Thermodynamics Properties Modeling Using Cryogenic Process

by

Carmen Lee Kar Mun

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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A project dissertation submitted to the
Chemical Engineering Programme
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Approved:

(DR. LAU KOK KEONG)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
DECEMBER 2010

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.

CARMEN LEE KAR MUN

ABSTRACT

This project aims to predict carbon dioxide composition in natural gas system using commercial fluid dynamics simulators (i.e FLUENT software). Currently, there is no fluid dynamics software that is able to capture phase change behavior of mixture components. Hence, this project involves incorporation of thermodynamics properties into FLUENT. This can be done by implementing coding using Peng Robinson model into FLUENT. Peng Robinson model is used because it has better behavior at critical point and thus, suitable to be used for vapor system. In this project, only a binary mixture of vapor phase is used for simplicity purposes. The scope of study also covers the operating condition to achieve desired separation using cryogenic process. The research started with literature review to investigate suitable model to be used, followed by development using C++ programming. The completed program is verified with HYSYS before further simulations are done. Once it is validated, simulation using a simple pipe is performed and results are validated with HYSYS again. Results obtained are almost as accurate as HYSYS and hence, this shows that thermodynamics properties using Peng Robinson model is able to be applied into FLUENT. This project has successfully produce computational code for vapor phase behavior studies to be implemented into FLUENT. This model in FLUENT is able to capture the phase change behavior and hence, enables the selection of the best design for intended separation.

ACKNOWLEDGEMENTS

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With Utmost Gratitude,

………………………………

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TABLE OF CONTENTS

LIST OF TABLES

LIST OF FIGURES

LIST OF ABBREVIATIONS

CFD	Computational Fluid Dynamic
CH_4	Methane
CO_2	Carbon Dioxide
EOS	Equation of State
HYSYS	Simulation software developed by ASPEN
JT	Joule Thomson
LNG	Liquid natural gas
PR	Peng-Robinson
SRK	Soave-Redlich-Kwong
VLE	Vapor-liquid equilibrium

NOMENCLATURE

Symbols

P_{BUBL}	Bubble-point pressure
P_{DEW}	Dew-point pressure
P_i^{sat}	Saturated pressure, species *i*
T	Absolute temperature, Kelvin
T_c	Critical temperature
R	Universal gas constant
x_i	Liquid fraction, species *i*
y_i	Vapor fraction, species *i*

Greek letters

Θ	Vapor phase fugacity coefficient of species *i*
γ_i	Liquid phase activity coefficient of species *i*
a	Molecules attraction parameter, cubic equation of state
b	Molecules repulsion parameter, cubic equation of state
ω	Acentric factor

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Natural gas is categorized as a non-renewable fossil fuel. Increasing energy demand and pricing trends have encouraged oil and gas companies to look at developing contaminated natural gas fields [1]. Natural gas is widely used as it is the cleanest and safest energy sources. Ample supplies from domestic resources also encouraged the usage of natural gas. It has become an important source since mid 1990s. Figure 1.1 shows the consumption of natural gas in Malaysia from year 2004 to year 2010. The total natural gas consumed is in cubic meter (cu m) [14]. It can be seen here that natural gas has become an important energy source usage in Malaysia as year passes by.

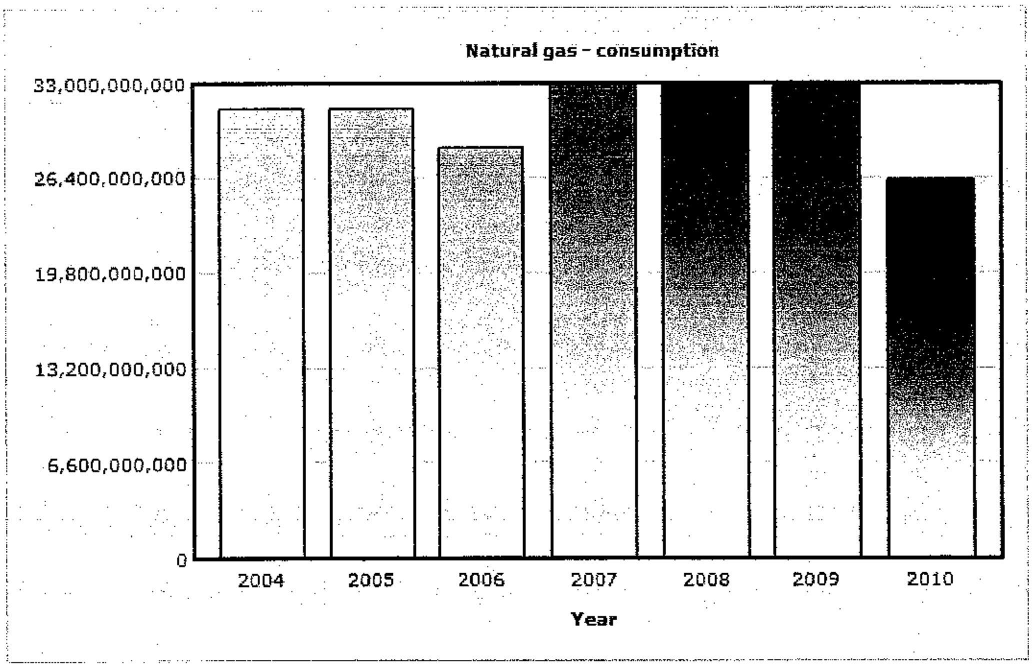


Figure 1.1 Consumption of natural gas in Malaysia (cubic meter)

Natural gas extracted from underground sources is saturated with heavier hydrocarbons and carbon dioxide. Before it can be used as fuel, it must go through several stages of processes to remove almost all components other than methane such as ethane, propane, higher molecular weight hydrocarbons, carbon dioxide and water vapor. The gas will then be transported in high-pressure pipelines from producing areas to industrial end users, storage areas and local distributing companies. As natural gas has low density, it is not easy to transport and store it. Usually natural gas will be turned into liquid at liquefaction plant. For example, LNG is used for long distance and high volume transportation.

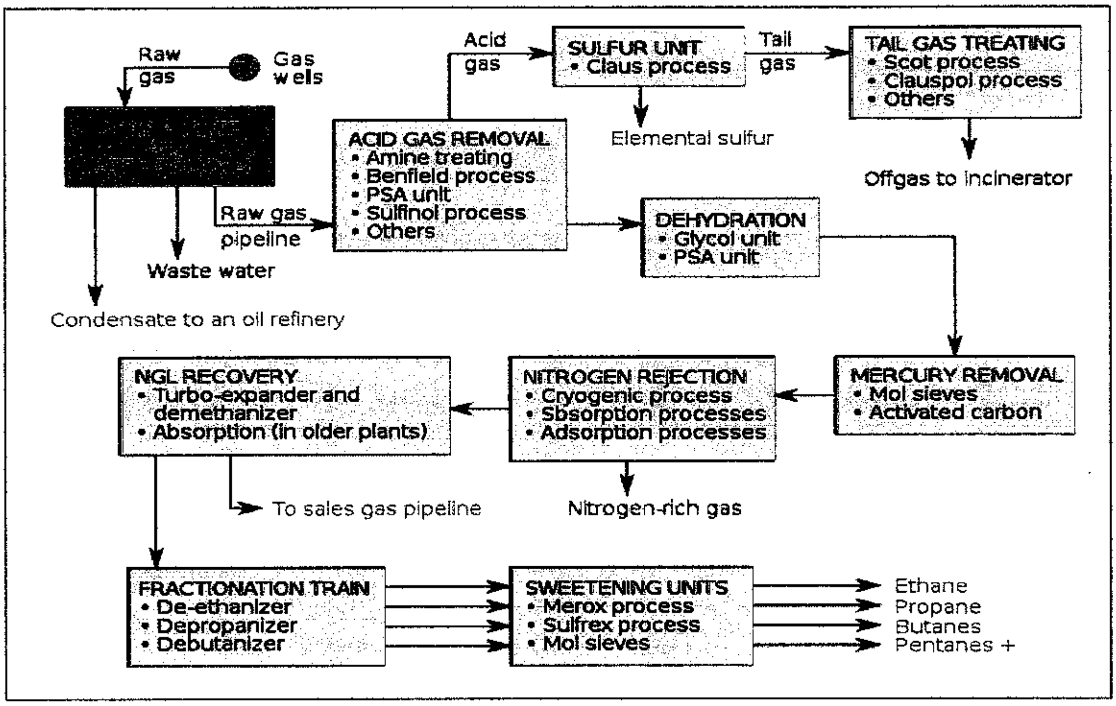


Figure 1.2 Natural gas processes

Figure 1.2 shows a common block flow diagram of natural gas process from the gas well to gas processing plant and finally, the final sales products. Raw natural gas collected from adjacent wells is processed to remove free water and natural gas condensate. It is then pipelined to gas processing plant in which initial purification is removal of acid gases (hydrogen sulfide and carbon dioxide). What this research project focuses here is the acid gas removal section, where carbon dioxide will be removed at the processing plant using cryogenic process. Next, if there is any acid gas present, it will then be routed into a sulfur recovery unit to convert hydrogen sulfide in acid gas into either elemental sulfur or sulfuric acid. Next step in gas processing plant is to remove water vapor from gas. Mercury and nitrogen are also removed before recovery of natural gas liquids (NGL), where the residue gas from NGL recovery section is pipelined to end-user markets. Most cryogenic plants do not include fractionation due to economic reasons.

Carbon dioxide is one of the byproducts exists in natural gas. Most industries demand for clean and pure natural gas for various applications such as generation of electricity, automobile fuel and domestic use. Hence, it has to be removed to an acceptable level as natural gas is highly contaminated by carbon dioxide. In addition, removal of high amount of carbon dioxide needs to be done as worldwide is concerned about the carbon emission to the air. This may lead to green house effect as carbon dioxide level is increasing due to excessive emission in natural gas production. For example, carbon dioxide removal from large scales industrial processes, such as production of ammonia from natural gas in fertilizer industry. In this production process, large quantities of carbon dioxide are produced and separated, but at present, most of it is vented to the atmosphere instead of captured and stored [9]. This emission can lead to green house effect.

There are three options for reducing total carbon dioxide emission into atmosphere. One, reduce energy intensity. Two, reduce carbon intensity and third, enhance sequestration of carbon dioxide. The first option requires efficient use of energy while the second option requires switching to using non-fossil fuels such as hydrogen and renewable energy [10]. The third option involves development of technologies to capture and sequester more carbon dioxide [10].

Removal of carbon dioxide is commonly done using adsorption, absorption, membrane separation and cryogenic. The choice of suitable technology to be used depends on the characteristics of flue gas stream. For example, in a coal IGCC (integrated gasification combined cycle) process, modified for capture, the carbon dioxide concentration would be about 35-40% at a pressure of 20 bars or more. In that case, physical solvents such as Selexol could be used for pre-combustion capture of carbon dioxide with the advantage that carbon dioxide can be released mainly by depressurization [10]. However, this research project focuses on cryogenic process whereby it involves separation of gas mixtures by fractional condensation and distillation at low temperature. Cryogenic involves cooling gases mixtures to a very low temperature to allow carbon dioxide to be liquefied and hence, separated from the mixtures. This process allows recovery of pure carbon dioxide in the form of liquid. This liquid carbon dioxide can be transported conveniently or pumped to the injection site for enhance oil recovery (EOR) or enhance coal-bed-methane (ECBM).

The removal of carbon dioxide from natural gas in this research project happens in almost similar process mentioned above. This research project will focus on pressure-temperature relationship to remove liquefied carbon dioxide. This explains why it is important to start off with the study of thermodynamics properties for natural gas. While natural gas flows into pipe, it is a must to ensure that the inlet temperature and wall temperature are suitable for condensation to occur so that liquefied carbon dioxide can be formed.

In addition, construction of mixture phase envelope is an important problem in phase equilibrium calculations, with many applications in chemical thermodynamics and hydrocarbon reservoir thermodynamics [9]. To correlate methane with carbon dioxide in natural gas, a phase envelope needs to be developed for this case study. This phase envelope is to determine the mixture's behavior in each phase of different operating conditions. It is important to know as the aim of this project is to remove high amount of carbon dioxide from natural gas.

1.2 Problem Statement

Natural gas extracted in Malaysia contains high carbon dioxide. However, the natural gas demand from most industries requires clean and pure natural gas. Hence, separation of carbon dioxide from natural gas is needed to meet this requirement. Current technologies can only extract a small percentage of carbon dioxide from natural gas but the demand of obtaining bulk carbon dioxide is increasing. The technologies available in market for natural gas treating may not be ideally suitable for treating highly contaminated natural gas where CO_2 geo-sequestration is required. Use of physical and chemical absorption solvents have been the most popular method for treating natural gas with high CO_2, and to lesser extent, membranes and adsorption methods. These technologies remove CO_2 at near ambient pressures thus requiring substantial amount of compression to levels needed for geo-sequestration [1].

Modeling of cryogenic separation for high CO_2 in natural gas field should consider thermodynamics properties. However, most fluid dynamics simulation processes do not take into account the thermodynamics properties of components. This is because simulation software does not have the ability to determine the phase change of components at each operating conditions. Hence, it is not possible for us to know the phase behavior if this study could not be incorporated into simulation software. What this research project focuses here is on how to develop and incorporate thermodynamics properties of binary mixtures (i.e. methane and carbon dioxide) into FLUENT to investigate the phase change behavior.

Besides that, as extraction has to be done at the platform, it is almost impossible to obtain large amount of carbon dioxide due to few disadvantages of current methods. The setbacks are they require relatively large facilities, huge investment and possibility of having a negative impact to the environment. Hence, new low-cost technologies have to be used to efficiently meet this requirement. Cryogenic process is able to overcome some of these disadvantages as it does not involve any chemicals or catalyst and equipments required are simple and small.

In addition, what this project is addressing is the issue of operating conditions that will result in an effective condensate separation of carbon dioxide from natural gas. Here, effective is defined as meeting separation requirement of liquid (in this case, carbon dioxide) by condensation so that the gas system exiting the separator device meets the desired specification. In practical sense, vapor and condensate ratio change in real time due to dynamic flow conditions (loss of heat and pressure during transmission). Hence, the unknown profile of natural gas flowing in a pipeline is function of at least, temperature, pressure and composition of components presents.

Apart from modeling, the study of temperature and pressure to achieve targeted vapor outlet content in the mixtures is also the focus of this research project. This part of research will help in developing and improving a technology whereby mechanical device, such as an expander is employed to condense gas stream passing through it. When gas is expanded, its temperature will inherently drop and this phenomenon brings down the liquid content in gas, resulting in lower liquid content of gas exiting the device.

1.3 Relevancy and Significance of Project

This project brings a contribution to the natural gas industry and its flow in pipeline as it utilizes thermodynamics studies from chemical engineering point of view. Modeling of natural gas behavior in thermodynamics properties and fluid dynamics enable the study of fluid flow and optimizing parameters such as pressure and temperature. This can ultimately contributes to economical and operational advantages of separation process for natural gas in processing network.

As the energy demand and pricing trends increases as well as worldwide concerns on carbon emissions, the transmission and distribution of natural gas commodity has to be done more economically while maintaining its technical feasibility. Hence, optimization of fluid flow in pipeline is important for this aspect. In natural gas transmission pipeline, risk of hydrocarbon condensation cannot be avoided. Hydrocarbon liquid resulted from condensation will increase pressure drop. Operational problems resulting from two-phase flow will occur. Thus, it is useful to study the optimal operating conditions applied to a separator device.

This project is a good start to support the use of new technology that can condense and remove carbon dioxide from natural gas. This technology is cost-effective, safe and environmental friendly. The benefits of using cryogenic process separation system are as below:

- Cost-effective in terms of capital and operating costs
- Environmental friendly with no chemical or catalyst involved
- Occupy small space. Such compact and low-weight facilities can be installed on minimum facilities platforms
- Simplicity of static device with no rotating parts
- Incremental cost of offshore facilities using new technology is generally more than balanced by savings on pipeline and onshore facilities, notably elimination of chemical-regeneration systems
- Novel separator is an attractive option for corrosive service. For example, gas compositions with high carbon dioxide fraction which may necessitate CRA export line.

1.4 Objectives of Project

The objectives of this research project are:

- To find out carbon dioxide composition in natural gas system
- To translate thermodynamics properties into computational codes
- To incorporate Peng Robinson model into FLUENT for phase change behaviour
- To investigate cooling effect in pipes

1.5 Scope of Work

The scope of study involves area of thermodynamics and fluid dynamics. As natural gas composes mainly of methane, the rest of other hydrocarbons usually present are disregarded. Light gases such as ethane, propane and other hydrocarbons are not included in the scope of study to reduce complexity when deals with programming and FLUENT. Hence, only methane and carbon dioxide are used for this project for simplicity purposes.

This research project focuses on the thermodynamics properties modeling. As mentioned in the problem statement section, thermodynamics properties are important to investigate the phase change behavior of components. However, currently most of fluid dynamics software or approach does not take into account the thermodynamics properties. Hence, FLUENT is used to capture this phase change for this case study. For simplicity purpose, only one single phase is solved here. Peng Robinson model is used, whereby a coding of operating conditions and vapor fraction from HYSYS is prepared. This coding is incorporated into FLUENT for simulation and then validated again with HYSYS to ensure that the phase change in FLUENT is correctly obtained.

This project also involves finding out operating conditions best for liquefaction of carbon dioxide from natural gas. Hence, it is important to know the typical pressure and temperature in gas pipeline and processing plant. The pressure of natural gas is typically 4 MPa to 8 MPa in processing plant and on-shore transmission while gas entering offshore pipelines is often compressed to 16 MPa or higher [11]. As carbon dioxide has a unique properties compared to other components, it is important to study its properties along side with methane. A phase envelope can be developed to correlate phase change with operating conditions.

In addition, it is important to ensure that the inlet temperature and wall temperature is sufficient for liquefaction of carbon dioxide to occur. The range of pressure is set to be 60 bar to 80 bar which cover well the range of pressure in processing plant. Temperature set should not be too high or too low because the design of separator device shall strive to minimize the need for coolant and heating medium to achieve separation.

CHAPTER 2

LITERATURE REVIEW

2.1 Carbon Dioxide

As carbon dioxide possesses unique thermodynamics properties, it is important to study and understand its properties on how the phase changes with different operating conditions. Carbon dioxide, CO_2 is a chemical compound of two oxygen atoms covalently bonded to a single carbon atom. It appears as gaseous phase at standard temperature and pressure.

Figure 2.1 shows the phase diagram of carbon dioxide. There is no liquid state of carbon dioxide at pressure lower than 5.11 atm. Sublimation process occurs at the pressure of 1 atm and temperature above -78°C. Sublimation is a process where carbon dioxide changes directly from solid phase to gaseous phase without going through liquid phase first. Solid carbon dioxide is known as dry ice. The triple point of carbon dioxide, where the three phases co-exist in thermodynamic equilibrium is at the pressure of 5.11 atm and -56.6°C.

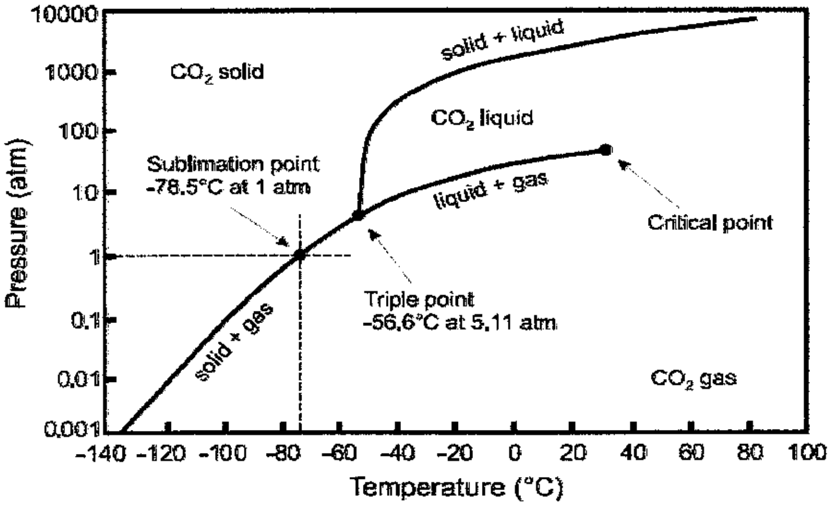


Figure 2.1 Pressure-Temperature phase diagram for CO_2

2.2 Phase Envelope

2.2.1 Natural gas

Phase envelope defines region between two-phase and single-phase fluids. It is useful to determine fluid's phase at certain operating conditions. Figure 2.2 shows the phase diagram of natural gas. The Y-axis indicates pressure and X-axis indicates temperature. Dew point curve (red curve) is the curve where liquid will begin to condensate. Bubble point curve (blue curve) is the curve that separates liquid region from two-phase region. It represents true vapor pressure (TVP) for a liquid.

For example, assume a pipeline is 800 psi and 50°F; the gas would be in gas phase. If temperature dropped to zero degrees, liquid would begin to form. If temperature decreased more, additional liquid would form as gas properties go deeper into two phase regions [10]. Liquid phase region exhibits low fluid compressibility and high mass density values. On the other hand, vapor phase region is an opposite of liquid phase region, where it exhibits high fluid compressibility and low mass density values [3]. Two-phase region is a region where the liquid and vapor states are formed simultaneously.

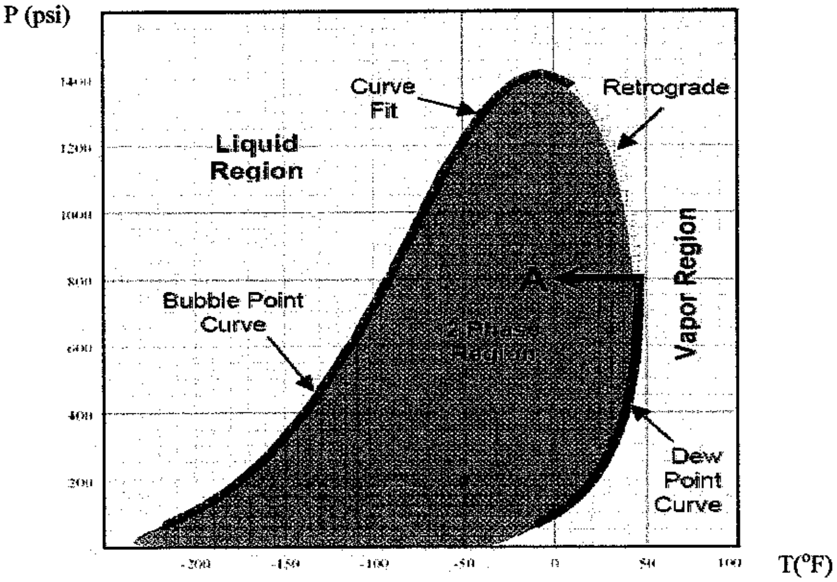


Figure 2.2 Typical phase envelope for natural gas

2.2.2 Two phase mixture

When two mixtures are mixed, their behaviors as pure components will not be the same anymore. This is due to the consequence of new fields of molecular interactions that has been created. For a two phase mixture, pressure increases as the system passes through from dew point to bubble point. The composition of liquid and vapor will change when operating condition changes but the overall composition of the system will remain the same. At dew point, composition of vapor is equal to the composition of the system. However, the infinitesimal amount of liquid that is condensed is more in the less volatile component. At bubble point, composition of liquid is equal to the composition of system. However, the infinitesimal amount of vapor remaining at bubble point is more in the more volatile component than the system in a whole.

Critical point is the common point between dew point and bubble point curves but this point does not represent the maximum pressure or minimum temperature for vapor-liquid coexistence. The range of temperature of the critical point locus is usually bounded by critical temperatures of pure components in binary mixtures. Due to this, the critical temperature for a binary mixture will never be below the lightest component's critical temperature or above the heaviest component's critical temperature. However, this concept is not applicable for critical pressures. The critical pressure for a binary mixture can be higher than the critical pressures for both pure components.

2.3 Equation of State (EOS)

Equation of state is needed to define the state of a system and also, to determine the properties of the system in that particular state. It is an important thermodynamic equation used to predict the states of liquids and gases. The study of EOS is important in this research project as this project focuses on thermodynamics properties for gases of binary mixtures.

Commercially, two equations of state, Peng-Robinson (PR) and Soave-Redlich-Kwong (SRK) are widely utilized for prediction and simulation of this natural gas reaction. These empirical EOS are the key component of any simulation packages in chemical and petroleum engineering [4]. Study of these EOS need to be done as HYSYS software required choosing any of these two packages to be used. Hence, detailed comparison of these two to determine which EOS fits best for this project. Comparisons of PR and SRK are done, as shown in Table 2.1.

Table 2.1 Properties of PR and SRK models

Peng- Robinson (PR) model	**Soave-Redlich-Kwong (SRK) model**
• Ideal for VLE calculations and calculating liquid densities for hydrocarbon systems	• Provides comparable results to Peng-Robinson
• Contains enhanced binary interaction parameters for all library hydrocarbon-hydrocarbon pairs and for most hydrocarbon-non-hydrocarbon binaries	• Should not be used for non-ideal chemicals such as alcohols, acids or other components. These chemicals are more accurately handled by the Activity Models (highly non-ideal) or the PR EOS (moderately non-ideal).
• Applicable over a wide range of conditions: - Temperature Range > -271°C or -456°F - Pressure Range < 100,000 kPa or 15,000 psia (high pressure)	• Range of application is significantly more limited: - Temperature Range > -143°C or -225°F - Pressure Range < 5,000 kPa or 750psia

Comparing PR and SRK EOS, both models are almost comparable except for a slightly better behavior by PR EOS at critical point. Due to this, PR EOS is suited to be used for gas or condensate system. Besides that, PR EOS is well-known to be used for carbon dioxide related case studies. Hence, PR EOS has become the most popular equation of state for natural gas systems in petroleum industry.

The general PR PVT relationship is described as below:

$$p = \frac{RT}{V-b} - \frac{a\alpha}{V(V+b)+b(V-b)}$$

where p = system pressure

T = system temperature

R = gas constant

V = volume (volume unit/mol)

a = molecules attraction parameters

b = molecules repulsion parameters

α = temperature correction parameter

Solving parameter *a* and *b* yields:

$$a = \Omega_a \frac{R^2 T_c^{\ 2}}{p_c}; \Omega_a = 0.45724$$

$$b = \Omega_b \frac{R\ T_c}{p_c}; \Omega_b = 0.07780$$

$$\alpha = \left[1 + m(1-\sqrt{T_r})\right]^2; m = 0.37464 + 1.54226\omega - 0.26992\omega^2$$

$$T_r = \frac{T}{T_c}$$

where Tr = critical temperature

m = PR parameter

ω = eccentric factor

2.4 Study of Thermodynamics Properties

Study of thermodynamics properties is important for this research project. As most simulation case study do not include in thermodynamics properties, this project focuses on how to incorporate this into FLUENT to investigate the phase change behavior.

For such, it is important to understand some thermodynamics terms. Thermodynamics deals with equilibrium states. Here, equilibrium is defined as a state of balance. In equilibrium state, there are no unbalanced potentials or driving forces within the system. A system is in equilibrium if it does not experience any changes when isolated from its surroundings. If a system involves two phases, it is in phase equilibrium when the mass of each phase reaches an equilibrium level and stays there [8].

The term steady refers to no change with time. Many engineering devices operate for long periods of time under the steady flow process. These devices are referred to as steady-flow devices. Process involving such devices can be represented in steady flow process, whereby it is a process in which a fluid flows through a control volume steadily. In other word, the fluid properties can change from one point to another within the control volume, but at any fixed point the properties remain the same during the entire process. Hence, volume, mass and total energy content of the control volume remain constant during a steady state flow process.

When dealing with steady state flow, what we are interested in is the mass flow rate, which is the amount of mass flowing per unit time. The conservation of mass principle for a general steady flow system states that the mass flow rate for inlet and outlet has to be equivalent.

$$\sum \dot{m}_{in} = \sum \dot{m}_{out}$$

2.5 Removal of Carbon Dioxide

Natural gas transported for usage contains almost entirely of methane. However, natural gas found at wellhead, although still composed primarily of methane, is not the pure methane as used by consumers. It contains water vapor, hydrogen sulfide, carbon dioxide, helium, nitrogen and other compounds. Some natural gas extracted contains carbon dioxide as high as 80%. Hence, carbon dioxide needs to be removed to obtain pure methane and reduce greenhouse effect as well as to reduce corrosion in the pipelines.

There are few methods currently available to effectively remove carbon dioxide from natural gas. The first method is by using membrane permeation. Gas treating membrane system provides a safe and efficient method to remove water vapor and carbon dioxide. This is especially useful for separation process done in remote locations. Membrane systems are adaptable to various gas volumes, carbon dioxide concentrations and/or product-gas specifications. For gas to permeate through a membrane surface, the gas must first dissolve in high pressure-side of the membrane. It will then diffuse across membrane wall and evaporate from low pressure side. However, there are limitations of this method such as the operating pressure has to be over 450 psig, availability of electricity and space and weight restrictions (i.e. offshore).

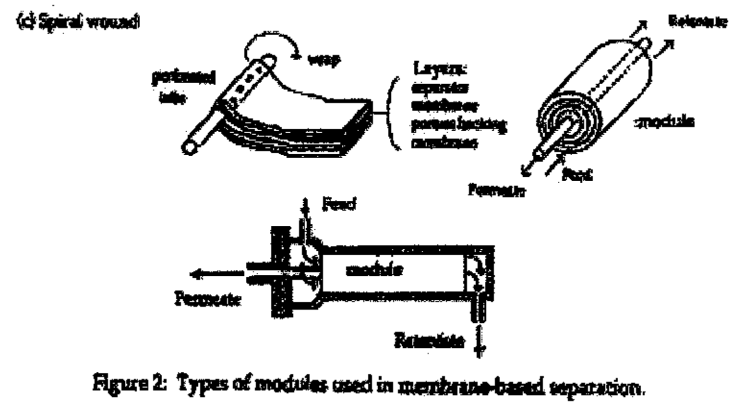


Figure 2.3 Types of modules used in membrane separation

The second method is using carbon ion pump by Lawrence Livermore National Laboratory (LLNL). This is a new method invented to separate carbon dioxide from flue gas. It has the potential to separate carbon dioxide from gas mixtures in natural gas fields. LLNL's ion pump method increases concentration of dissolved carbonate ion solution and this increases the vapor pressure of carbon dioxide gas [15]. Carbon dioxide is then to be removed from downstream side of ion pump as pure gas [15]. Ion pumping may be obtained from reverse osmosis or electro dialysis.

The third method is absorption in solvents. This method is used at industrial scales treatment and in experimental plants for carbon capture. After the process of particle filtering, removal of sulphur and nitrous compounds, the dilute gas is continuously contacted with solvents flowing counter-currently through a packed bed. Desorption of carbon dioxide from this solvent is done in stripping using steam-heat. Physical solvents are used pure and take up carbon dioxide by physical solubility. The operation has to be done after cooling of gas below ambient, which can reach up to negative temperature. However, the limitation of this method is that it requires large energy requirement. The largest energy penalty in chemical absorption is the heat required for desorption process.

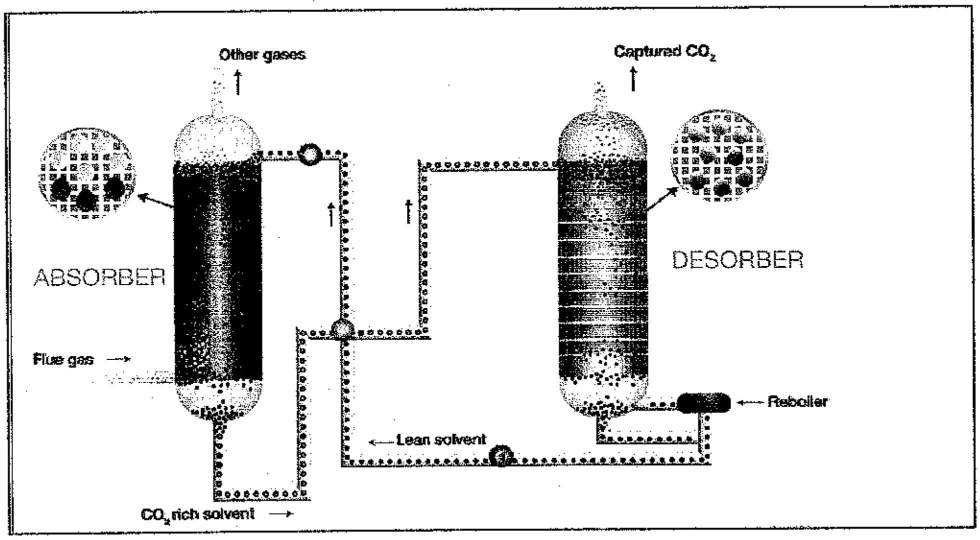


Figure 2.4 Example of absorption method for removal of CO_2

2.6 Cryogenic Process

Section 2.5 describes the common methods used in industry to remove carbon dioxide from natural gas. However, this research process focuses on cryogenic process for the same purposes. Cryogenics involves study of production of materials at very low temperatures, usually below -150°C (123K) and behaviors of those materials at the specified temperature. It is not a substitute for heat treatment, but an extension cycle of heating, quenching and tempering. In most cases, when a material is quenched, the final temperature is at ambient. This is due to the reason that most heat treaters do not have cooling equipments. The process continues this action from ambient temperature to -196°C (78K).

Cryogenic process is used for various applications in industry such as:

- Cryogenic air separation to produce highly purified gases/liquids
- Cryogenic operations to produce liquid natural gas (LNG)
- Production of argon from cryogenic air separation process
- Hydrogen cryogenic purification system
- Hybrid re-purifier for cryogenic air separation plants

In natural gas field, cryogenic process is used to extract natural gas liquid from natural gas. Absorption process is commonly used to extract almost all heavier natural gas liquids but the lighter hydrocarbons (i.e. ethane) are more difficult to recover from natural gas stream. This process usually consists of temperature drop of gas stream to around -120°F.

There are few methods of chilling gas to these temperatures. One of the most effective methods is known as turbo expander process. In this process, external refrigerants are used to cool down natural gas stream. An expansion turbo is then used to rapidly expand the chilled gas. This will cause a significant temperature drop. The rapid temperature drop condenses ethane, hydrocarbons and carbon dioxide in gas stream while maintaining methane in gaseous form. While the process occurring, this expansion turbine is able to convert some of the energy released when natural gas steam is expanded into recompressing gaseous methane effluent, thus saving energy cost [12].

This type of gas separation technology has few benefits as below:

- Achieve step change reduction in both capital and operating costs as compared to using other separation methods
- Simplicity and reliability of a static device with no rotating parts and operates without chemicals
- Occupy small space which is suitable for offshore
- Eliminating chemical-regeneration systems avoids environmentally and harmful emissions

2.7 Joule Thomson Effect

Joule-Thomson effect describes temperature change of fluid when it flows through an insulated valve. Enthalpy remains constant in this process. In practice, Joule Thomson effect is achieved by allowing gas to expand through a well insulated throttling device to prevent heat exchange to environment. The effect of pressure drop on temperature changes along the pipeline. This happens as there is no heat loss to environment and hence, it does not control these temperature variations. Ratio of $\Delta T/\Delta P$ is known as Joule Thomson coefficient. It is the change in temperature upon expansion without any heat transfer.

Joule Thomson effect happens by two mechanisms. For the first mechanism, as gas expands, average distance between molecules grows. This increases potential energy of gas due to intermolecular attractive forces. Increase in potential energy will decrease the kinetic energy and temperature. As there is no heat transfer occurs, total energy remains the same due to conservation of energy.

The second mechanism has the opposite effect from the first mechanism. When gas molecules collide, kinetic energy is converted into potential energy. The collision increases the average intermolecular distance and hence, a decrease in average potential energy. As total energy is conserved, there will be an increase in kinetic energy in terms of temperature. Below Joule Thomson inversion temperature, free expansion causes decrease in temperature. Above inversion temperature, gas molecules move faster and collide more often, hence, decrease in temperature.

2.8 Joule Thomson Nozzle System

The main part of a supersonic separation process is the supersonic (converging-diverging) nozzle. Supersonic nozzles do not contain any moving parts. The nozzle has three main sections; converging section, throat and diverging section.

Gas flow through nozzle is isentropic, which means that gas enthalpy is constant. The gas flowing through the nozzle inlet has subsonic flow. The gas is compressible with small pressure wave propagating through it. As the gas flows into the throat section, gas velocity becomes sonic where this condition is called as choked wave (Mach number = 1.0). Here, the cross sectional are of throat is small. As gas flows into section where nozzle cross sectional area increases, gas begins to expand to supersonic velocities. When this happens, sound wave will not propagate backwards through gas.

It is important to take note that nozzle will only choke at throat if pressure and mass flow rate through nozzle is sufficient to reach sonic speeds. The industry rule of thumb mentioned that ambient pressure must be no higher than 2-3 times the pressure in supersonic gas at nozzle outlet for the supersonic flow to leave nozzle.

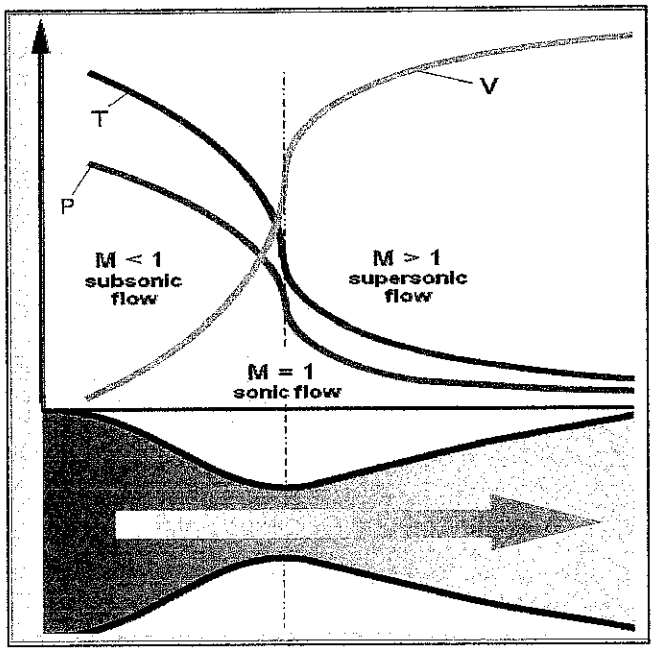


Figure 2.5 Graph of flow velocity, temperature and pressure as gas flows across the nozzle

Figure 2.5 shows diagram of the nozzle, in which it shows the effect of temperature and pressure as well as flow velocity within flow across the nozzle. Sudden expansion after the throat section causes temperature and pressure to drop drastically while the velocity of supersonic flow increases. Mach number at throat equals to 1 while the Mach number after the throat will be larger than 1, defining supersonic gas flow.

CHAPTER 3

METHODOLOGY/PROJECT WROK

3.1 Description of Methodology

The first step involves selecting the best EOS to use as the model to incorporate thermodynamics properties into FLUENT. Literature review is done to select a suitable model. Once the EOS is determined, a range of operating conditions for a simple case study is selected. HYSYS is used together with the EOS to obtain vapor fraction of methane and carbon dioxide. The thermodynamics table for these operating conditions and vapor fraction is formed. For this research project, only a single phase of binary mixtures is used for simplicity purposes. These properties are then developed into codes in C++ language. The code is validated with HYSYS to ensure the accuracy of data. Once the program based on C++ has been finalized and validated, the codes are then modified into FLUENT structure so that it can be incorporated into FLUENT. When this user defined function is successfully implemented into FLUENT, simulation can be commenced. Simulation of a simple pipe with cooling effect is tested to ensure that FLEUNT is able to read the user defined function to investigate the phase change behavior. The data obtained from FLUENT is again validated with HYSYS to ensure accuracy of readings. Once the data is validated, design of different finned pipes is drawn using GAMBIT and later on used in FLUENT to investigate the relationship of different design with cooling effect. Comparisons between energy used to remove carbon dioxide between the best finned pipe and Joule Thomson valve is also done.

3.2 Summary of Methodology Used

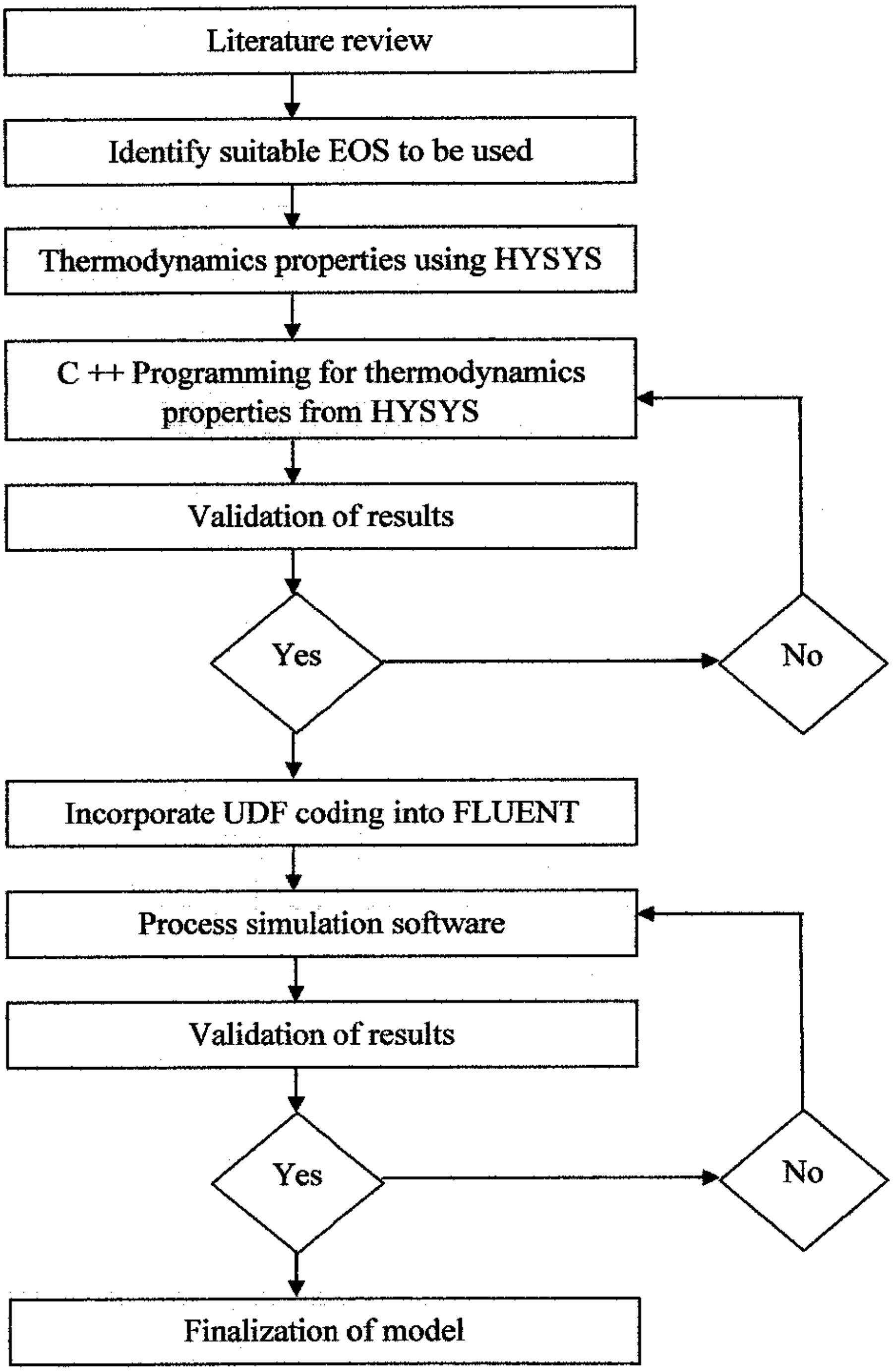


Figure 3.1 Flow Chart

No.	Task/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Selection of project topic	■	■												
2	Understanding problem			■											
3	Research and literature review				■	■									
4	Learn FLUENT and GAMBIT						■	■							
5	Submission of progress report							■							
6	Development of phase envelope								■	■					
7	Identifying suitable EOS model										■	■			
8	Development of case study using HYSYS											■	■	■	
9	Development of thermodynamics table											■	■	■	
10	Programming of model using C language													■	■
10	Validation of code with HYSYS													■	■
11	Interim report submission														■
12	Oral presentation														■

Figure 3.2 Gantt Chart for FYP I

No.	Task/Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Modification of code into FLEUNT structure	■	■												
2	Incorporate UDF into FLUENT			■											
3	Submission of progress report 1				■										
4	Development of simple pipe				■										
5	Run simulation					■									
6	Validation of results with HYSYS						■								
7	Development of finned pipes design using GAMBIT							■	■						
8	Run simulation									■	■				
9	Interpretation of results										■	■			
10	Pre-EDX and poster exhibition												■		
11	Submission of progress report 2												■		
12	Final report softcopy													■	
11	Final oral presentation														■
12	Submission of hardbound report														■

Figure 3.3 Gantt Chart for FYP II

3.3 Software Required

1. HYSYS
2. GAMBIT
3. FLUENT
4. Bloodshed Dev C++
5. Microsoft Visual Studio 6.0
6. Microsoft Office

CHAPTER 4
RESULTS AND DISCUSSION

4.1 Development of Phase Envelope

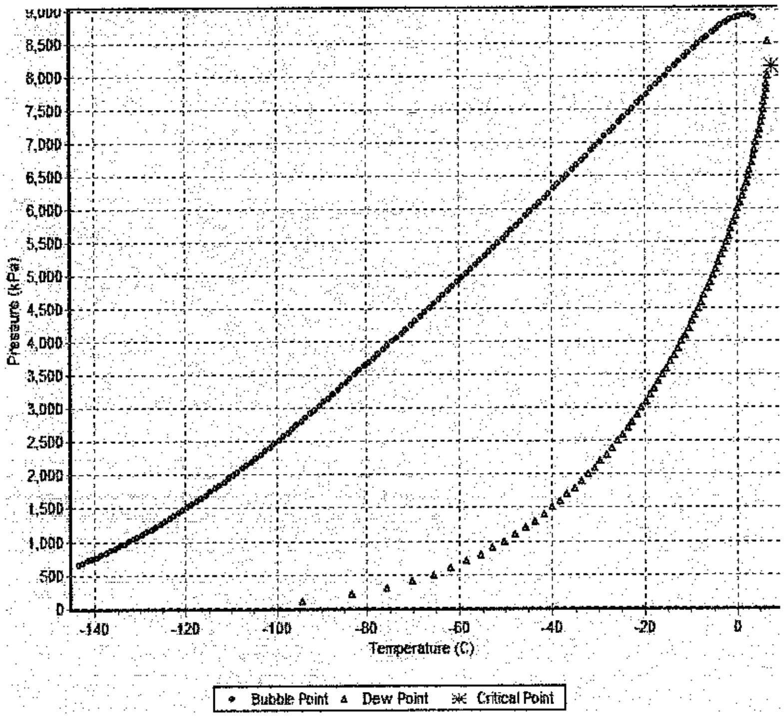


Figure 4.1 Phase envelope for binary mixtures

Phase envelope is developed to investigate phase envelope of binary mixtures of methane and carbon dioxide, with fraction of 0.3 CH_4 and 0.7 CO_2. Figure 4.1 shows the phase envelope developed using VLEFlash. This phase envelope allows us to determine the mixture phase whether it's in liquid, vapor or mixture phase for different operating conditions.

The region near the dew point line (right hand side) is the vapor phase region. Dew point curve is the point where liquid will begin to condense. The region between the dew point and bubble point curve is the two phase region, in which it is a mixture of liquid and vapor phase. Moving towards the left hand side is the bubble point curve where the first drop of bubble is formed. The critical point as shown in Figure 4.1 is approximately at 10°C and 8100 kPa. Critical point is the point where liquid and vapor phase co-exist together.

VLEFlash uses Raoult's Law, Modified Raoult's Law with Wilson Interaction parameters, Soave Redlich Kwong (SRK) and Peng Robinson (PR) EOS. The equations to calculate P_{bubble} and P_{dew} are as below:

$$P_{BUBL} = \sum \frac{x_i \gamma_i p_i^{sat}}{\Theta_i} \qquad (1)$$

$$P_{DEW} = \frac{1}{\sum y_i \Theta_i / \gamma_i P_i^{sat}} \qquad (2)$$

where x_i = Liquid fraction for species *i*

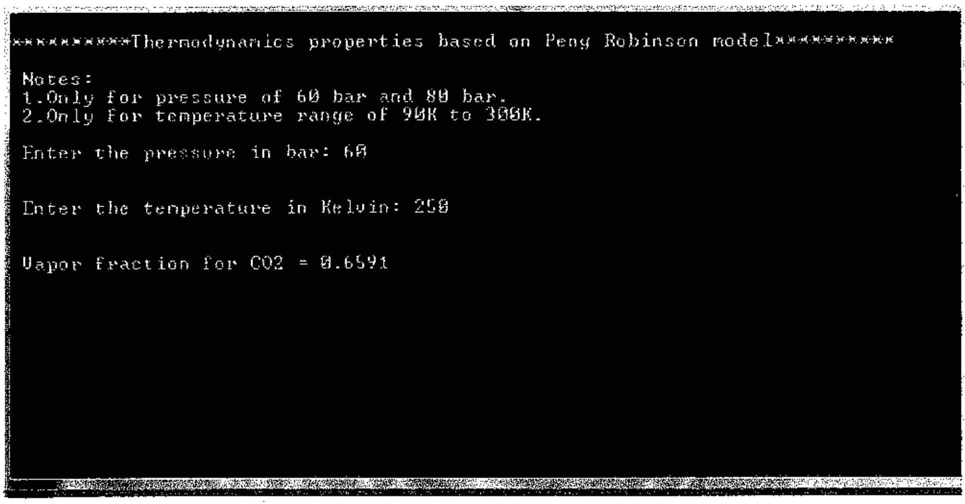
y_i = Vapor fraction for species *i*

γ = Liquid phase activity coefficient for species *i*

Θ = Vapor phase fugacity coefficient of species *i*

4.2 Validation of C++ Programming with HYSYS

C++ Programming coding based on Peng Robinson model is written for two different pressures, 60 bar and 80 bar for a temperature range of 90K to 300K. This coding is then validated with HYSYS to ensure that the vapor fraction of CO_2 at each operating conditions is almost similar with data in HYSYS. Table 4.1 shows the percentage error between the C++ programming coding with HYSYS. Once these values are validated, the coding is changed into FLUENT structure to incorporate it with FLUENT. Sample of coding is attached in Appendix C.



```
**********Thermodynamics properties based on Peng Robinson model**********

Notes:
1.Only for pressure of 60 bar and 80 bar.
2.Only for temperature range of 90K to 300K.

Enter the pressure in bar: 60


Enter the temperature in Kelvin: 250


Vapor fraction for CO2 = 0.6591
```

Figure 4.2 Sample of coding based on Peng Robinson model

Table 4.1 shows the validation values between C++ programming with HYSYS. Ten randomly selected data is used for such comparison. It shows that the percentage error is small enough and hence, validation is successfully done. With this, the code in C++ programming can be modified into FLUENT structure to be incorporated with FLUENT for simulation purposes.

Table 4.1 Comparison of data for pressure of 60 bar

Temperature	C++ Programming	HYSYS	% error
246.11	0.62235	0.62233	2.732E-05
247.30	0.63365	0.63362	4.577E-05
247.59	0.63641	0.63637	5.657E-05
248.70	0.64688	0.64686	2.473E-05
249.66	0.65590	0.65591	1.220E-05
249.87	0.65788	0.65789	1.368E-05
250.00	0.65910	0.65911	1.365E-05
255.25	0.68057	0.70000	2.775E-02
290.50	0.70000	0.70000	0.000E+00
330.15	0.70000	0.70000	0.000E+00

4.3 Results of Simulation for Different Pressure

Two different pressures are used for validation purposes. A simple pipe with wall cooling is used for two pressures of 60 bar and 80 bar. Here, UDF coding is incorporated into FLUENT. Validation with HYSYS is done again to ensure that the Peng Robinson model has been successfully incorporated into FLUENT to investigate the phase change behavior.

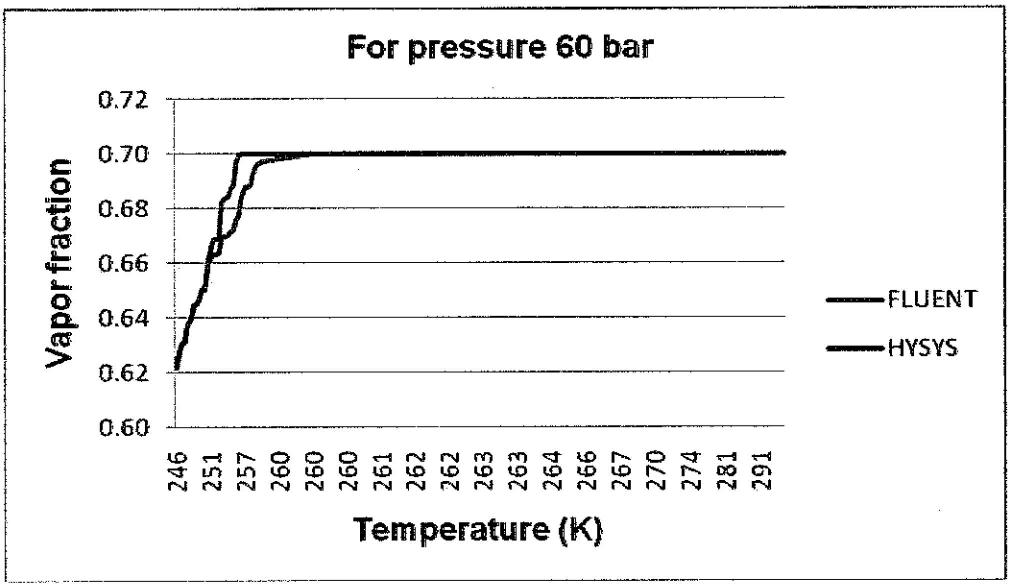


Figure 4.3 Comparison of vapor fraction at 60 bar for FLUENT and HYSYS

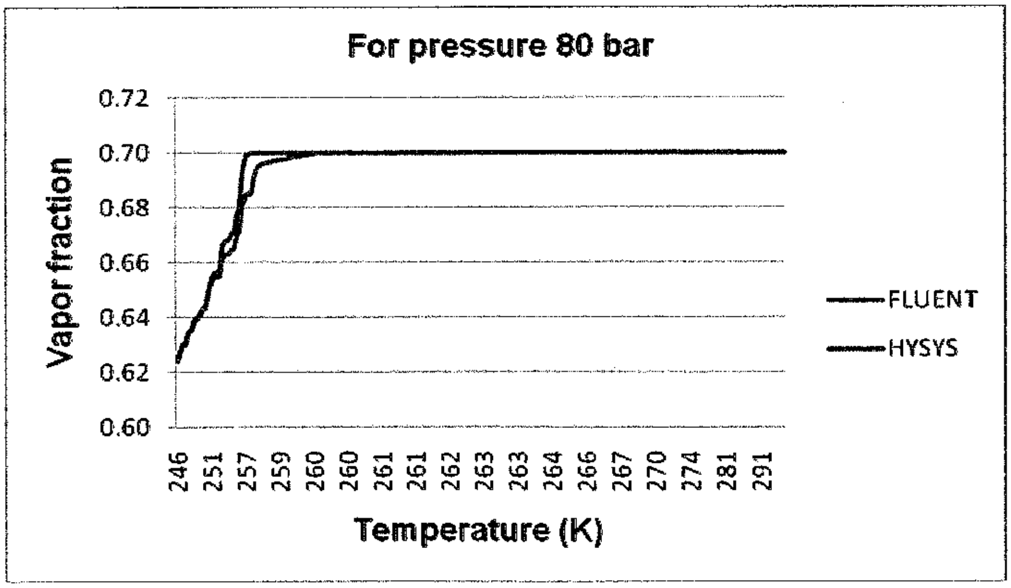


Figure 4.4 Comparison of vapor fraction at 80 bar for FLUENT and HYSYS

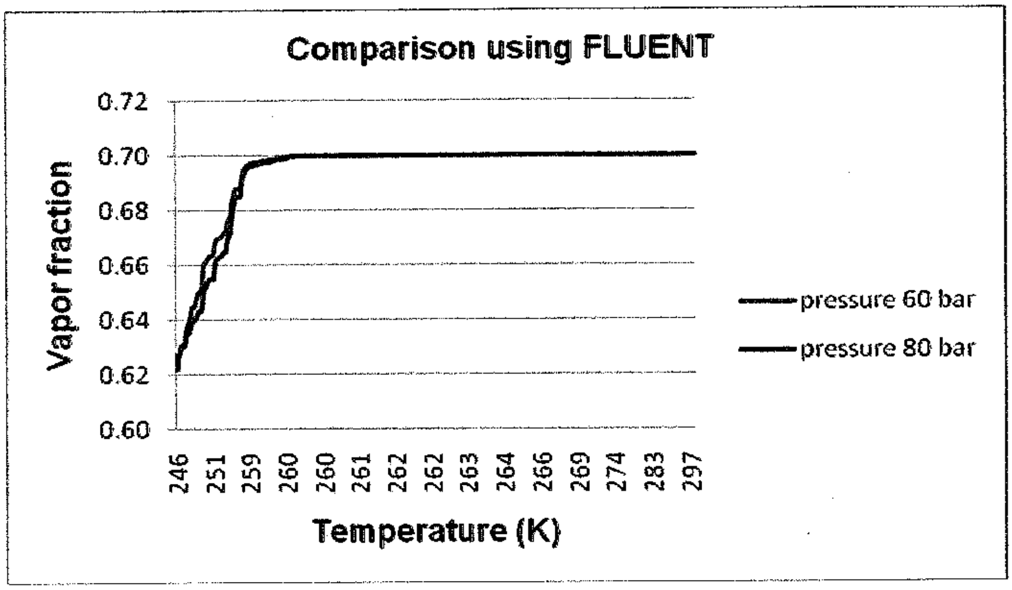


Figure 4.5 Comparison for pressure 60 bar and 80 bar from FLUENT

Figure 4.3 and Figure 4.4 shows carbon dioxide vapor fraction obtained using FLUENT and HYSYS for pressure of 60 bar and 80 bar. Validation with HYSYS shows that vapor fraction obtained from FLUENT simulation when thermodynamics properties are embedded in, are successfully done. It is predicted that vapor fraction estimated using FLUENT performs well against HYSYS because for natural gas containing only CH_4 and CO_2, system is gaseous in many operating conditions in pipeline.

Figure 4.5 shows the comparison of carbon dioxide vapor fraction for both pressure of 60 bar and 80 bar from FLUENT simulation. Here, it can be seen that higher pressure is able to liquefied carbon dioxide at a same temperature compared to lower pressure. This is because at a higher pressure, the intermolecular forces between molecules are stronger. Hence, when forces are applied to the molecules, the molecules are able to attract one another and reduce the distance between molecules to form liquid. Due to this, the pressure of 80 bar is chosen to be used for further simulation purposes.

It is clearly shown here that the higher the pressure, the more desirable is the outcome, which is the separation of liquefied carbon dioxide. Lower pressure to meet separation can be achieved by lowering temperature but it must be mindful that at low temperature, the whole system might be condensed into liquid or go into solid states.

4.4 FLUENT Simulation for Different Pipe Designs

4.4.1 Simple Pipe with Wall Cooling

There are many varieties of design for cryogenic process and through this pipe simulation, one can choose the best design and operating conditions to suit the separation process.

Table 4.2 shows simulation of a simple pipe with species mass fraction input of methane and carbon dioxide. These mass fractions for each component will be used as the input for other subsequent simulations.

Table 4.2 Information for simulation purposes

Temperature (K)	300
Pressure (bar)	80
Species	Input Mass Fraction
Methane (CH_4)	0.3
Carbon dioxide (CO_2)	0.7

Figure 4.6 and figure 4.7 shows the temperature change and carbon dioxide concentration for wall temperature of 150K.

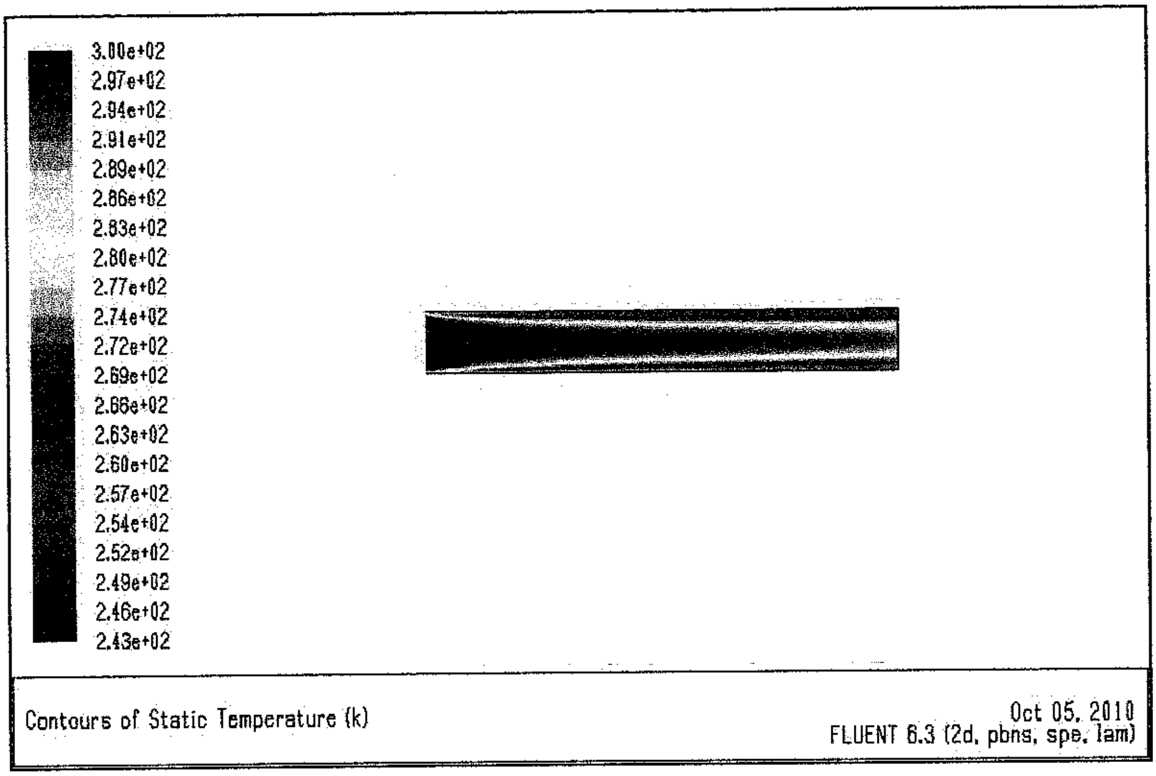


Figure 4.6 Temperature change for simple pipe (A0)

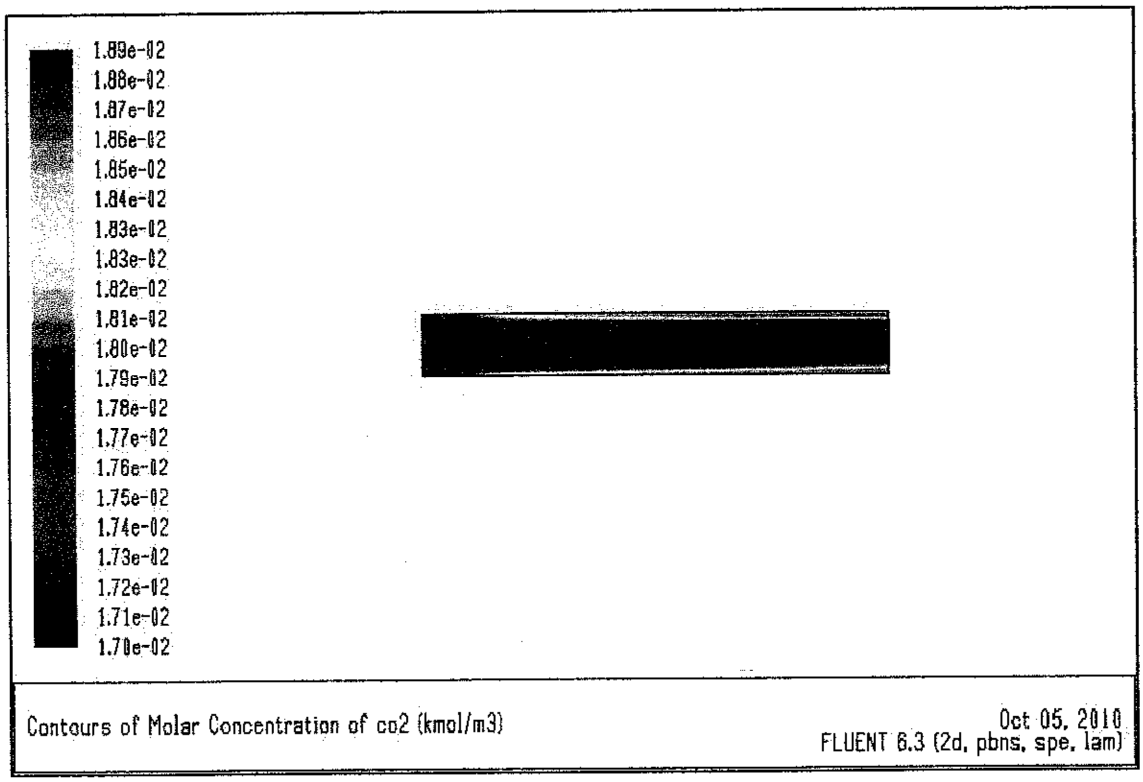


Figure 4.7 Molar concentration of CO_2 for simple pipe (A0)

4.4.2 Finned Pipe with Wall Cooling

Simulation for this section runs similar simulation as section 4.4.1 but with finned pipe. Simulation shows how cooling affects the temperature change and stream component concentration for different design. Each simulation is set to 10,000 iterations or achieves convergence; whichever comes first. Stream inlet flow velocity has to be set to low velocity to allow sufficient time for energy transfer. Hence, a flow velocity of 0.01 m/s is used for these simulations. Each pipe is 32m by 1m with buffer length of 10 m before the first fin.

Table 4.3 Designs for finned pipes

Design	Fin spacing (m)	Fin width (m)	Fin length (m)
A1	2	0.20	0.50
A2	4	0.20	0.50
B1	2	0.40	0.50
B2	2	0.60	0.50
C1	2	0.20	0.25
C2	2	0.20	0.75

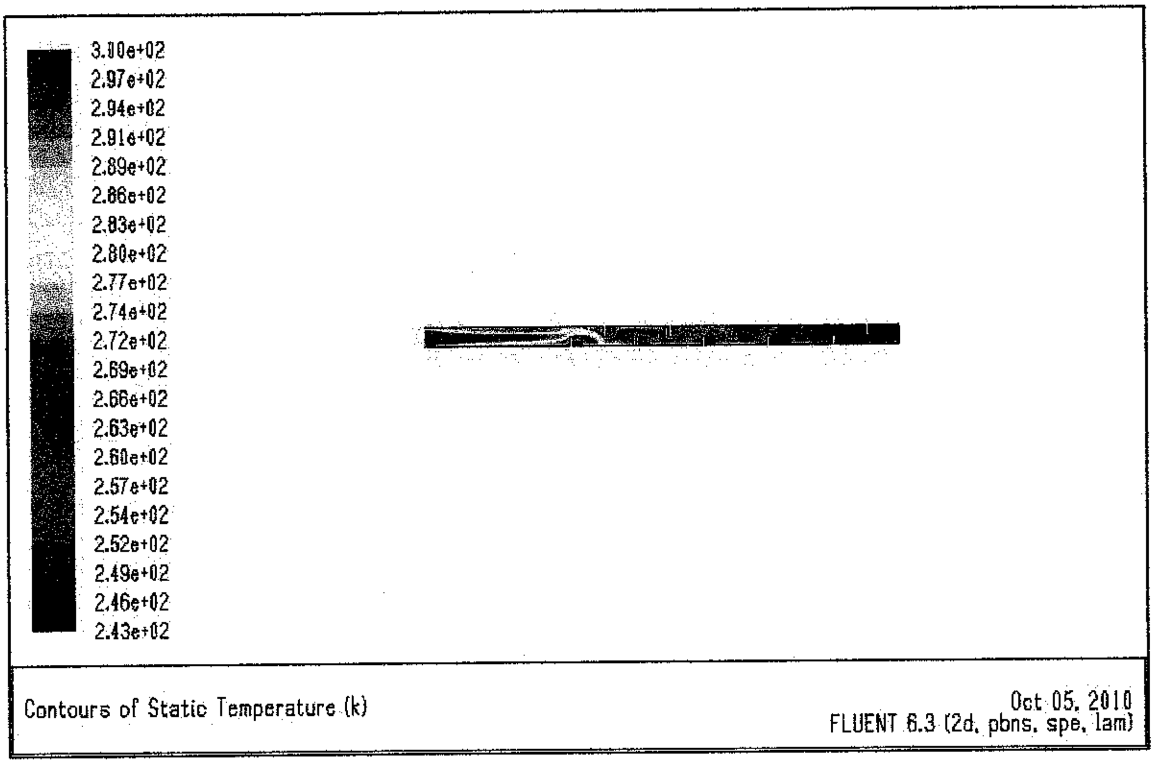


Figure 4.8 Temperature change for A1

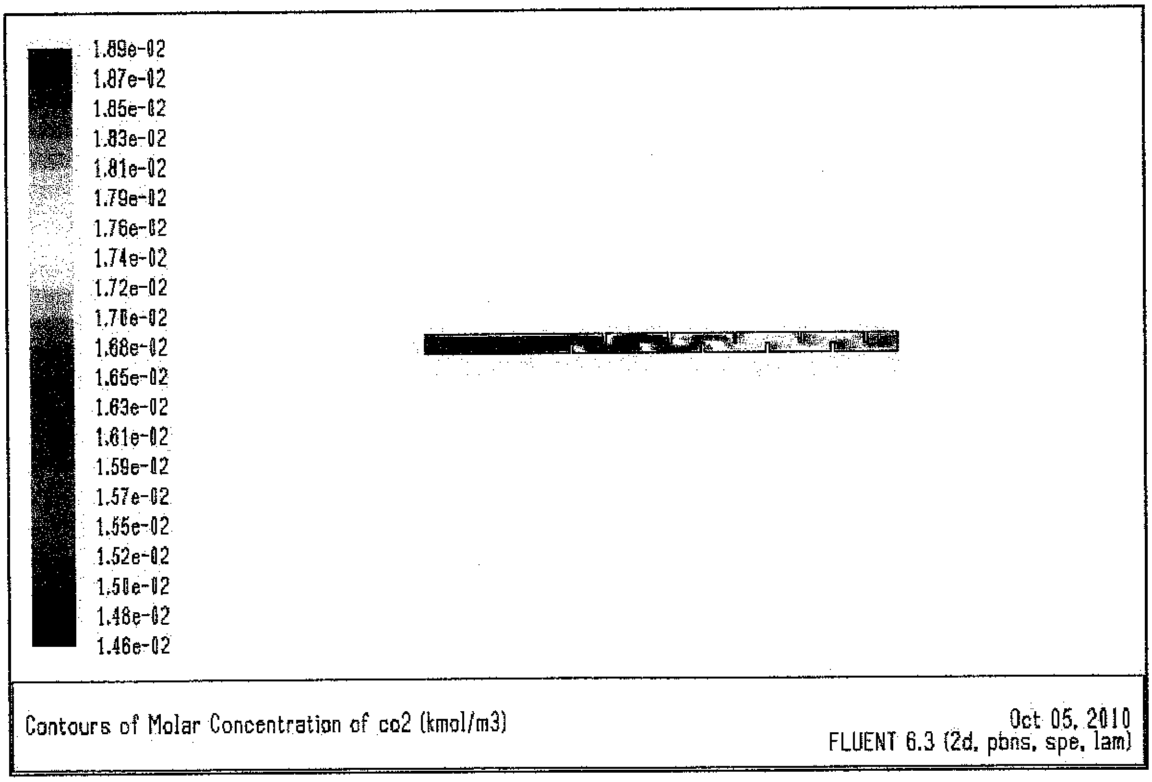


Figure 4.9 Molar concentration of CO_2 for A1

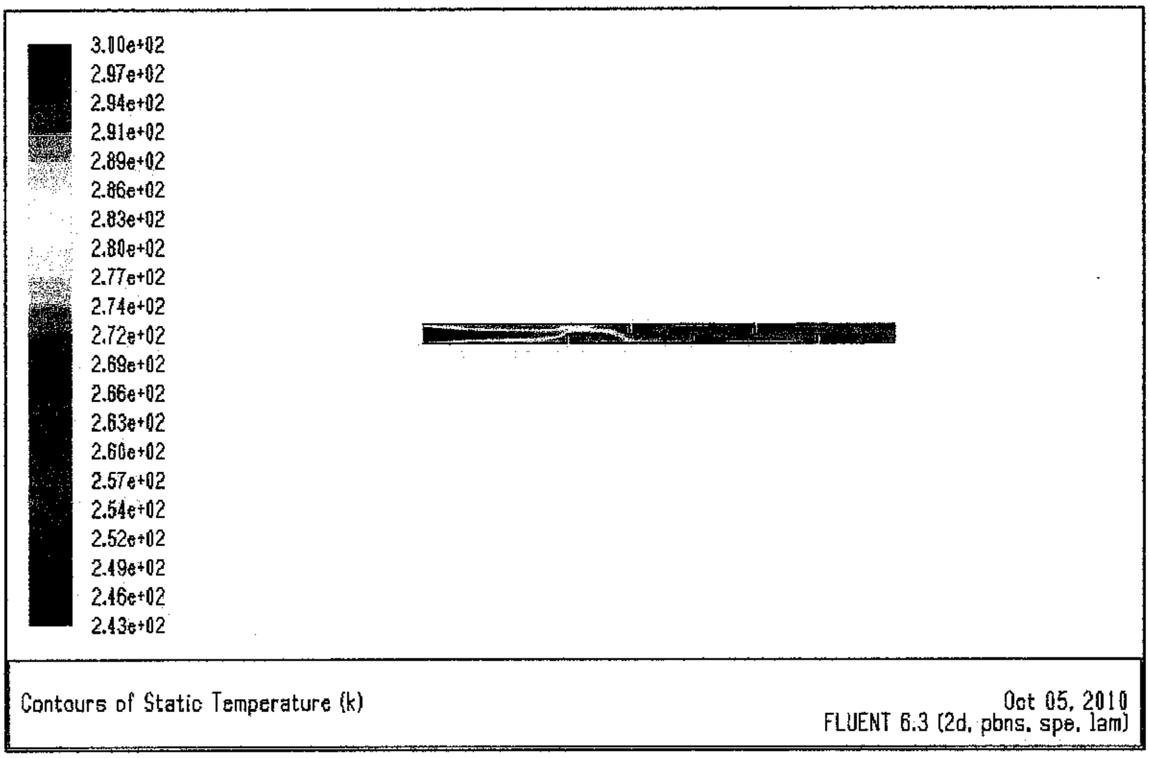


Figure 4.10 Temperature change for A2

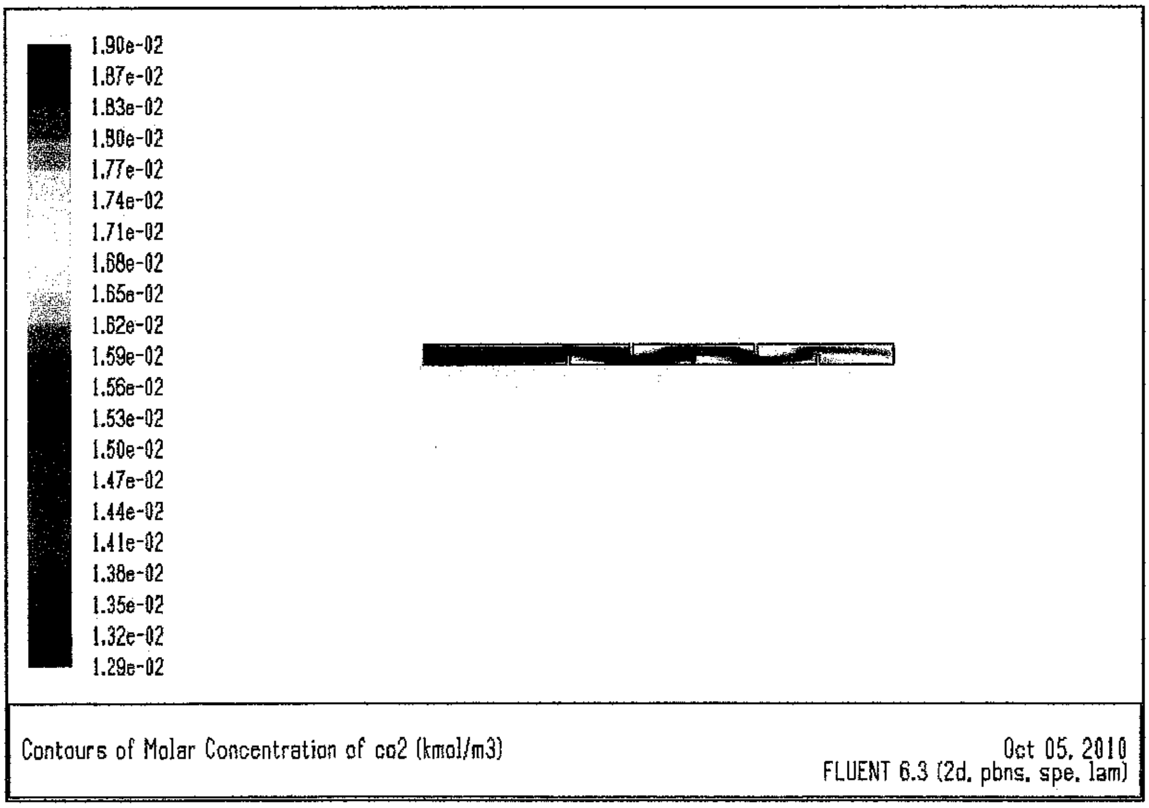


Figure 4.11 Molar concentration of CO_2 for A2

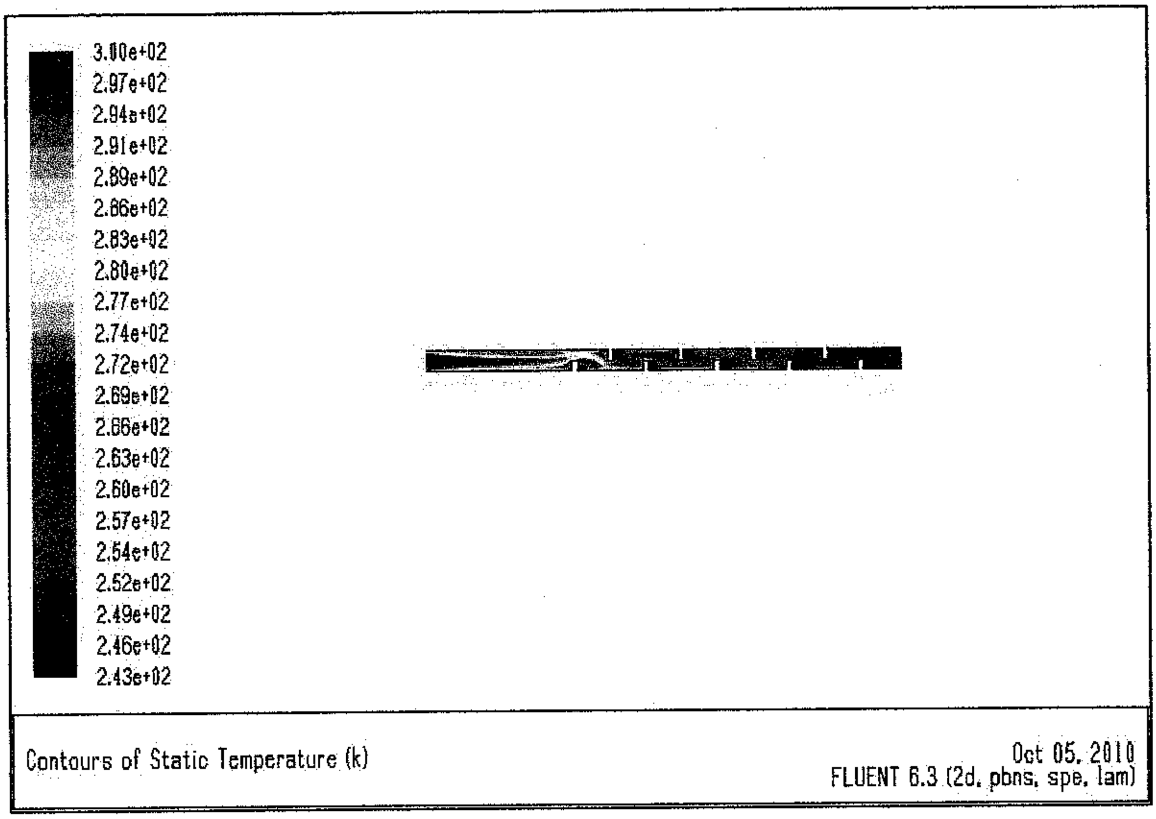


Figure 4.12 Temperature change for B1

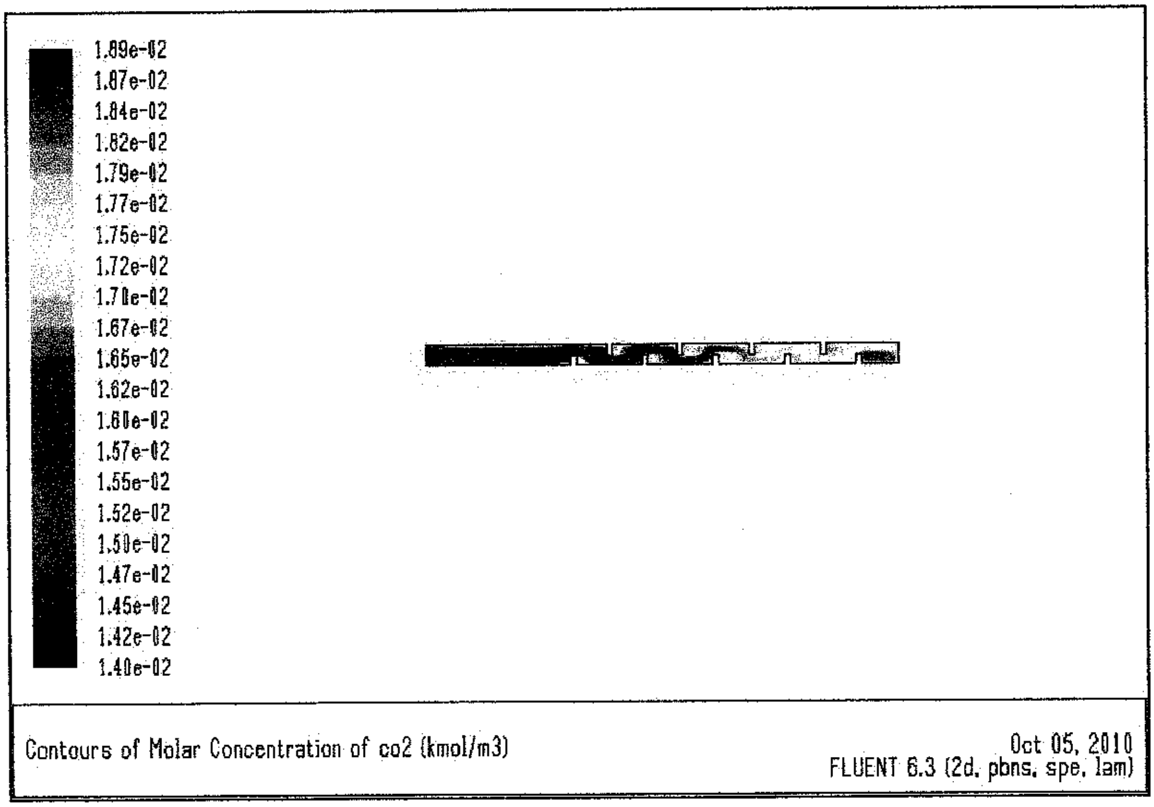


Figure 4.13 Molar concentration of CO_2 for B1

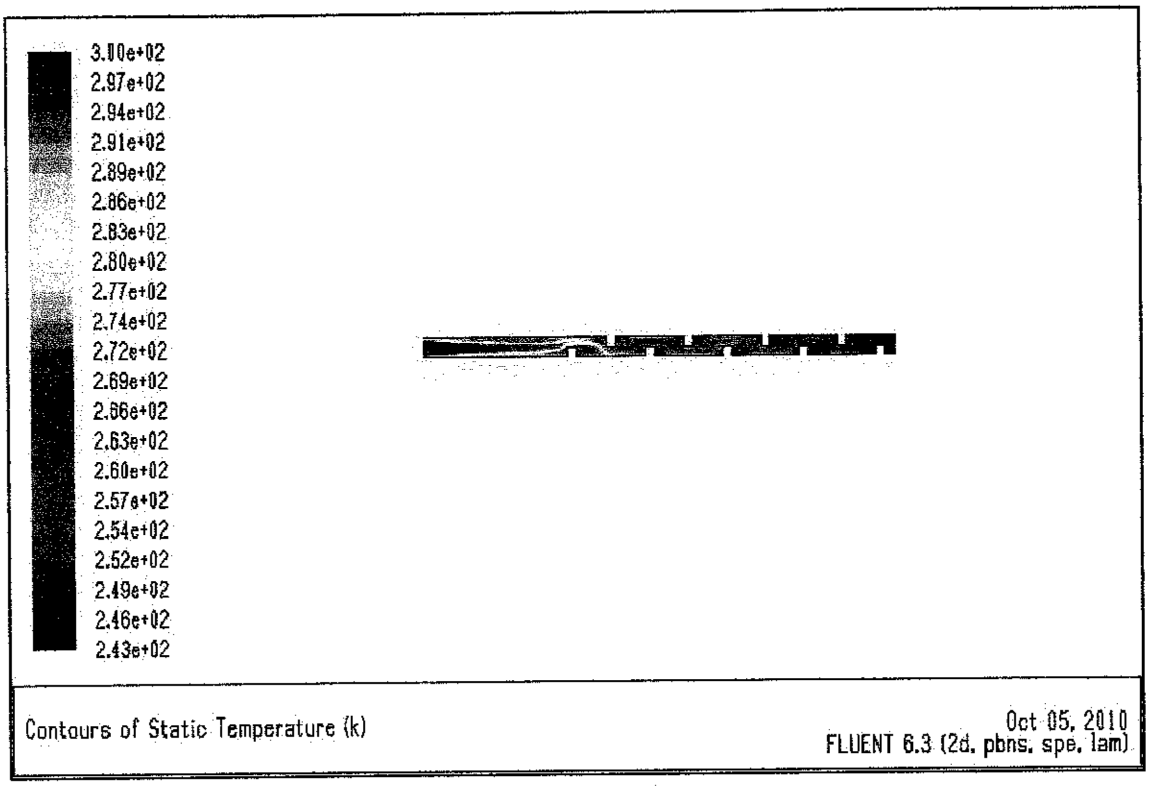


Figure 4.14 Temperature change for B2

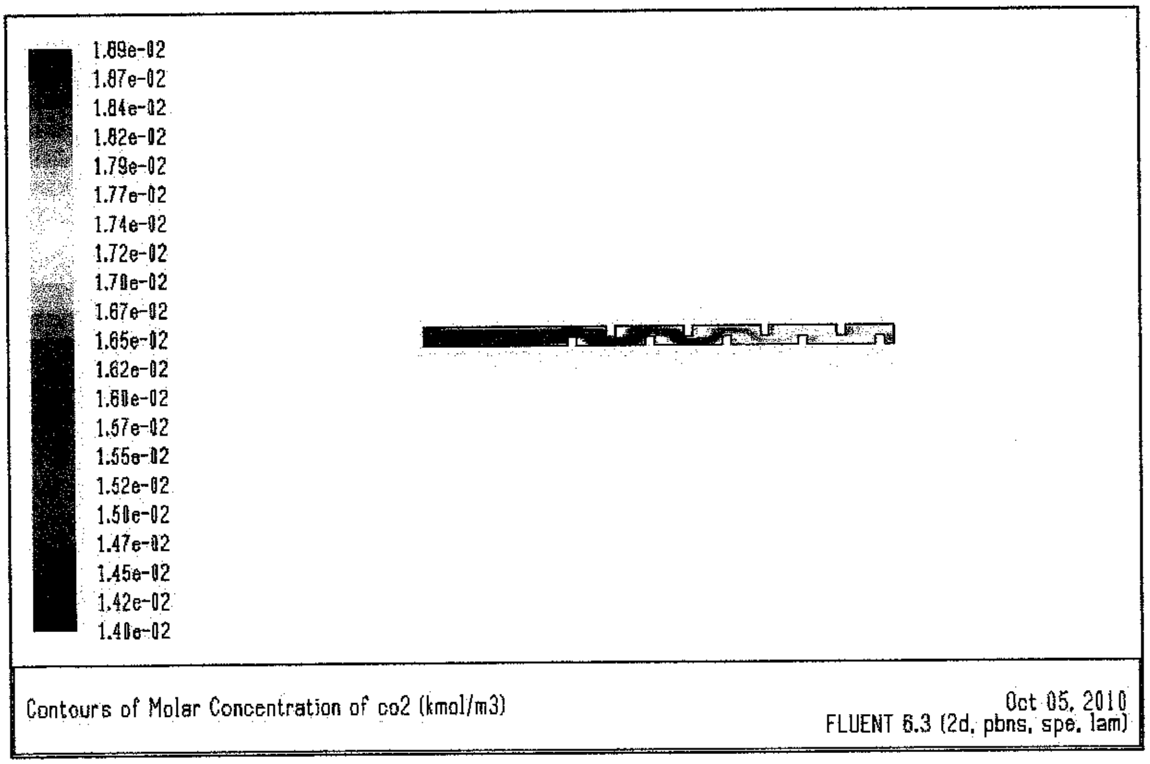


Figure 4.15 Molar concentration of CO_2 for B2

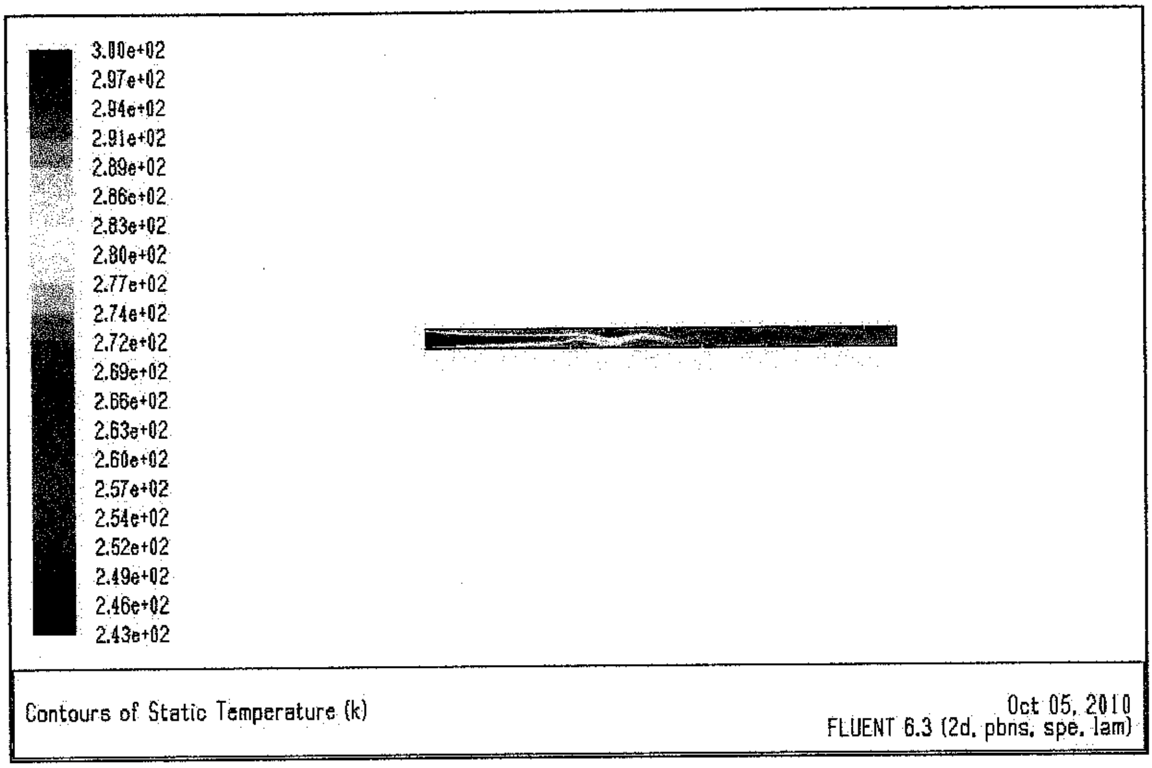


Figure 4.16 Temperature change for C1

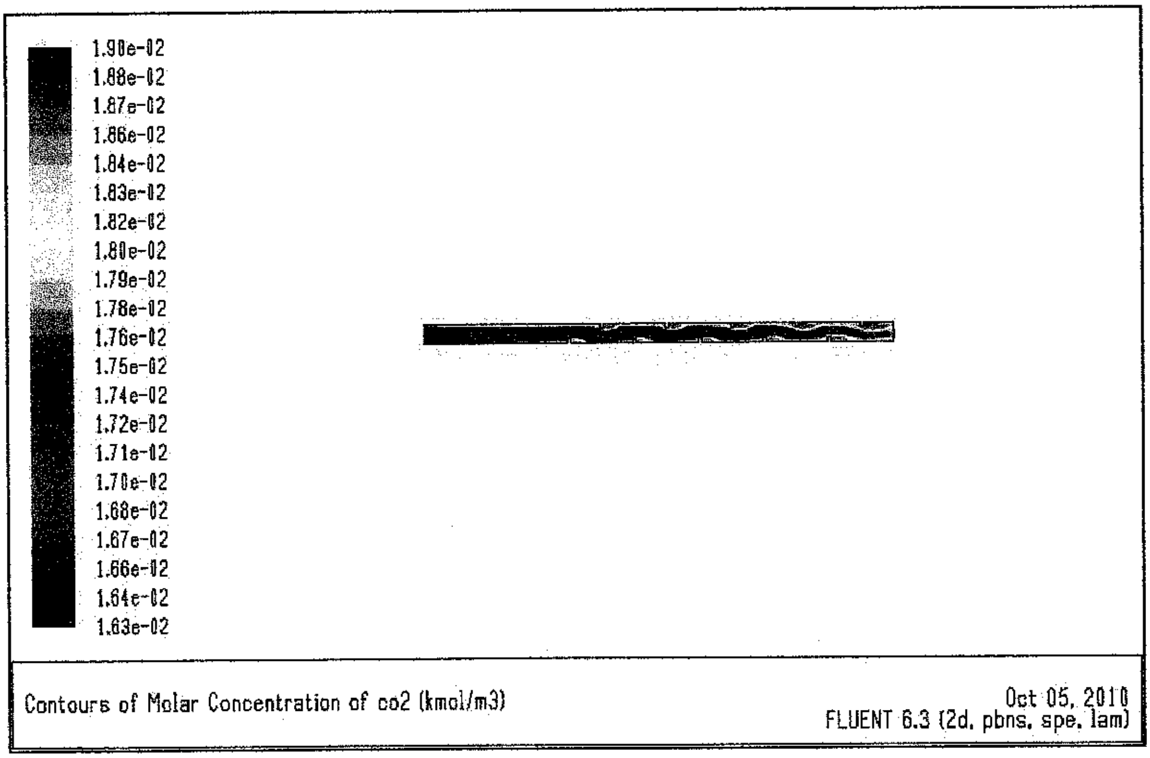


Figure 4.17 Molar concentration of CO_2 for C1

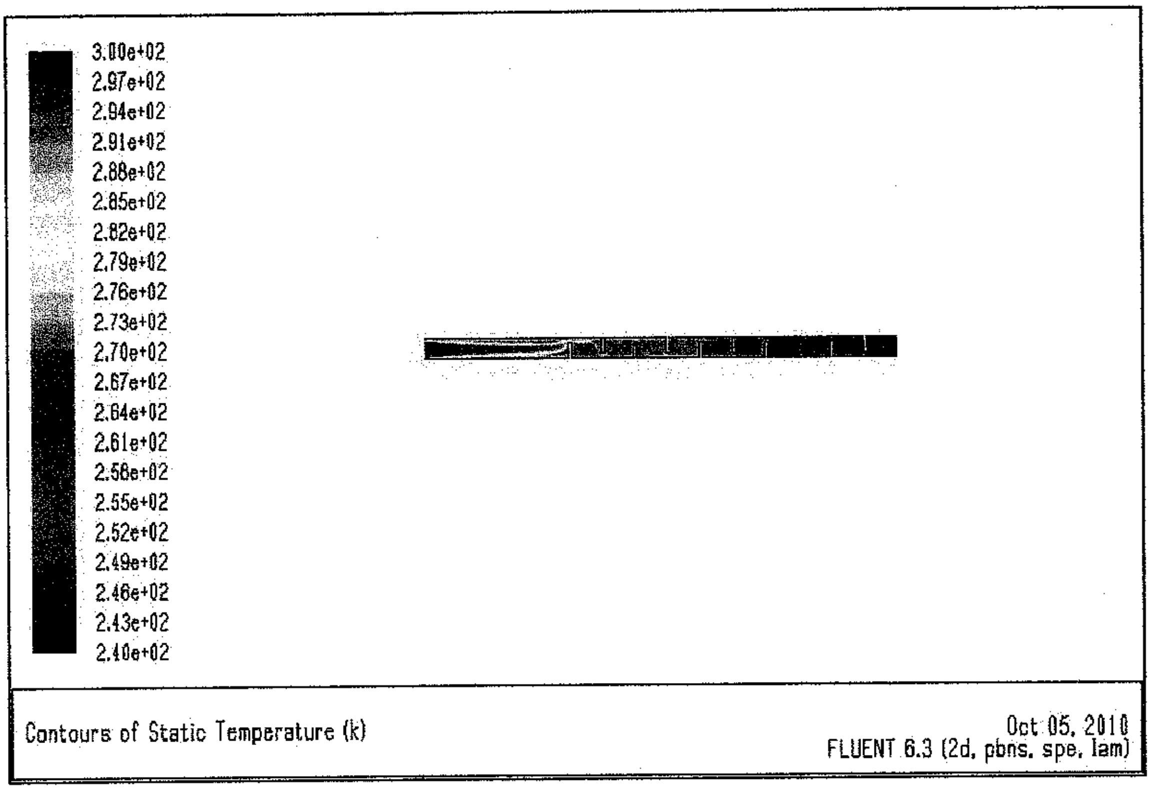


Figure 4.18 Temperature change for C2

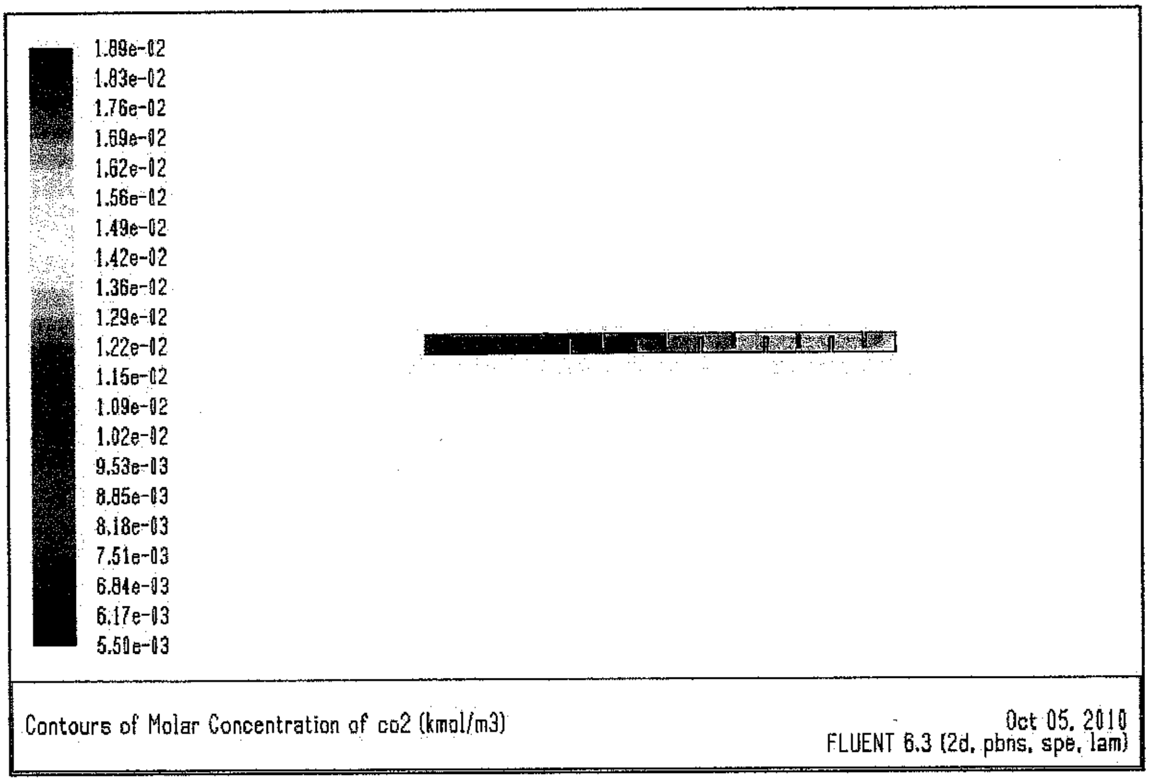


Figure 4.19 Molar concentration of CO_2 for C2

4.4.3 Summary of Simulation

From the simulations above, it can be seen that there are few factors that affect the cooling effect as the design of finned pipe changes:

1. Number of fins: As number of fins increases, cooling effect increases.
2. Width of fin: The lager the width, the higher the cooling effect.
3. Length of fin: The longer the fin, the higher the cooling effect.

Table 4.4 shows the arrangement of design that provide the least to the highest cooling effect starting from A0, followed by C1, A2, B1, A1, B2, and C2. Pipe with higher cooling effect should be able to remove more carbon dioxide.

Table 4.4 Pipe Design Analysis

Design	Fin spacing (m)	Fin width (m)	Fin length (m)	Remarks
A0	n/a	n/a	n/a	Pipe with no fin. Hence, it has least cooling effect.
C1	2	0.20	0.25	Small fin spacing with 10 fins. However, due to short fin length, stream passes through the middle with least resistance or contact with fin.
A2	4	0.20	0.50	Moderate fin spacing with 5 fins for cooling effect. It gives moderate cooling effect.
B1	2	0.40	0.50	Small fin spacing gives 9 fins for cooling. Larger fin width results in slightly more cooling effect than A2.
A1	2	0.20	0.50	Small fin spacing results in 10 fins for cooling. One additional number of fin has more cooling effect than increased in width size.

B2	2	0.60	0.50	Almost comparable with A1. Cooling effect slightly better due to increase in width size.
C2	2	0.20	0.75	Have 10 fins and longer fins. Stream encounters most resistance when flows through all the 10 fins for cooling effect.

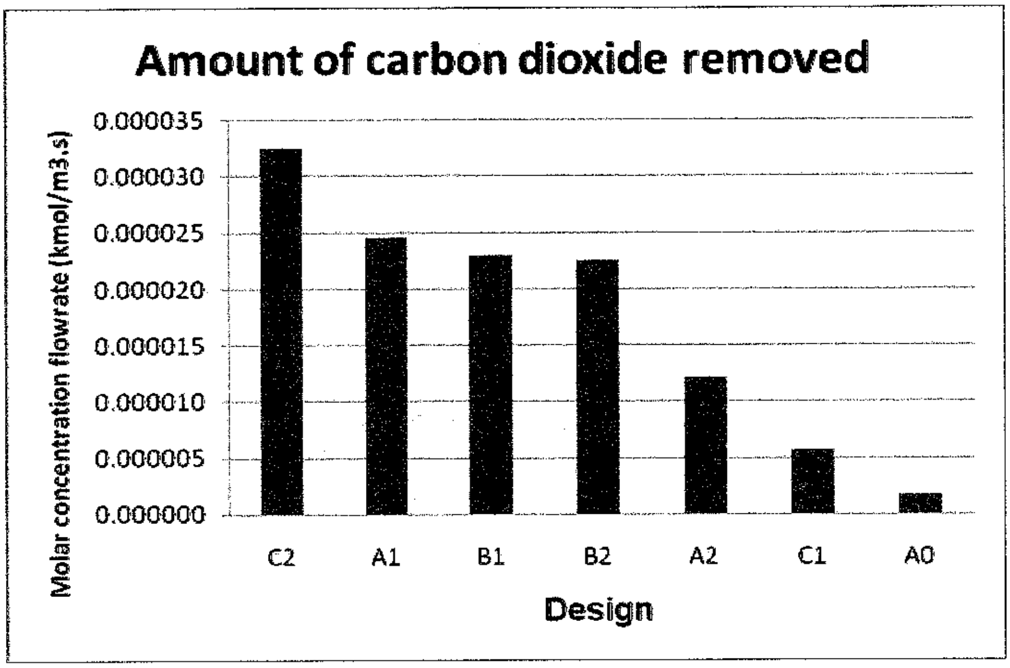


Figure 4.20 Amount of carbon dioxide removed for different pipe design

Amount of carbon dioxide removed increases with increasing cooling effect as per shown in Figure 4.20. The trend is almost similar as shown in Table 4.4 but not entirely the same. The cooling effect for different pipe design in Table 4.4 is compared based on qualitative method. However, Figure 4.20 is based on quantitative method. Simple pipe of A0 gives the lowest cooling effect as it removed the least amount of carbon dioxide compared to other finned pipe designs. Finned pipe of B1 and B2 are rather comparable with each other base on both qualitative and quantitative point of view. Finned pipe of C2 removed the most carbon dioxide and hence, has the best cooling effect. From quantitative analysis, the arrangement of design that offers the most cooling effect to the least is C2, A1, B1, B2, A2, C1, and A0. This quantitative view is the same as qualitative view as it shows in Table 4.4 that C2 gives the highest cooling effect. Based on both qualitative and quantitative methods, it is clear that finned pipe is able to liquefied more carbon dioxide in cryogenic process and hence, better removal compared to simple pipe.

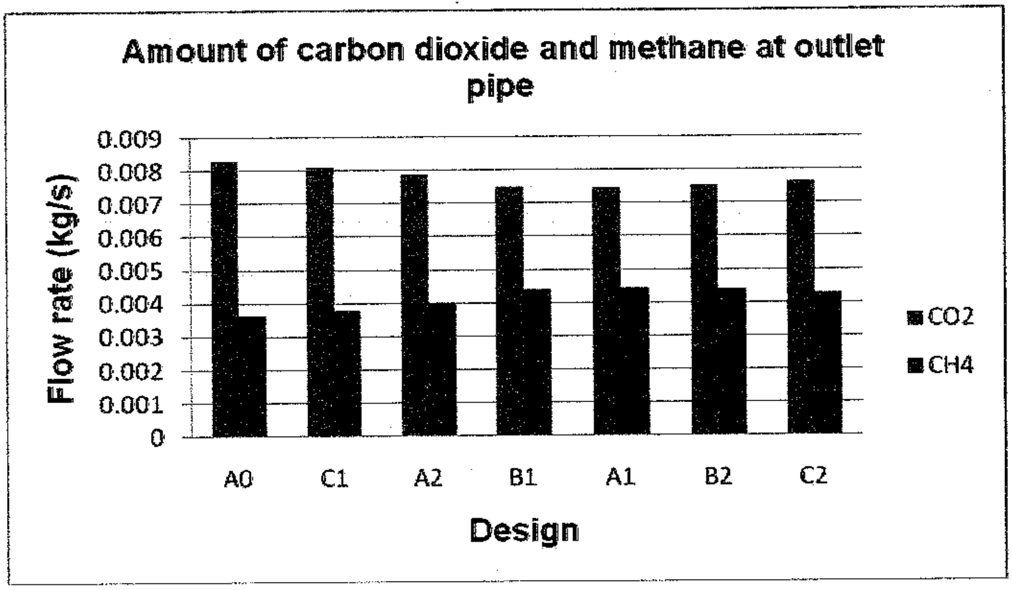


Figure 4.21 Amount of CO_2 and CH_4 at outlet pipe

Even though it is preferred to choose a design with the most cooling effect, the components mass fraction at the pipe outlet has to be checked to ensure that methane recovered is sufficient enough to meet specific requirement. In order to meet pipeline specification, mass fraction of carbon dioxide shall not exceed certain value. There has to be an optimum design in which it can remove large amount of carbon dioxide while meeting the specification.

Figure 4.21 shows the flow rate of both methane and carbon dioxide at the pipe outlet. Higher cooling effect is capable of liquefying more carbon dioxide compared to designs with low cooling effect. However, this phenomenon is not desirable if the objective is to meet maximum allowable carbon dioxide content with maximum recovery of methane at gas outlet stream. Higher cooling effect removes carbon dioxide as well as the valuable methane which should be recovered as much as possible at the gas outlet stream. This shows that providing more cooling effect may not be a wise decision for separation process. Hence, optimum design shall be chosen instead. As such, designs of A1 and B1 may be better for liquefaction of carbon dioxide with minimum methane loss.

4.5 FLUENT Simulation for JT valve

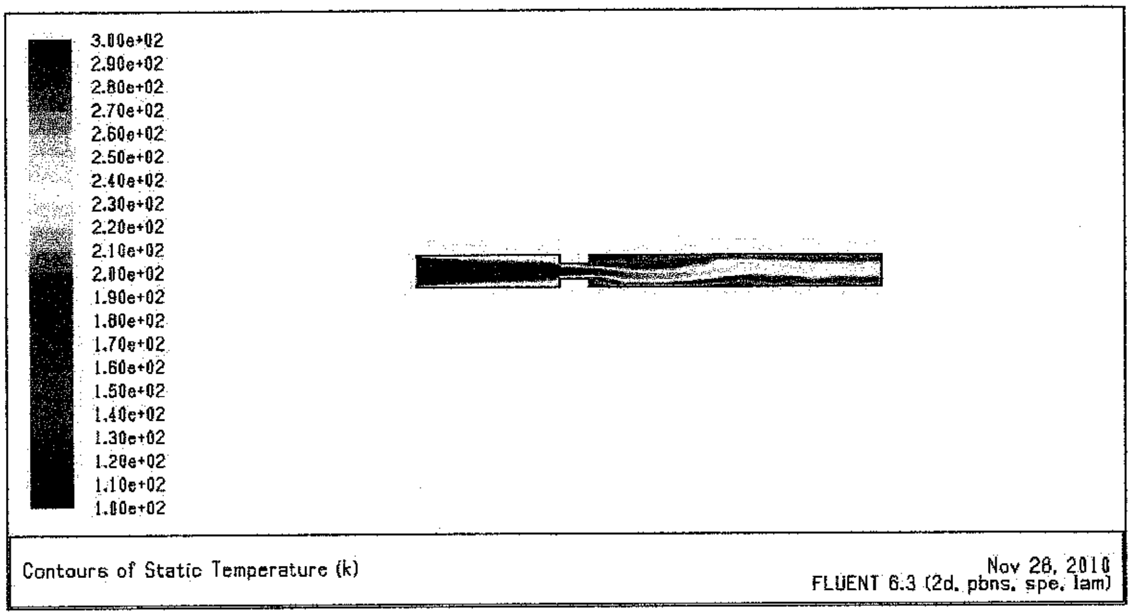


Figure 4.22 Temperature change for JT valve

Simulation using JT valve is done to see how the cooling effect occurs in the valve. The valve is of dimension 32 m length with 2 m width. The throat area is 2 m length and 1 m width. JT valve is a supersonic flow valve with Joule Thomson effect. JT effect happens in a way that there will be a drastic temperature change when it flows through an insulated valve as shown in Figure 4.22. The simulation for JT valve is done with the same information and method as section 4.4.

As the fluid flows from diverging section to throat area, the flow changed from subsonic flow to sonic flow. The sudden expansion from throat area to converging section causes temperature to drop drastically while the velocity of fluid increases. Here, supersonic flow is able to be achieved. Finned pipe is able to remove more carbon dioxide than JT valve. This is because fluid encounters more resistance when flows through fins for cooling effect while JT valve is mainly based on pressure and temperature drop when fluid flows through the throat area.

4.6 Comparison of work produced by JT valve and finned pipes

Finned pipe of A1 is used to make a comparison with a JT valve with dimension of 32 m length with 2 m width. Table 4.5 shows the work produced by finned pipe A1 and JT valve.

Table 4.5 Comparison between finned pipe A1 and JT valve

Design	CO_2 inlet (kg/s)	CO_2 outlet (kg/s)	Work produced (kW)
Finned pipe A1	0.008326	0.007451	14 400
JT valve	0.008326	0.007451	15 314

The comparison of finned pipe A1 and JT valve is done in a way that the inlet and outlet amount of carbon dioxide for both designs are the same. Based on Table 4.5, it can be seen that JT valve is able to produce more power compared to finned pipe A1, which means that JT valve uses very little work to remove carbon dioxide compared to finned pipe A1. The efficiency for JT valve is higher as fluid flows through the valve and hence, heat can be transferred to fluid evenly.

Cryogenic effect is able to be applied to the entire fluid that is flowing through it. On the other hand, efficiency for finned pipe is lower. Cryogenic process in finned pipe happens in a way that the refrigerant has to be cooled first followed by cooling at the wall area before cooling of the fluid (i.e. liquefaction of carbon dioxide). Due to these many process, heat transferred is less and hence, a lower efficiency. This explains why a JT valve has a better efficiency than finned pipe and is able to remove carbon dioxide with less work.

CHAPTER 5

CONCLUSION AND RECOMMENDATIONS

5.1 Recommendations

Some suggestions can be done to further improve the scope of the project and accuracy of results:

1. Model using FLUENT can be tested for many other pipe designs. More pipe designs can be created for simulation and vary the variables such as temperature, pressure and fluid velocities to study the cooling effect.
2. Create more components for simulation purposes instead of using binary components of methane and carbon dioxide. This can improve the accuracy of results as natural gas is actually composed of many other components.
3. Create two phase (vapor and liquid phase) simulation to see how much vapor is condensed into liquid and how much liquid is vaporized. With this, absolute amount of loss for each component can be obtained.
4. For validation of results, the project should be done experimentally to compare with simulation results rather than just verifying with HYSYS.
5. Cost of refrigerants used in finned pipe should be taken into consideration as industry emphasizes on the efficiency of the pipe as well as the total cost needed for such design.

5.2 Conclusion

Understanding thermodynamics properties is important in developing new type of gas separation technology. As most fluid dynamics software or approach does not consider thermodynamics properties, it is important to incorporate this into the simulation. In this research, vapor phase of methane and carbon dioxide is studied. Peng Robinson model is used for this case study as it has a slightly better behavior at critical point and hence, suitable for gaseous phase. The program developed which includes in thermodynamics properties obtained from HYSYS is embedded into FLUENT for simulation purposes. Validation of carbon dioxide vapor fraction from FLUENT with HYSYS shows that these properties are successfully incorporated into FLUENT software.

Looking at normal pipeline operating condition, temperature of 300 K with pressure 80 bar can be used to liquefied carbon dioxide and separate it from mixture to obtain purer methane. Model is highly flexible when it is incorporated into FLUENT as it can predict flow behavior for any pipe design as long as boundary conditions are specified. With the success of incorporating thermodynamics properties into FLUENT, one can choose the best design for the desired separation of carbon dioxide from methane (natural gas).

Cooling effect of pipes, for both simple pipe and finned pipe is affected by three factors; number of spacing, length of fin and width of fin. As the number of fin increases, the cooling effect increases. The larger and longer the fin, the cooling effect increases as well. Comparing the amount of work produced for the optimum design of finned pipe (finned pipe A1) and JT valve, the latter produces more work. This is due to the fact that heat is able to be transferred evenly to the whole fluid and hence, cryogenic effect can be applied thoroughly to the entire fluid.

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APPENDICES

Appendix A	Result Data for Pressure of 60 bar
Appendix B	Result Data for Pressure of 80 bar
Appendix C	The C Code in FLUENT Structure for pressure 60 bar
Appendix D	The C Code in FLUENT Structure for pressure 80 bar
Appendix E	Result Data for FLUENT Simulation
Appendix F	Calculation for Work Produced

APPENDIX A

RESULTS DATA FOR PRESSURE 60 BAR

Comparison for CO_2 mass fraction between FLUENT and HYSYS

Temperature (K)	FLUENT	HYSYS	% error
246.03	0.62159	0.62157	0.00003
246.56	0.62660	0.62660	0.00000
246.99	0.63070	0.63068	0.00002
247.00	0.63080	0.63080	0.00000
247.65	0.63693	0.63694	0.00001
247.90	0.63931	0.63930	0.00001
248.44	0.64444	0.64441	0.00004
248.51	0.64511	0.64507	0.00007
248.67	0.64660	0.64658	0.00003
249.03	0.64999	0.64998	0.00002
249.05	0.65021	0.65017	0.00006
250.26	0.66017	0.66155	0.00208
250.68	0.66188	0.66549	0.00543
251.00	0.66321	0.66849	0.00789
251.01	0.66324	0.66858	0.00799
251.08	0.66353	0.66924	0.00853
252.44	0.66909	0.68192	0.01882
252.62	0.66980	0.68359	0.02017
252.69	0.67010	0.68424	0.02067
253.01	0.67140	0.68721	0.02300
253.11	0.67183	0.68813	0.02370
254.00	0.67547	0.69636	0.03000
254.34	0.67685	0.69949	0.03237
256.09	0.68401	0.70000	0.02284
256.96	0.68757	0.70000	0.01776
257.00	0.68774	0.70000	0.01752
257.06	0.68799	0.70000	0.01716
258.11	0.69227	0.70000	0.01104
258.80	0.69509	0.70000	0.00701
259.10	0.69633	0.70000	0.00525
259.25	0.69692	0.70000	0.00439
259.30	0.69714	0.70000	0.00408
259.35	0.69733	0.70000	0.00381
259.39	0.69751	0.70000	0.00356

259.43	0.69767	0.70000	0.00334
259.47	0.69782	0.70000	0.00311
259.51	0.69798	0.70000	0.00289
259.54	0.69813	0.70000	0.00267
259.58	0.69828	0.70000	0.00245
259.62	0.69843	0.70000	0.00224
259.65	0.69858	0.70000	0.00203
259.69	0.69873	0.70000	0.00181
259.73	0.69888	0.70000	0.00159
259.77	0.69904	0.70000	0.00137
259.80	0.69919	0.70000	0.00116
259.84	0.69935	0.70000	0.00093
259.88	0.69950	0.70000	0.00071
259.92	0.69966	0.70000	0.00049
259.95	0.69981	0.70000	0.00027
259.99	0.69997	0.70000	0.00004
260.03	0.70000	0.70000	0.00000
260.07	0.70000	0.70000	0.00000
260.11	0.70000	0.70000	0.00000
260.15	0.70000	0.70000	0.00000
260.19	0.70000	0.70000	0.00000
260.23	0.70000	0.70000	0.00000
260.27	0.70000	0.70000	0.00000
260.31	0.70000	0.70000	0.00000
260.35	0.70000	0.70000	0.00000
260.39	0.70000	0.70000	0.00000
260.44	0.70000	0.70000	0.00000
260.48	0.70000	0.70000	0.00000
260.52	0.70000	0.70000	0.00000
260.56	0.70000	0.70000	0.00000
260.60	0.70000	0.70000	0.00000
260.65	0.70000	0.70000	0.00000
260.69	0.70000	0.70000	0.00000
260.73	0.70000	0.70000	0.00000
260.78	0.70000	0.70000	0.00000
260.82	0.70000	0.70000	0.00000
260.87	0.70000	0.70000	0.00000
260.91	0.70000	0.70000	0.00000
260.95	0.70000	0.70000	0.00000
261.00	0.70000	0.70000	0.00000
261.04	0.70000	0.70000	0.00000
261.09	0.70000	0.70000	0.00000
261.14	0.70000	0.70000	0.00000

261.18	0.70000	0.70000	0.00000
261.23	0.70000	0.70000	0.00000
261.27	0.70000	0.70000	0.00000
261.32	0.70000	0.70000	0.00000
261.37	0.70000	0.70000	0.00000
261.41	0.70000	0.70000	0.00000
261.46	0.70000	0.70000	0.00000
261.51	0.70000	0.70000	0.00000
261.55	0.70000	0.70000	0.00000
261.60	0.70000	0.70000	0.00000
261.65	0.70000	0.70000	0.00000
261.70	0.70000	0.70000	0.00000
261.74	0.70000	0.70000	0.00000
261.79	0.70000	0.70000	0.00000
261.84	0.70000	0.70000	0.00000
261.89	0.70000	0.70000	0.00000
261.94	0.70000	0.70000	0.00000
261.99	0.70000	0.70000	0.00000
262.03	0.70000	0.70000	0.00000
262.08	0.70000	0.70000	0.00000
262.13	0.70000	0.70000	0.00000
262.18	0.70000	0.70000	0.00000
262.23	0.70000	0.70000	0.00000
262.27	0.70000	0.70000	0.00000
262.32	0.70000	0.70000	0.00000
262.37	0.70000	0.70000	0.00000
262.42	0.70000	0.70000	0.00000
262.47	0.70000	0.70000	0.00000
262.52	0.70000	0.70000	0.00000
262.56	0.70000	0.70000	0.00000
262.61	0.70000	0.70000	0.00000
262.66	0.70000	0.70000	0.00000
262.71	0.70000	0.70000	0.00000
262.76	0.70000	0.70000	0.00000
262.81	0.70000	0.70000	0.00000
262.85	0.70000	0.70000	0.00000
262.90	0.70000	0.70000	0.00000
262.95	0.70000	0.70000	0.00000
263.00	0.70000	0.70000	0.00000
263.05	0.70000	0.70000	0.00000
263.10	0.70000	0.70000	0.00000
263.15	0.70000	0.70000	0.00000
300.00	0.70000	0.70000	0.00000

APPENDIX B

RESULTS DATA FOR PRESSURE 80 BAR

Comparison of CO_2 mass fraction for FLUENT and HYSYS

Temperature (K)	FLUENT	HYSYS	% error
246.03	0.62418	0.62419	0.00001
246.56	0.62735	0.62732	0.00004
246.99	0.62993	0.62993	0.00001
247.00	0.63000	0.63000	0.00000
247.65	0.63406	0.63403	0.00005
247.90	0.63564	0.63562	0.00005
248.44	0.63912	0.63908	0.00005
248.51	0.63958	0.63954	0.00006
248.67	0.64059	0.64058	0.00002
249.03	0.64291	0.64294	0.00005
249.05	0.64306	0.64307	0.00002
250.26	0.65072	0.65119	0.00072
250.68	0.65283	0.65405	0.00188
251.00	0.65448	0.65626	0.00271
251.01	0.65451	0.65633	0.00276
251.08	0.65486	0.65681	0.00296
252.44	0.66175	0.66632	0.00686
252.62	0.66263	0.66759	0.00743
252.69	0.66300	0.66809	0.00762
253.01	0.66462	0.67036	0.00857
253.11	0.66514	0.67107	0.00884
254.00	0.66964	0.67744	0.01152
254.34	0.67135	0.67989	0.01256
256.09	0.68022	0.69260	0.01788
256.96	0.68462	0.69897	0.02054
257.00	0.68483	0.69927	0.02065
257.06	0.68514	0.69971	0.02082
258.11	0.69044	0.70000	0.01366
258.80	0.69393	0.70000	0.00867
259.07	0.69527	0.70000	0.00676
259.21	0.69601	0.70000	0.00570
259.26	0.69628	0.70000	0.00532
259.31	0.69651	0.70000	0.00498

259.35	0.69672	0.70000	0.00468
259.39	0.69692	0.70000	0.00439
259.43	0.69712	0.70000	0.00412
259.47	0.69730	0.70000	0.00385
259.50	0.69749	0.70000	0.00359
259.54	0.69768	0.70000	0.00332
259.58	0.69786	0.70000	0.00305
259.61	0.69805	0.70000	0.00279
259.65	0.69823	0.70000	0.00252
259.69	0.69842	0.70000	0.00226
259.73	0.69861	0.70000	0.00199
259.76	0.69880	0.70000	0.00172
259.80	0.69899	0.70000	0.00145
259.84	0.69918	0.70000	0.00117
259.88	0.69937	0.70000	0.00090
259.91	0.69956	0.70000	0.00062
259.95	0.69976	0.70000	0.00035
259.99	0.69995	0.70000	0.00007
260.03	0.70000	0.70000	0.00000
260.07	0.70000	0.70000	0.00000
260.11	0.70000	0.70000	0.00000
260.15	0.70000	0.70000	0.00000
260.19	0.70000	0.70000	0.00000
260.23	0.70000	0.70000	0.00000
260.27	0.70000	0.70000	0.00000
260.31	0.70000	0.70000	0.00000
260.35	0.70000	0.70000	0.00000
260.39	0.70000	0.70000	0.00000
260.44	0.70000	0.70000	0.00000
260.48	0.70000	0.70000	0.00000
260.52	0.70000	0.70000	0.00000
260.56	0.70000	0.70000	0.00000
260.61	0.70000	0.70000	0.00000
260.65	0.70000	0.70000	0.00000
260.69	0.70000	0.70000	0.00000
260.74	0.70000	0.70000	0.00000
260.78	0.70000	0.70000	0.00000
260.82	0.70000	0.70000	0.00000
260.87	0.70000	0.70000	0.00000
260.91	0.70000	0.70000	0.00000
260.96	0.70000	0.70000	0.00000
261.00	0.70000	0.70000	0.00000
261.05	0.70000	0.70000	0.00000

261.09	0.70000	0.70000	0.00000
261.14	0.70000	0.70000	0.00000
261.19	0.70000	0.70000	0.00000
261.23	0.70000	0.70000	0.00000
261.28	0.70000	0.70000	0.00000
261.32	0.70000	0.70000	0.00000
261.37	0.70000	0.70000	0.00000
261.42	0.70000	0.70000	0.00000
261.47	0.70000	0.70000	0.00000
261.51	0.70000	0.70000	0.00000
261.56	0.70000	0.70000	0.00000
261.61	0.70000	0.70000	0.00000
261.66	0.70000	0.70000	0.00000
261.70	0.70000	0.70000	0.00000
261.75	0.70000	0.70000	0.00000
261.80	0.70000	0.70000	0.00000
261.85	0.70000	0.70000	0.00000
261.90	0.70000	0.70000	0.00000
261.94	0.70000	0.70000	0.00000
261.99	0.70000	0.70000	0.00000
262.04	0.70000	0.70000	0.00000
262.09	0.70000	0.70000	0.00000
262.14	0.70000	0.70000	0.00000
262.19	0.70000	0.70000	0.00000
262.23	0.70000	0.70000	0.00000
262.28	0.70000	0.70000	0.00000
262.33	0.70000	0.70000	0.00000
262.38	0.70000	0.70000	0.00000
262.43	0.70000	0.70000	0.00000
262.48	0.70000	0.70000	0.00000
262.53	0.70000	0.70000	0.00000
262.57	0.70000	0.70000	0.00000
262.62	0.70000	0.70000	0.00000
262.67	0.70000	0.70000	0.00000
262.72	0.70000	0.70000	0.00000
262.77	0.70000	0.70000	0.00000
262.82	0.70000	0.70000	0.00000
262.86	0.70000	0.70000	0.00000
262.91	0.70000	0.70000	0.00000
262.96	0.70000	0.70000	0.00000
263.01	0.70000	0.70000	0.00000
263.06	0.70000	0.70000	0.00000
263.11	0.70000	0.70000	0.00000

263.16	0.70000	0.70000	0.00000
263.22	0.70000	0.70000	0.00000
263.28	0.70000	0.70000	0.00000
263.34	0.70000	0.70000	0.00000
263.40	0.70000	0.70000	0.00000
263.47	0.70000	0.70000	0.00000
263.55	0.70000	0.70000	0.00000
263.63	0.70000	0.70000	0.00000
263.71	0.70000	0.70000	0.00000
263.80	0.70000	0.70000	0.00000
263.89	0.70000	0.70000	0.00000
263.99	0.70000	0.70000	0.00000
264.08	0.70000	0.70000	0.00000
264.18	0.70000	0.70000	0.00000
264.29	0.70000	0.70000	0.00000
264.39	0.70000	0.70000	0.00000
264.50	0.70000	0.70000	0.00000
264.61	0.70000	0.70000	0.00000
264.72	0.70000	0.70000	0.00000
264.84	0.70000	0.70000	0.00000
264.96	0.70000	0.70000	0.00000
265.08	0.70000	0.70000	0.00000
265.20	0.70000	0.70000	0.00000
265.33	0.70000	0.70000	0.00000
265.46	0.70000	0.70000	0.00000
265.59	0.70000	0.70000	0.00000
265.73	0.70000	0.70000	0.00000
265.87	0.70000	0.70000	0.00000
266.01	0.70000	0.70000	0.00000
266.15	0.70000	0.70000	0.00000
266.30	0.70000	0.70000	0.00000
266.45	0.70000	0.70000	0.00000
266.61	0.70000	0.70000	0.00000
266.77	0.70000	0.70000	0.00000
266.93	0.70000	0.70000	0.00000
267.10	0.70000	0.70000	0.00000
267.27	0.70000	0.70000	0.00000
267.45	0.70000	0.70000	0.00000
267.63	0.70000	0.70000	0.00000
267.82	0.70000	0.70000	0.00000
268.01	0.70000	0.70000	0.00000
268.21	0.70000	0.70000	0.00000
300.00	0.70000	0.70000	0.00000

APPENDIX C

THE C CODE FOR FLUENT STRUCTRE FOR PRESSURE 60 BAR

```
#include <udf.h>

    float co2_vap_massfrac;


DEFINE_EXECUTE_AT_END (thermo2
{

Domain *d;
Thread *t;
cell_t c;

d = Get_Domain(1);

thread_loop_c (t,d)
{

begin_c_loop (c,t)


        if(C_T(c,t) <= 350 && C_T(c,t) >= 260)
        {
        co2_vap_massfrac = 0.7;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 260 && C_T(c,t) > 250)
        {
        co2_vap_massfrac = (C_T(c,t)-260)/(250-260)*(0.6591-
 0.7000)+0.7000;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 250)
        {
        co2_vap_massfrac = 0.6591;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 250 && C_T(c,t) > 249)
        {
        co2_vap_massfrac = (C_T(c,t)-250)/(249-250)*(0.6497-
 0.6591)+0.6591;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 249)
        {
        co2_vap_massfrac = 0.6497;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
```

```
        }
        else if(C_T(c,t) < 249 && C_T(c,t) > 248)
        {
        co2_vap_massfrac = (C_T(c,t)-249)/(248-249)*(0.6403-
0.6497)+0.6497;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 248)
        {
        co2_vap_massfrac = 0.6403;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 248 && C_T(c,t) > 247)
        {
        co2_vap_massfrac = (C_T(c,t)-248)/(247-248)*(0.6308-
0.6403)+0.6403;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 247)
        {
        co2_vap_massfrac = 0.6308;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 247 && C_T(c,t) > 246)
        {
        co2_vap_massfrac = (C_T(c,t)-247)/(246-247)*(0.6213-
0.6308)+0.6308;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 246)
        {
        co2_vap_massfrac = 0.6213;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 246 && C_T(c,t) > 245)
        {
        co2_vap_massfrac = (C_T(c,t)-246)/(245-246)*(0.6118-
0.6213)+0.6213;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 245)
        {
        co2_vap_massfrac = 0.6118;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 245 && C_T(c,t) > 244)
        {
        co2_vap_massfrac = (C_T(c,t)-245)/(244-245)*(0.6022-
0.6118)+0.6118;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 244)
        {
```

```
        co2_vap_massfrac = 0.6022;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 244 && C_T(c,t) > 243)
        {
        co2_vap_massfrac = (C_T(c,t)-244)/(243-244)*(0.5927-
0.6022)+0.6022;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 243)
        {
        co2_vap_massfrac = 0.5927;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 243 && C_T(c,t) > 242)
        {
        co2_vap_massfrac = (C_T(c,t)-243)/(242-243)*(0.5832-
0.5927)+0.5927;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 242)
        {
        co2_vap_massfrac = 0.5832;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 242 && C_T(c,t) > 241)
        {
        co2_vap_massfrac = (C_T(c,t)-242)/(241-242)*(0.5737-
0.5832)+0.5832;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 241)
        {
        co2_vap_massfrac = 0.5737;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 241 && C_T(c,t) > 240)
        {
        co2_vap_massfrac = (C_T(c,t)-241)/(240-241)*(0.5641-
0.5737)+0.5737;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 240)
        {
        co2_vap_massfrac = 0.5641;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 240 && C_T(c,t) > 239)
        {
        co2_vap_massfrac = (C_T(c,t)-240)/(239-240)*(0.5546-
0.5641)+0.5641;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
```

```
        }
        else if(C_T(c,t) == 239)
        {
        co2_vap_massfrac = 0.5546;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 239 && C_T(c,t) > 238)
        {
        co2_vap_massfrac = (C_T(c,t)-239)/(238-239)*(0.5452-
0.5546;)+0.5546;;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 238)
        {
        co2_vap_massfrac = 0.5452;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 238 && C_T(c,t) > 237)
        {
        co2_vap_massfrac = (C_T(c,t)-238)/(237-238)*(0.5357-
0.5452)+0.5452;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 237)
        {
        co2_vap_massfrac = 0.5357;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 237 && C_T(c,t) > 236)
        {
        co2_vap_massfrac = (C_T(c,t)-237)/(236-237)*(0.5263-
0.5357)+0.5357;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 236)
        {
        co2_vap_massfrac = 0.5263;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 236 && C_T(c,t) > 235)
        {
        co2_vap_massfrac = (C_T(c,t)-236)/(235-236)*(0.5170-
0.5263)+0.5263;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 235)
        {
        co2_vap_massfrac = 0.5170;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 235 && C_T(c,t) > 234)
        {
```

```
        co2_vap_massfrac = (C_T(c,t)-235)/(234-235)*(0.5076-
0.5170)+0.5170;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 234)
        {
        co2_vap_massfrac = 0.5076;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 234 && C_T(c,t) > 233)
        {
        co2_vap_massfrac = (C_T(c,t)-234)/(233-234)*(0.4984-
0.5076)+0.5076;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 233)
        {
        co2_vap_massfrac = 0.4984;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 233 && C_T(c,t) > 232)
        {
        co2_vap_massfrac = (C_T(c,t)-233)/(232-233)*(0.4892-
0.4984)+0.4984;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 232)
        {
        co2_vap_massfrac = 0.4892;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 232 && C_T(c,t) > 231)
        {
        co2_vap_massfrac = (C_T(c,t)-232)/(231-232)*(0.4801-
0.4892)+0.4892;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 231)
        {
        co2_vap_massfrac = 0.4801;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 231 && C_T(c,t) > 230)
        {
        co2_vap_massfrac = (C_T(c,t)-231)/(230-231)*(0.4710-
0.4801)+0.4801;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 230)
        {
        co2_vap_massfrac = 0.4710;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
```

```
        }
        else if(C_T(c,t) < 230 && C_T(c,t) > 229)
        {
        co2_vap_massfrac = (C_T(c,t)-230)/(229-230)*(0.4621-
0.4710)+0.4710;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 229)
        {
        co2_vap_massfrac = 0.4621;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 229 && C_T(c,t) > 228)
        {
        co2_vap_massfrac = (C_T(c,t)-229)/(228-229)*(0.4533-
0.4621)+0.4621;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 228)
        {
        co2_vap_massfrac = 0.4533;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 228 && C_T(c,t) > 227)
        {
        co2_vap_massfrac = (C_T(c,t)-228)/(227-228)*(0.4445-
0.4533)+0.4533;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 227)
        {
        co2_vap_massfrac = 0.4445;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 227 && C_T(c,t) > 226)
        {
        co2_vap_massfrac = (C_T(c,t)-227)/(226-227)*(0.4360-
0.4445)+0.4445;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 226)
        {
        co2_vap_massfrac = 0.4360;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 226 && C_T(c,t) > 225)
        {
        co2_vap_massfrac = (C_T(c,t)-226)/(225-226)*(0.4275-
0.4360)+0.4360;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 225)
        {
```

```
     co2_vap_massfrac = 0.4275;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) < 225 && C_T(c,t) > 224)
     {
     co2_vap_massfrac = (C_T(c,t)-225)/(224-225)*(0.4192-
0.4275)+0.4275;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) == 224)
     {
     co2_vap_massfrac = 0.4192;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) < 224 && C_T(c,t) > 223)
     {
     co2_vap_massfrac = (C_T(c,t)-224)/(223-224)*(0.4111-
0.4192)+0.4192;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) == 223)
     {
     co2_vap_massfrac = 0.4111;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) < 223 && C_T(c,t) > 222)
     {
     co2_vap_massfrac = (C_T(c,t)-223)/(222-223)*(0.4031-
0.4111)+0.4111;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) == 222)
     {
     co2_vap_massfrac = 0.4031;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) < 222 && C_T(c,t) > 221)
     {
     co2_vap_massfrac = (C_T(c,t)-222)/(221-222)*(0.3954-
0.4031)+0.4031;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) == 221)
     {
     co2_vap_massfrac = 0.3954;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
     }
     else if(C_T(c,t) < 221 && C_T(c,t) > 220)
     {
     co2_vap_massfrac = (C_T(c,t)-221)/(220-221)*(0.3879-
0.3954)+0.3954;
     C_YI (c,t,0) = co2_vap_massfrac;
     C_YI (c,t,1) = 1-co2_vap_massfrac;
```

```
        }
        else if(C_T(c,t) == 220)
        {
        co2_vap_massfrac = 0.3879;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 220 && C_T(c,t) > 219)
        {
        co2_vap_massfrac = (C_T(c,t)-220)/(219-220)*(0.3805-
0.3879)+0.3879;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 219)
        {
        co2_vap_massfrac = 0.3805;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 219 && C_T(c,t) > 218)
        {
        co2_vap_massfrac = (C_T(c,t)-219)/(218-219)*(0-
0.3805)+0.3805;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) <= 218 && C_T(c,t) > 100)
        {
        co2_vap_massfrac = 0;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }


end_c_loop (c,t)

}
}
```

APPENDIX D

THE C CODE FOR FLUENT

STRUCTRE FOR PRESSURE 80 BAR

```
#include <udf.h>

    float co2_vap_massfrac;


DEFINE_EXECUTE_AT_END (thermo1)
{

Domain *d;
Thread *t;
cell_t c;

d = Get_Domain(1);

thread_loop_c (t,d)
{

begin_c_loop (c,t)


        if(C_T(c,t) <= 350 && C_T(c,t) >= 260)
        {
        co2_vap_massfrac = 0.7;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 260 && C_T(c,t) > 250)
        {
        co2_vap_massfrac = ((C_T(c,t)-260)/(250-260)*(0.6494-
0.7000))+0.7000;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 250)
        {
        co2_vap_massfrac = 0.6494;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 250 && C_T(c,t) > 249)
        {
        co2_vap_massfrac = ((C_T(c,t)-250)/(249-250)*(0.6427-
0.6494))+0.6494;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 249)
        {
        co2_vap_massfrac = 0.6427;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
```

```
        }
        else if(C_T(c,t) < 249 && C_T(c,t) > 248)
        {
        co2_vap_massfrac = ((C_T(c,t)-249)/(248-249)*(0.6363-
0.6427))+0.6427;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 248)
        {
        co2_vap_massfrac = 0.6363;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 248 && C_T(c,t) > 247)
        {
        co2_vap_massfrac = ((C_T(c,t)-248)/(247-248)*(0.6300-
0.6363))+0.6363;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 247)
        {
        co2_vap_massfrac = 0.6300;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 247 && C_T(c,t) > 246)
        {
        co2_vap_massfrac = ((C_T(c,t)-247)/(246-247)*(0.6240-
0.6300))+0.6300;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 246)
        {
        co2_vap_massfrac = 0.6240;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 246 && C_T(c,t) > 245)
        {
        co2_vap_massfrac = ((C_T(c,t)-246)/(245-246)*(0.6184-
0.6240))+0.6240;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 245)
        {
        co2_vap_massfrac = 0.6184;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 245 && C_T(c,t) > 244)
        {
        co2_vap_massfrac = ((C_T(c,t)-245)/(244-245)*(0.6132-
0.6184))+0.6184;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 244)
        {
```

```
        co2_vap_massfrac = 0.6132;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 244 && C_T(c,t) > 243)
        {
        co2_vap_massfrac = ((C_T(c,t)-244)/(243-244)*(0.6086-
0.6132))+0.6132;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 243)
        {
        co2_vap_massfrac = 0.6086;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 243 && C_T(c,t) > 242)
        {
        co2_vap_massfrac = ((C_T(c,t)-243)/(242-243)*(0.6048-
0.6086))+0.6086;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 242)
        {
        co2_vap_massfrac = 0.6048;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 242 && C_T(c,t) > 241)
        {
        co2_vap_massfrac = ((C_T(c,t)-242)/(241-242)*(0.6021-
0.6048))+0.6048;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 241)
        {
        co2_vap_massfrac = 0.6021;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 241 && C_T(c,t) > 240)
        {
        co2_vap_massfrac = ((C_T(c,t)-241)/(240-241)*(0.6011-
0.6021))+0.6021;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) == 240)
        {
        co2_vap_massfrac = 0.6011;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
        }
        else if(C_T(c,t) < 240 && C_T(c,t) > 239)
        {
        co2_vap_massfrac = ((C_T(c,t)-240)/(239-240)*(0-
0.6011))+0.6011;
        C_YI (c,t,0) = co2_vap_massfrac;
        C_YI (c,t,1) = 1-co2_vap_massfrac;
```

```
          }
          else if(C_T(c,t) <= 239 && C_T(c,t) >= 90)
          {
          co2_vap_massfrac = 0.000;
          C_YI (c,t,0) = co2_vap_massfrac;
          C_YI (c,t,1) = 1-co2_vap_massfrac;
          }

end_c_loop (c,t)

}
}
```

APPENDIX E
RESULT DATA FOR FLUENT SIMULATION

Pipe design	Molar concentration of CO_2 (kmol/m^3.s)		
	inlet	outlet	removed
C2	0.00023	0.00019	3.2528E-05
A1	0.00023	0.00020	2.4554E-05
B1	0.00023	0.00020	2.2992E-05
B2	0.00023	0.00020	2.2480E-05
A2	0.00023	0.00021	1.2098E-05
C1	0.00023	0.00022	5.7408E-06
A0	0.00023	0.00022	1.7585E-06

Pipe design	Flowrate (kg/s)	
	CO2	CH4
A0	0.00828	0.00361
C1	0.00811	0.00379
A2	0.00788	0.00401
B1	0.00749	0.00441
A1	0.00745	0.00444
B2	0.00752	0.00437
C2	0.00763	0.00427

APPENDIX F
CALCULATION FOR WORK PRODUCED

Finned pipe

Assumptions:

1. Refrigerator concept is applied here where the refrigerant used is R 134-a.
2. Steady state operating condition

$$W_{in} = (264.68 kJ/kg)(0.011895 kg/s) = 3.15 kW$$

COP for refrigerator is between 2.6 and 3. Hence, take COP as 3.

$$COP = \frac{\dot{Q}_L}{W_{in}}$$

$$\dot{Q}_L = (3)(3.15 kW) = 9.45 kW$$

$$\dot{Q}_H = \dot{Q}_L + Wi_n = 3.15 kW + 9.45 kW = 12.6 kW$$

For 0.000875 kg/s carbon dioxide removed, total work produced is 14 400 kW.

Joule Thomson valve

Assumptions:

1. Steady flow process
2. JT valve is adiabatic and hence, no heat transfer
3. ΔPE and ΔKE are negligible

$$W_{out} = (0.5 kg/s)(249.6 - 222.8) kJ/kg = 13.4 kW$$

For 0.000875 kg/s carbon dioxide removed, total work produced is 15 314 kW.