MODELING OF NATURAL GAS DEHYDRATION IN A SUPERSONIC SEPARATOR: CONDENSATION PROCESS

By

MOHD SAFWAN BIN MUHAMAD DIAH
10774

Dissertation submitted in partial fulfillment of the requirements for the

Bachelor of Engineering (Hons)
(Chemical Engineering)

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Universiti Teknologi PETRONAS
Bandar Seri Iskandar
31750 Tronoh

CERTIFICATION OF APPROVAL

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(CHEMICAL ENGINEERING)

Approved by,

(DR. LAU KOK KEONG)

UNIVERSITI TEKNOLOGI PETRONAS
TRONOH, PERAK
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.

MOHD SAFWAN BIN MUHAMAD DIAH

ABSTRACT

The purpose of this report is to provide an overview of the author's Final Year Project. Natural gas, as it is used by consumers, is much different from the natural gas that is brought from underground up to the wellhead. The natural gas used by consumers is composed almost entirely of methane. However, natural gas found at the wellhead, is by no means as pure. The gas commonly exists in mixtures with hydrocarbons, water vapor, hydrogen sulfide (H_2S), carbon dioxide (CO_2), helium, nitrogen and other compounds.

Most of the liquid, free water associated with extracted natural gas is removed by separation methods at or near the wellhead. However, the removal of the water vapor that exists in solution in natural gas requires a more complex treatment. This treatment consists of 'dehydrating' the natural gas, which usually involves one of two processes: either absorption, or adsorption. Absorption occurs when the water vapor is taken out by dehydrating agent while adsorption occurs when the water vapor is condensed and collected on the surface.

The research started with literature review to investigate suitable model to be used, followed with the construction of nozzle geometry with specified meshes. The project describes a conservative two-dimensional compressible numerical model for supersonic spontaneous condensing steam flow based on the classical nucleation theory.

The project aims to model the condensation behavior of liquid water in a supersonic convergent-divergent nozzle separator. Currently, there is no research has been done to study the behavior of the water vapor to water liquid formation and growth in relation with the oil and gas field. Quantitative validation of the numerical model was accomplished and the results showed a good agreement between numerical simulation and the result from published literature.

ACKNOWLEDGEMENT

Throughout the whole period of conducting the Final Year Project, many have provided immeasurable amount of guidance, ideas, assistance, support and advice. Foremost, I am indebted to my supervisor, Dr Lau Kok Keong for the continuous support of my final year project, for his patience, motivation, enthusiasm, and immense knowledge. His guidance helped me in all the time of research and writing of this thesis.

Also to the Final Year Project Coordinators, Dr Lau Kok Keong, Pn. Anis Suhaila Bt Shuib and Dr. Lukman Ismail for providing all the necessary information required to conduct the project.I also want to thanks all the lecturers and staffs of Chemical Engineering Department, Universiti Teknologi Petronas for their cooperation, suggestions and guidance in the compilation and preparation this final year project thesis.

Deepest thanks and appreciation to my parents, family, and others for their cooperation, encouragement, constructive suggestion and full of support for the thesis completion, from the beginning till the end. Also thanks to all of my friends and everyone, that has been contributed by supporting my work and helps myself during the final year project progress till it is fully completed.

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CHAPTER 1

INTRODUCTION

1.1 Background of Study

The dwindling high quality crude oil reserves around the globe have motivated the oil and gas industry to discover natural gas reservoirs in remote areas. Currently, over 95% of natural gas used in the United States moves from well to market entirely via pipelines (American Petroleum Institute, 2011). Natural gas is widely used as it is the cleanest and safest energy sources. Figure 1.1 shows the consumption of natural gas in Malaysia from year 1980 till the year 2009. It can be seen here that natural gas has become an important energy source in Malaysia as the year passes by.

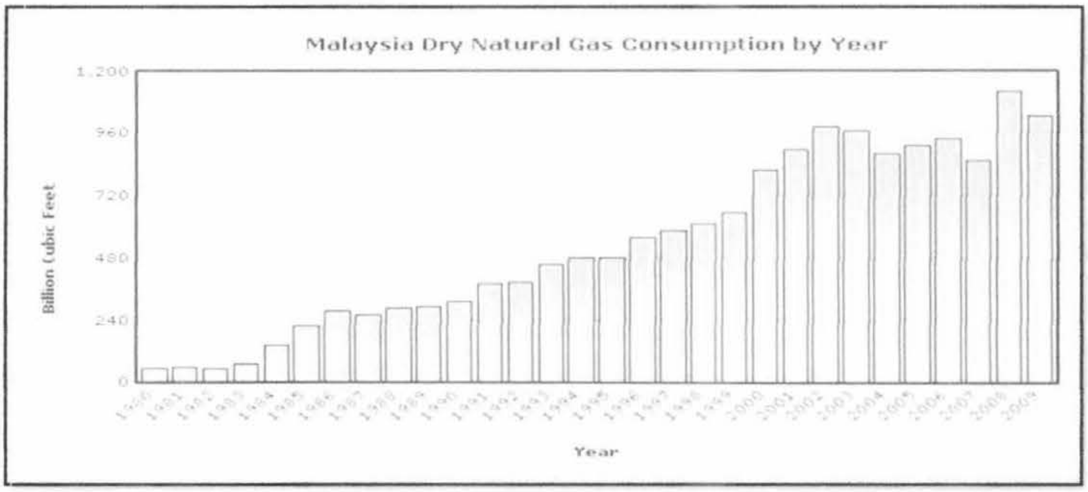


Figure 1.1: Malaysia Dry Natural Gas Consumption by Year
(Taken from Gas Malaysia SDN.BHD)

In order to meet the requirements for a dry, wholly gaseous fuel suitable for transmission through pipelines and distribution for burning by end users, the gas must go through several stages of processing, including separation to avoid the existence of impurities. Current separation techniques are absorption, separation to avoid the existence of impurities. Current separation techniques are absorption, adsorption, and membrane separation. The choice of suitable technology to be used depends on the characteristics of flue gas stream. For an example, absorption process occurs when the water vapor is taken out by dehydrating agent while adsorption occurs when the water vapor is condensed and collected on the surface.

Water is a common impurity in natural gas streams, and removal of it is necessary because water vapor becomes liquid water under low temperature and/or high pressure conditions. The presence of moisture in a pipeline will govern the rate at which corrosion may occur particularly when carbon dioxide and hydrogen sulfide are present in the natural gas. Moreover, the formation of hydrates can reduce pipeline flow capacities, even leading to pipe blockage. Besides, liquid water in a natural gas pipeline potentially causes slugging flow conditions resulting in lower flow efficiency of the pipeline.

The dehydration of water content from natural gas streamline in this research project will focus on the nucleation and growth of liquid water particles due to the supersonic condition in the pipeline that result from the temperature drop of the gas stream. Water vapors from the gas stream condense to water liquid due to the tremendous cooling effect of the pipeline supersonic conditions coupled with de Laval nozzle geometry. 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 water can be formed.

1.2 Research Problem Definition

Natural gas extracted in Malaysia contains high moisture content. However, the natural gas demand from most industries requires clean and pure natural gas. Hence, separation of water content from natural gas is needed to meet this requirement. Current technology used in industrial to remove the water vapour in natural gas is not efficient whereby it can only extract a small percentage of water content from the gas but the demand for clean and pure bulk natural gas is increasing.

The current separation techniques are absorption and membrane separation. The setbacks are they occupy large floor space, high maintenance thus will leads to high capital cost. Compactness of production systems is the most challenging design criteria for offshore applications whereby the available space is limited.

In this research project, a fresh method of separation is proposed - separation using high centrifugal force or known as Cryogenic process is able to overcome some of the disadvantages as it does not involve any chemicals or catalyst. In addition, the equipments required are simple and small compared to the equipments of membrane and adsorption technology.

This project is addressing the supersonic separation of natural gas as it passing through a converging-diverging nozzle that travels at supersonic flow and having swelling effect. As the fluid flows through the nozzle-expander, the water vapour will condensed and separated while the methane will be dehydrated. Before the prototype is build, the feasibility of this separation technique needs to be studied first.

Modeling of cryogenic separation for high water content in natural gas field should consider nucleation and growth model. However, most fluid dynamics simulation processes do not take into account the nucleation and growth rate of a particle. This research will be now focusing on how to develop and incorporate nucleation model into FLUENT simulator to investigate the nucleation and growth distribution and behavior.

1.3 Objectives of the Study

The objectives of the study are:

- To incorporate condensation model into Computational Fluid Dynamic
- To simulate natural gas flow through De Laval nozzle (supersonic separator)
- To validate the results of particle nucleation predicted by the developed models with other results obtained from published literature.

1.4 Scope of Study

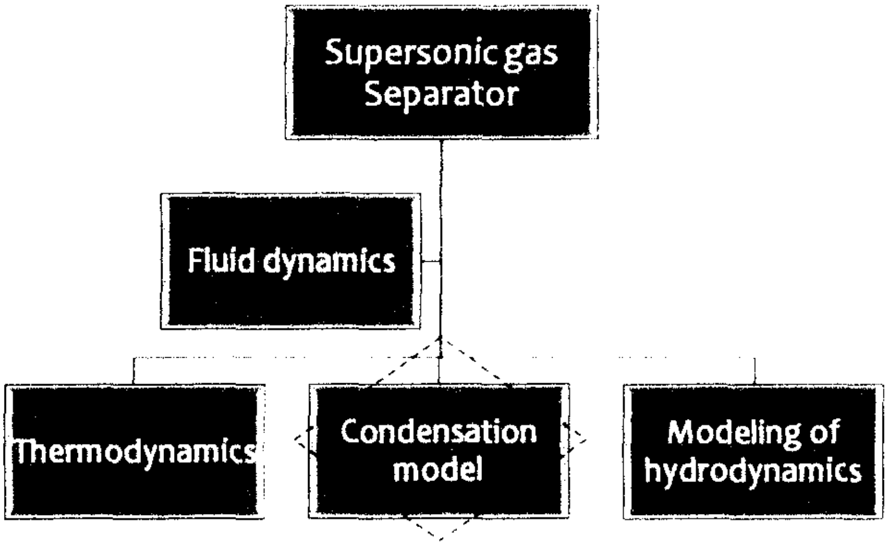


Figure 2.2: Scope of study

The case studies are mainly about cooling and condensation of a mixture of water vapor and natural gas in supersonic gas processing separator technology. Classical nucleation and growth theory will be applied extensively to model the condensate formation and growth of particles under supersonic conditions.

The software used in this research is Ansys Fluent 12.0. The model can be drawn in any shape, depends on the real model in Ansys workbench-geometry. The file is exported as mesh file and is opened in fluent whereby it simulate the separation process thus giving the solutions and results as what needed.

CHAPTER 2

LITERATURE REVIEW

2.1 Introduction

As water possesses unique thermodynamic properties, it is important to study and understand its properties on how the phase changes with different operating conditions. Water, H_2O is a chemical compound of two oxygen atoms covalently bonded to a single hydrogen atom. It appears as liquid phase at standard temperature and pressure

Figure 2.1 taken from (David Mogk, Montana State University) shows the phase diagram of water. It shows that at low temperature, (solid) ice is the stable phase. At moderate temperatures and high pressure, (liquid) water is the stable phase, and at high temperature and low pressure, (gas) vapour is the stable phase. The sublimation curve separates the solid from the gas. This line indicates the vapour pressure of ice as a function of temperature. Note that the vapour pressures for ice and water at 273 K (0°C) are the same 4.579 mm Hg (torr). At this temperature, all the three phases (ice, water and vapor) coexist.

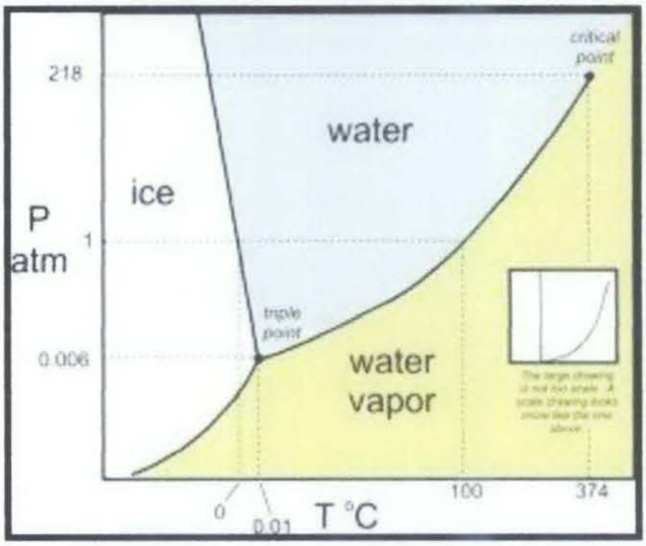


Figure 2.1: Pressure-Temperature phase diagram for H_2O
(Taken from David Mogk, Montana State University)

At temperature greater than 647 K, water cannot be liquefied. The fluid shares the properties of gas. Thus no vapor pressure beyond this temperature is measured. The temperature of 647 K is called the critical temperature, and the vapor pressure at this temperature is called the critical temperature. The melting curve or fusion of ice/water is very special. It has a negative slope due to the fact that when ice melts, the molar volume decreases. Ice actually melts at lower temperature at higher pressure (D.A. Simpson, 2005).

One feature of the diagram is the boiling line separating liquid and gaseous water ends at one point. At high enough pressure, the distinction between liquid and gas gets lost – essentially, the difference in density between gas and liquid becomes zero, and the latent heat of condensation/ evaporation vanishes. The end point of the boiling line, marked by the grey dot, is called the critical point. If temperature and pressure can be chosen such that the fluid is very close to the critical point, it will develop bubbles of gas containing small droplets of liquid.

2.2 Dehydration Methods

Removal of water from natural gas can be achieved by several alternatives methods, which are discussed in the following part

2.2.1 Adsorption of Water by a Solid

Adsorption is the adhesion of atoms, ions, bio molecules or molecules of gas, liquid, or dissolved solids to a surface. This process creates a film of the adsorbate (the molecules being accumulated) on the surface of the adsorbent. It differs from absorption, in which a fluid permeates or is dissolved by a liquid or solid. The term sorption encompasses both process, while desorption is the reverse of adsorption. It is a surface phenomenon.

i. Calcium chloride

Calcium Chloride ($CaCl_2$) is a bulk chemical widely used throughout industry. Calcium chloride is quite often referred as a desiccant, which is a substance that promotes drying to dehydrate natural gas but is more accurately describe as a deliquescent as it will eventually turn to liquid id it is absorbs enough moisture. It will dissolve in its own lattice structure of the resulting hydrate, leaving a puddle of liquid when left in contact (Johannes Bruining, 2007).

As water absorption continues, brine solution will be formed. In this unit calcium chloride pellets are placed in a fixed bed. The units might show poor performance under some conditions if $CaCl_2$ pellets bond together and form a solid bridge in the tower. These units produce a waste stream that has to be taken care of appropriately. The reaction to produce $CaCl_2.2H_2O$ (calcium chlorides dehydrate) from anhydrous $CaCl_2$ is really exothermic. The dehydrate is much more thermodynamically favourable, and more likely to exist.

There are at least 4 levels of hydration of Calcium Chloride – 1, 2, 4 and 6-hydrate. As water is absorbed, the hydration level increases until the Calcium Chloride will dissolve and become a highly concentrated liquid.

ii. Activated alumina

Activated alumina is manufactured from aluminium hydroxide by dehydroxylating it in a way that produces a highly porous material. This material yields a surface area of between 120-250 square meters per gram of material. Activated alumina does not soften or disintegrate when immersed in liquids. A high internal surface area through the presence of pores or micropores is necessary to create adsorption sites.

Alumina is used as desiccants because it possesses both high water adsorption capacities as well as favourable water adsorption isotherm shapes. Also it is alkaline and cannot be used in the presence of acid gases, or acidic chemicals used for well treating (Yan-Hui Li, 2003). The tendency to adsorb heavy hydrocarbons is high, and it is difficult to remove these during regeneration. It has good resistance to liquids, but little resistance to disintegration due to mechanical agitation by the flowing gas.

2.2.2 Absorption of Water in Glycols

In glycol dehydration, a liquid desiccant dehydrator serves to absorb water vapour from the gas stream. Glycol the principal agent in this process has a chemical affinity for water. This means that, when in contact with a stream of natural gas that contains water, glycol will serve to 'steal' the water out of the gas stream.

Essentially, glycol dehydration involves using a glycol solution, usually either diethylene glycol (DEG) or triethylene glycol (TEG), which is brought into contact with the wet gas stream in what is called the 'contactor'. The glycol solution will absorb water from the wet gas. Once absorbed, the glycol particles become heavier and sink to the bottom of the contactor where they are removed. The natural gas, having been stripped of most of its water content, is then transported out of the dehydrator.

The treated gas leaves the top of the absorber; the spent ethanolamine glycol mixture enters the reactivator tower, where heat drives off the absorbed acid gases and water. This technology needs a large facility and due to the need for glycol, it is a possibility for some operational problems such as corrosion, foaming in contactor device, fouling of heat transfer surfaces, glycol contamination and loss.

2.2.3 Membrane Separation

In membrane separation technology feed stream into two effluent streams-the permeate and the concentrate. The stream that is rejected by the membrane is called as concentrate whereas the liquid that passes through the semi-permeable membrane is called as permeate. Current membranes used for natural gas separation applications are produced as hollow fibers or flat sheets packaged as spiral-wound modules Hollow-fibres modules allow large areas of membrane to be packaged into compact membrane molecule

Membrane separation is relatively expensive (especially for large gas flow rates) and can be easily fouled by gas contaminants. They also need high pressure for efficient operation. However, they have a low-pressure drop through the process and do not need any chemical reagents. The installation and change of the membrane cartridges are relatively easy and the maintenance cost is low. The membrane's capability to remove water vapour is not selective and part of the gas is always wasted through co-permeation.

Separation through membrane takes place by either convection or diffusion. Transportation is affected by using electric field or by using pressure or temperature gradient. The thickness of the membrane varies from 100 micron to several mms. It is the application that decides the type of the membrane to be used.

2.3 The Cryogenic Expansion Process

Cryogenic processes are also used to extract water vapour and light hydrocarbons from natural gas. While absorption methods can extract almost all of the heavier hydrocarbons, the lighter hydrocarbons and water vapour are often more difficult to recover from the natural gas stream. However, if it is economic to extract ethane and other lighter hydrocarbons, cryogenic processes are required for high recovery rates. Essentially, cryogenic processes consist of dropping the temperature of the gas stream to around 120 degrees Fahrenheit.

There are a number of different ways of chilling the gas to these temperatures, but one of the most effective is known as the turbo expander process. In this process, external refrigerants are used to cool the natural gas stream. Then, an expansion turbine is used to rapidly expand the chilled gases, which causes the temperature to drop significantly. This rapid temperature drop condenses ethane and other hydrocarbons in the gas stream, while maintaining methane in gaseous form. This process allows for the recovery of about 90 to 95 percent of the ethane originally in the gas stream. In addition, the expansion turbine is able to convert some of the energy released when the natural gas stream is expanded into recompressing the gaseous methane effluent.

2.4 Joule -Thomson Effect

Joule-Thomson effect is also known as the Joule-Kelvin effect. When a gas expands through a porous plug, a change of temperature occurs, proportional to the pressure difference across the plug. The Joule-Thomson coefficient is the change of temperature per unit change of pressure. The temperature change is due to a departure of the gas from Joule's law, the gas performing internal work in overcoming the mutual attractions of the molecules and thus cooling itself and partly to deviation of the gas from Boyle's law.

The latter effect can give rise either to cooling or heating, depending upon the initial temperature and pressure difference used. For a given mean pressure, the temperature at which the two effects balance, resulting in no alteration of temperature is called the inversion temperature. Gasses expanding through a porous plug below their inversion temperature are cooled otherwise they are heated. Joule-Thomson cooling occurs when a non-ideal gas expands from high to low pressure at constant enthalpy. The effect can be amplified by using the cooled gas to pre-cool the incoming gas in the heat exchanger.

In practice, the Joule-Thomson effect is achieved by allowing the gas to expand through a throttling device (usually a valve) which must be very well insulated to prevent any heat transfer to or from the gas. No external work is extracted from the gas during the expansion. Only when the Joule-Thomson coefficient for the given gas at the given temperature is greater than zero can the gas be liquefied at that temperature by the Linde cycle. In other means, a gas must be below its inversion temperature to be liquefied by the cycle.

2.5 Supersonic Flow

Supersonic speed is a rate of travel of an object that exceeds the speed of sound (Mach 1). Sounds greater than five times the speed of sound (Mach 5) is often referred to as hypersonic. In natural gas, the value required for an object to be travelling at a supersonic speed is approximately 460 m/s. Supersonic flow behaves very differently from subsonic flow. Fluids react to differences in pressure; pressure changes are how a fluid is "told" to respond to its environment.

Sounds are travelling vibrations (pressure waves) in an elastic medium. In gases sound travels longitudinally at different speeds, mostly depending on the molecular mass and temperature of the gas (Chuang wen, 2010). In water at room temperature, supersonic can be considered as any speed greater than 1,440 m/s (4,724 ft/s). In solids, sound waves can be longitudinal or transverse and have even higher velocities. Supersonic fracture is crack motion faster than the speed of sound in a brittle material.

2.6 De Laval Nozzle

A de Laval nozzle or converging – diverging nozzle as in Figure 2.2 below taken from (en.citizendium) is a tube that is pinched in the middle, making a carefully balanced, asymmetric hourglass-shape. It is used to accelerate a hot, pressurized gas passing through it to a supersonic speed, and upon expansion, to shape the exhaust flow so that the heat energy propelling the flow is maximally converted into directed kinetic energy. Because of this, the nozzle is widely used in some types of steam turbines.

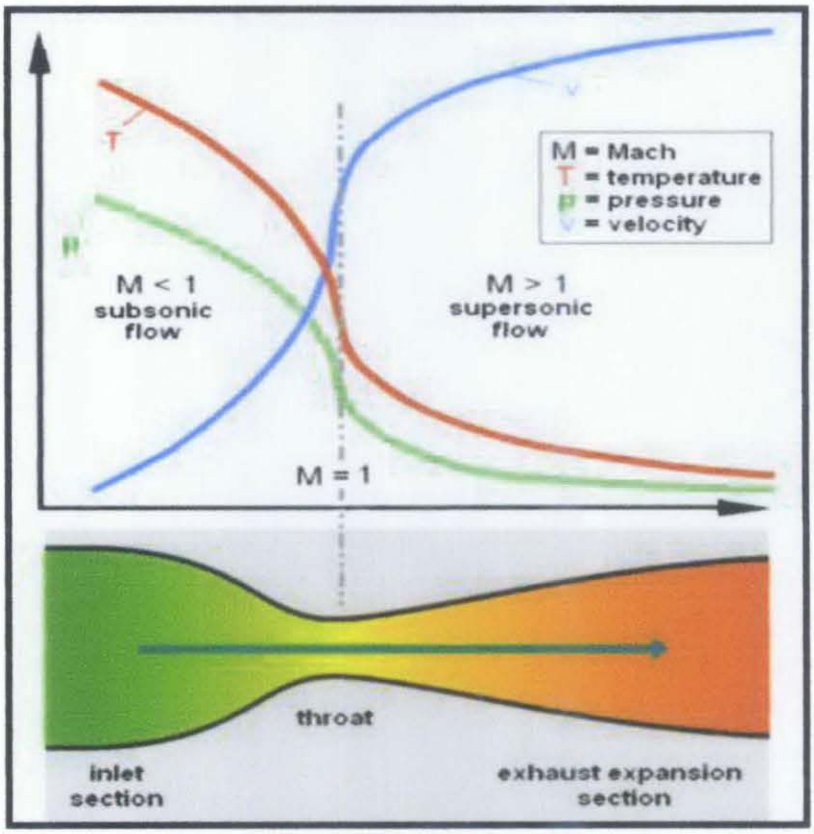


Figure 2.2: Graph of velocity, temperature and pressure with the flow across nozzle (*Taken from en.citizendium*)

Its operation relies on the different properties of gases flowing at subsonic and supersonic speeds. The speed of a subsonic flow of gas will increase if the pipe carrying it narrows because the mass flow rate is constant (P. Jain, 2003). The gas flow through a de Laval nozzle is isentropic (gas entropy is nearly constant). At subsonic flow the gas is compressible; sound, a small pressure wave, will propagate through it. At the "throat", where the cross sectional area is a minimum, the gas velocity locally becomes sonic (Mach number = 1.0), a condition called choked flow. As the nozzle cross sectional area increases the gas begins to expand and the gas flow increases to supersonic velocities where a sound wave will not propagate backwards through the gas as viewed in the frame of reference of the nozzle (Mach number > 1.0).

De Laval nozzle will only choke at the throat if the pressure and mass flow through the nozzle is sufficient to reach sonic speeds, otherwise no supersonic flow is achieved and it will act as a Venturi tube; this requires the entry pressure to the nozzle to be significantly above ambient at all times (equivalently, the stagnation pressure of the jet must be above ambient).

In addition, the pressure of the gas at the exit of the expansion portion of the exhaust of a nozzle must not be too low. Because pressure cannot travel upstream through the supersonic flow, the exit pressure can be significantly below ambient pressure it exhausts into, but if it is too far below ambient, then the flow will cease to be supersonic, or the flow will separate within the expansion portion of the nozzle, forming an unstable jet that may 'flop' around within the nozzle, possibly damaging it.

2.7 Supersonic Separator

The Twister Supersonic Separator is a unique combination of known physical processes combining aero-dynamics, thermo-dynamics and fluid-dynamics to produce an innovative gas conditioning process. Condensation and separation at supersonic velocity is the key to achieving a significant reduction in both capital and operating cost.

The simplicity and reliability of Twister technology enables de-manned, or not normally manned, operation in harsh onshore and offshore environments and is expected to prove to be a key enabler for sub-sea gas processing (Dr. Fred T. Okimoto, 2000). In addition, the compact and low weight Twister system design enables de-bottlenecking of existing space and weight constrained platforms. The diagram of twister supersonic is shown below in Figure 2.3.

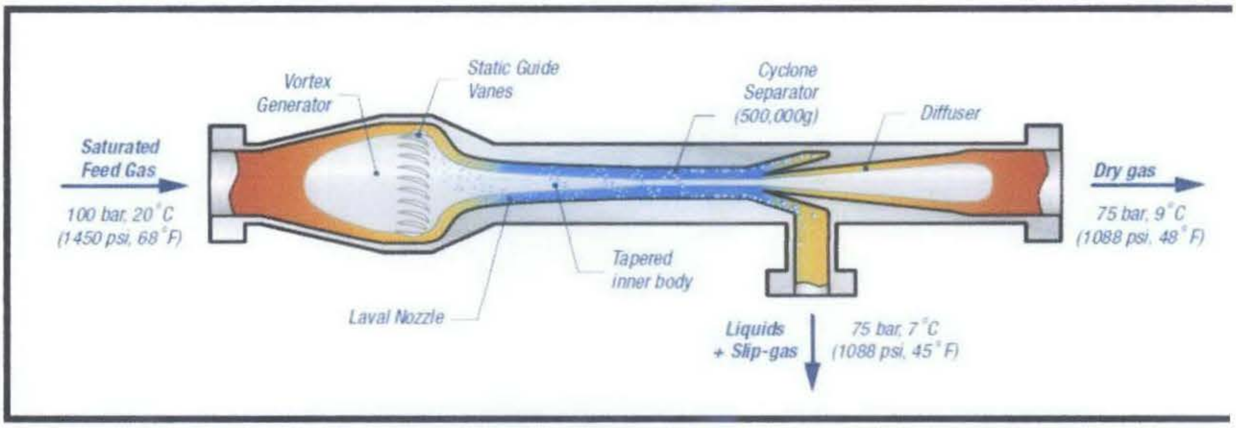


Figure 2.3: Twister supersonic separator (*Taken from Twister®BV homepage*)

The Twister Supersonic Separator has thermodynamic similar to a turbo-expander and combines the following process steps into a compact, tubular device:

- Expansion
- Cyclonic gas/liquid separation
- Re-compression

Twister achieves temperature drop by transforming pressure to kinetic energy. The centrifugation force generated by the cyclonic flow in the twister can go up to 500,000g in order to achieve supersonic flow and swelling effect (Johannes Bruining, 2007). A laval nozzle is used to expand the saturated feed gas to supersonic velocity, which results in a low temperature and pressure. This results in the formation of a mist of water and hydrocarbon condensation droplets (Dr. Fred T. Okimoto, 2000).

The high vorticity swirl centrifuges the droplets to the wall. The liquids are split from the gas using a cyclonic separator. The separated streams are slowed down in separate diffusers, typically recovering 70-75 % of the initial pressure. The liquid stream contains slip-gas, which will be removed in a compact liquid de-gassing vessel and recombined with the dry gas stream. For Natural Gas Liquid recovery applications, the gas will typically expand to around 20% of the feed pressure mid-Twister and recompress to around 50-65% of the gas feed pressure when exiting the tube.

The Twister^{TM} Supersonic Separator efficiently condenses and separates water and hydrocarbons from natural gas in a chemical free, environmentally-friendly, safe, compact process with minimal operating cost as no moving parts are required in the Twister tube. Twister gas conditioning technology offers the solution of unmanned operation for offshore dehydration facilities, which is not only a cost-effective solution but also a safe and environmentally friendly alternative, whilst eliminating many of the flow assurance risks and limitations involved with Wet Gas Evacuation

2.8 Navier-Stokes Equations

Navier-stokes equations describe the motion of fluid substances. These equations arise from applying Newton's second law to fluid motion, together with the assumption that the fluid stress is the sum of a diffusing viscous term (proportional to the gradient of velocity), plus a pressure term. The Navier–Stokes equations dictate not position but rather velocity (Beam, 1977). A solution of the Navier–Stokes equations is called a velocity field or flow field, which is a description of the velocity of the fluid at a given point in space and time. Once the velocity field is solved for, other quantities of interest (such as flow rate or drag force) may be found.

The Navier–Stokes equations are nonlinear partial differential equations in almost every real situation. In some cases, such as one-dimensional flow and Stokes flow (or creeping flow), the equations can be simplified to linear equations. The nonlinearity makes most problems difficult or impossible to solve and is the main contributor to the turbulence that the equations model.

The nonlinearity is due to convective acceleration, which is an acceleration associated with the change in velocity over position. Hence, any convective flow, whether turbulent or not, will involve nonlinearity. An example of convective but laminar (non turbulent) flow would be the passage of a viscous fluid (for example, oil) through a small converging nozzle (Beam, 1977). Such flows, whether exactly solvable or not, can often be thoroughly studied and understood.

2.9 Classical Nucleation Theory

Nucleation is the extremely localized budding of a distinct thermodynamic phase. Some examples of phases that may form via nucleation in liquids are gaseous bubbles, crystals or glassy regions. Creation of liquid droplets in saturated vapor is also characterized by nucleation. Most nucleation processes are physical, rather than chemical, but a few exceptions do exists (e.g. electrochemical nucleation). Nucleation normally occurs at nucleation sites on surfaces contacting the liquid or vapor (Donald, 1953). Nucleation without preferential nucleation sites is homogeneous nucleation that occurs spontaneously and randomly but requires superheating or super cooling of the medium.

The nucleation rate depends on the average number of critical clusters and the diffusion of molecules to the cluster. The number of clusters of a certain size is a function of the total number of atoms in the system (W.Koalling, 2007). At a very low temperature, rate of diffusion is low but the greater the super cooling, the smaller the critical radius will be and less energy needed to form a nucleus. In present study, the non-equilibrium flow calculations consider only homogeneous nucleation in pure substance (Yong Yang, 2009).

Classical nucleation theory estimates the free energy barrier to nucleation by treating the droplet of the phase which is forming, here the nematic phase, as composed of a bulk core surrounded by an interface. The change in the Gibbs free energy when a nucleus forms is the sum of a bulk term and surface term. Nucleation takes place at constant pressure and temperature. The bulk term is equal to the number of rods in the nucleus (Seunghwa Ryu, 2010)

CHAPTER 3

METHODOLOGY

3.1 Description of Methodology

Literature review is done thoroughly to select a suitable nucleation model that matches with the project aims. The geometry of the converging-diverging nozzle was drawn using Ansys workbench with specified meshes and its boundary conditions.

In the study, the non-equilibrium condensation model has been implemented within the commercial CFD program FLUENT 12.0, which provides the framework for the solution of the hydrodynamic equations. The liquid and gas phase conservation are discretized using conservative finite-volume integration over a control volume.

Initially simulation of a simple nozzle with constant parameters is tested to ensure that FLUENT is able to read the user define function to investigate the nucleation rate. Once the initial data was validated, the meshes of the nozzle need to be improved towards more fine as well as introducing variable parameters rather than constant parameters that fit to the project case.

3.2 Summary of Methodology Used

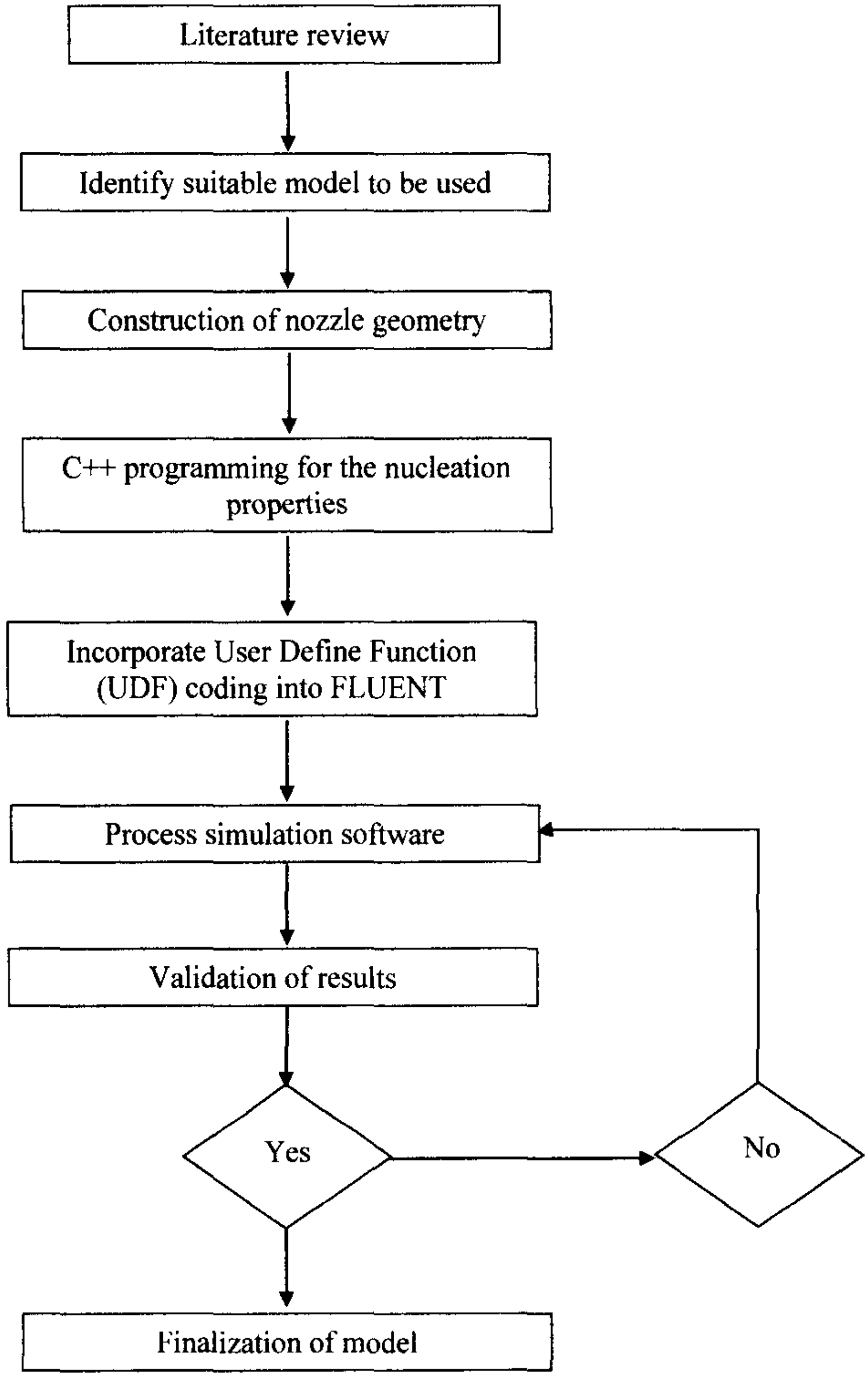
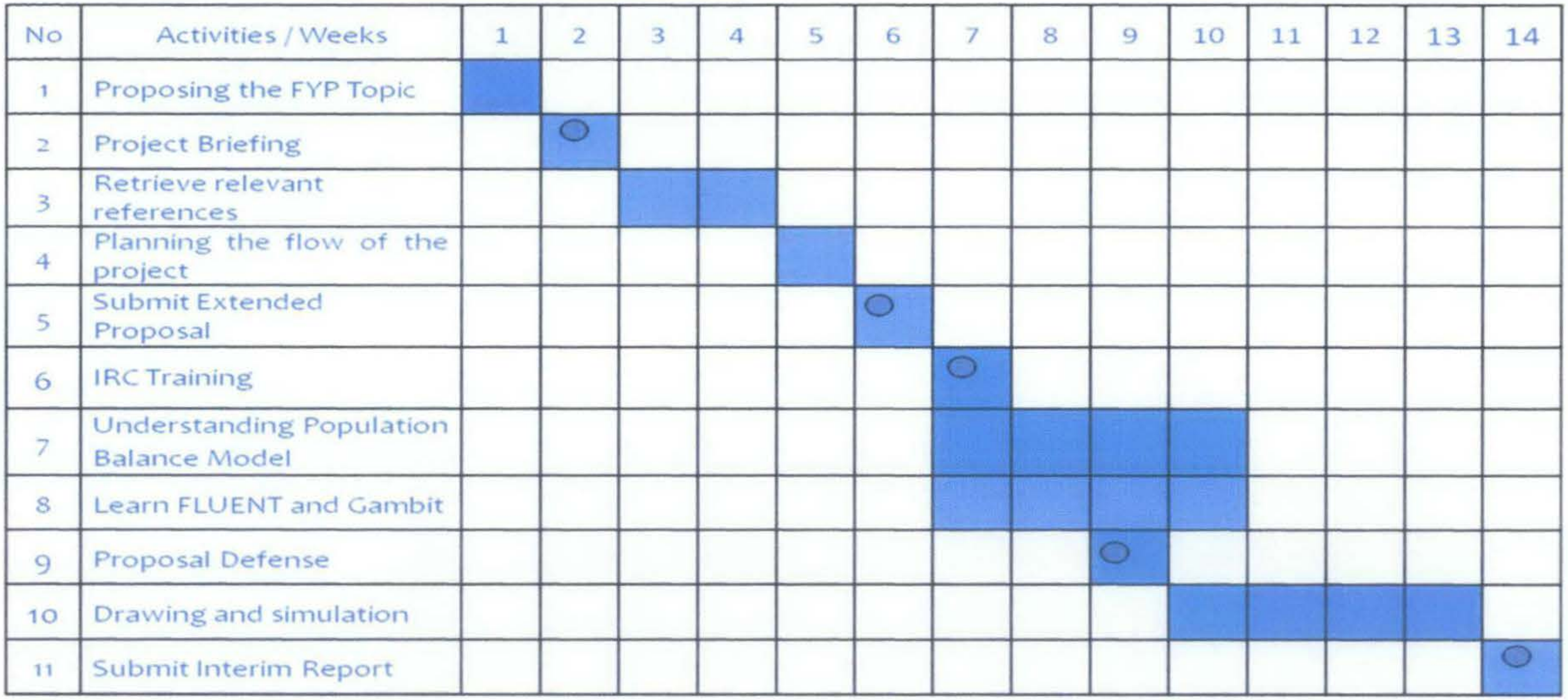
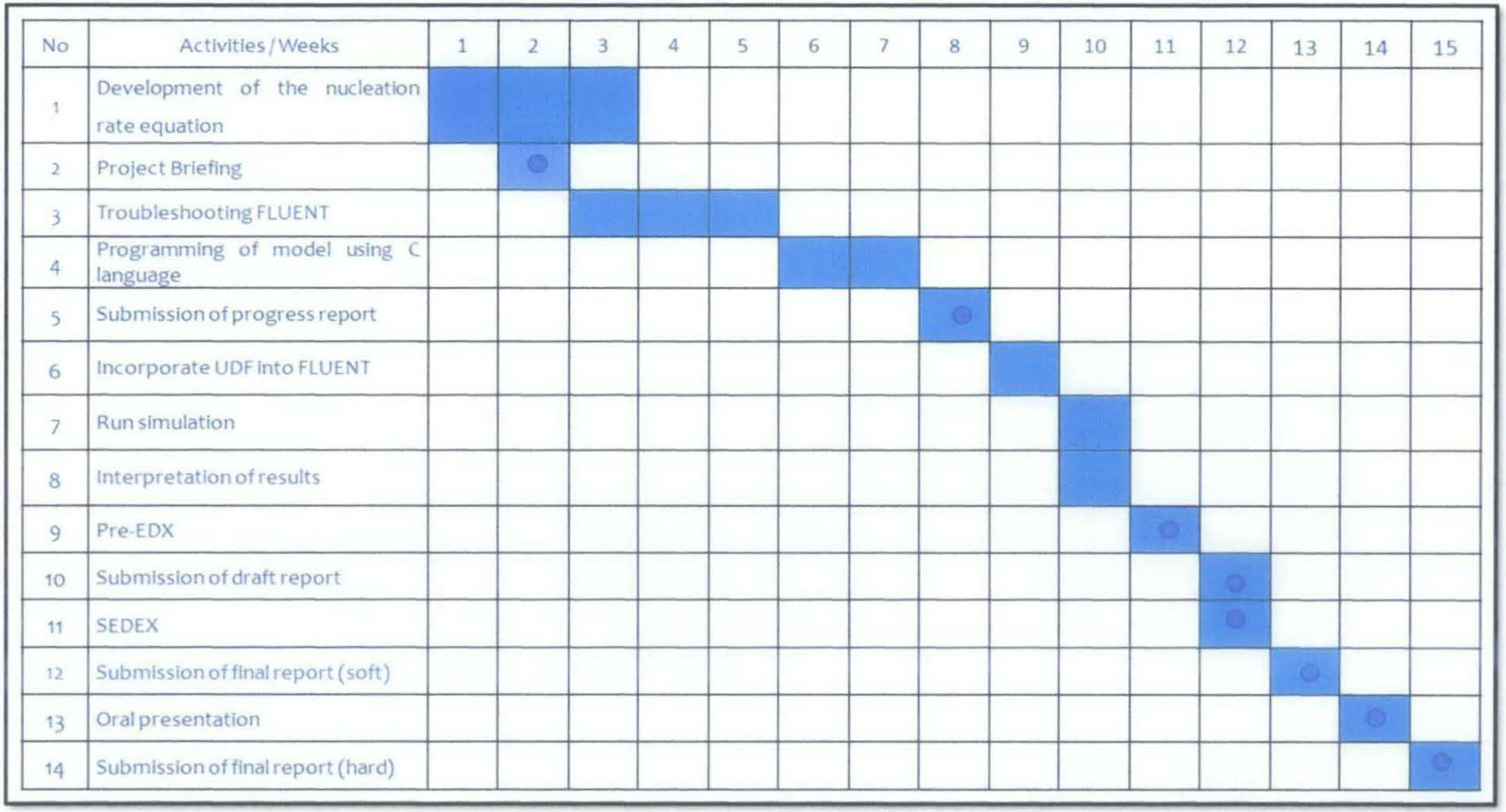


Figure 3.1: Project flow chart



No	Activities / Weeks	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Proposing the FYP Topic	■													
2	Project Briefing		■ ○												
3	Retrieve relevant references			■	■										
4	Planning the flow of the project					■									
5	Submit Extended Proposal						■ ○								
6	IRC Training							■ ○							
7	Understanding Population Balance Model							■	■	■	■				
8	Learn FLUENT and Gambit							■	■	■	■				
9	Proposal Defense									■ ○					
10	Drawing and simulation										■	■	■	■	
11	Submit Interim Report														■ ○

Figure 3.2: Gantt chart for FYP 1



No	Activities / Weeks	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15
1	Development of the nucleation rate equation	■	■	■												
2	Project Briefing		●													
3	Troubleshooting FLUENT			■	■	■										
4	Programming of model using C language						■	■								
5	Submission of progress report								●							
6	Incorporate UDF into FLUENT									■						
7	Run simulation										■					
8	Interpretation of results										■					
9	Pre-EDX											●				
10	Submission of draft report												●			
11	SEDEX												●			
12	Submission of final report (soft)													●		
13	Oral presentation														●	
14	Submission of final report (hard)															●

Figure 3.3: Gantt chart for FYP 2

3.3 Software Required

1. Ansys Fluent 12.0

   This software is used to draw the pipe designs and simulation of the flow. Functions include geometry drawing of an object, meshing of the geometry, defining faces such as inlet, outlet, and wall and provide fluid dynamics solutions and results.

2. Bloodshed Dev C++

   This is a C++ compiler to compile C++ codes into an executable program. This is used in the process for the development of program under C language in which compatible with FLUENT environment.

3. Thermo Solver

   Software which accompanies the textbook *Engineering and Chemical Thermodynamics by Milo Koretsky*. This software is used to perform complex thermodynamics calculations, and explore thermodynamics for systems which would be impossible to solve without a significant investment in programming.

4. Microsoft Office

   Including words, excel, project and power point.

CHAPTER 4
RESULTS AND DISCUSSIONS

4.1 Nucleation Model

Experimental and theoretical studies of expansion of steam through supersonic nozzles have been conducted by various investigators. While several theories have been proposed for obtaining the nucleation rate during spontaneous condensation, the two main theories of interest are the classical theory and the theory developed by (M.E. Deich, 1969). In the present study, the non-equilibrium flow calculation considers only homogeneous nucleation in pure substance and relies on the classical theory corrected for non-isothermal effects by (Yong Yang, 2009).

The nucleation rate is given by:

$$I = \frac{q_c}{1+\theta}\left(\frac{\rho v^2}{\rho l}\right)\sqrt{\frac{2\pi RT}{M_m^3 \pi}}exp\left(-\frac{4\pi r_*^2 \sigma}{3K_b T}\right)$$

Where,

q_c = Condensation coefficient

K_b = the Boltzmann constant
Mm = the mass of one molecule
σ = the liquid surface tension
θ = a non-isothermal correction factor

In the model, the classical homogeneous nucleation theory describes the formation of a liquid-phase in the form of droplets from a supersaturated phase in the absence of impurities or foreign particles.

The non-isothermal correction factor is given by:

$$\theta = \frac{2(\gamma - 1)}{(\gamma + 1)} \left(\frac{h_{lv}}{RT}\right)\left(\frac{h_{lv}}{RT} - 0.5\right)$$

h_{lv} = latent heat of evaporation at pressure P

γ = The ratio of specific heat capacities

r_* = Kelvin-Helmholtz critical droplet radius

The droplet will grow as its radius is larger than r_* otherwise the droplet will evaporate. And r_* is given as follows:

$$r_* = \frac{2\sigma}{\rho_l RT Ln S}$$

Where S is the super saturation ratio defined as the ratio of vapour pressure to the equilibrium saturation pressure:

$$S = \frac{P}{P_{sat}(T)}$$

4.2 Calculation of Nucleation Rate

Different calculation methods for condensing steam flow have been presented in the published literature. In the present research, the mathematical model describing the condensing steam consist of the continuous vapour phase at temperature T and pressure P, interspersed with a large number of spherical liquid droplets. It is assumed that the liquid is monodispersed; that is, that all liquid droplets are of the same size at one point in the flow and the interactions between droplets are neglected (Yong Yang, 2009). The nucleation rate calculated expression is a function of the temperature, fluid density, and super saturation ratio.

Properties	**Value**
Condensation coefficient, q_c	0.84 – 0.71
Water liquid density, ρl	970. 53 kg/m^3
Gas Constant, R	0.008314 kJ/Kmol K
Boltzmann constant, K_b	1.38066 x 10^-23 m^{2}kgs^{-2}
Liquid surface tension, σ	5.89 x 10^-2 N/m
Avogadro's number, N_A	6.0221 x 10^23/mol
Mass of one molecule, M_m	2.99 x 10^-23 kg
The ratio of specific heat capacities, γ	1.33

Table 4.1: Water properties

i. Critical Droplet Radius, r_*

$$r_* = \frac{2\sigma}{\rho_l RTLnS}$$

$$= \frac{2\ (5.89 \text{ x } 10\text{^}-2)}{(970.53)(0.008314)TLnS}$$

$$r_* = \frac{0.0146}{TLnS} \text{ ------------ } (1)$$

ii. Correction factor, θ

$$\theta = \frac{2(\gamma - 1)}{(\gamma + 1)}\left(\frac{h_{lv}}{RT}\right)\left(\frac{h_{lv}}{RT} - 0.5\right)$$

$$\theta = \frac{2(1.33 - 1)}{(1.33 + 1)}\left(\frac{2257}{(0.008314)T}\right)\left(\frac{2257}{(0.008314)T} - 0.5\right)$$

$$\theta = (0.2833)\left(\frac{271470}{T}\right)\left(\frac{271470}{T} - 0.5\right) \text{-----------} (2)$$

Substitute equation (1) and (2) into nucleation rate formula

Nucleation Rate I

$$= \frac{0.84}{1 + \left(\frac{76907}{T}\right)\left(\frac{271470}{T} - 0.5\right)}\left(\frac{\rho v^2}{970.53}\right)\sqrt{(6.2407x10^{65})T}exp\left(-\frac{1.88x10^{22}}{T}\left(\frac{0.0146}{TLnS}\right)^2\right)$$

4.3 Geometry of Supersonic Separator

In our supersonic swirling separator, the Laval nozzle was designed to be a new annular nozzle, which incorporates a central body, allowing the principle of conservation of angular momentum to be harness. The geometries dimensions of the converging-diverging nozzle as Figure 4.1 were taken to be the same as the Nozzle B used in the experiment of (M.J. Moore, 1973). The channel, between the wall and the central body, forms a Laval nozzle, which is composed of three sections: the convergent (subsonic zone), throat section (critical zone) and divergent section (supersonic zone) as seen in Figure 4.1 from (Yong Yang, 2009)

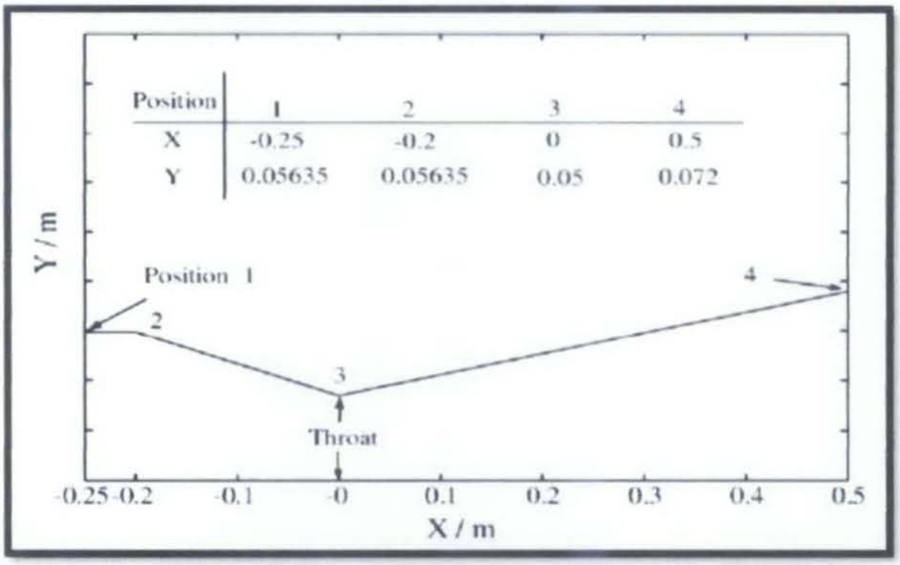


Figure 4.1: Geometry of the converging-diverging nozzle
Taken from (Yong Yang, 2009)

Based on the asymmetric points given by the literature, the supersonic nozzle was drawn and meshed using Ansys workbench geometry 12.0. The model was drawn with finer mesh at area nearer to the convergent and divergent section and to its wall as the fluids properties changes are significant there. A total number of 276,720 number of grid elements was constructed. The quality of the mesh plays a significant role in the accuracy and stability of the numerical calculation. Figure 4.2 shows the simulated drawing of the nozzle.

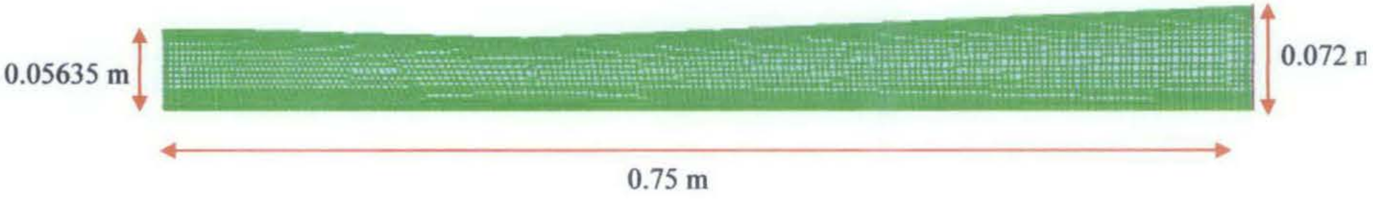


Figure 4.2: Simulated geometry of the converging-diverging nozzle

4.4 Modelling and Simulation Results

In the supersonic swirling separator, the strong swirling flow is generated by the swirling vanes. Therefore, the standard k- ε turbulence model is used here, because it provides an option to account for the effects of swirl by modifying the turbulent viscosity appropriately (Bart Prast, 2006). In a supersonic swirling separator, the gas phase is treated as continuous and the locally averaged Navier-Stokes equation is used to describe the mass, momentum and energy conservation equations for the continuous phase (Chuang wen, 2010).

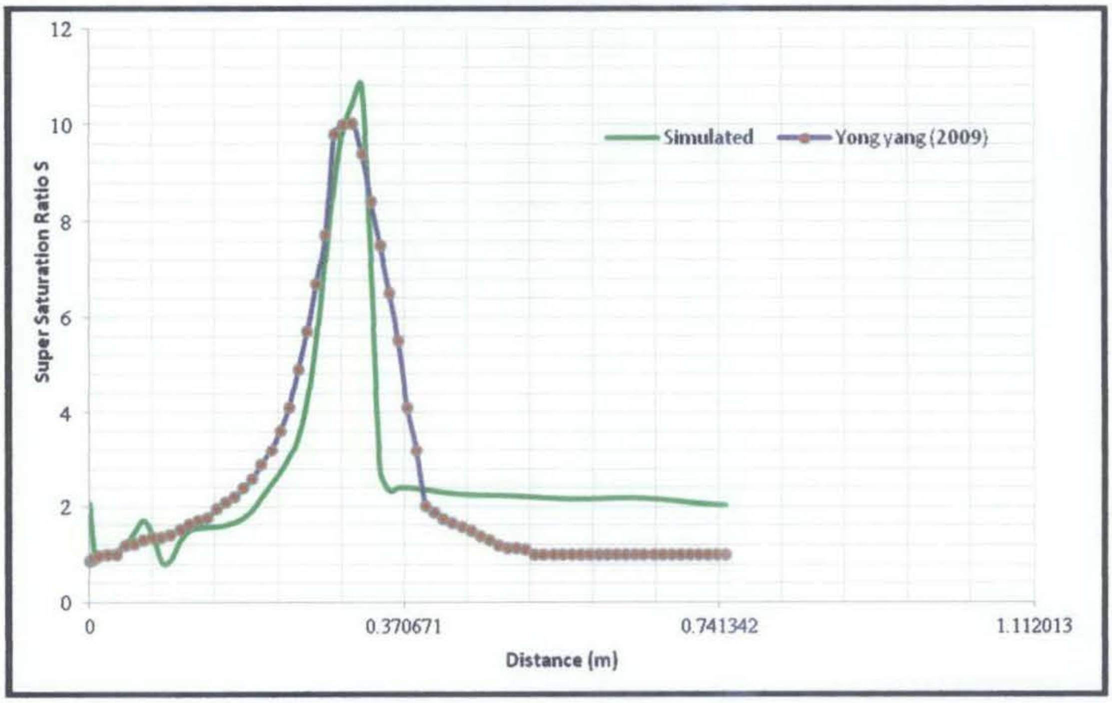
The velocity of the flow is expected to increase when it passes through the converging part until it achieves the supersonic flow, 460m/s (Mach = 1) at the throat. After the throat, it will flows through divergence part and the natural gas will experience swelling effect which causes temperature and pressure drop. The water will be condensed into water droplets; hence reducing water vapour content in the pipe

The boundary conditions and the assumptions made were as follows:

1) At the nozzle inlet, subsonic flow was specified using gauge total pressure (P_{TI}), initial gauge pressure (P_{gI}), and total temperature (T_{TI}). In addition, a turbulent intensity of 0.05, and an eddy length scale of 0.0084525 m of the nozzle inlet diameter were used.
2) At the wall, a stationary wall motion was specified with no slip adiabatic wall condition.
3) Assuming that the flow is axisymmetric about the nozzle centreline, symmetry conditions were enforced for all flow variables along this plane.
4) At the nozzle outlet, supersonic outflow conditions were applied, and all of the flow parameters were extrapolated from the interior of the domain to the exit plane. In addition, a backflow turbulent intensity of 0.05, and a backflow hydraulic diameter of 0.0108 m of the nozzle were applied.

To qualitatively describe the physics of supersonic steam flow with or without non-equilibrium condensation, a sample of the calculated results for the converging-diverging nozzle are shown in Figure 4.3 to Figure 4.11. The boundary conditions for the results were P_{oin} = 25 kPa and T_{oin} = 354.6 K at the inflow with supersonic condition.

With comparison to the proposed model by (Yong Yang, 2009), Figure 4.3 gives the distribution of super saturation ratio along the nozzle centreline, in which the solid-line corresponds to the super saturation ratio of condensing steam flow with homogeneous nucleation, and the dotted-line corresponds to the super saturation ratio profile of the proposed model in literature. One can see in Figure 4.3 that the simulated model used in this study predicts close distribution of the super saturation ratio over the nozzle length, in particular the location of the condensation shock whereby water liquid starts to form downstream of the throat. Therefore, the simulation model is considered valid.



.**Figure 4.3: Supersaturation ratio distribution along the nozzle centreline compared with the models from (Yang, 2009)**

Velocity of fluid increased as it is forced to converge to go through the smaller cross sectional area. Figure 4.4 and Figure 4.5 below shows a sharp increase in velocity at 0.06m x-direction, which is after the throat position at 0m where the fluid achieved its highest velocity of 532m/s. Increase in flow area at divergent section reduces the velocity of fluid to flow

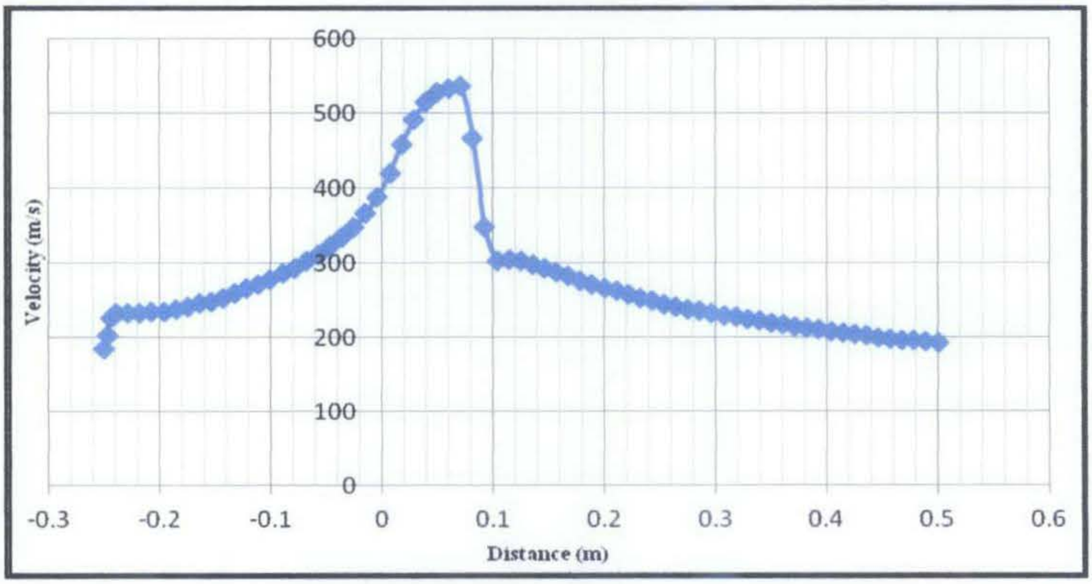


Figure 4.4: Centreline values for the fluid velocity

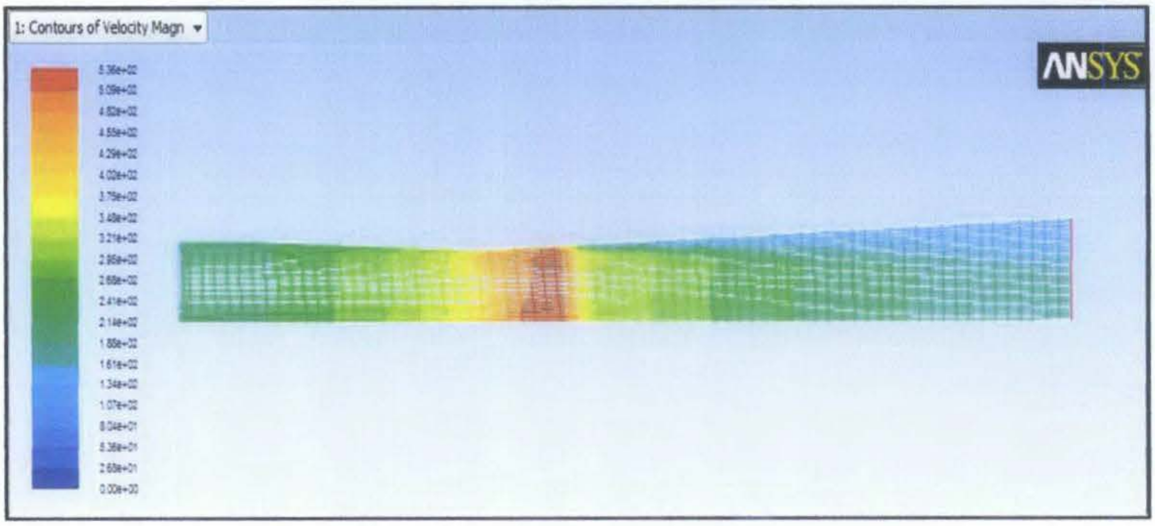


Figure 4.5: Velocity profile of fluid flow in unit m/s

Figure 4.5 and Figure 4.6 below shows the centreline values distribution for the fluid Mach number and the Mach number profile. The steam flow through the nozzle approaches supersonic fluid flow near the choke, where its Mach number is equal to 1.38 higher than the speed of sound at Mach number 1.0. The fluid achieve the highest Mach number at the position of 0.07m from the throat position.

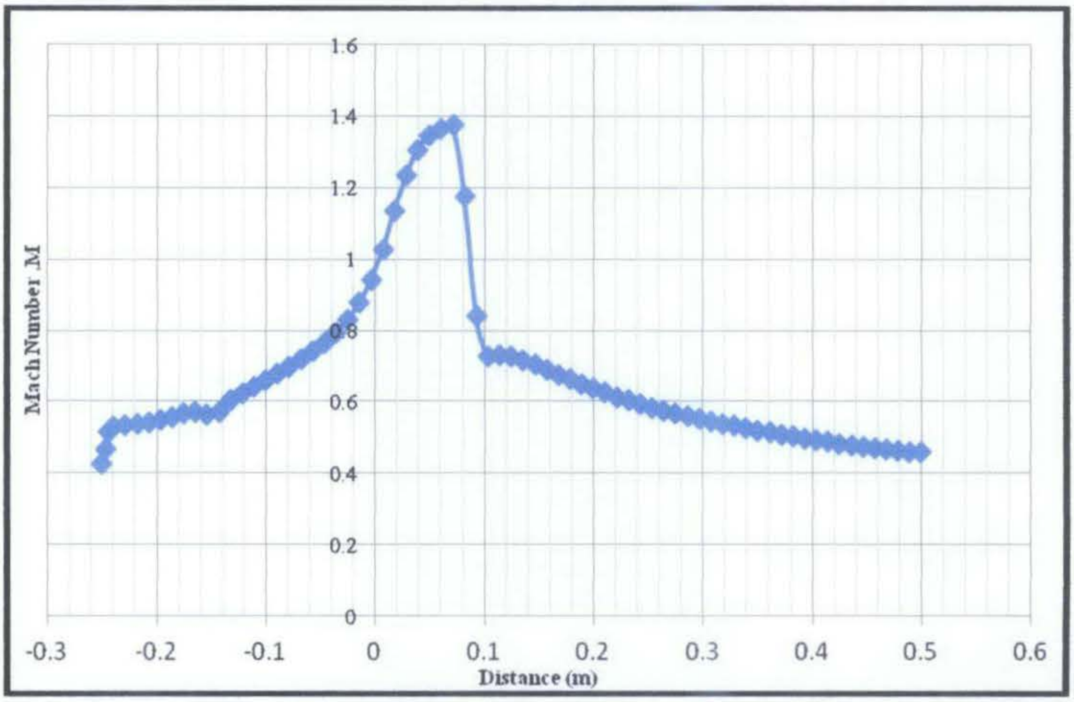


Figure 4.6: Centreline values for the fluid Mach number

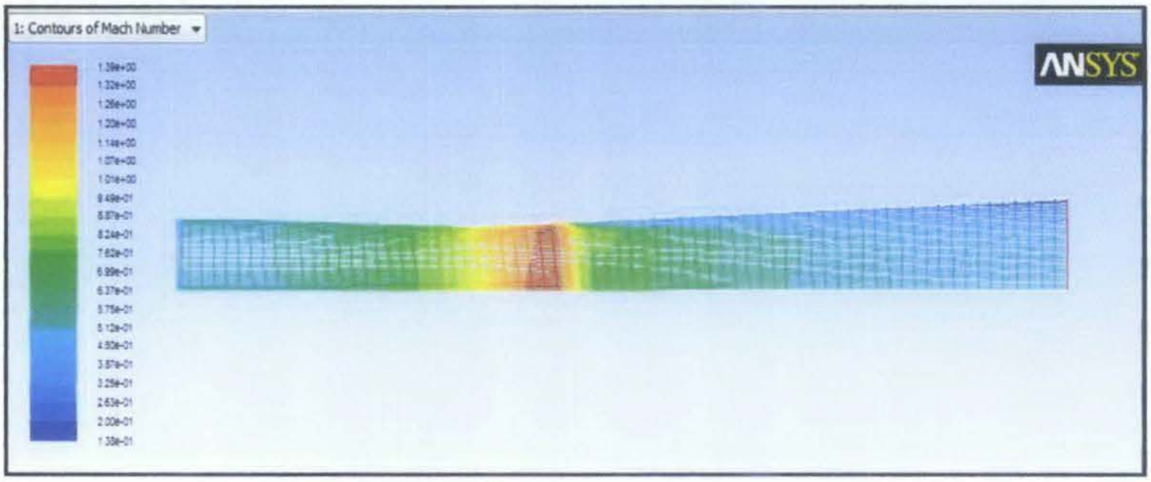


Figure 4.7: Mach number profile of fluid flow

Figure 4.8 and Figure 4.9 below shows the centreline values for the fluid temperature drop distribution and the fluid temperature drop profile. As the velocity of the fluid increases, the temperature will drop rapidly from 370K to 300K at 0.07m after the nozzle throat. This demonstrates Joule-Thompson effect when gas is forced through a much smaller area.

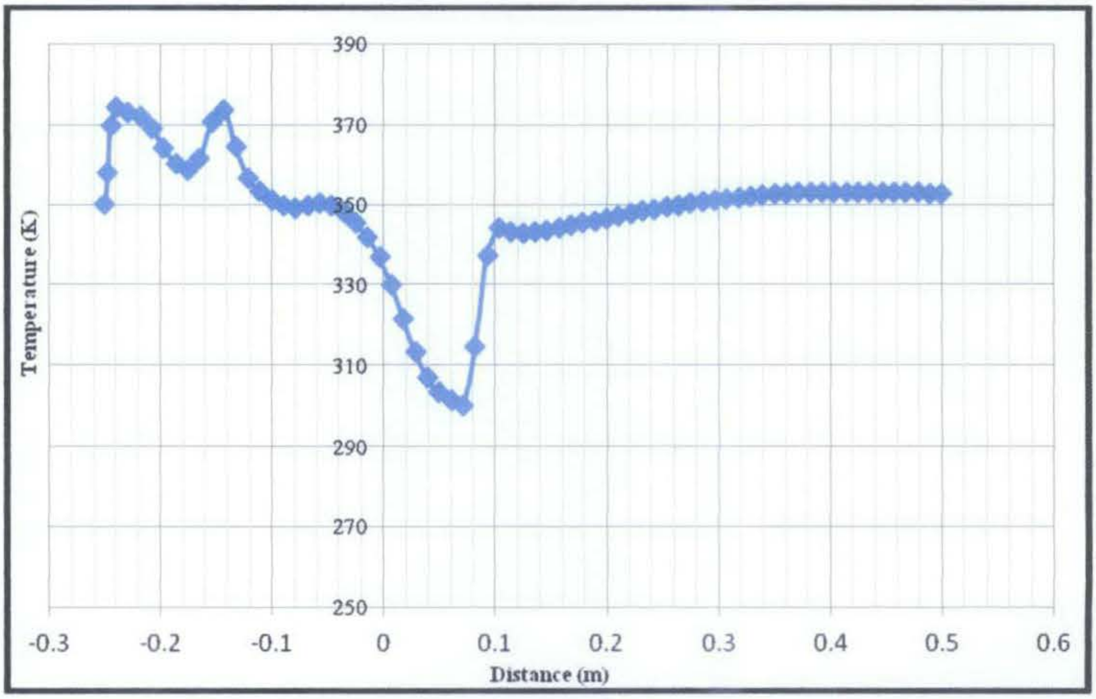


Figure 4.8: Centreline values for the fluid temperature drop

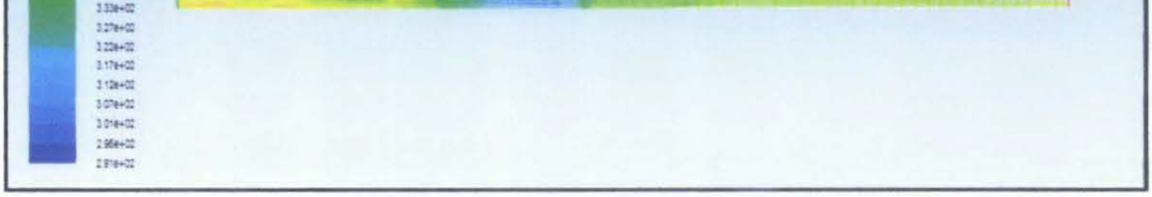


Figure 4.9: Temperature profile of fluid flow unit Kelvin

Figure 4.10 and Figure 4.11 below shows the centreline values for the fluid nucleation rate distribution and the nucleation profile. As the critical conditions are approached the supersaturation ratio and the nucleation rate increases dramatically as seen in below figure with the peak of nucleation rate approaching the order of 10^{25} at the same location of X = 0.061m downstream the nozzle throat.

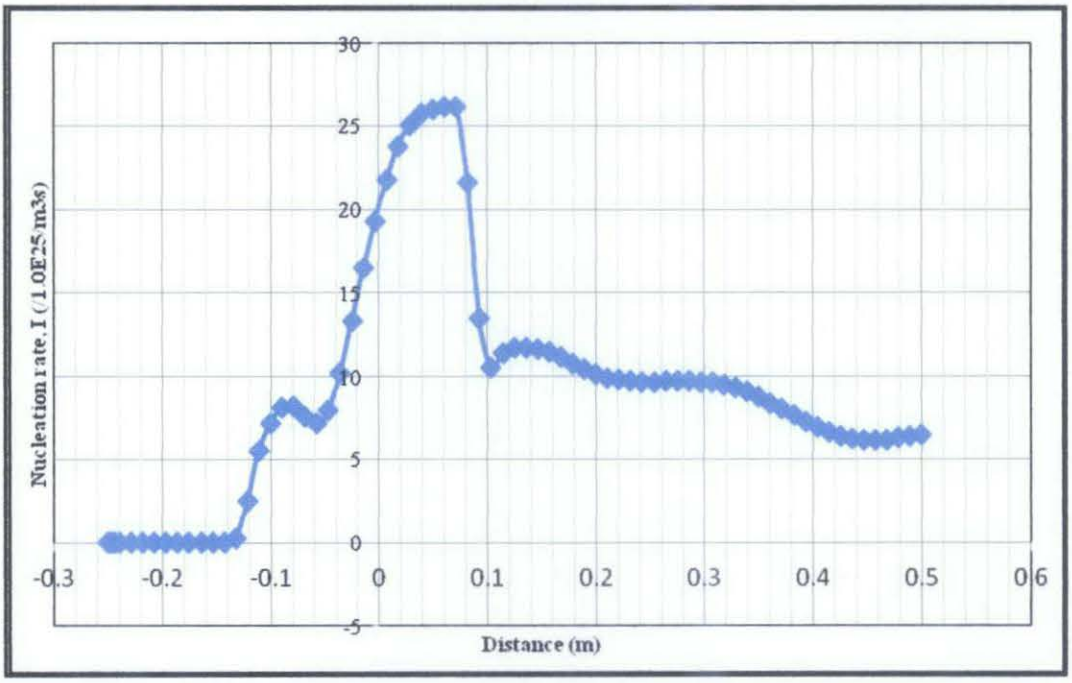


Figure 4.10: Centreline values for the fluid nucleation rate

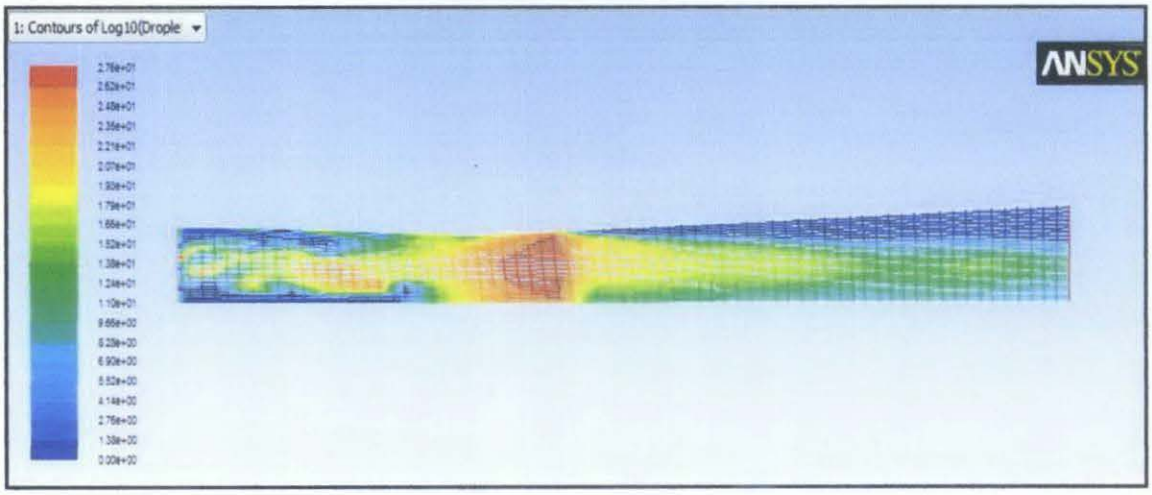


Figure 4.11: Nucleation rate profile of fluid flow

4.5 Simulation Summary

The concept of liquid-vapor separation using supersonic condition by applying Joule Thomson cooling effect is feasible. It is because when the steam enters the convergence section, the velocity of the flow will increase and supersonic flow will be created.

Down the throat, it will flow through divergence part and the steam will undergo swelling effect which causes sudden temperature and pressure drop. This phenomenon will condense the water vapor to become water droplets and fallout from the stream. The condensed water will flow out through a small pipe outlet connected to the end of the pipe while the saturated steam will continue to flow out from the separator at high speed.

Since the critical conditions are approached the super saturation ratio and the nucleation rate increases dramatically as seen in Figure 4.3 and Figure 4.10, with the biggest super saturation ratio of more than 10 and the peak of nucleation rate approaching the order of 10^{25} downstream of the nozzle throat. The release of latent heat to the flow induces a shock at the location causing an increase in temperature as well as pressure and as a result the particle nucleation pulse is terminated abruptly (Yong Yang, 2009). With the latent heat of condensation, the temperature rises back along the pipeline, and the pressure drop was recovered.

CHAPTER 5

CONCLUSION & RECOMMENDATION

5.1 Recommendation

Recommendation for future work to improvise the scope of the project and accuracy of the results are listed below:

1. Create more components for simulation purposes instead of using binary components of water vapor and water liquid. This can improve the accuracy of results as natural gas is actually composed of many other components.
2. Include heat of condensation to the problem by generating energy balance equation in user defined functions (UDF) codes and incorporate it into the simulation to obtain the temperature drop, super saturation ratio, as well as the nucleation actual distribution.
3. This project should be done experimentally as well to compare the result with the simulation result. Small prototype of Joule-Thompson valve can be build to study its feasibility and efficiency.
4. Optimizing geometry grid whereby size and mesh element are effectively define.

5.2 Conclusion

Understanding nucleation theory and growth is important in developing new type of gas separation technology. As most fluid dynamics software or approach does not consider the particle nucleation theory, it is important to incorporate this into the simulation. In this research, vapor phase of water and liquid water is studied. Corrected classical homogeneous nucleation model is used for this case study as it describe the quantity of droplets at a location in the continuous gas phase can be known.

The numerical simulation for the prediction of the non-equilibrium steam flow with spontaneous condensation in the supersonic separator is completed. The success of the simulation was measured by the validation based on the experiment from published literature. The objectives of this project which are to incorporate condensation model into CFD, and simulate gas flow through supersonic separator was achieved.

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APPENDICES

APPENDIX A

NUCLEATION UDF CODES

```
#include "udf.h"
#include "sg_pb.h"
#include "sg_mphase.h"

DEFINE_PB_NUCLEATION_RATE (nuc_rate, cell, thread)

{
        double T,I, f_term, s_term, t_term, fr_term;

         double Qc = 0.8 ;              /* condensation coefficient */
        double kb = 1.38066e-23 ;     /* Boltzmann constant */
        double u  = 62.112e-3 ;        /* liquid surface tension */
        double Mm = 1.33175e-23 ;  /* Mass of one molecule */
        double pv = 958.35 ;            /* vapor density */
        double pl = 970.253 ;            /* liquid density */
        double r  = 1.616e-9 ;          /* critical droplet radius */
        double R  = 8.314e-3 ;          /* Gas Constant */

        Thread *tc = THREAD_SUPER_THREAD(thread);
        Thread **pt = THREAD_SUB_THREADS(tc);
        Thread *tp = pt[P_PHASE];

        T = C_T(cell,tp);

        //double f_term = Qc;
        s_term = pow(pv,2)/ pl;
        t_term = sqrt( ( (2*3.142*R*T) / (pow(Mm,3)*3.142) ) );
        fr_term = exp ( ( (4*3.142*pow(r,2)*u) / (3*kb*T) ) );


              I = Qc*s_term*t_term*fr_term;

                    return I;

}
```

APPENDIX B

Classical Nucleation Theory

A. Homogeneous Nucleation

Nucleation generally occurs with much more difficulty in the interior of a uniform substance, by a process called *homogeneous nucleation*. The creation of a nucleus implies the formation of an interface at the boundaries of a new phase.

Liquids cooled below the maximum heterogeneous nucleation temperature (melting temperature), but which are above the homogeneous nucleation temperature (pure substance freezing temperature) are said to be supercooled. This is useful for making amorphous solids and other metastable structures, but can delay the progress of industrial chemical processes or produce undesirable effects in the context of casting. Supercooling brings about supersaturation, the driving force for nucleation. Supersaturation occurs when the pressure in the newly formed solid is less than the liquid pressure, and brings about a change in free energy per unit volume, G_v, between the liquid and newly created solid phase. This change in free energy is balanced by the energy gain of creating a new volume, and the energy cost due to creation of a new interface. When the overall change in free energy, ΔG is negative, nucleation is favoured.

Some energy is consumed to form an interface, based on the surface energy of each phase. If a hypothetical nucleus is too small (known as an unstable nucleus or "embryo"), the energy that would be released by forming its volume is not enough to create its surface, and nucleation does not proceed. The critical nucleus size can be denoted by its radius, and it is when r=r* (or r critical) that the nucleation proceeds.

For example in the classic case of a spherical cluster that liberates $-G_v$ Joules per cubic centimeter during formation (here G_v is a negative quantity), but which must pay the positive cost of σ Joules per square centimeter of surface interfacing with the surrounding, the free energy needed to form a spherical cluster of radius r is,

$$\Delta G = \frac{4}{3}\pi r^3 G_v + 4\pi r^2 \sigma$$

Where the first term shows the energy gain of creating a new volume and the second term shows the energy loss due to surface tension (σ) of the new interface.

It costs free energy to add molecules to this cluster (because $\frac{dG}{dr} > 0$) until the radius reaches,

$$r^* = -\frac{2\sigma}{G_v}$$

Where,

$$\frac{dG}{dr} = 0$$

Addition of new molecules to clusters larger than this critical radius releases, rather than costs, available work. In other words at that point growth of the cluster is no longer limited by nucleation, but perhaps by diffusion (i.e. the supply of molecules) or by reaction kinetics instead.

The free energy needed to form this critical radius can be found by

$$\Delta G^* = \frac{16\pi\sigma^3}{3(G_v)^2}$$

which occurs at the maximum ΔG where $dG / dr = 0$
The term ΔG_v can be related to the equilibrium temperature, enthalpy of fusion (ΔH_v), and the degree of under cooling (ΔT) as follows,

$$\Delta G_v = \Delta H_v - T\Delta S_v$$

By evaluating this equation at the equilibrium point ($\Delta G_V = 0$) at the melting temperature T_m we achieve,

$$\Delta S_v = \frac{\Delta H_v}{T_m}$$

Substitution of ΔS_v into the first equation leads to,

$$\Delta G_v = \Delta H_v - T(\frac{\Delta H_v}{T_m})$$

Which by using common denominators and the definition of $\Delta T = T_m - T$ provides,

$$\Delta G_v = \frac{\Delta H_v}{T_m}\Delta T$$

As the phase transformation becomes more and more favourable, the formation of a given volume of nucleus frees enough energy to form an increasingly large surface, allowing progressively smaller nuclei to become viable. Eventually, thermal activation will provide enough energy to form stable nuclei. These can then grow until thermodynamic equilibrium is restored. A greater degree of super cooling favours phase transformation, and we can relate ΔG^* to super cooling and find r* and ΔG * as a function of ΔT by the substitution of ΔG_v,

$$r^* = \frac{2\sigma T_m}{\Delta H_s}\frac{1}{\Delta T}$$

and

$$\Delta G^* = \frac{16\pi\sigma^3 T_m^2}{3\Delta H_s^2}\frac{1}{(\Delta T)^2}$$

The greater the super cooling, the smaller the critical radius and the less energy needed to form it. The spontaneous nucleation rate in, say, water changes very rapidly with temperature, so the spontaneous nucleation temperature can be quite well defined. 'Film boiling' on very hot surfaces and the Leidenfrost effect are both believed to be stabilized by spontaneous nucleation phenomena.

B. Heterogeneous Nucleation

Heterogeneous nucleation occurs much more often than homogeneous nucleation. It forms at preferential sites such as phase boundaries or impurities like dust and requires less energy than homogeneous nucleation. At such preferential sites, the effective surface energy is lower, thus diminishing the free energy barrier and facilitating nucleation. Surfaces promote nucleation because of wetting – contact angles greater than zero between phases encourage particles to nucleate. The free energy needed for heterogeneous nucleation is equal to the product of homogeneous nucleation and a function of the contact angle:

$$\Delta G_{\text{heterogeneous}} = \Delta G_{\text{homogeneous}} * f(\theta)$$

Where,

$$f(\theta) = \frac{1}{2} - \frac{3}{4}\cos\theta + \frac{1}{4}\cos^3\theta$$

Rate of Nucleation

The nucleation rate, I, depends on the average number of critical clusters, n* and the diffusion of molecules to the cluster, β.

$$I = n^*\beta$$

Where the average population of critical nuclei is

$$n^* = N \exp\left(\frac{-\Delta G^*}{k_B T}\right)$$

Where:

- ΔG^* is critical free energy needed corresponding to that of the critical radius.
- N is the number of potential nucleation sites per unit volume
- k_B is the Boltzmann constant

The number of clusters of a certain size formed is a function of the total number of atoms in the system, the free energy to create a cluster (of that size), and the temperature. The number of clusters increases with increasing temperature.

Plugging in for ΔG^*, we get

The rate of addition of one extra atom to the critical nucleus as estimated by the Volmer-Weber theory is

$$\mathrm{B} = A \exp\left(\frac{-(Q + \Delta G^*)}{k_B T}\right)$$

where A is a term that incorporates the shape factor of the atoms and the area to which atoms can join, and the vibrational frequency of the particles. And Q is the activation energy for atomic migration.

This term gives us the diffusion of the atoms to the site of nucleation. However, a problem with the Volmer Weber theory is that it ignores formation of particles of r>r* and assumes that size distribution is maintained (fluctuations are occurring fast)

The rate of nucleation can be expressed as:

$$I(T) = A \exp\left(\frac{-Q}{kT}\right) \exp\left(\frac{-16\pi\gamma_{sl}^3}{3\Delta H_s^2} \cdot \frac{1}{kT} \cdot \frac{T_m^2}{\Delta T^2} \cdot f(\theta)\right)$$

Where:

- γ is the surface tension.
- ΔH_s is the enthalpy per unit volume.
- Tm is the melting temperature.
- Θ is the wetting angle.

APPENDIX C

Navier-Stokes equations

The derivation of the Navier–Stokes equations begins with an application of Newton's second law: conservation of momentum (often alongside mass and energy conservation) being written for an arbitrary portion of the fluid. In an inertial frame of reference, the general form of the equations of fluid motion is:

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)=-\nabla p+\nabla\cdot\mathbb{T}+\mathbf{f},$$

where $\mathbf{v}$ is the flow velocity, ρ is the fluid density, p is the pressure, $\mathbb{T}$ is the (deviatoric) stress tensor, and $\mathbf{f}$ represents body forces (per unit volume) acting on the fluid and ∇ is the del operator. This is a statement of the conservation of momentum in a fluid and it is an application of Newton's second law to acontinuum; in fact this equation is applicable to any non-relativistic continuum and is known as the Cauchy momentum equation.

This equation is often written using the material derivative *D*v/*Dt*, making it more apparent that this is a statement of Newton's second law:

$$\rho\frac{D\mathbf{v}}{Dt}=-\nabla p+\nabla\cdot\mathbb{T}+\mathbf{f}.$$

The left side of the equation describes acceleration, and may be composed of time dependent or convective effects (also the effects of non-inertial coordinates if present). The right side of the equation is in effect a summation of body forces (such as gravity) and divergence of stress (pressure and shear stress).

Incompressible flow of Newtonian fluids.

A simplification of the resulting flow equations is obtained when considering an incompressible flow of a Newtonian fluid. The assumption of incompressibility rules out the possibility of sound or shock waves to occur; so this simplification is invalid if these phenomena are important. The incompressible flow assumption typically holds well even when dealing with a "compressible" fluid — such as air at room temperature — at low Mach numbers (even when flowing up to about Mach 0.3). Taking the incompressible flow assumption into account and assuming constant viscosity, the Navier–Stokes equations will read, in vector form:

$$\rho\left(\frac{\partial \mathbf{v}}{\partial t}+\mathbf{v}\cdot\nabla\mathbf{v}\right)=-\nabla p+\mu\nabla^2\mathbf{v}+\mathbf{f}.$$

Here **f** represents "other" body forces (forces per unit volume), such as gravity or centrifugal force. The shear stress term $\nabla\mathbb{T}$ becomes the useful quantity $\mu\nabla^2\mathbf{v}$(∇^2 is the vector Laplacian) when the fluid is assumed incompressible, homogeneous and Newtonian, where μ is the (constant) dynamic viscosity. It's well worth observing the meaning of each term (compare to the Cauchy momentum equation):

$$\rho\Bigg(\overbrace{\underbrace{\frac{\partial \mathbf{v}}{\partial t}}_{\text{Unsteady acceleration}} + \underbrace{\mathbf{v}\cdot\nabla\mathbf{v}}_{\text{Convective acceleration}}}^{\text{Inertia (per volume)}}\Bigg) = \overbrace{\underbrace{-\nabla p}_{\text{Pressure gradient}} + \underbrace{\mu\nabla^2\mathbf{v}}_{\text{Viscosity}}}^{\text{Divergence of stress}} + \underbrace{\mathbf{f}}_{\text{Other body forces}}.$$

Note that only the convective terms are nonlinear for incompressible Newtonian flow. The convective acceleration is an acceleration caused by a (possibly steady) change in velocity over position, for example the speeding up of fluid entering a converging nozzle. Though individual fluid particles are being accelerated and thus are under unsteady motion, the flow field (a velocity distribution) will not necessarily be time dependent.

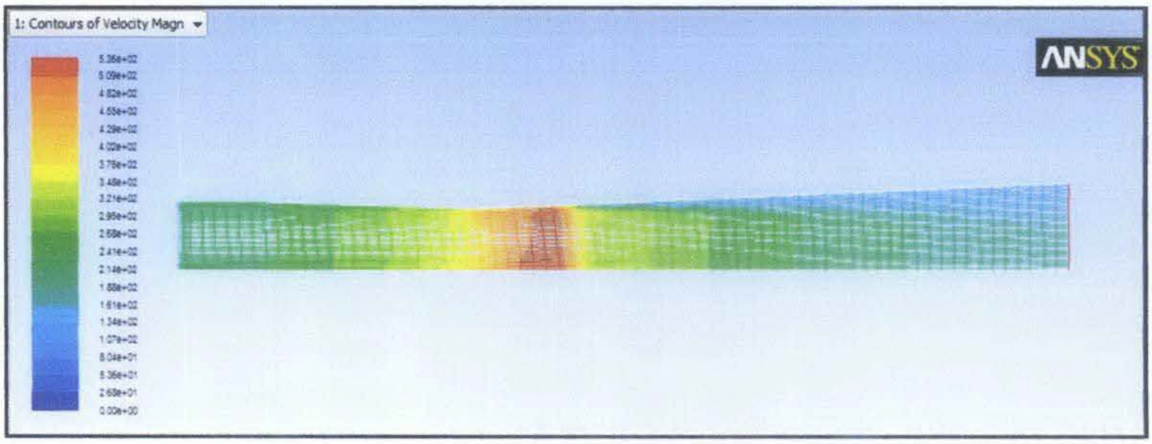
Another important observation is that the viscosity is represented by the vector Laplacian of the velocity field (interpreted here as the difference between the velocity at a point and the mean velocity in a small volume around). This implies that Newtonian viscosity is diffusion of momentum, this works in much the same way as the diffusion of heat seen in the heat equation (which also involves the Laplacian).

This is more specifically a statement of the conservation of volume. These equations are commonly used in 3 coordinates systems: Cartesian, cylindrical, and spherical. While the Cartesian equations seem to follow directly from the vector equation above, the vector form of the Navier–Stokes equation involves some tensor calculus which means that writing it in other coordinate systems is not as simple as doing so for scalar equations (such as the heat equation).

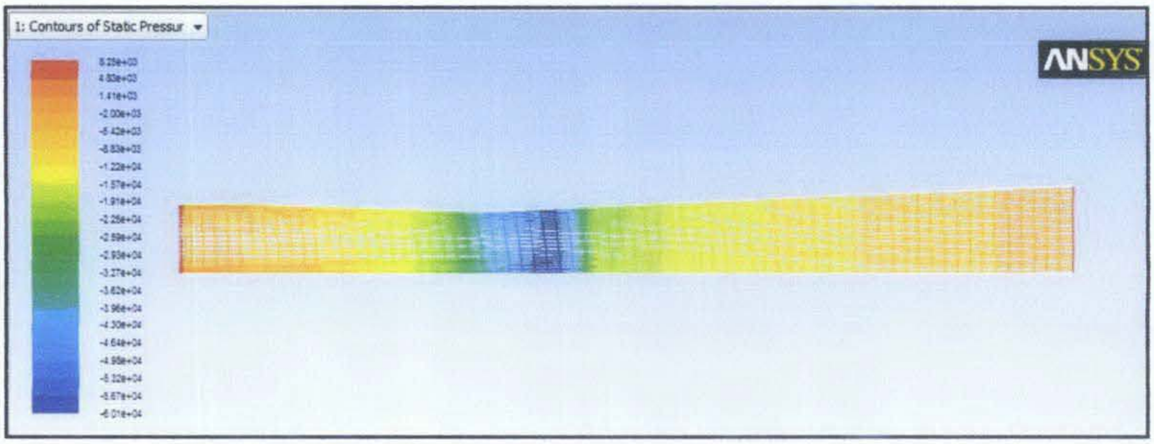
APPENDIX D

SIMULATION RESULTS

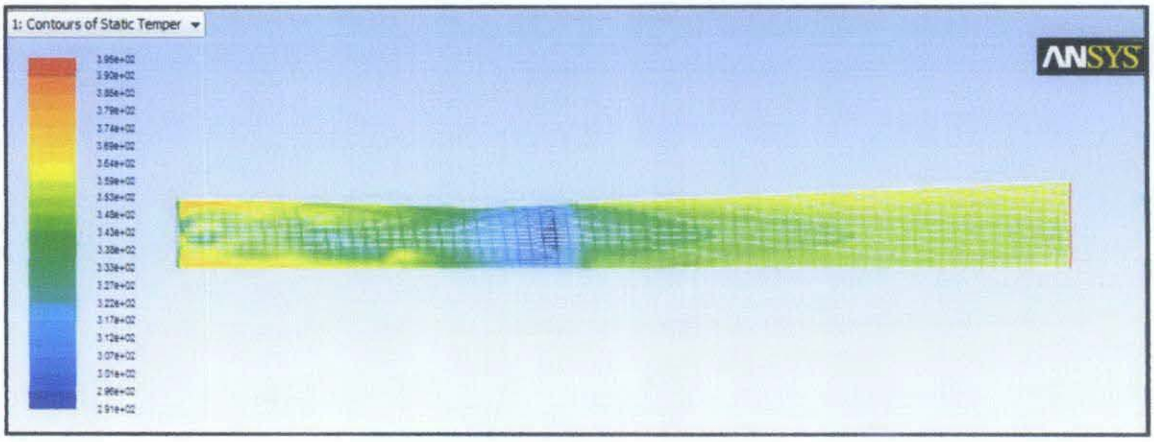
Velocity profile



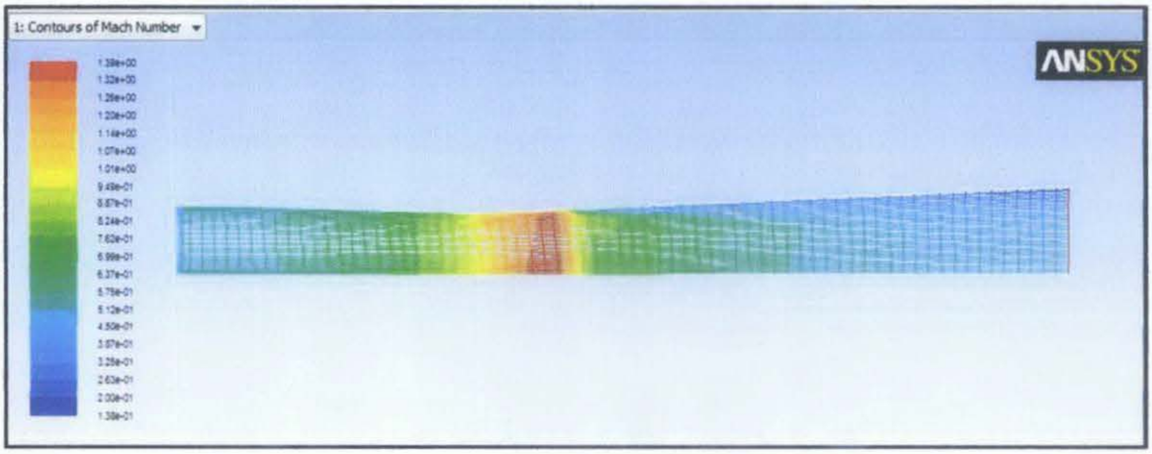
Pressure profile



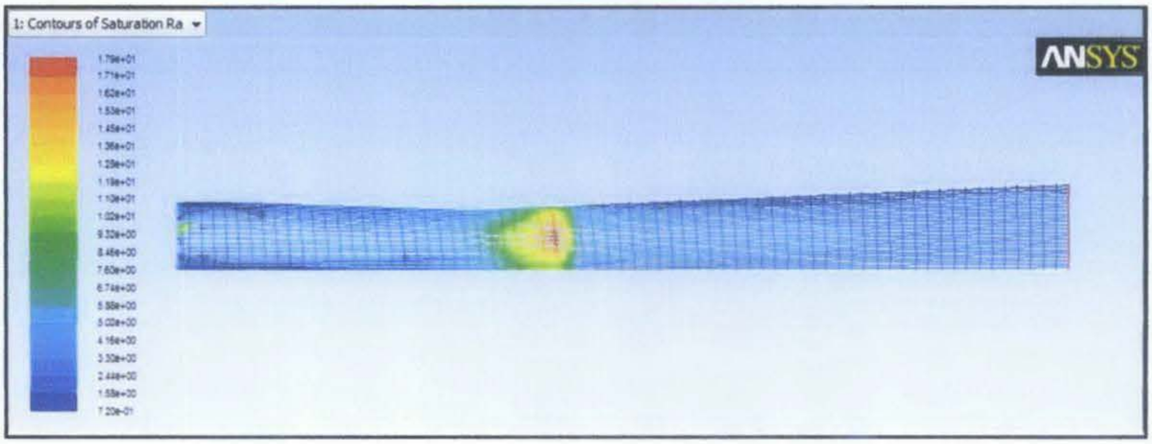
Temperature profile



Mach number profile



Saturation ratio profile



Nucleation rate profile