the relationship between cement plug length and the density in the system.

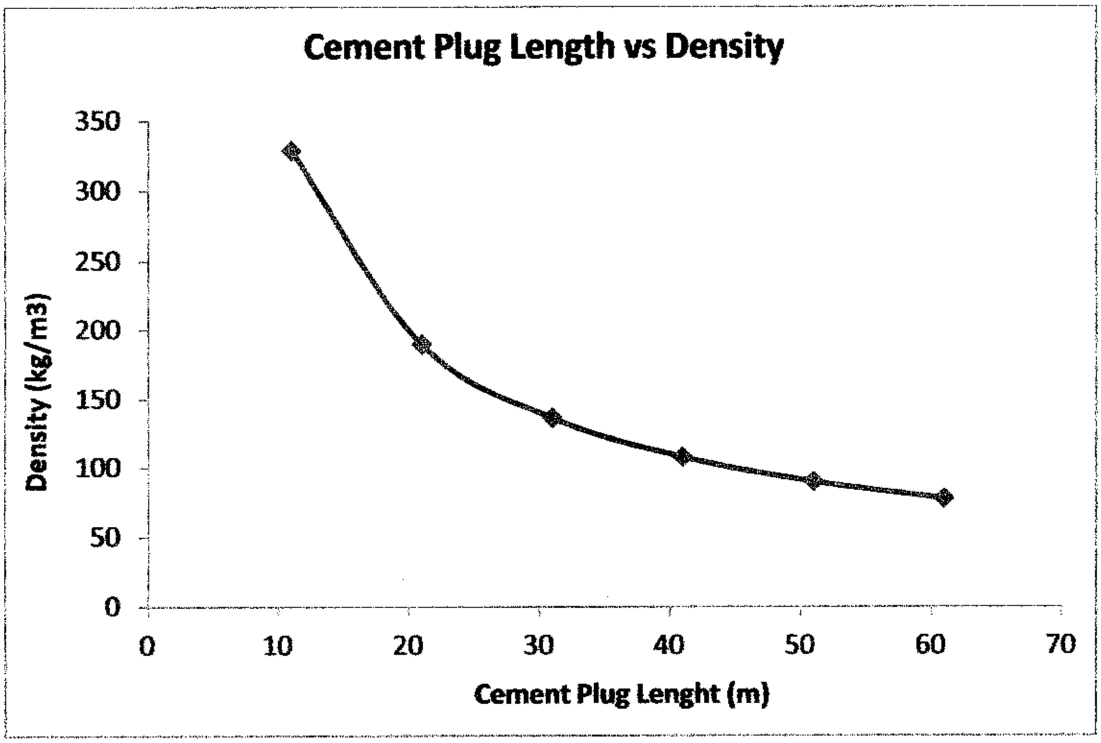

Figure 17: Graph of cement plug length against the density

In order to study the permeability involved in the reaction, density is identified as one of the parameter in Darcy Equation. Thus the value of the density obtained from Table 8 above is used in order to determine the permeability of the mixture. The value of permeability at given density is clearly tabulated in table below.

Table 8: Value of the permeability at different density

Density (kg/m^3)	**Permeability (m^2)**
329.177	5.32635E-09
190.066	9.22476E-09
136.831	1.28137E-08
108.453	1.61666E-08
90.6633	1.93387E-08
78.389	2.23668E-08

The data is plotted as graph below to show the effect of density in changing of the permeability.

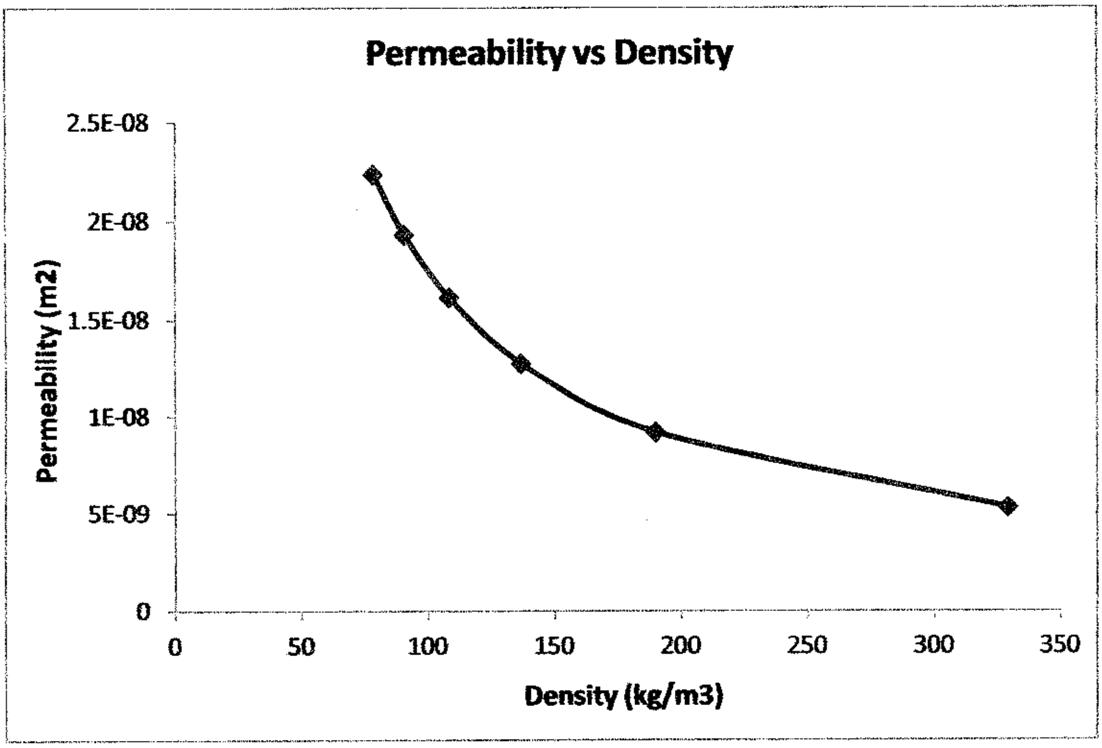

Figure 18 : Graph of permeability against the density

In order to show the relationship between the permeability at different high and changed in density at the particular cement plug length, the data is clearly tabulated as shown in table below.

Table 9: Value of the comparison between density and permeability and different cement plug length

Density (kg/m^3)	**Cement plug length (m)**	**Permeability (m^2)**
329.177	10.96	5.32635E-09
190.066	20.96	9.22476E-09
136.831	30.96	1.28137E-08
108.453	40.96	1.61666E-08
90.6633	50.96	1.93387E-08
78.389	60.96	2.23668E-08

The graph of cement plug length against the permeability is plotted as shown in Figure 19 below.

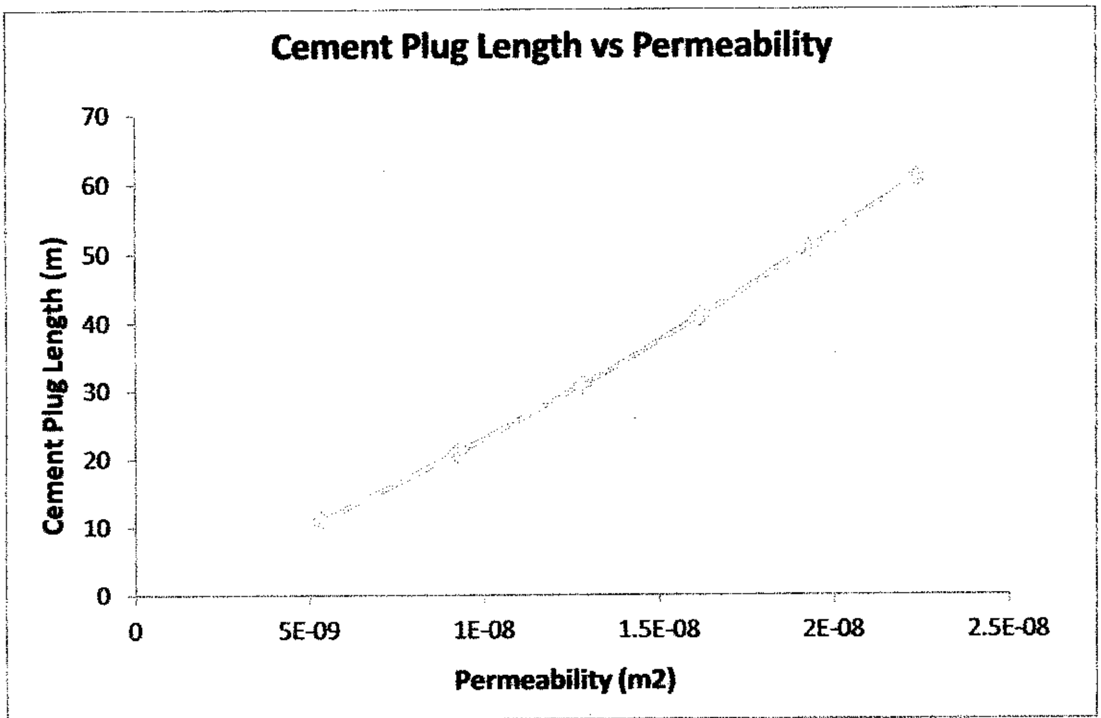

Figure 19 : Graph of cement plug length against the permeability

From all three graphs, we can summarize that the density of the cement plug is changing at different length across the vertical direction. The density is declining when the length of cement plug is increasing. Different situation shows in the second graph where the permeability is proportionally inversed to the density. Calcium bicarbonate that produced from the reaction has 73.756 kg/m^3 of density, which is lower in comparison with the calcium hydroxide that having the density of 2210 kg/m^3. As the density of the calcium bicarbonate is lower, thus the permeability is higher. According to Santra et al (2009), the permeability of the Portland cement is increasing after the dissolution of calcium bicarbonate took place in the Portland cement. Initially the permeability is of the Portland cement is equal to 7.8874e-10 m^2 which is equal to permeability to calcium hydroxide and after the reaction is completed the permeability is increasing to 2.2377e-8 m^2. Thus, the result has been validated by the theory that the permeability of Portland cement increase as the reaction is completed.

It also proves that the lower part of cement plug has lower permeability due to the high density value. However, with middle part and the upper part of the cement plug has higher permeability due to lower density value. As a result, the CO_2 can easily move through the more permeable system of which the domain element is calcium hydroxide. Thus, it leads to the leakage through the system.

CHAPTER 5

CONCLUSION & RECOMMENDATION

5.1 CONCLUSION

As a conclusion, the cement plug environment constitutes a key element to consider in the long term integrity performance of a well. Darcy law in a homogenous porous medium are the most significant equations throughout the project span. Not to forget, in order to develop the Computational Fluid Dynamic modelling, Darcy Law equation becomes a vital knowledge in designing the model. These equations describe the relationship between the densities with the value of the permeability. Eddy-Dissipation model and K-epsilon model is used in order to complete the reaction in Portland cement. Some assumptions have been formulated on the permeability values to solve the numerical simulations. Improvements in the modelling will have to be performed to take into account the significant differences between some parameters values.

The numerical simulations have highlighted the competition between the permeability of Portland cement (cement plug) and the volume of CO_2 leakage dispersed to the surface. The reaction model in Portland cement has been successfully developed using ANSYS Fluent. The reaction model was developed in order to obtained the data for determining the permeability value at given density.

From the result, the permeability of the cement plug is increased after the iteration is completed. It is due to the high number of calcium bicarbonate produced in the system that reducing the value of the density. Hence, the value of the permeability of the cement plug is increasing when the Darcy Law is applied. It clearly shows that this may harm the geological storage environment because there is possible of CO_2 leakage within the wellbore due to permeability change in the Portland cement. Thus, future research is necessary in order to improve the sustainability of Portland cement as the plug for the abandoned well.

5.2 RECOMMENDATION AND FUTURE WORK FOR EXPANSION

Since this research is kind of new thing, thus no reference data or simulation can be used in for validation purposes. This report is based on engineering theory and it relies 100% from the information that have been discussed earlier in this dissertation in order to validate the data. Below are several recommendations on the future work in order to complete the objectives and increase the relevancy of this project:

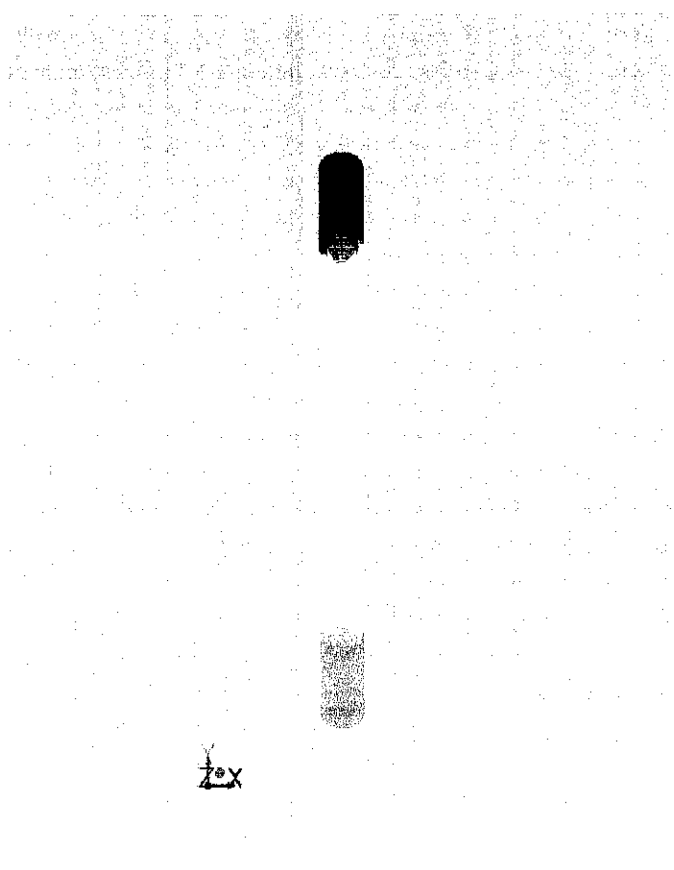

Figure 20: 3-D geometry result from Ansys Fluent

- Introduce the porous media function along with the reaction involved in Portland cement instead of simulating the reaction model in hollow space. 3-D model is constructed and the boundary condition is identified as wellbore inlet, porous zone inlet, porous zone, porous zone outlet and wellbore outlet as shown in Figure 20 above. The density of porous zone is set as 73.756 kg/m^3 and CO_2 is defined as inlet material. Both K-epsilon model and porous media function is enabled in order to obtain the desired result.
- The relevancy of the result may improve by considering different CO_2 leakage potential pathway. Thus, different boundary condition must be selected.
- To relate the effect of high level of Calcium Bicarbonate in the system with changing of permeability of Portland Cement

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APPENDICES

Final year project 2 planning

NO.	ACTIVITY / WEEK	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1.	Define modelling goal															
2.	Perform the simulation															
3.	Discuss the outcome with supervisor															
4.	Reiterate the modelling															
5.	Examine & finalize the result															
6.	Consider revision to the model															
7.	Compiling all material for final report FYP 2															
8.	Submission of final report															

Key milestone

NO.	ACTIVITY / WEEK	1	2	3	4	5	6	7		8	9	10	11	12	13	14
1.	Selection of Project Title		X													
2.	Preliminary Research Work					X										
3.	Submission of Extended Proposal						X									
4.	Preparation for Oral Proposal Defence							X								
5.	Oral Proposal Defence Presentation									X						
6.	Detailed Literature Review													X		
7.	Learn Modelling Software (FLUENT 14)															X
8.	Preparation of Interim Report															
9.	Submission of Interim Draft Report														X	
10.	Submission of Interim Final Report															X