A Thermodynamics Study for a Mixture of

Natural Gas & Water Flowing Through a Supersonic Nozzle

by

Chan Yen Pinng

Dissertation submitted in partial fulfillment 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
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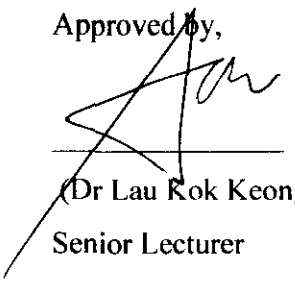
Approved by,



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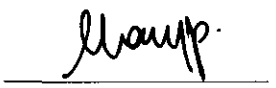
September 2011

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.



CHAN YEN PINNG

ABSTRACT

In order to meet the specifications of transportation of natural gas in pipelines, there is a need for efficient separation of water from natural gas mixture. To date, supersonic separation has proven to be efficient in such a physical separation, yet there is limited study on the thermodynamic of the system. Lack of suitable equation of state in fluid flow simulation software ANSYS FLUENT 12.0 to model the non negligible density changes in the compressible flow also calls for a source code that can introduce real gas equations, that's also appropriate for hydrocarbon systems.

With that, the objective of this Final Year Project will focus on understanding the thermodynamics of natural gas dehydration and producing a solution scheme based on Soave-Redlich-Kwong equation of state using user defined functions in computational fluid dynamics (CFD) software ANSYS FLUENT 12.0 to predict flow behaviour and changes in other thermodynamic properties. Therefore, scope of study for this project includes thermodynamics, real gas equation of state to accurately study the compressible, turbulent, high velocity, single phase water vapour flow behaviour and solution by means of computational fluid dynamics (CFD) software ANSYS® FLUENT 12.0 in two-dimension. This will be done through extensive literature review, identification of validation literature, writing of solution mechanism, performing CFD simulation and finally post-processing for analysis.

Here, validation of simulation was done against Yang et al's (2009) paper on numerical simulation of non equilibrium spontaneous condensation in supersonic steam flow. Main findings showed that density change in compressible, high velocity flow does significantly influence the thermodynamic properties of the fluid flow system and super cooling resulting from isentropic expansion was also observed. This further verified that the source code written for using Soave-Redlich-Kwong equation of state to model density changes is successful. It was also proven that Soave-Redlich-Kwong equation of state is more accurate and reliable when it comes to modelling a system with high pressure variation, compared to ideal gas law.

This dissertation thus presents the results from literature review, solution methodology, findings of this project and analysis. It is believed that such a study will aid in understanding the system in order to achieve efficient separation of impurities from natural gas in the future.

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Last but not least, I want to extend my gratitude to my family and friends who have supported me throughout the entire course of my Final Year Project, all the way until completion, of which I cannot do without. Thank you.

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ABBREVIATIONS & NOMENCLATURE

CFD	Computational Fluid Dynamics
EOS	Equation of State
NASA	National Aeronautics and Space Administration
PRSV	Peng-Robinson-Stryjek-Vera Equation of State
SRK	Soave-Redlich-Kwong Equation of State
UDF	User Defined Function
UTP	Universiti Teknologi PETRONAS

a	Substance specific constant 1 for SRK EOS
b	Substance specific constant 2 for SRK EOS
T_c	Critical temperature (K)
P_c	Critical pressure (Pa)
T_R	Reduced temperature (K)
T	Temperature (K)
P	Pressure (Pa)
R	Universal gas constant (m^3.Pa/gmol.K)
m	Constant for SRK EOS
k-ε	Semi-empirical model based on model transport equations for the turbulence kinetic energy (k) and its dissipation rate (ε)
ω	Accentric factor for SRK EOS
α	Function for SRK EOS
$\tilde{V}$	Molar volume

CHAPTER 1

INTRODUCTION

1.1 Background of Study

Natural gas that is extracted from the ground usually comes out in the form of multi-components- mixture of hydrocarbons, reservoir water, carbon dioxide and other impurities. In fact, it is most likely in a supercritical dense phase in which water and hydrocarbon components form liquid phase. Pre-processing in natural gas is therefore needed because presence of water in natural gas not only reduces its calorific value; it also causes operational problems such as corrosion, slug formation and decrease in pressure drop which in turn affects the transportability of the natural gas. While the more common natural gas dehydration technique includes liquid desiccant absorption, solid desiccant absorption or dehydration by refrigeration and membrane permeation, these methods involve use of chemicals and bulky equipments in large facilities which require supervision and extensive control strategy. Not to mention, these techniques are also relatively expensive since regeneration of material is needed and heavy equipments are usually involved *(Karimi et al, 2009)*.

Supersonic gas separation is one of the modern technologies applied in the natural gas industry today. The main mechanism of supersonic separation system takes place in a supersonic nozzle in which both condensation and separation occur at supersonic velocities, leaving hydrate no time to deposit on the wall surfaces due to the short residence time and the high velocity of the fluid *(Karimi et al, 2009)*. This opens up a possibility to separate condensed water droplets from natural gas effectively without use of complex and costly facilities unlike the conventional dehydration techniques.

In supersonic gas separation, gas is forced through a tube, the gas molecules are deflected by the walls of the tube. As the speed of the flow approaches the speed of sound, compressibility effects on the gas must be considered. The density of the gas now basically varies from one location to the next. Considering flow through a converging-diverging nozzle, if the flow is very gradually compressed due to decreasing tube area and then gradually expanded due to increasing area, the flow conditions basically return to their original values. Such a process is termed

reversible. Considering the second law of thermodynamics, a reversible flow maintains a constant value of entropy, or in other words, isentropic flow takes place. This isentropic expansion basically brings about a significant change in the thermodynamics of the flow that cannot be ignored *(NASA, 2008)*. While most of the studies done on this technology revolves around the design parameters, lack of studies has been conducted for natural gas dehydration using principles of supersonic separation in a supersonic nozzle, from a thermodynamic point of view using computational fluid dynamics (CFD) techniques, which would be worth investigating considering the advantages and efficiency of the separation technology.

1.2 Problem Statement

To date, there is limited number of research on natural gas dehydration using supersonic technology. In fact, those who do study this system mainly focus on the boundary conditions and shockwave locations as an after result of isentropic expansion. Research particularly on the thermodynamics of this system is needed because in a converging-diverging nozzle, also known as Laval nozzle, sudden decrease and increase in the flow area leads to isentropic expansion, immediate cooling and pressure drop, along with condensation and creation of shock waves. This rapid expansion often leads to a non equilibrium thermodynamic condition that is often neglected due to complexity and difficulty in quantifying.

This justifies the need for research on real thermodynamics for this system, especially in the condition where ideal gas assumptions will not stand since we are dealing with a high velocity compressible flow. Density significantly varies from one point to another in the flow system and ideal gas assumption does not reflect this thermodynamic behaviour precisely. With that, cubic equation of states must be utilized to portray the thermodynamics environment in which the system will undergo to accurately present the phase change phenomena in the nozzle. This area of study is crucial in order to fully understand the phase equilibrium of the system for optimizing water separation from natural gas mixture. Coming as close as possible to the real thermodynamics condition which will affect the phase conditions, mixture flow behaviour, hydrodynamics, condensation and nucleation phenomena in the supersonic nozzle, it will help us in find out whether thermodynamics of the real flow system will have a significant effect on the efficiency of natural gas dehydration.

However, there is no readily written solution scheme in ANSYS® FLUENT 12.0 that allows usage of cubic equation of state to influence the density computation. While some models are available, the density models that are proposed are either not suitable for the vapour-liquid phase system or not suitable if the codes were to be used for complex simulation that involves heavy hydrocarbons in the future. With that said, there is a need to produce a solution scheme to suit the high velocity compressible flow through introduction of Soave-Redlich-Kwong equation of state into ANSYS FLUENT 12.0, which leads to the objective of this Final Year Project, followed by validation of scientific work.

1.3 Objectives

The aim of this Final Year Project is:

- To produce a solution scheme that incorporates cubic equation of state to predict and validate real flow behaviour under real gas conditions inside the supersonic nozzle- solution scheme that can be validated by simple water-steam flow and used for complex carbon dioxide-natural gas mixture system
- To predict the fluid flow profile and other thermodynamics properties for supersonic flow of natural gas mixture containing water flowing in a supersonic nozzle through determination of the most appropriate equation of state

1.4 Scope of Study

Study on the supersonic flow of substances through a nozzle can cover a broad area of detailed researches. The scope of study is hereby determined as follows:

- Thermodynamics:
    - Thermodynamics phenomena in supersonic vapor flow under non ideal gas conditions i.e. real gas conditions
    - Changes in thermodynamic properties that occur in the system under non ideal gas conditions while going through changes at supersonic condition in the converging-diverging nozzle
    - Varying density due to compressibility of vapor flowing at supersonic conditions, followed by isentropic expansion

- Equation of state:
    - Determination of the most suitable equation of state for flash calculation that can accurately reflect the thermodynamics changes in a supersonic water-natural gas mixture system
    - Comparison between accuracy and suitability of Soave-Redlich-Kwong equation of state and ideal gas equation of state
- Computational fluid dynamics (CFD):
    - Modeling of turbulence in the flow system
    - Inclusion of user defined functions to introduce real gas equation of state to ANSYS FLUENT 12.0
    - Model and portray thermodynamic changes by means of CFD calculations and post-processing

1.5 Relevancy of the Project

Relevancy of the project is justified as follows:

- The study involves the study of thermodynamics, fluid mechanics, and separation process and transport phenomena in the mixture systems, which are all core of chemical engineering studies. This project will be able to challenge the knowledge obtained throughout undergraduate years.
- Natural gas is a valuable clean fossil fuel. Understanding of its components, effects of components and their fraction towards natural gas behavior, properties, flow behavior and phase change while exploring its dehydration technology can improve the performance of oil and gas industry.
- Study of thermodynamics of flow in a supersonic nozzle is lacking. This research will surely help in discovering more about the realities of the process.
- Real gas conditions have long been neglected in studying dehydration of natural gas. Studying this area of thermodynamics can improve the understanding of supersonic flow, leading to positive modification and troubleshooting of this process.
- There is a need to improve the utilization of computational fluid dynamics (CFD) techniques in understanding the thermodynamics and fluid dynamics of such a challenging system.

1.6 Feasibility of Project

The feasibility of carrying out the project is justified as follows:

- Study on thermodynamics of complex fluid flow is not completely novel. There are extensive documents and papers that can help in understanding and learning about the phenomena and its effects.
- There are available resources and journals documenting the researches done on flow inside a supersonic nozzle on selective dehydration and accurate geometry details available for simulation, thereby providing credible sources for validation of theories and simulation results.
- Computational Fluid Dynamics (CFD) is a reliable and high performance engineering method in which fluid flow fields can be evaluated for a domain of interest relatively accurately.

CHAPTER 2

LITERATURE REVIEW

This Final Year Project revolves around four engineering study fields, namely supersonic turbulence modelling, thermodynamics, natural gas-water system and numerical solution in computational fluid dynamics.

Supersonic turbulence modelling

Supersonic turbulence modelling for one, has taken the interest of many scientists. Extensive research done in predicting flow behaviour in dehydration and extraction of heavy natural gas liquids in natural gas using supersonic nozzle has given confidence that selective separation of components using this technology is plausible. Karimi et al. (2009) have simulated the performance of supersonic nozzle in removing water in supercritical conditions. On the other hand, Ma et al. (2009) in their research to improve the separation performance of a supersonic gas separation device for the treatment of gas mixture with a single heavy component, have carried out a series of experiments in the improved separation device under various conditions, using air-ethanol vapour as the medium and micro water droplets as nucleation centres. These works have shown that the plausibility of the separation technology in removing selected substances from the system.

Basically, supersonic separation works like this:

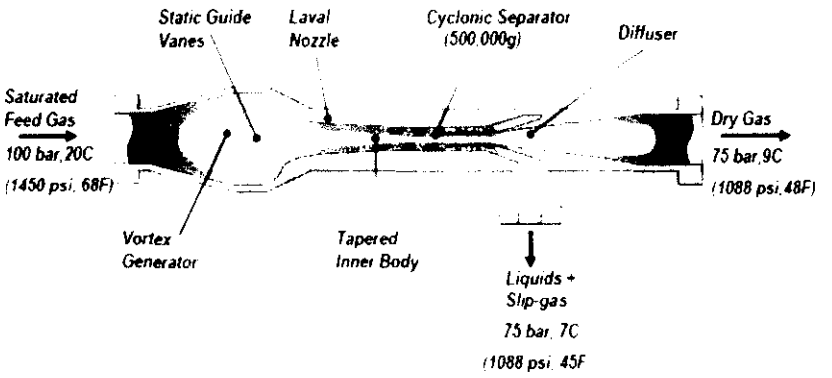


Figure 1: Cross-section view of the tube shows separation elements (*Retrieved from Twister B.V., 2011*)

In a Laval nozzle, cyclonic separation under adiabatic condition takes place in a single, compact device. Adiabatic cooling is accomplished through isentropic

expansion that takes place due to the converging-diverging characteristic of the tube. The swirling motion is generated by a fixed static vane ring at the entrance of the Laval nozzle. Here, the swirl strength increases strongly due to the contraction in the nozzle. The fine dispersed liquids formed during the adiabatic expansion thanks to condensation from rapid cooling are separated as a result of the centrifugal forces exerted by the strong swirling flow, and removed from the dry flow at minimum temperature and pressure with significantly high separation efficiency. At the point where liquid/gas separation takes place, a proven by Twister B.V., the total fluid velocity can be around 1,312 ft/second (400 m/second) resulting in a maximum gas residence time inside the tube of less than 2 milliseconds (Twister B.V., 2011). The remaining kinetic within the tube is then transformed to increased static pressure in the diffuser sections. The design incorporates an inner body which allows the principle of conservation of angular momentum to be harnessed and it is indeed highly favourable since no mechanical parts or additional chemicals are needed for this dehydration technology.

When it comes to supersonic turbulence modelling, thermodynamically the system is affected, since at such a high Mach number flow vibrational energies cannot be neglected. While sophisticated techniques such as Large Eddy Simulation (LES) have been used to simulate jet flow, high degree of accuracy is not yet possible. This is due to the requirement of large computational grids and very long computer run time. Large temperature and pressure fluctuations have a profound effect on turbulence as well. With that said, ideal gas law cannot be met where density changes are simply not negligible. Therefore, real gas equations must be used, which leads to the next point about significance of thermodynamics in this Final Year Project.

Thermodynamics

In theory, real gases require more complex equations than ideal gases. Ideal gases are highly favoured in chemical engineering calculations because of its easy correlation with almost any thermodynamics system. However, as a gas is forced through a tube, if the speed of the gas is much less than the speed of sound of the gas, the density of the gas remains constant and the velocity of the flow increases. Here, ideal gas assumption might still be valid. However, as the speed of the flow approaches

the speed of sound, compressibility effects must be taken into account. The density of the gas varies from one location to the next and cannot be termed as a constant as in ideal gas assumption anymore. If the flow is very gradually compressed (area decreases) and then gradually expanded (area increases), the flow conditions return to their original values. We say that such a process is reversible. From Second Law of Thermodynamics, this reversible flow maintains a constant value of entropy or in other words, this condition is also referred to as isentropic (*NASA, 2008*). Isentropic flows occur when the change in flow variables is small and gradual. The generation of sound waves is an isentropic process. In such a nozzle, isentropic expansion and cooling takes place (*NASA, 2008*). We can see from here that many significant thermodynamic related conditions will take place from the reaction of flow towards the changing geometry of the nozzle in which the flow goes through. Real gas equation therefore comes in handy to fully describe the thermodynamic environment.

The equation of state of Peng and Robinson (1976) and the modification of the Redlich-Kwong equation of state by Soave (1972) have been applied successfully to the vapour- liquid equilibria of hydrocarbon-hydrocarbon and some hydrocarbon-non-hydrocarbon systems (Graboski et al. 1978). The advantage of these equations over Virial equations is that they can represent the thermodynamic systems where both liquid and vapour are present. Soave-Redlich-Kwong equation of state includes volume correction and a molecular interaction parameter, adding more advantage to its usage.

In Kabadi et al. (1985)'s research, the use of modified SRK equation of state for phase equilibrium calculations for water-hydrocarbon system has given fairly good results in all the regions of the phase diagram. It predicted the instability in the liquid phase and the liquid-liquid equilibrium data with a fair degree of accuracy. With that we have the confidence that cubic equation of states can be considered as solution scheme for our case, since for validation we are dealing with steam system. The equation of state will also be usable for a hydrocarbon system, proven by Kabadi et al.'s work.

Natural gas-water system

Natural gas being a precious energy source does attract the attention of many scientists and researchers worldwide. Karimi et al. (2009) for one have simulated selective water removal from natural gas by controlling design parameters such as inlet pressure and temperature and controlling the backpressure. Their research successfully simulated the performance of supersonic nozzle in removing water in supercritical conditions. Simulation of natural gas with other components has also been carried out previously. One of it that was reviewed is one written by Munkejord et al. (2009). This paper calculated the transportation and depressurization of a 2D phase multi-component CH_4-CO_2 mixture using Soave-Redlich-Kwong Equation of State. Specifically with respect to natural gas system, Chuang et al. (2011) on the other hand, investigated effects of the supersonic swirling flow on the radial distribution of main parameters of gas flow and the effects of shock position. Compared to the many other researchers, Chuang at al. (2011) were among the few that investigated natural gas system flowing through supersonic separator, however using less accurate ideal gas equation of state where effects of compressibility were also taken into consideration. Specifically with respect to natural gas system, Chuang et al. (2011) investigated effects of the supersonic swirling flow on the radial distribution of main parameters of gas flow and the effects of shock position. However, Chuang et al. (2011) also used a less accurate ideal gas equation of state where effects of compressibility was not considered. Therefore we can see the importance of investigating natural gas system flowing under real condition.

Numerical solution in computational fluid dynamics (CFD)

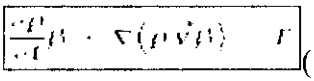
Since we are dealing with simulation, literature review was done with respect to numerical solutions proposed by other researchers as well. Zeitoun (1997) performed a numerical study on hypersonic viscous flow fields by solving unsteady laminar Navier-Stokes equations, coupled with those describing the chemical and vibrational non-equilibrium processes in real air mixture. It was suggested that thermodynamics and chemical states of flow resulting from a convergent-divergent nozzle are typically in non- equilibrium, due to the freezing resulting from the rapid expansion in the nozzle. This shows the importance of investigating the thermodynamics environment in supersonic flow. Vandromme et al. (1996) upon starting a supersonic turbulence modelling work also commented on the difficulties in modelling complex

compressible flow expected in a supersonic nozzle. It was noted that the turbulence model should consider the turbulence variables as field quantities which are transported in space and time; turbulence model must be modified through modelling of pressure correlations and must take into account the energy transfer between turbulent and mean motions. Vandromme's suggestions were later strengthened by Mallinger (1997) who also agreed that vibrational energy transfer between diatomic molecules must be taken into account since high Mach number flows will bring about strong non equilibrium effects. With that, as mentioned earlier, Mallinger introduced Master Equations that are coupled with classical flow equations such as Navier-Stokes or Euler of gas dynamics while governing the particle motion among different quantum states, which serves as a great reference in numerical calculations. This however, involved much complex equations and extension understanding.

Validation Literature

Regarding numerical modelling of compressible fluid flow, Yang et al. (2009) has done a validation work by computing a conservative two-dimensional compressible numerical model for supersonic non-equilibrium spontaneous condensing steam flow in the conventional Laval nozzle, based on the classical nucleation theory and the equation of state based on Virial coefficients. In the paper. the difference between the dry isentropic expansion and the non-equilibrium flow with spontaneous condensation has been investigated particularly. It was found that in supersonic steam flow, non-equilibrium spontaneous condensation will occur in the form of "condensation shock"-which is the release of latent heat resulting in a deceleration of the flow and arise in pressure, downstream of the nozzle throat at a certain value when the super cooling and the super saturation ratio achieve a high level.

In solving, Yang et al. (2009) has adopted the Eulerian–Eulerian approach for modelling the condensing steam flow. The two-phase flow is modelled using the conservation-type two-dimensional compressible Navier-Stokes equations, with transport equations for the liquid-phase mass-fraction (β) and the number of liquid droplets per unit volume (η):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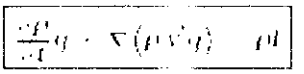
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(Retrieved from Yang et al., 2009)

This recent piece of research could be a good source for validation since for the system investigated for this final year project, it is desired that the thermodynamics be able to be investigated where condensation and nucleation are expected due to the non equilibrium rapid expansion through the nozzle structure as well. Yang's research was also supported by Gerber et al. (2004) who modelled homogeneous nucleation in high speed transonic flow using Eulerian multiphase equations, governing both the vapour and liquid phases, which are also formulated utilizing Classical nucleation theory and the concept of droplet interfacial area density. These equations were applied to predict the moisture distribution in low- and high pressure steam flow in a Laval nozzle and 2D rotor-tip section of a stage turbine.

Both Yang and Gerber however, have employed an equation of state proposed by Vukalovich (1958) which utilized Virial formulation to account for the thermodynamic conditions of super cooled states in the nozzle, which is something to be improved on since Virial equations does not represent both vapour and liquid mixture phase well. This of course, has been covered in the objective of this Final Year Project. Focus will thereby be put on the simulation of single phase steam flow through the supersonic nozzle, validated against the experimental and simulated results presented by Yang et al. (2009).

CHAPTER 3

METHODOLOGY

3.1 Research Methodology & Workflow

Since this project is not suitable to be carried out in a pilot plant scale, nor it is feasible to experimentation in a lab due to lack of technical expertise, computational fluid dynamics (CFD) simulation has been carried out to investigate the thermodynamic condition of fluid mixture flowing through a supersonic nozzle. The research methodology employed for completion of this Final Year Project is summarized in the following flow chart:

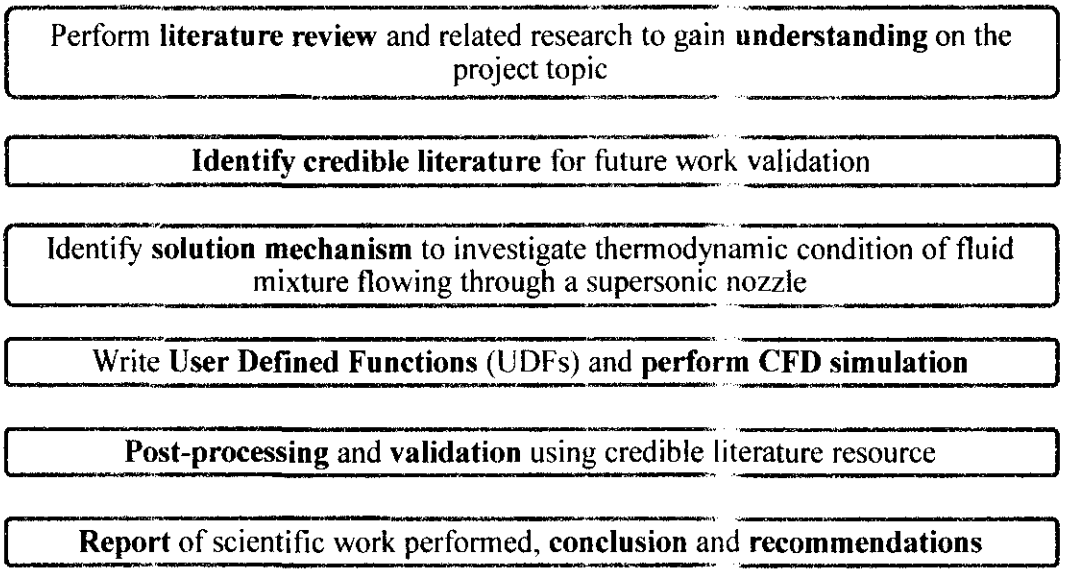

Figure 2: Flow chart of project activities

In whole, the research process involves investigation, prediction and validation of the flow behaviour by means of CFD. Therefore, there is a need to pay close attention to the numerical solution methodology that will be employed in the simulation. The research started with understanding of the topic thoroughly which includes intensive literature review on the topic of thermodynamics, modelling and supersonic separation. This is then followed by identification of the journal or paper that is in line and best suits the objective of the Final Year Project in order to be the validation literature for whatever simulation results to be obtained. With that done, planning of the solution mechanism in CFD to investigate thermodynamic condition of fluid flowing through a supersonic nozzle is done. This includes identifying the most suitable equation of state to reflect the thermodynamics condition, translating the equation of state and its numerical solution method into C programming codes to be

defined as user-defined function in ANSYS FLUENT 12.0. This is then followed by simulation work after defining the most suitable settings that can help study the cas for this Final Year Project and in line with the validation literature. Once that is done, validation of results against journal to confirm and analyse the simulation results is then performed through post-processing in ANSYS FLUENT 12.0 before finally documenting and concluding the scientific work.

3.2 Software

Since this final year project is of simulation work, instead of chemicals, only software will be involved in the project. In this case, state of the art computational fluid dynamics software ANSYS Workbench® and ANSYS FLUENT® has been used. These software are able to model different mesh conditions and allow a good variety of parameter settings suitable for the flow conditions set by user while providing appropriate solution scheme.

Figure 3: Logo of ANSYS Incorporation ***(Retrieved from ANSYS Inc., 2011.)***

ANSYS® Workbench™ was used because it gives an innovative project schematic view that ties together the entire simulation process, guiding the user every step of the way throughout multiphysics analyses (*ANSYS homepage, 2011*). It is also flexible in a sense that many trials and errors can be performed using this software without interrupting another simulation solution trial and updates in any of the software of the platform will immediately be done for all the other related software in the project simulation platform, providing utmost modeling convenience. Within ANSYS Workbench™, Fluid Flow package which includes Design Modeler, ANSYS Meshing and state of the art CFD software ANSYS FLUENT® 12.0 can be activated.

As CFD software, ANSYS FLUENT® provides broad modelling capabilities needed to model flow, turbulence, heat transfer, and reactions for industrial applications. Especially suitable in modelling fluid flow, ANSYS FLUENT® 12.0 is most convenient for this Final Year Project because it allows fluid flow simulations under a good variety of settings that can fit my case, for example turbulence and high

velocity compressible fluid flow can all be simulated. Not to mention, it also allows the use of User Defined Functions (UDF) to introduce equation of state to suit the project purposes, thus producing highly precise results. ANSYS FLUENT 12.0 having a reputation in providing accurate and speedy simulation that are helpful for validation work, proved the choice to be favorable. These software have indeed been of good use throughout this entire Final Year to conduct the study and produce the research results desired most effectively.

3.3 Gantt Chart

With reference to the timeline provided and research methodologies that has been determined, Gantt chart and the key milestones for Final Year Project II is as follows:

No	Details	1-7	8	9	10	11	12	13	14	15
1	Start simulation in CFD software									
2	Submission of Progress Report									
3	Validation of results with literature									
4	Documentation of scientific work									
5	Pre-EDX preparation									
6	Pre-EDX									
7	Dissertation and report writing									
8	Submission of Draft Report									
9	Submission of Dissertation (soft)									
10	Submission of Technical Paper									
11	Oral Presentation									
12	Submission of Project Dissertation									

It is of great delight to say that all of the planned project activities have been carried out right on time with most favorable results and deliverables. Although simulation work has been rather challenging, the progress was good throughout the entire project and the allocated time span listed out in the Gantt Chart also proved itself to be sufficient and appropriate because the work were able to be accomplished and submitted on time.

3.4 Key Milestones and Project Activities

In developing the software module to achieve the project objectives in simulating fluid flow to study thermodynamics in a supersonic natural gas dehydration unit, a general work flow has been followed. Key milestones for this Final Year Project are listed as follows:

- Literature review and identification of validation literature
- Project simulation work
- Post-processing, validation and analysis of results
- Documentation, conclusion and presentation of deliverables

This means that all the above steps should be accomplished before moving on to the next and it also marks the advancement of the project towards completion. Following shows a simple graphical representation of the key project activities executed:

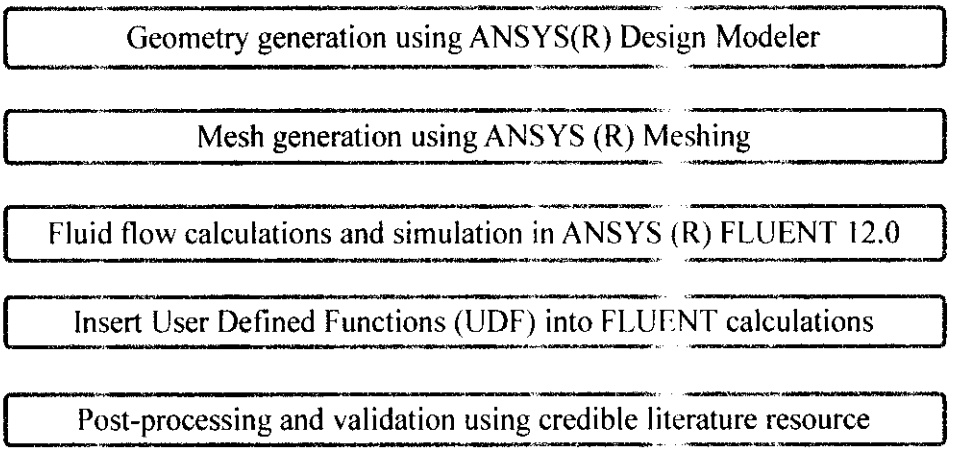

Figure 4: Key project activities

To begin with, ANSYS Workbench™ was activated and tutorial on this software was followed to learn the functions and graphical user interface. Within this software, a platform was set up for the simulation work of my Final Year Project. Following shows a print screen figure of the platform in ANSYS ® Workbench:

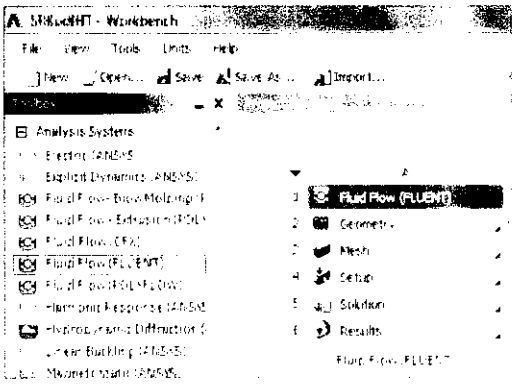

Figure 5: Project schematic view in ANSYS® Workbench™

To generate geometry, ANSYS® Design Modeler was used to specify the dimensions and details of the two dimension symmetrical converging diverging tube with reference to the specification provided by Yang et al. (2009). This work was then followed by tetrahedral mesh generation using ANSYS® Meshing. After setting up the boundary conditions, the meshed geometry was transferred to ANSYS FLUENT® within the ANSYS® Workbench™ platform for CFD calculation setup and solution.

Additional physical models for example turbulence, steady state and axisymmetrical model that are required for calculations in ANSYS FLUENT® are then set up. At the same time, user defined function that gives the equation of state to be introduced to the software was also written in C programming language, interpreted and hooked to the software. Boundary conditions and operating conditions that influence the process are input using the interactive graphical user interface (GUI) as well. This is then followed by setting of solver parameters such as under-relaxation factor, convergence criterion and the most suitable discretization schemes before running the simulation.

For verification, result from ANSYS FLUENT® is first observed graphically. Reasonable plots will be followed by further post-processing steps which include generation of graphical displays showing grids and contours to analyse the reaction results. Otherwise, troubleshooting will begin with observing the convergence of the equations in FLUENT®, and shall continue until a plausible result is obtained.

If results are validated to be plausible and logic according to the journal written by Yang et al. (2009) on the numerical simulation on non equilibrium spontaneous condensation in supersonic steam flow, further work will be done to compare between the efficiency and accuracy of gas models used in the simulation by altering the inlet pressure values, since pressure is of great influence towards the thermodynamics of the system. This is then followed by detailed documentation and conclusion of scientific results. The execution of these project activities basically determined the success of this Final Year Project.

CHAPTER 4

RESULTS AND DISCUSSION

4.1 Governing Equations

Being a fluid flow modelling software, basically ANSYS ® FLUENT 12.0 solves conservation equations to mathematically solve and model transport phenomena in a geometry. In fact, the advantage of this software is that it allows a broad range of mathematical models for transport phenomena for example heat transfer or even chemical reactions.

For all flows, ANSYS ® FLUENT solves conservation equations for mass and momentum. For flows involving heat transfer or compressibility, an additional equation for energy conservation is also solved, which is precisely the case of this Final Year Project. Besides, additional transport equations are also solved when the flow is turbulent. In fact, all these equations were studied as part of this Final Year Project to understand the thermodynamic properties that are influenced and influencing these conservation equations. Therefore, this part of the results will present the understanding about the governing equations that are involved in this project, namely mass conservation, momentum conservation, energy conservation in heat transfer, compressible flow and turbulence.

4.1.1 Mass Conservation Equation

With reference to the ANSYS FLUENT Theory Guide (2009), the equation for conservation of mass, or continuity equation, can be written as follows, applicable for both incompressible and compressible flows:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \vec{v}) = S_m \tag{3}$$

For 2D axisymmetric geometries, the continuity equation is given by

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x}(\rho v_x) + \frac{\partial}{\partial r}(\rho v_r) + \frac{\rho v_r}{r} = S_m \tag{4}$$

(Retrieved from ANSYS FLUENT 12.0 Theory Guide, 2009)

where x is the axial coordinate, r is the radial coordinate, v_x is the axial velocity, and v_r is the radial velocity. In the case where condensation is expected from the supersonic separation, source term S_m can be added to include the influence of mass transfer on the fluid flow. From the equations, we can see that indeed the density of

the fluid flow has a significant influence on the mass conservation equation. Since we are dealing with compressible flow, density changes must be scrutinized.

4.1.2 Momentum Conservation Equation

For 2D axisymmetric geometries, the axial and radial momentum conservation equations are given by

$$\frac{\partial}{\partial t}(\rho v_x) + \frac{1}{r}\frac{\partial}{\partial x}(r\rho v_x v_x) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v_r v_x) = -\frac{\partial p}{\partial x} + \frac{1}{r}\frac{\partial}{\partial x}\left[r\mu\left(2\frac{\partial v_x}{\partial x} - \frac{2}{3}(\nabla \cdot \vec{v})\right)\right] + \frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\left(\frac{\partial v_r}{\partial x} + \frac{\partial v_x}{\partial r}\right)\right] + F_x \tag{5}$$

and

$$\frac{\partial}{\partial t}(\rho v_r) + \frac{1}{r}\frac{\partial}{\partial x}(r\rho v_x v_r) + \frac{1}{r}\frac{\partial}{\partial r}(r\rho v_r v_r) = -\frac{\partial p}{\partial r} + \frac{1}{r}\frac{\partial}{\partial x}\left[r\mu\left(\frac{\partial v_r}{\partial x} + \frac{\partial v_x}{\partial r}\right)\right] + \frac{1}{r}\frac{\partial}{\partial r}\left[r\mu\left(2\frac{\partial v_r}{\partial r} - \frac{2}{3}(\nabla \cdot \vec{v})\right)\right] - 2\mu\frac{v_r}{r^2} + \frac{2}{3}\frac{\mu}{r}(\nabla \cdot \vec{v}) + \rho\frac{v_x^2}{r} + F_r \tag{6}$$

where

$$\nabla \cdot \vec{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_r}{\partial r} + \frac{v_r}{r} \tag{7}$$

(Retrieved from ANSYS FLUENT 12.0 Theory Guide, 2009)

and v_z is the swirl velocity (ANSYS FLUENT Theory Guide, 2009). Here since swirling flow is not included, this term will be zero while the rest of the equation will be solved by FLUENT in transport phenomena calculations.

4.1.3 Energy Conservation in Heat Transfer

For this Final Year Project, the fluid flow involved is one that goes through a Laval nozzle at high Mach number condition and with that, isentropic expansion that leads to rapid cooling is also expected of the compressible flow. Therefore, energy conservation equation must be included in the calculations as well. ANSYS FLUENT solves the energy equation in the following form:

$$\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\vec{v}(\rho E + p)) = \nabla \cdot \left(k_{\text{eff}}\nabla T - \sum_j h_j \vec{J}_j + (\bar{\bar{\tau}}_{\text{eff}} \cdot \vec{v})\right) + S_h \tag{8}$$

(Retrieved from ANSYS FLUENT 12.0 Theory Guide, 2009)

where k_{eff} is the effective conductivity ($k + k_t$, where k_t is the turbulent thermal conductivity, defined according to the turbulence model being used), and J_j is the diffusion flux of species j. The first three terms on the right-hand side of the above equation represent energy transfer due to conduction, species diffusion, and viscous

dissipation, respectively. The term S_h on the right hand side, includes the heat of chemical reaction, and any other volumetric heat sources one defines. However, for this case, energy transfer due to conduction, species diffusion, viscous dissipation and heat of chemical reaction will not be computed since it is not part of the system's conditions. It should also be noted that from the above energy equation:

$$E = h - \frac{p}{\rho} + \frac{v^2}{2} \tag{9}$$

where sensible enthalpy h is defined for ideal gases as

$$h = \sum_j Y_j h_j \tag{10}$$

(Retrieved from ANSYS FLUENT 12.0 Theory Guide, 2009)

Since we are talking about compressible flow, the energy equation above actually also includes pressure work and kinetic energy terms which are often negligible in incompressible flows. For this reason, the pressure-based solver by default does not include the pressure work or kinetic energy when one is solving incompressible flow (ANSYS FLUENT Theory Guide, 2009). Therefore, inclusion of pressure work and kinetic energy in energy equation is actually manually done since my project is simulated with pressure based solver and pressure work and kinetic energy always needs to be accounted for when you are modelling compressible flow.

4.1.4 Compressible Flow

With further reference to the Theory Guide, it has been confirmed that compressibility effects are encountered in gas flows at high velocity and/or in which there are large pressure variations. This means that variation of the gas density with pressure has a significant impact on the flow velocity, pressure and temperature. Compressible flows thereby create a unique set of flow physics for which one must be aware of the special input requirements and solution techniques. Basically, compressible flows can be characterized by the value of the Mach number:

$$\mathrm{M} \equiv v/c \tag{11}$$

Here, c is the speed of sound in the gas given by:

$$c = \sqrt{\gamma RT} \tag{12}$$

(Retrieved from ANSYS FLUENT 12.0 Theory Guide, 2009)

where γ is the ratio of specific heats (cp/cv). As the Mach number approaches 1.0 which is in transonic flow regime, compressibility effects become important. When the Mach number exceeds 1.0, the flow is termed supersonic, and may contain shocks and expansion fans which can impact the flow pattern significantly. This I turn affects the thermodynamic properties of the fluid flow as well. For an ideal gas, these quantities can be related to the static pressure and temperature by the following:

$$\frac{P_0}{P} = exp\left(\frac{\int_T^{T_0} \frac{C_p}{T} dT}{R}\right) \tag{13}$$

For constant Cp, the ideal gas law reduces to

$$\frac{P_0}{P} = \left(1 + \frac{\gamma - 1}{2} M^2\right)^{\gamma/(\gamma-1)}$$
$$\frac{T_0}{T} = 1 + \frac{\gamma - 1}{2} M^2 \tag{14}$$

(Retrieved from ANSYS FLUENT 12.0 Theory Guide, 2009)

These relationships describe the variation of the static pressure and temperature in the flow as the velocity changes under isentropic conditions. Choked flow condition can also be predicted under certain conditions. This choked flow condition will be established at the point of minimum flow area which is usually the throat of a nozzle. As for the conservation equations solved for compressible flow, they are described by the standard continuity and momentum equations solved by ANSYS FLUENT as described in the previous sections. The temperature, T, however will be computed from the energy equation.

4.1.5 Turbulence

For this Final Year Project, turbulence setting was set to be RNG k-ε model. Almost similar to standard k-ε model, RNG model is of refinement, giving more reliable and accurate results for a wider range of flows:

- Has an additional term in its ε equation that significantly improves the accuracy for rapidly strained flows
- Provides an analytical formula for turbulent Prandtl numbers
- Provides an analytically-derived differential formula for effective viscosity that accounts for low-Reynolds-number effects.

Transport equation for RNG k-ε model is as shown below (ANSYS FLUENT Theory Guide, 2009):

$$\frac{\partial}{\partial t}(\rho k) + \frac{\partial}{\partial x_i}(\rho k u_i) = \frac{\partial}{\partial x_j}\left(\alpha_k \mu_{eff} \frac{\partial k}{\partial x_j}\right) + G_k + G_b - \rho\varepsilon - Y_M + S_k \quad (15)$$

Where Gk= generation of turbulence kinetic energy due to the mean velocity gradients; Gb= generation of turbulence kinetic energy due to buoyancy; Y_M= contribution of the fluctuating dilatation in compressible turbulence to the overall dissipation rate; α_k and α_ε are the inverse effective Prandtl numbers for k and ε; Sk and Sε are user-defined source terms.

4.2 Equation of State

Equation of state relates pressure, molar or specific volume and temperature for any pure homogeneous fluid in equilibrium states. The simplest of all is the ideal gas law, which is valid usually for the low pressure gas region of the PT and PV diagrams. Ideal gas behaviour can be expected when

$$P/Pc << 1 \text{ or } T/Tc > 2 \text{ and } P/Pc < 1$$

For incompressible fluid, constant density could be a good option. However, this does not apply to our case. As the speed of the flow approaches the speed of sound, density of the gas will vary from one location to the next therefore we must consider compressibility effects on the gas. Therefore, the real gas model allows us to solve accurately for the fluid flow and heat transfer problems where the working fluid behavior deviate from the ideal-gas assumption (ANSYS FLUENT Theory Guide, 2009). Research results on the equation of state will be discussed here.

Yang et al. (2009) in their numerical simulation used the equation of state reported in the study of Vukalovich, which was tested for extrapolation into supercooled states. This equation of state, utilizing a Virial formulation, is reported to be reliable for both high and low pressure conditions ranging from 0.01 to 100 bar, and over a temperature range of 273.15–1000 K. The steam equation of state used in the study, which relates the pressure to the vapor density and the temperature, is given by:

$$p = \rho_v RT (1 + B\rho_v + C\rho^2_v) \quad (16)$$

(Retrieved from Yang et al., 2009)

where B and C are the second and the third virial coefficients. This formulation however might not be so suitable for complex hydrocarbon system in which this simulation results will be used in the future. ANSYS FLUENT basically provides two real gas options for solving these types of flows: the Aungier-Redlich-Kwong Real Gas Model and NIST Real Gas Models. With reference to the Theory Guide,

the summary of density options available in FLUENT, conditions in which they can be used and suitability for our case of study can be found in Appendix A.

To be highlighted here is that unfortunately none of these equations can be used because the thermodynamic conditions of our supersonic flow system will not be accurate since both models are not suitable for use in two-phase flows where liquid and vapour coexist. With that, a better equation of state must be introduced through user defined functions (UDF) to correct the density changes in FLUENT's calculations. Many equation of state are available for consideration. Their brief descriptions are listed in the table below:

Table 1: Comparison between equation of states

Equation of State	Descriptions
Soave-Redlich-Kwong	• Results will be a cubic equation in P, T, and V. • Solution typically requires an iterative ("trial-and- error") solution. • Serve similar functions as the Redlich-Kwong EOS but require more parameters. • For polar systems, SRK always makes a better prediction. • Suitable in simulating vapour and liquid phase that co-exist. • Proven to be high accuracy in representing thermodynamic conditions in hydrocarbon system and natural gas processes.
Peng-Robinson	• Provides reasonable accuracy near the critical point, particularly for calculations of the compressibility factor and liquid density. • Equation applicable to all calculations of all fluid properties in natural gas processes. • For the most part the Peng–Robinson equation exhibits performance similar to the Soave equation, although it is generally superior in predicting the liquid densities of many materials, especially non-polar ones.
Peng-Robinson-Stryjek-Vera 2	• A subsequent modification published in 1986 (PRSV2) further improved the model's accuracy by introducing two additional pure component parameters to the previous attraction term modification. • PRSV2 is particularly advantageous for vapour-liquid equilibrium calculations
Virial Equation	• The simplest extension of the ideal gas equation where the compressibility factor is assumed to depend on the pressure or the volume. • Reid caution against using this equation for polar compounds (such as water).

The Soave-Redlich-Kwong (SRK) EOS is a cubic equation of state, i.e., third order with respect to volume and density. It is a relatively simple equation with only a few adjustable parameters and it is easily applicable for mixtures and phase-equilibrium calculations. Munkejord et al.'s paper (2009) has demonstrated the usability of SRK in calculating the thermodynamic and transport properties for CO_2-CH_4 mixture. In fact, SRK has always been commended as suitable and able to accurately describe both liquid and vapour phase for hydrocarbon systems. With that, SRK EOS has been chosen to correct the density changes in our mixture system due to supersonic flow conditions. Soave-Redlich-Kwong equation of state and its parameters are given as follows (Soave, 1972):

$$P = \frac{RT}{\tilde{V} - b} - \frac{\alpha a}{\tilde{V}\left(\tilde{V} + b\right)} \tag{17}$$

where the constants a, b, m, and α are determined by:

$$a = 0.42748 \cdot \frac{R T_c^2}{P_c}, \quad b = 0.08664 \cdot \frac{R T_c}{P_c}, \quad \alpha = \left[1 + m\left(1 - \sqrt{T_R}\right)\right]^2, \quad m = 0.48508 + 1.55171 \cdot \omega - 0.1561 \cdot \omega^2$$

(Retrieved from Soave, 1972)

where T=temperature, P=pressure, R= universal gas constant, T_c= critical temperature, P_c= critical pressure, $\tilde{V}$= molar volume and ω= accentric factor.

4.3 Numerical Methods

Since the equation of state to be used is Soave-Redlich-Kwong equation of state, which is a cubic equation, numerical methods must be used to solve it. Many good methods are available but out of the many, Secant Method is chosen and this part of the report will discuss the features, advantages of this method and the application to this project.

Compared to the most common root finding method- Newton Raphson, Secant Method does have its advantages. The Newton-Raphson method of solving a nonlinear equation $f(x) = 0$ is given by the iterative formula

$$x_{i+1} = x_i - \frac{f(x_i)}{f'(x_i)} \tag{18}$$

(Retrieved from University of South Florida, 2011)

Here, the Jacobian matrix is a matrix of the first derivatives of the functions. First, the functions are evaluated at that point to get f_{x0}, then the Jacobian is calculated at that point. Using the above equation, x_1 values are then calculated. These x_1 values

are then used as x_0 values for a new iteration and the whole process is repeated until either the equations converge. However, one of the drawbacks of the Newton-Raphson method is that one has to evaluate the derivative of the function. For cubic equations like PRSV or SRK equation of state, complicated equations such as these may be difficult to differentiate and inconvenient to calculate. This can be a laborious process, and even intractable if the function is derived as part of a numerical scheme. To overcome these drawbacks, the derivative of the function, $f(x)$ is approximated as:

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{x_i - x_{i-1}} \tag{19}$$

Substituting Equation (2) in Equation (1) gives

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})} \tag{20}$$

(Retrieved from University of South Florida, 2011)

The above equation is called the Secant method. This method now requires two initial guesses, but unlike the bisection method, the two initial guesses do not need to bracket the root of the equation, therefore it is not considered as simple bracketing method. Another advantage is that once secant method converges, it will typically converge faster than the bisection method. Geometrically, it can be represented as follows *(University of South Florida, 2011)*:

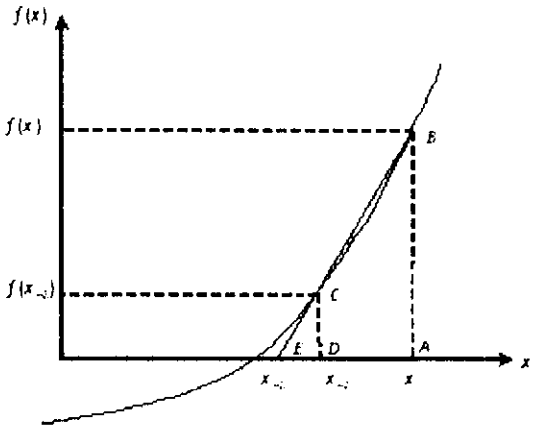

Figure 6: Geometrical representation of the secant method (*Retrieved from University of South Florida, 2011*)

Taking two initial guesses, x_{i-1} and x_i, one draws a straight line between $f(x_i)$ and $f(x_{i-1})$ passing through the x-axis at x_{i+1}. ABE and DCE are similar triangles. Hence,

$$\frac{AB}{AE} = \frac{DC}{DE}; \frac{f(x_i)}{x_i - x_{i+1}} = \frac{f(x_{i-1})}{x_{i-1} - x_{i+1}} \tag{21}$$

On rearranging, the secant method is thereby given as

$$x_{i+1} = x_i - \frac{f(x_i)(x_i - x_{i-1})}{f(x_i) - f(x_{i-1})} \tag{22}$$

(Retrieved from University of South Florida, 2011)

With reference to my case, x refers to the initial guess given to molar volume which is to be calculated from the function $f(x_i)$, which is the Soave-Redlich-Kwong equation of state itself. X_{i-1} on the other hand is the other initial guess determined by a small difference constant set from the beginning of the calculation which is 0.01, denoted by delta in the user defined function.

4.4 User Defined Function

Now that the equation of state and numerical methods for cubic equation solution to be used has been determined, user defined function (UDF) must be used to introduce the equation to FLUENT for solution. UDFs are used for the reaction model import. Basically, UDFs are functions that user programs, which are then dynamically loaded into the ANSYS FLUENT® solver to enhance features of the code.

Here the model specific DEFINE macro used is DEFINE_PROPERTY, used to specify density (ANSYS FLUENT 12.0 UDF Manual 2009). DEFINE_PROPERTY is basically used to specify a custom material property in ANSYS FLUENT for single-phase and multiphase flows. There are three arguments to DEFINE PROPERTY: name, c, and t. Here, the name given is SRK_density while c and t are variables that are passed by the ANSYS FLUENT solver to the UDF.

The UDF will need to compute the real density property only for a single cell and return it to the solver. This is because the function, like source term UDFs, property UDFs (defined using DEFINE_PROPERTY) are called by ANSYS FLUENT from within a loop on cell threads. The solver passes all of the variables needed to allow a DEFINE PROPERTY UDF to define a custom material, since properties are assigned on a cell basis. Consequently, the UDF will not need to loop over cells in a zone since ANSYS FLUENT is already doing it.

Since density is not a constant but is instead a function of the pressure field, to stabilize the pressure solution for compressible flows in ANSYS FLUENT, an extra term related to the speed of sound is also needed in the pressure correction equation. Consequently, the model also included a speed of sound function (ANSYS FLUENT 12.0 UDF Manual 2009). Therefore, my UDF source code shall contain two concatenated functions: a density function named SRK_density that is defined in terms of pressure and a custom speed of sound function named sound_speed. Further discussion on the details of the UDF will be discussed in later sections of this dissertation.

4.5 CFD Solution Scheme in ANSYS® FLUENT 12.0

According to White (2008), if density changes are significant, it follows from the equation of state that the temperature and pressure changes are also substantial. With that large temperature change, energy equation can no longer be neglected. Therefore, solution will now need to include continuity equation, momentum equation, energy equation and equation of state. In fact, all these equations will be solved simultaneously. The flow chart of the solution mechanism identified is shown below:

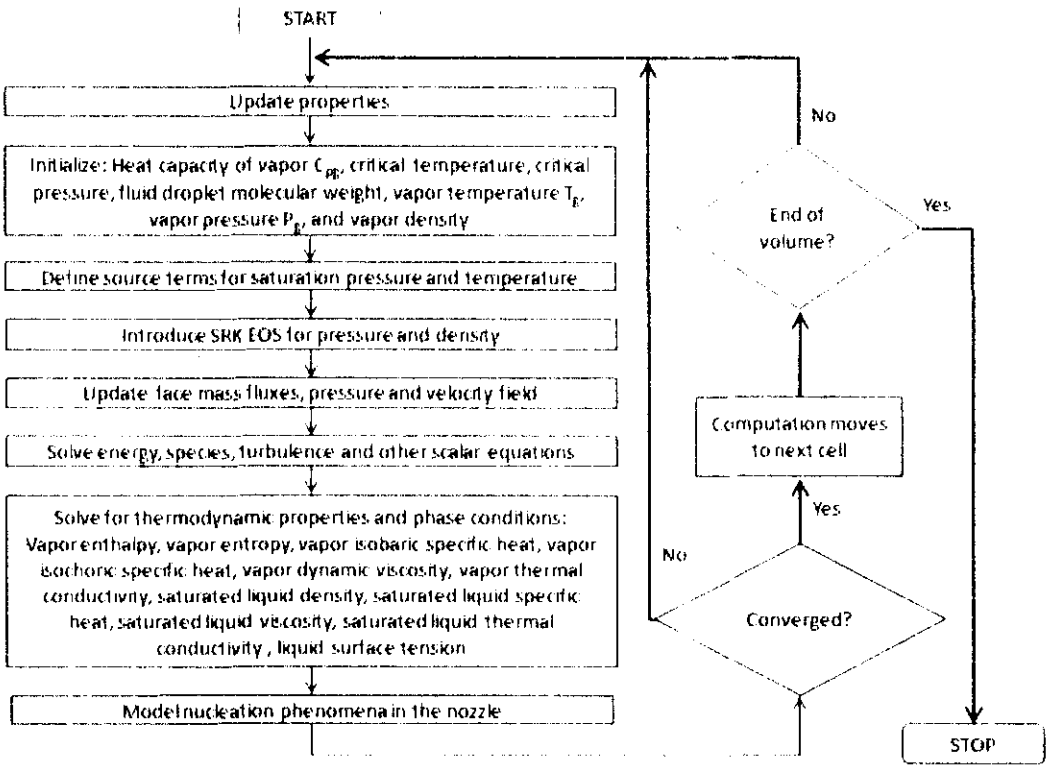

Figure 7: Flow chart of numerical solution in ANSYS FLUENT® 12.0

For the numerical solution in FLUENT, as shown in the flow chart, it starts with updating the properties upon initialization. There, all of the related flow parameters will be initialized based on inputs that are keyed in. Source terms pre-defined in FLUENT will also be used to compute the saturation pressure and temperature, alongside the user defined function which will alter the density property, thus influencing the conservation equations. As mentioned previously, the numerical method employed here is the Secant method. Although the intent of this Final Year Project is focused on investigating dehydration of natural gas and explore its thermodynamic conditions, here a single phase water vapour is being simulated. This less complex system is being used because it will help in possible troubleshooting and in understanding the most fundamental of the thermodynamics condition in the converging-diverging nozzle. This helps to effectively prove the feasibility of the coupling of SRK equation of state that determines density changes due to supersonic flow conditions in the nozzle. Not to mention, this choice is also backed up by Yang et al. (2009) in the validation paper that simulated wet steam system. In other words, validation of the source code containing Soave-Redlich-Kwong equation of state is done against the research paper published by Yang et al. (2009).

4.6 Results

This part of the dissertation will present the results obtained from using Soave-Redlich-Kwong equation of state to determine the density changes in a single phase, compressible water vapor flow system, in validation with Yang et al.'s paper in simulating steam flow through a Laval nozzle. This simulation was done to understand the thermodynamic condition in a supersonic nozzle in order to prove the workability of user-defined function written in C language, for use to study the real conditions in dehydration process from natural gas. Three main deliverables will be presented here, which are:

- Geometry and mesh generated
- User Defined Function written for Soave-Redlich-Kwong equation of state and the corresponding speed of sound function
- Graphical and numerical results and discussion

4.6.1 Geometry and Mesh Generation

Following figure shows the meshed geometry that has been reproduced using ANSYS® Design Modeler and ANSYS® Meshing with the following geometry specifications according with Yang et al.'s (2009) paper:

- Diameter of inlet= 0.05635m *2
- Hydraulic length=0.75m
- Diameter of throat= 0.1m
- Distance from inlet to throat= 0.05m

Following figure gives a graphical representation of the geometry used, which is also the same geometry used by Moore et al. (1973):

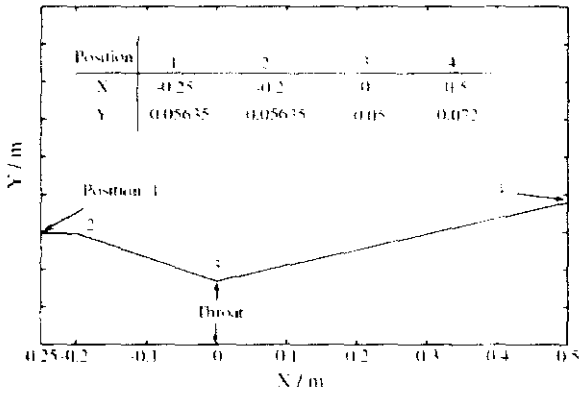

Figure 8: Nozzle geometry as used by Yang et al. (2009)

This following figure on the other hand, shows the geometry and mesh that has been generated for this Final Year Project:

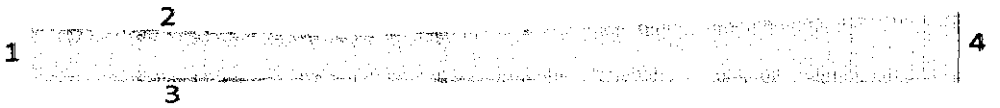

Figure 9: Mesh and geometry

For meshing work, it was done using ANSYS® Meshing software available in ANSYS Workbench. Quadrilateral method was used for the meshing work of this two dimensional geometry and the total mesh number was 4225 cells, which is fine enough for accurate and converging solution yet not too fine that it leads to high computational time. Besides, in terms of edge sizing, bias factor was also utilized in order to have smaller mesh size for boundaries which have higher constraints, which are at the near-wall region and throat region. This was necessary in order to improve computational fluid dynamics calculations and convergence in FLUENT software.

Basically, finer near wall region meshes was required here because near wall region and throat gives higher constrain to the numerical solution and turbulence occurs due to constraints given by the wall towards the fluid flow. Not to mention, near the throat region, expansion was expected to occur rapidly and fluid velocity gradient is very likely to be large. When velocity gradient is large, FLUENT® might take longer solution time because convergence takes longer with the large gradient or divergence might even occur. Therefore, by refining, mesh density is increased at the near wall region and throat while mesh density is decreased at the interior of the pipe, thereby obtaining sufficient information to characterize the gradients in both regions and helps in the numerical solution of conservation equations in FLUENT®. For the boundary conditions and the mesh refinement details, they are listed as follows in accordance to the numbering given in the figure above:

1. Inlet: pressure inlet
    - Bias factor was set to be 5 in order to refine near wall region
2. Outlet: pressure outlet
    - Bias factor was set to be 5 in order to refine near wall region
3. Wall: wall
    - Bias factor was set to be 2 in order to refine throat region
4. Axis: axis

4.6.2 User Defined Function for Soave-Redlich-Kwong Equation of State

For this Final Year Project, in order to study the thermodynamics of natural gas and water mixture flowing through a supersonic nozzle, two comparisons of results were actually made in order to check the suitability of SRK in modeling water vapor through its accuracy of results. The comparisons were between:

- Results of SRK model with results of ideal gas law model
- Results of SRK model with simulation results by Yang et al. (2009)

Despite the fact that ideal gas model can be activated in ANSYS FLUENT's graphical user interface, a user defined function was written in order to test the hooking of user defined function to ANSYS FLUENT and test the transfer of data in order that the same setting may be used for a more challenging UDF which involves SRK equation of state. Here, main discussion will focus on the UDF defining Soave-Redlich-Kwong equation of state. The logic of the user defined function will be explained here. In the density function, basically Soave-Redlich-Kwong equation is

rearranged and put into C language format after its constants have been calculated. Here are the constants used for the SRK model:

- Critical temperature for water (Tcwater)= 647.4K
- Critical pressure for water (Pcwater)= 22119.25kPa
- Accentric factor (omega) for water= 0.344
- Gas constant R= 8.314 m^3.Pa/gmol.K

After defining the necessary parameters which includes specifying the initial guess of the molar volume to be zero and the second initial guess difference to be δ=0.01, basically a 'for' function loop is used to ensure looping or iteration until convergences is achieved numerically with an error difference of 0.001%. Within this 'for' loop, pressure and temperature is actually obtained from the cells in the finite volume using FLUENT macros- C_P(c,t) for temperature and C_T(c,t) for temperature. These macros basically will loop through all the cells in the mesh of the geometry and feedback thermodynamic property values to calculate the density using Soave-Redlich-Kwong equation defined here in this C source code. Constants for SRK defined are listed below:

- m=0.48+(1.574*omega)-(0.176*pow(omega,2))
- alpha= pow(1+m*(1-pow(Tr,0.5)),2)
- a=alpha*0.42748*(pow(R,2))*(pow(Tcwater, 0.5))/Pcwater
- b=0.08664*R*Tcwater/Pcwater

Here, Secant method described previously is used to perform the numerical solution for this UDF. When the condition is fulfilled, 'break' will end the looping process and feed a final value of molar volume to calculate the density. Otherwise, iteration will continue from the top of the codes.

As for the functions related to speed of sound, a simple speed of sound function was used in which the value of pressure and density is obtained from FLUENT using a cell looping macro- C_P(c,t) for pressure and C_R(c,t) for density. The relation of

$$Speed\ of\ sound, a = \sqrt{dp/d\rho} \tag{23}$$

was translated into C language and included in the user defined function file. The user defined function has been tested and worked well through the results obtained which will be show in the coming sections of this dissertation. The source code

written for ideal gas law and Soave-Redlich-Kwong equation of state, which were successfully hooked to FLUENT respectively, can be found in Appendix-C. It should be noted that these codes were rather challenging to produce since it involves many trials and errors into improving and obtaining a result that can be validated with the validation journal. Nonetheless, the user defined functions were indeed successful since it produced the desired results which can be found in the following section.

4.6.3 CFD Simulation Results and Discussion

This section of the dissertation includes all the CFD simulation results and the discussion plus analysis of the results. There are two main parts:

i. Validation of results against the validation literature by Yang et al. (2009) entitled numerical simulation on non-equilibrium spontaneous condensation in supersonic steam flow:
   - The importance of this part of the project is to prove that the written UDF for SRK equation of state is functioning optimally and able to produce reliable results, validated against data provided in published journal.

ii. Comparison of the accuracy of using Soave-Redlich-Kwong equation of state against ideal gas law in simulating the thermodynamic environment in a Laval nozzle under high pressure condition:
   - The importance of this part of the project is to prove the accuracy and reliability of using Soave-Redlich-Kwong, a real gas equation of state to reflect the thermodynamics condition through density property for a high velocity compressible in contrast to ideal gas law.

i. Validation of results against the validation literature by Yang et al. (2009)

To validate the results and accuracy of the UDF source code done, simulation has been carried out in ANSYS FLUENT and compared with that was provided by Yang et al. (2009) in their numerical simulation on non equilibrium spontaneous condensation in supersonic steam flow. Yang et al.'s paper was good because they have completed not only a numerical model but also compared with experimental results, provided not only the geometry that was used, in which was reproduced, but also some graphical plots for validation.

As mentioned earlier, mesh was first generated in ANSYS Workbench using its Design Modeler™ and ANSYS® Meshing. After passing the model to ANSYS® FLUENT 12.0, the solution case was setup. Following shows the general solution setup:

- Pressure based solver
- Steady solver
- 2D axisymmetric
- Energy equation: activated
- Viscous model setting: RNG k-ε with standard wall functions without viscous heating but with pressure term and kinetic term activated for solution of energy conservation equation
- Material: single phase water vapor with varying density determined by Soave-Redlich-Kwong equation of state

To verify the accuracy of results, two comparisons of results were made to prove the workability of the C codes written for Soave-Redlich-Kwong in predicting the thermodynamic behavior of high velocity fluid flow:

- Results of SRK model with results of ideal gas law model
- Results of SRK model with simulation results by Yang et al. (2009)

Here, Table 2 shows the boundary condition setting for the case in discussion:

Table 2: Boundary condition settings

Specifications	Values
Inlet temperature	354.6 K
Inlet Gauge Total Pressure	25000 Pa
Inlet turbulence intensity	5%
Inlet turbulent length scale	0.0085m
Pressure-Velocity Coupling Scheme	SIMPLE
Spatial Discretization	First Order Upwind

Simulation results were most desirable because convergence was actually achieved for the simulations in single phase. This shows that the numerical methods employed in solving the ideal gas law and cubic equation of state are suitable and the numerical solution of all the related conservation equations went well using the solver provided by ANSYS FLUENT 12.0. The assumptions that apply for this modeling work are:

- Effects of condensation are neglected, assuming that the volume fraction of liquid produced is small enough compared to the volume of the water vapour system
- •No swirling effect.
- •Adiabatic

The figures below show that for simulation using ideal gas law, convergence was achieved at 417th iteration while for simulation using Soave-Redlich-Kwong equation of state, convergence was achieved at the 438th iteration.

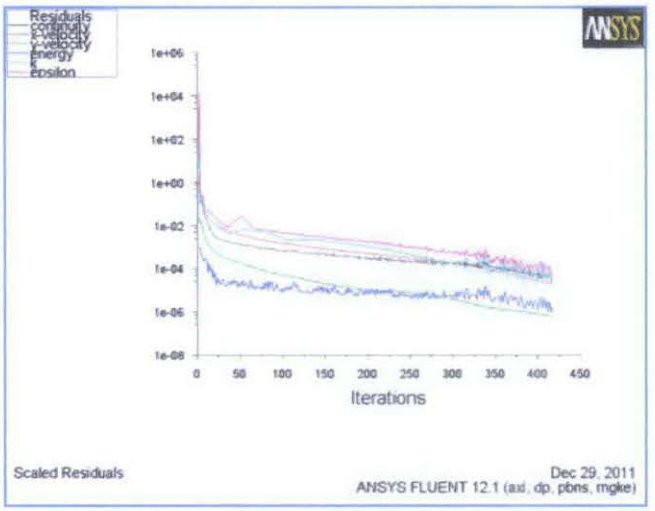

Figure 10: Residual plot for simulation using ideal gas law

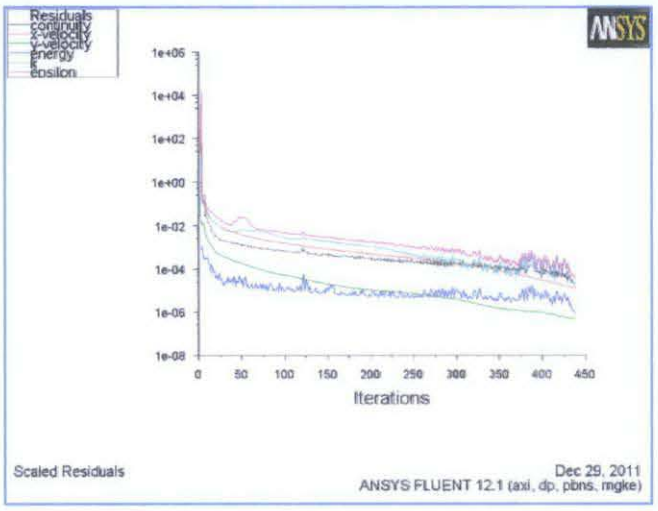

Figure 11: Residual plot for simulation using Soave-Redlich-Kwong equation of state

Following also shows the results of the simulation, showing comparison of the temperature curve between all the models which is most significant because cooling is expected to be observed as a result of isentropic expansion in the Laval nozzle.

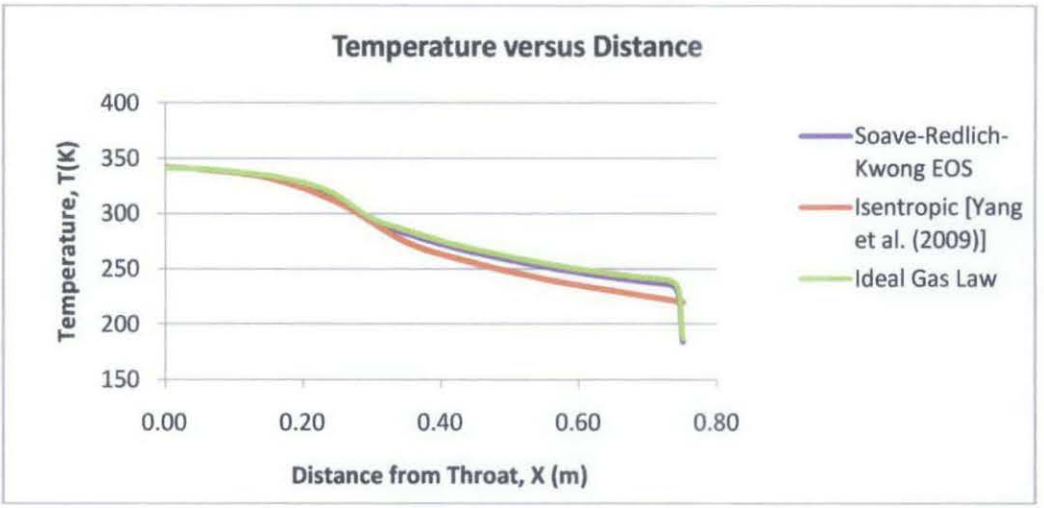

Figure 12: Comparison of temperature profile between isentropic model by Yang et al. (2009), Soave-Redlich-Kwong EOS and Ideal Gas Law

Temperature profile is validated here. This is because when it comes to supersonic turbulence modeling, fluid flow that passes through the converging-diverging part of the nozzle at such a high Mach number will surely experience an isentropic expansion and a super cooling phenomenon. This super cooling phenomenon can therefore be verified through the temperature profile in order to confirm that the flow is indeed in supersonic condition and condensation have possibly occurred. In fact, it is sufficient because temperature profile will rightfully reflect the pressure and density profile as well since they are all thermodynamically related. With relation through the Soave-Redlich-Kwong equation of state, temperature decrease will reflect decrease in pressure and density.

As seen in the above graph, both ideal gas law and Soave-Redlich-Kwong gives a decrease in the temperature profile, which are both agreeable compared to the isentropic temperature profile plot, proving that the user defined functions did a fine job in modeling the density change in the system which in turn determined the cooling effect in the fluid flow through the nozzle. Since my case is also modeling of steam flow, comparison can indeed be made between these models. From the above plot, one can also observe closely that the purple line which reflects the Soave-Redlich-Kwong EOS is slightly closer to the isentropic temperature profile that Yang et al. presented in their paper from simulating wet steam flow. This shows that SRK equation of state could possibly be more accurate in representing this compressible flow at high velocity.

Besides, the fact that results from ideal gas law and SRK equation of state are agreeable with one another without much difference could also be due to the fact that the inlet pressure is rather small which is only at 25kPa. It is expected that results will deviate for the case using ideal gas law once there is a high pressure difference in the fluid flow. This speculation is further verified in the following section.

ii. Comparison of the accuracy of using Soave-Redlich-Kwong equation of state against ideal gas law under high pressure condition

For this part of the project, what was accomplished was the comparison between the performances of using ideal gas law versus Soave-Redlich-Kwong equation of state in modelling a compressible high velocity single phase steam flow. Previously, we have seen that indeed both gas laws were usable and give desirable results regarding the density change and temperature profile of the fluid flow at low inlet pressures. However, here, there is also a need to verify that Soave-Redlich-Kwong equation of state is more suitable for this kind of flow conditions especially at high pressure condition. This is important since the results of this Final Year Project are expected to be applicable when it comes to modelling of a complex system of natural gas containing water. Under real life conditions, natural gas transportation system will be under high pressure condition as well therefore the simulation should be done as close to real life conditions as possible to be deem as reliable.

With that, inlet pressure was actually manipulated alongside under relaxation factors while other boundary conditions are kept constant to study the effects of pressure magnitude on the simulation results using the different thermodynamic models. The pressure magnitudes investigated were:

- 25kPa
- 50kPa
- 100kPa
- 500kPa

The following few pages will show the temperature and density profiles of the fluid flow under the different inlet pressure magnitude and changes, compared between plots from using ideal gas law and simulation done using user defined density using Soave-Redlich-Kwong equation of state. Analysis and discussion will also be done alongside the presentation of results. First, the following Figure 13 and 14 shows the

temperature profile in comparison between ideal gas law and Soave-Redlich-Kwong EOS under different inlet total pressures.

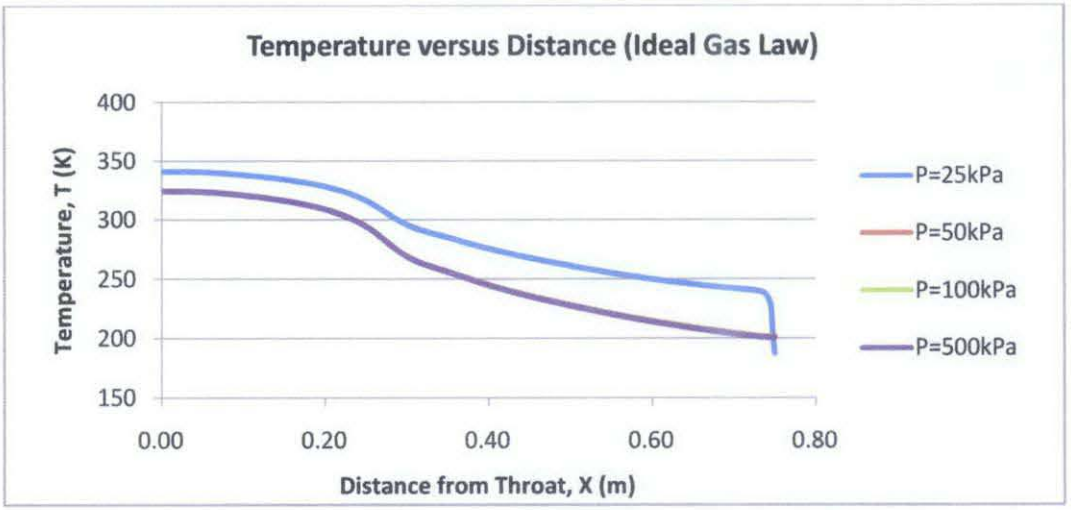

Figure 13: Graph of temperature versus distance using ideal gas law

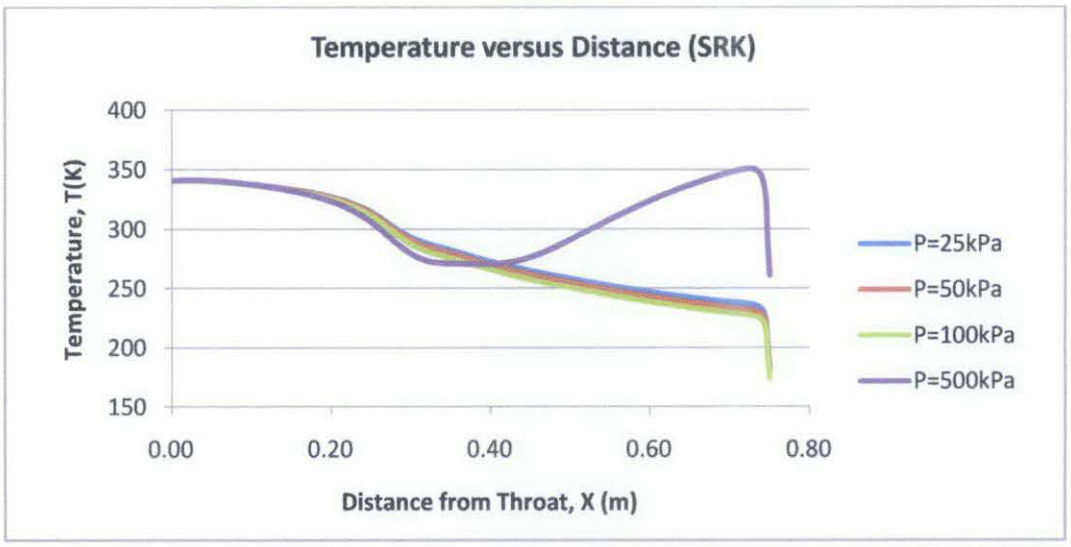

Figure 14: Graph of temperature versus distance using Soave-Redlich-Kwong equation of state

From the temperature profile, we can see that using ideal gas law, once the pressure is above 50kPa, not much temperature changes are observed. By right, the temperature profile should change since inlet pressure magnitude is increased and pressure influences the temperature profile since they are thermodynamically related and are both influenced by density changes resulting from the compressible, high Mach number flow. This shows that ideal gas law might not be able to accurately represent the fluid flow's phase change behaviour once pressure variation is big. However, for simulation using Soave-Redlich-Kwong equation of state, although the changes in temperature is minimal, decrease and differences corresponding to the

change in pressure can be observed. In fact, the influence on the temperature change is even more obvious when inlet pressure is set to be at 500kPa. This gives verification that Soave-Redlich-Kwong equation of state might be better than ideal gas law in predicting phase change and fluid flow behaviour of natural gas-water mixture system under high pressure condition.

The following Figure 15 and Figure 16 now show the density profile.

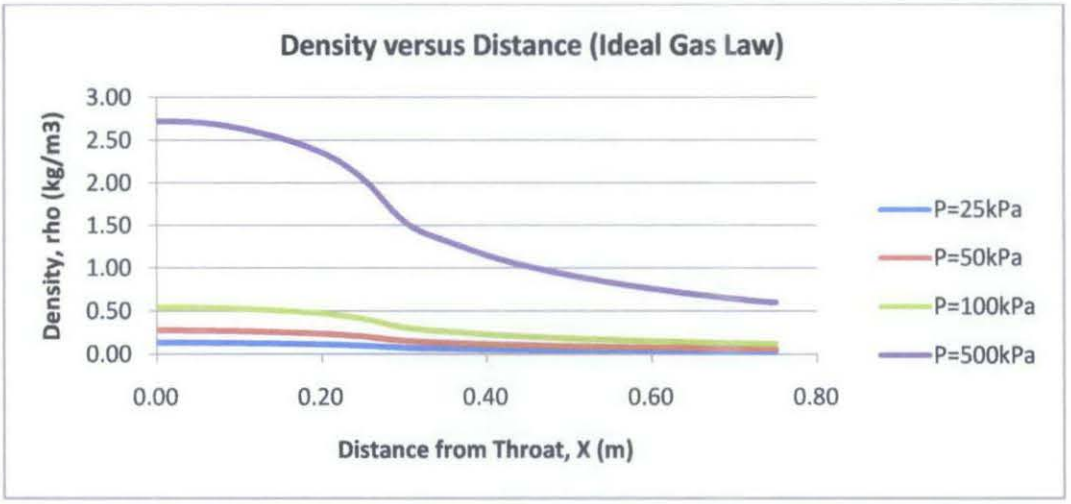

Figure 15: Graph of density versus distance using ideal gas law

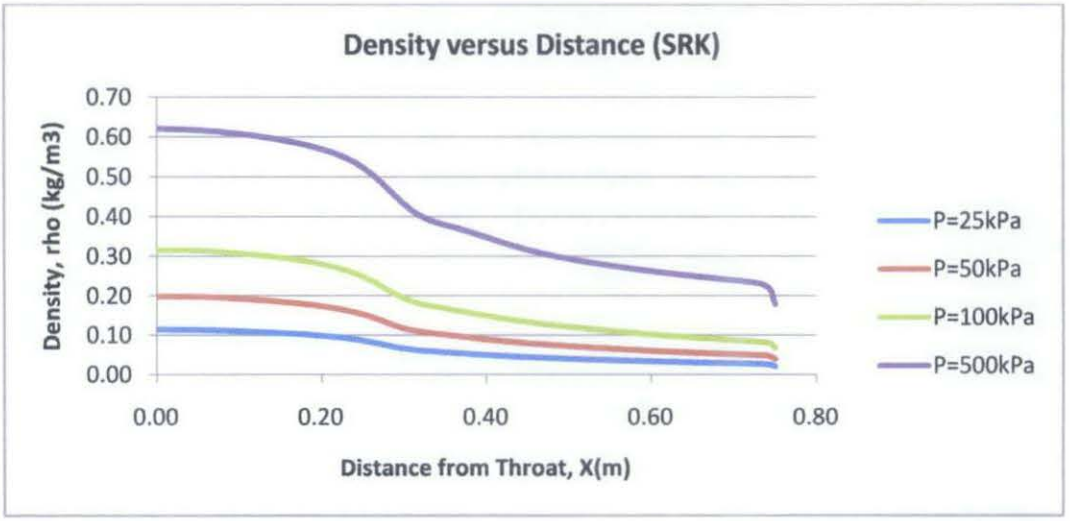

Figure 16: Graph of density versus distance using Soave-Redlich-Kwong equation of state

From the density profile, one can observe a greater deviation in the property when one uses ideal gas law to model the density changes for a compressible high velocity flow. As mentioned previously, density changes cannot be neglected nor assumed constant in a highly compressible flow since it will significantly affect the temperature and pressure of the fluid flow as well. We can observe from the density

profile for modelling using ideal gas law that the density values obtained are deviating further and further away from reality- up till 2.7kg/m^3 as inlet total gauge pressure is increased till 500kPa. This value of density is hardly possible for a single phase water vapour flow since at standard condition density of water vapour is to be around 0.55kg/m^3 only.

In contrast, we can see that the CFD simulation using Soave-Redlich-Kwong equation of state has proven itself to be most reliable for simulation of this type of complex compressible flow under highly turbulent conditions since the density changes computed are not only reasonable- which is around the range of 0.1-0.65kg/m^3 but it also gave an increasing trend as the inlet total gauge pressure is increased, thus proving its reliability for modelling of fluid flow under compressible, high Mach number conditions. This gives much confidence that Soave-Redlich-Kwong equation of state can be employed when it comes to modelling of system involving water vapour phase under high pressure difference conditions, which is the case in natural gas processing processes in the industry.

CHAPTER 5

CONCLUSION & RECOMMENDATIONS

5.1 Conclusion

In conclusion, the objectives of this Final Year Project have indeed been achieved with most desirable deliverables to be presented. In terms of the thermodynamics of the separation of water vapour from natural gas mixture through supersonic separation, it has been identified that indeed, in a compressible, turbulent flow under high velocity approaching supersonic condition, density changes are non negligible. Use of real gas equation to model the density changes that basically affects all the other thermodynamic properties such as temperature and pressure was most appropriate. With that, the fluid flow profile was accurately predicted as well, since isentropic expansion was simulated through the super cooling effects observed from the decrease in temperature and changes in the pressure and density profile along with supersonic velocity observed at the throat region of the converging-diverging nozzle.

A suitable real gas equation of state has also been identified for numerical simulation of water vapour system which will be applicable for simulation of hydrocarbon components, which is the Soave-Redlich-Kwong equation of state that can be solved using Secant Method. The results have been validated with temperature profile of simulation results presented by Yang et al. (2009) with the same dimension and solution setup, thus proving that the solution scheme and user defined function development was successful and can indeed be used to study the thermodynamics of natural gas dehydration. Test on the reliability of using Soave-Redlich-Kwong equation of state for numerical simulation of single phase water vapour compared to ideal gas law in compressible high velocity flow in system with high pressure changes, application to natural gas transportation, has also proven that Soave-Redlich-Kwong equation of state was indeed more accurate and will not deviate at high pressure environment.

In all, this Final Year Project was most successful and the results can surely serve well in understanding dehydration of high pressure natural gas-water vapour system under real gas conditions.

5.2 Recommendations

Further recommendations suggested to continue on issues related to this Final Year Project for further improvement and understanding are:

- Refinement on the mesh quality to improve computational accuracy, along with refinement especially at the most constrained areas of the geometry, which is at inlet, outlet and near wall region. Three-dimension geometry can also be modeled and simulated to further investigate this fluid flow system, nearer to its real life environment.
- Multiphase simulation can be done, along with inclusion of heat of condensation and nucleation process that might have taken place due to the isentropic expansion and rapid cooling at the shockwave region after the nozzle throat. This could help in understanding the non equilibrium thermodynamics and phase changes of this complex fluid flow system.
- Multi-component simulation can be executed as well, which means inclusion of other components available in natural gas mixture such as methane, carbon dioxide or even sulfur and water, to study the effects of concentration of different components on the fluid flow and thermodynamic condition of the system.

All these recommended work will surely help in understanding more about dehydration of natural gas from a thermodynamic point of view.

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APPENDIX

APPENDIX-A: Density Options Available in Pressure Based Solver

Table A1: Density options available in pressure based solver

Density Options	Description	Suitability
Constant	• If density is not to be a function of temperature • For incompressible flow	NO. Flow is compressible
Ideal gas law	For compressible flow that meets the ideal gas law	NO. Ideal gas law is not met since in compressible flow at high Mach number, density changes are not negligible. Ideal gas assumption cannot be used.
Incompressible ideal gas law	• When pressure variations are small enough that the flow is fully incompressible but ideal gas law is to be used to express the relationship between density and temperature. • Density depends only on the operating pressure and no on the local relative pressure field.	NO. Flow is compressible.
Real gas Aungier-Redlich-Kwong	• Can be used to solve problems in the gas and supercritical fluid regimes • Not available for use with fluids in the liquid state, or two-phase flows where liquid and vapour coexist.	NO. Two phase flow where liquid and vapour exists.
Boussinesq equation	For natural convection problems involving small changes in temperature	NO. Not a natural convection problem
Polynomial Piecewise-linear Piecewise-polynomial	When density is a function of temperature, where heat transfer is involved in a natural convection problem.	NO. Not a natural convection problem
User defined	Solve problems in all regimes, as long as appropriate relationships are provided through the User-Defined real gas functions.	YES. Can be employed

APPENDIX-B: Additional Results

Contours for changes of properties in the fluid flow given in ANSYS ® FLUENT 12.0 are shown below:

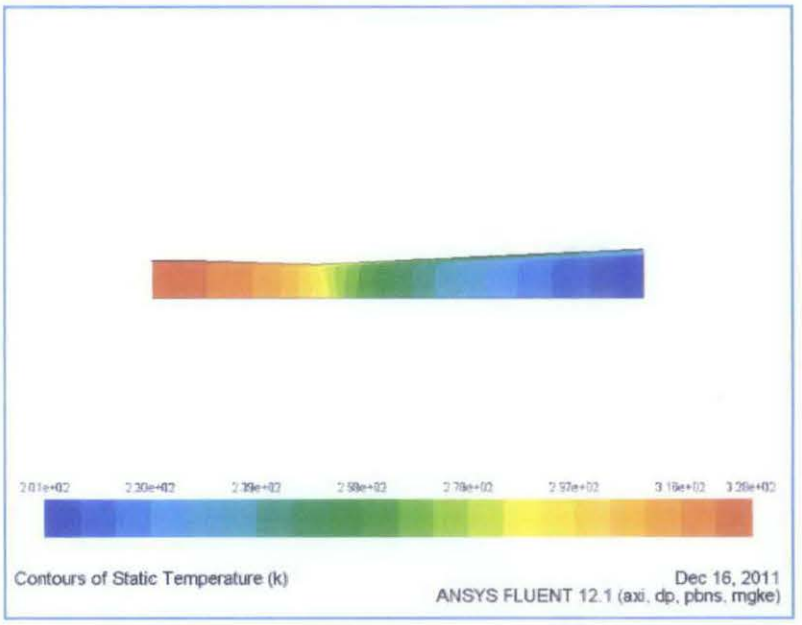

Figure A: Contours of static temperature for simulation using ideal gas law

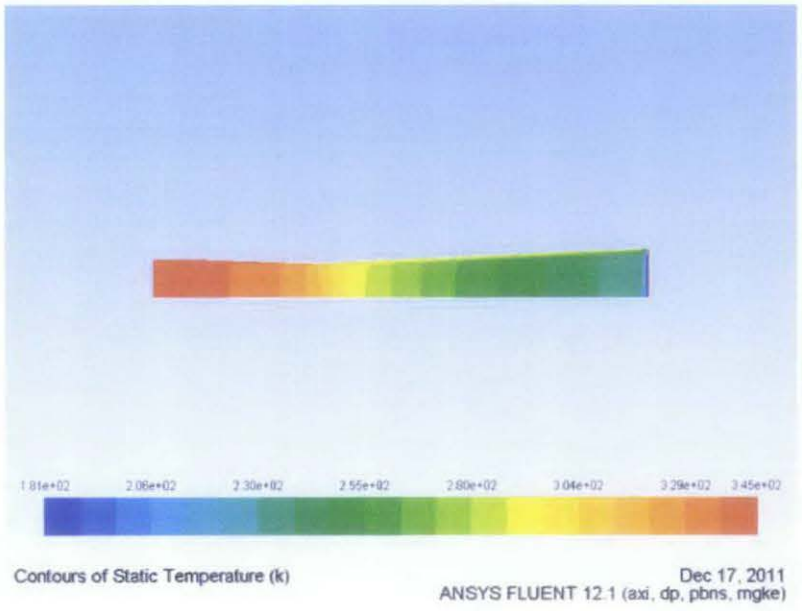

Figure B: Contours of static temperature for simulation using Soave-Redlich-Kwong equation of state

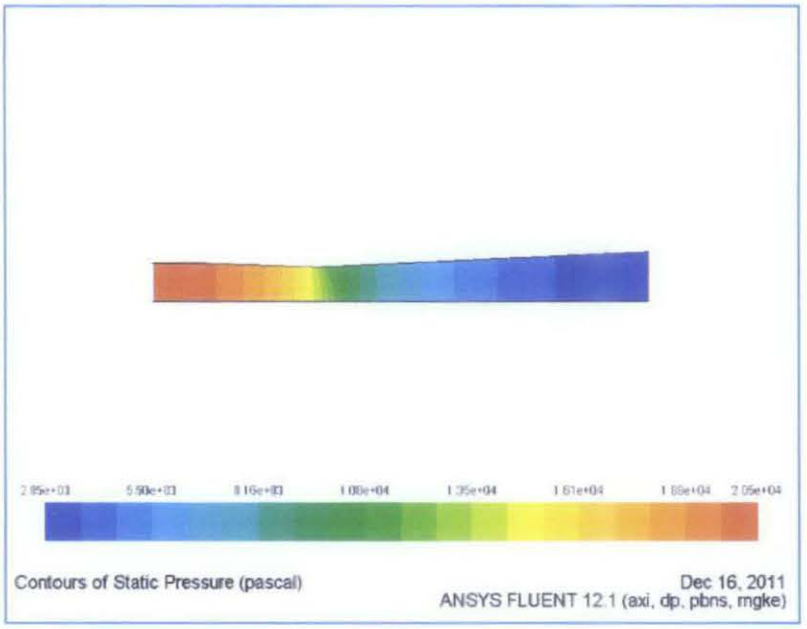

Figure C: Contours of static pressure for simulation using ideal gas law

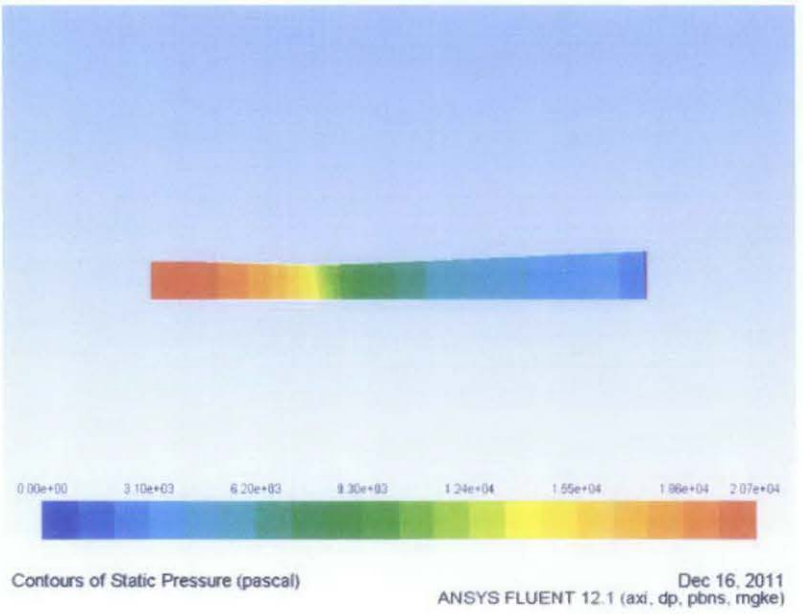

Figure D: Contours of static pressure for simulation using Soave-Redlich-Kwong equation of state

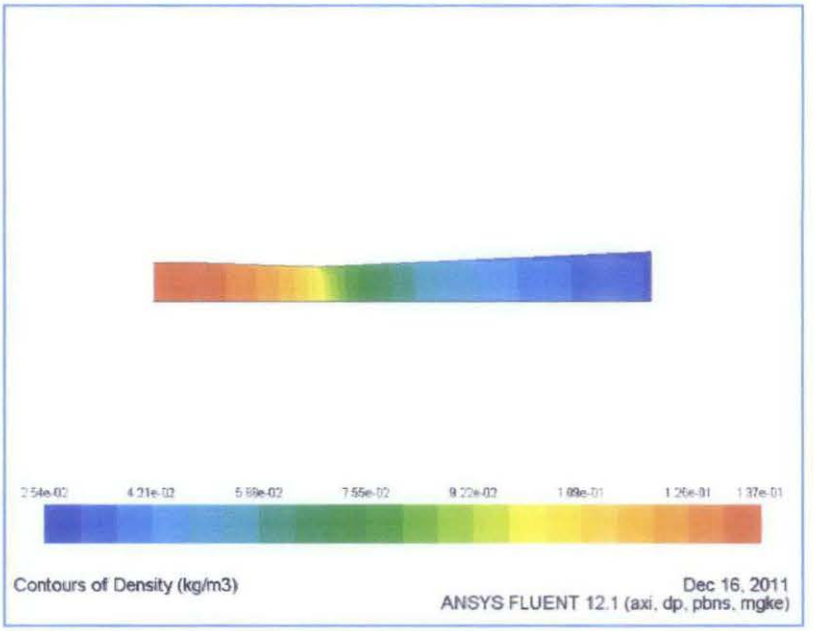

Figure E: Contours of density for simulation using ideal gas law

Figure F: Contours of density for simulation using Soave-Redlich-Kwong equation of state

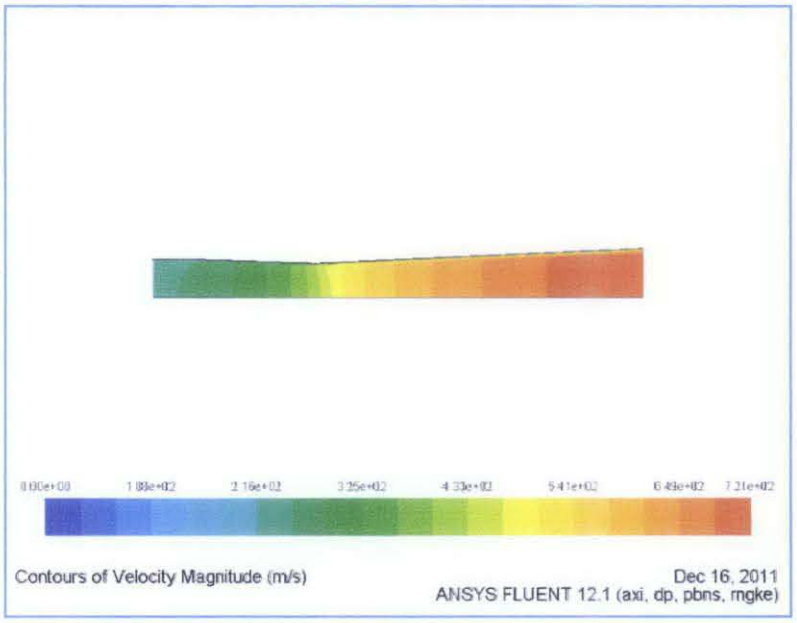

Figure G: Contours of velocity magnitude for simulation using ideal gas law

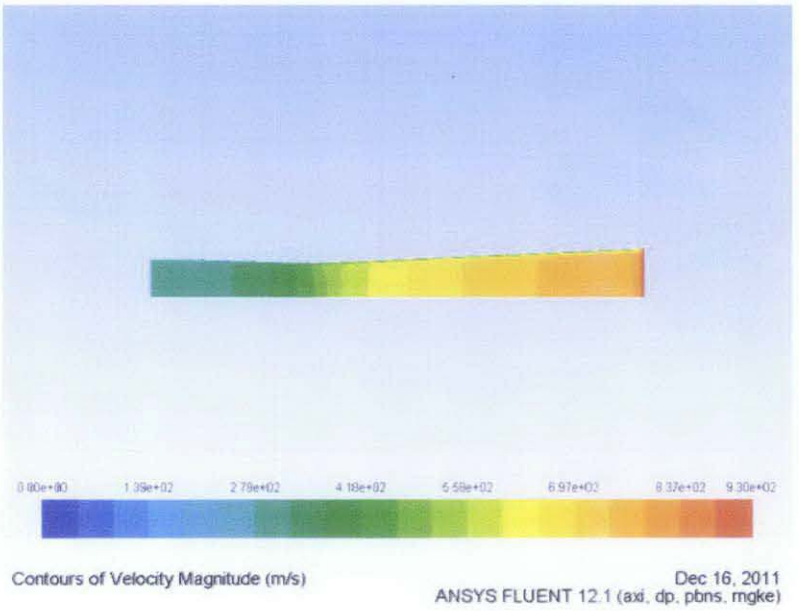

Figure H: Contours of velocity magnitude for simulation using Soave-Redlich-Kwong equation of state

APPENDIX-C: User Defined Function source codes for Ideal Gas Law and Soave-Redlich Kwong equation of state

Following shows the user defined function written for the Ideal Gas Law:

```
DEFINE_PROPERTY(igl_density,c,t)
{
int i;
double rho;
double dp;
double Ftemp;


dp = C_P(c,t);
Ftemp= C_T(c,t);

rho=(dp*18.0)/(R*Ftemp);

return rho;

}



DEFINE_PROPERTY(speed_sound,c,t)
{
double dp, density.
double x,a;


density= C_R(c,t);
dp = C_P(c,t);
x=dp/density;
a=pow(x,0.5);

return a;

}
```

User defined function for use of Soave-Redlich-Kwong equation is needed since this EOS is not readily available to be used in ANSYS FLUENT 12.0 to model density changes that can cater to vapor and liquid phase equilibria. Following shows the source code written in C language and hooked to define the density and speed of sound property in FLUENT:

```
DEFINE_PROPERTY(SRK_density,c,t)
{

int i;
double rho, alpha, a, b, m;
double f, f2, diff;
double Vm,Vm_new, Vm2;
double Tr,dp;
double Ftemp;
double final;
double delta;

Vm_new=0.;
Vm=100.0;
delta=0.01;

for(i=1;i<1000;i++)
{

dp = C_P(c,t);
Ftemp= C_T(c,t);
Tr= Ftemp/Tcwater;

m=0.48+(1.574*omega)-(0.176*pow(omega,2));
alpha= pow(1+m*(1-pow(Tr,0.5)),2);
a=alpha*0.42748*(pow(R,2))*(pow(Tcwater, 0.5))/Pcwater;
b=0.08664*R*Tcwater/Pcwater;

Vm2=Vm+(delta*Vm);
f=(R*Ftemp*Vm)+((a*b*alpha)/Vm)-(dp*pow(Vm,2))+ (dp*(pow(b,2)))+(R*Ftemp*b)-(alpha*a);
f2=(R*Ftemp*Vm2)+((a*b*alpha)/Vm2)-(dp*pow(Vm2,2))+ (dp*(pow(b,2)))+(R*Ftemp*b)-(alpha*a);
Vm_new = Vm-((delta*Vm*f)/(f2-f));
diff= (fabs(Vm-Vm_new)/Vm_new)*100.0;

if(diff >= 0.001)
{
  Vm=Vm_new;
}

else
{
 final=Vm_new;
  break;
}
}
rho= 18.0/final;
return rho;

}

DEFINE_PROPERTY(sound_speed, c,t)
{
real a;
real p, dp;
real density;

dp = C_P(c,t);
density= C_R(c,t);
a = pow((dp/density),0.5);

return a;
}
```