



UNIVERSITI
TEKNOLOGI
PETRONAS

**MODELING AND SIMULATION OF SUPERSONIC GAS
DEHYDRATION USING JOULE THOMSON VALVE**

by

Ho Chia Ming

7720

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

JULY 2009

Universiti Teknologi PETRONAS

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CERTIFICATION OF APPROVAL

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A project dissertation submitted to the
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Approved by,

(DR. LAU KOK KEONG)

UNIVERSITI TEKNOLOGI PETRONAS

TRONOH, PERAK

JULY 2009

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.

(HO CHIA MING)

ABSTRACT

Entitled “Supersonic gas dehydration in pipeline using Joule Thomson Valve”, this project ultimately aims to introduce a new technology, Joule Thomson valve to separate water from natural gas (from reservoir) using supersonic flow and joule Thomson cooling effect. Due to time and financial constraints, this project is only being done in simulation, not in term of experiment. Gas dehydration in pipeline is essential because water content in the gas system could cause large pressure drop and corrossions that will be enhanced by the presence of H₂S and CO₂ typically associated in sour gas. The current technologies used are membrane and absorption separation technique. However, they required high CAPEX, OPEX and maintenance works. Separation using Joule Thomson valve is technically and economically feasible.

ACKNOWLEDGEMENTS

I would like to take this opportunity to thank everyone whom had given their support and help throughout the whole period of completing this project.

First and foremost, I would like acknowledge the endless help and support received from my supervisor, Dr. Lau Kok Keong throughout the whole period of completing this final year project. His guidance has really been the main source of motivation and has driven me in completing this project successfully.

Special thanks goes to FYP 1 and 2 coordinators, for their systematic approach and timely arrangement for this project. Genuine gratitude goes to the examiners and evaluators both internal and external.

Finally, I would like to thank my classmate, Wong Mee Kee for her encouragement, comment and input on my simulation result.

Thank you.

With Utmost Gratitude

.....
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LIST OF ABBREVIATION

EOS	Equation of state
FYP	Final year project
HYSYS	Simulation software developed by ASPEN
PR	Peng-Robinson, equation of state
PVT	Pressure; Volume; Temperature
VLE	Vapour-liquid equilibrium
J-T	Joule Thomson
UDF	User Defined Function

NOMENCLATURE

n	Number or moles
P	Absolute pressure
P _c	Critical pressure
p _i	Partial pressure, species i
R	Universal gas constant
T	Absolute temperature, Kelvins or Rankines
T _{bi}	Normal boiling point, species i
T _c	Critical temperature
V	Molar or specific volume
W	Water content in lb/MMscf
x _i	Liquid fraction, species i,
y _i	Vapour fraction, species i,
z	Compressibility factor $\equiv PV/RT$

CHAPTER 1: INTRODUCTION

1.1 Background of Study

The petroleum industry spends millions of dollars every year to combat the formation of hydrates, the solid, crystalline compounds that form from water and small molecules that cause problems by plugging transmission lines and damaging equipment. They are a problem in the production, transmission and processing of natural gas and it is even possible for them to form in the reservoir itself if the conditions are favorable.

Basically, it is impossible to avoid the existence of water vapor in the natural gas. The water vapor can be formed due to condensation of gas in the pipeline or by natural existence in the natural gas itself. Existence of water in the pipeline can cause corrosion at the inner pipe surface, affect the heat transfer process and the quality of exported dry gas (product)

Water vapor always exists in the natural gas produced from the well head in the platform. In the reservoir fluid, the pores contain both oil and gas, and water liquid. It is difficult to separate them in the reservoir together. When the reservoir fluid is produced from the well, the mixture contains both water and oil. Thus, water need to be extracted from the gas/oil to ensure the fluid is dry enough for further production. In most of the platforms, the natural gas is being treated through gas dehydration system using glycol as an absorbent. Glycol will absorb water from the natural gas in glycol contactor.

1.2 Problem Statement

Current technology used in industrial to remove the water vapour in the natural gas is not efficient. The current separation techniques are absorption and membrane separation. However, membrane separation occupies large floor space, requires high maintenance and high CAPEX. Membrane has to be changed periodically to maintain high efficiency of separation.

Meanwhile, most of the adsorption separation technology uses glycol as absorbent to absorb the water from the gas in glycol tower. After that, the glycol will be sent to glycol regeneration system to remove the water from glycol so that the glycol can be used again. Though the separation efficiency is high, the CAPEX (for the equipment) , maintenance and operating cost are high.

In this project, a new method of separation is proposed – separation using high centrifugation force. This is a new technology in industry. The main advantage of this new technology is low CAPEX (capital expenditure) and operating cost because it does not involve any chemicals or catalyst. The equipments required are simple and small compared to the equipments of membrane and adsorption technique.

Before the experiment is carried out or the prototype is built, the feasibility of this separation technique needs to be studied first. This can be done by predict the behaviour of the particles before and after simulation using *Fluent and Gambit* software. From the simulation the feasibility and the efficiency can be determined.

1.3 Objectives

1. Understanding thermodynamics and phase behavior of water and natural gas in a pipeline under high pressure
2. Model thermodynamics properties of water and natural gas under high pressure
3. Integrate Wilson model with CFD simulator to simulate supersonic separation process using J-T valve

1.4 Scope of Study

Basically, the scope for study for FYP1 and 2 can be summarized as below

- Understand Wilson Model for thermodynamics properties
- Model Joule Thomson valve in natural gas pipeline using gambit software.
- Simulate dehydration process in natural gas using Joule-Thomson Valve
- Incorporate Wilson Model Coding to calculate water fraction

The case study is mainly about separation process between water and gas. The existence of water vapour in the gas pipeline affects the methane purity. Thus, removal of water from the gas by using high centrifugation force is proposed

In the pipeline, the fluid consists of methane gas and water vapour. After flow through the nozzle-expander, the water vapour will condense and separated. Gas methane will be dehydrated.

The twister supersonic separator is integrated into the pipeline to create supersonic flow and swelling effect to separate the water vapour from natural gas efficiently without using any chemical. Equipment similar to twister supersonic separator is De Laval nozzle, which is also studied in this project.

Some of the important terms and principle applied in this project are principle of centrifugation, Mach number, super sonic flow, de Laval nozzle experiment, Joule-thomson cooling effect, Melewar 3S technology, Twister BV equipment.

The software used to draw the model is *gambit*. The model can be draw in any shape, depends on the real model and it serves as a platform for simulation. The file is exported as mesh file. The exported file is opened in *fluent*. *Fluent* is the software used to simulate the separation process.

CHAPTER 2: LITERATURE REVIEW

2.1 Orifice Plate

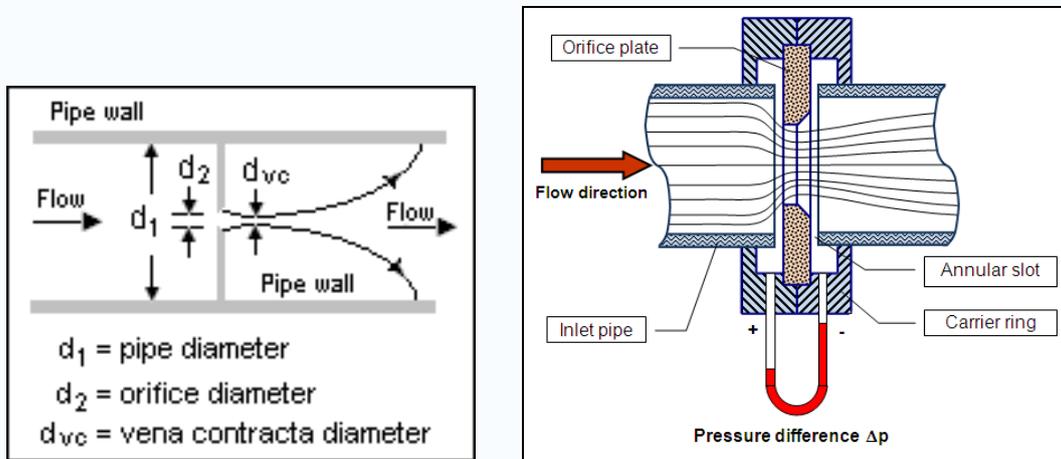


Figure 2.1 Dimension of orifice plate in a pipeline

Joule Thomson valve can also be a valve with an **orifice plate** in the middle. It is a device used to measure the rate of fluid flow. It uses the same principle as a Venturi nozzle, namely Bernoulli's principle which says that there is a relationship between the pressure of the fluid and the velocity of the fluid. When the velocity increases, the pressure decreases and vice versa.

An orifice plate is basically a thin plate with a hole in the middle. It is usually placed in a pipe in which fluid flows. As fluid flows through the pipe, it has a certain velocity and a certain pressure. When the fluid reaches the orifice plate, with the hole in the middle, the fluid is forced to converge to go through the small hole; the point of maximum convergence actually occurs shortly downstream of the physical orifice, at the so-called vena contracta point (see the figure above). As it does so, the velocity and the pressure changes. Beyond the vena contracta, the fluid expands and the velocity and pressure change once again. By measuring the difference in fluid pressure between the normal pipe section and at the vena contracta, the volumetric and mass flow rates can be obtained from Bernoulli's equation.

2.2 Joule Thomson Effect

In this project, the separation process is based on Joule Thomson effect. The water is removed from the natural gas when the gas flows through a nozzle-expander. The nozzle will increase the speed of the stream while the expander will cause temperature and pressure drop. It is called Joule Thomson Cooling effect. Due to the sudden pressure and temperature drop, the water vapour will condense and fall out of the stream as liquid droplet. The pure methane gas stream will continue to flow.

The effect is named for James Prescott Joule and William Thomson, 1st Baron Kelvin who discovered it in year 1852 following earlier work by Joule on Joule expansion, in which a gas undergoes free expansion in a vacuum.

In thermodynamics, the Joule-Thomson effect, also addressed as Joule-Kelvin effect or Kelvin- Joule effect describes the temperature changes of a gas or liquid when it is forced through a valve or porous plug while being insulated so that no heat is lost to the environment. This procedure is called throttling process or Joule Thomson process. At room temperature, all gases except hydrogen, helium and neon cool upon expansion by Joule Thomson process.

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 (the gas must not be expanded through a turbine) 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

words, a gas must be below its inversion temperature to be liquefied by the Linde cycle. For this reason, simple Linde cycle liquefiers cannot normally be used to liquefy helium, hydrogen, or neon.

The detail of derivation of Joule Thomson coefficient is shown in Appendix A. The coefficient and its equation might be used in defining the correlation and boundary condition for the simulation later on.

The figure below compares the degree of natural gas cooling at the same differential. The green color curve indicates the cooling efficiency of Joule Thomson Valve.

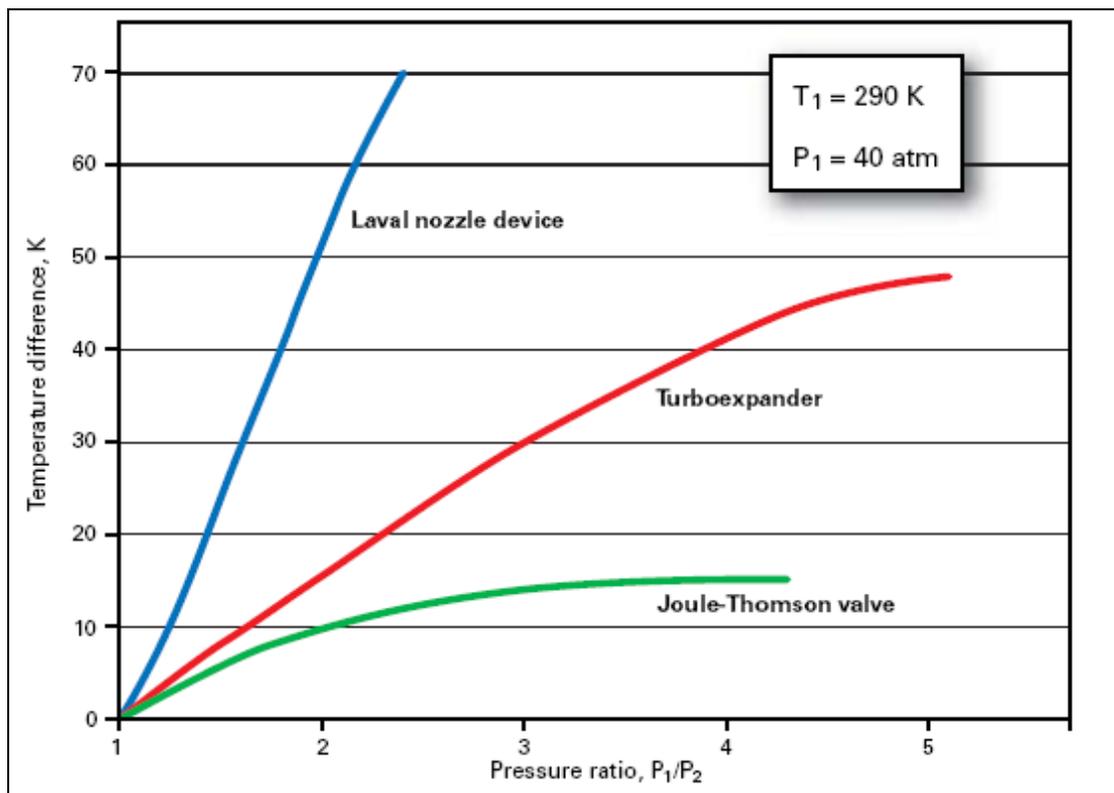


Figure 2.2 Cooling curve for Joule Thomson Valve

2.3 Joule Thomson Coefficient

A throttling process produces no change in enthalpy; hence for an ideal gas the temperature remains constant. For real gases, however, the throttling process will cause the temperature to increase or decrease.

The rate of change of temperature T with respect to pressure P in a Joule–Thomson process (that is, at constant enthalpy H) is the Joule–Thomson (Kelvin) coefficient μ_{JT} . This coefficient can be expressed in terms of the gas's volume V , its heat capacity at constant pressure C_p , and its coefficient of thermal expansion α as:

$$\mu_{JT} \equiv \left(\frac{\partial T}{\partial P} \right)_H = \frac{V}{C_p} (\alpha T - 1)$$

The value of μ_{JT} is typically expressed in °C/bar (SI units: K/Pa) and depends on the type of gas and on the temperature and pressure of the gas before expansion.

A positive value of μ indicates that the temperature decreases as the pressure decreases; a cooling effect is thus observed. This is true for almost all gases at ordinary pressures and temperatures. The exceptions are hydrogen (H_2), neon, and helium, which have a temperature increase with a pressure decrease, hence $\mu < 0$. Even for these gases there is a temperature above which the Joule-Thomson coefficient changes from negative to positive. At this inversion temperature, $\mu = 0$.

$$\mu = + \frac{1}{c_p} \left[\underbrace{- \left(\frac{\partial u}{\partial p} \right)_T}_{\text{deviation from Joul's law}} - \underbrace{\left(\frac{\partial(pv)}{\partial p} \right)_T}_{\text{deviation from Boyle's law}} \right]$$

The first term in the brackets denotes the deviation from Joule's law, which states that the internal energy is a function only of temperature. On expansion, there is an increase in the molecular potential energy, and hence is negative. This results in a positive μ and a temperature decrease. The second term in the brackets indicates the derivation from Boyle's law (that v varies inversely with p) for a real gas. For most gases at low temperatures and pressures, is negative; however, it changes sign at higher temperatures and pressures.

The following figures indicate the curve of u in T-P and T-S graphs. The value of u is affected by the values of temperature, pressure, enthalpy and entropy.

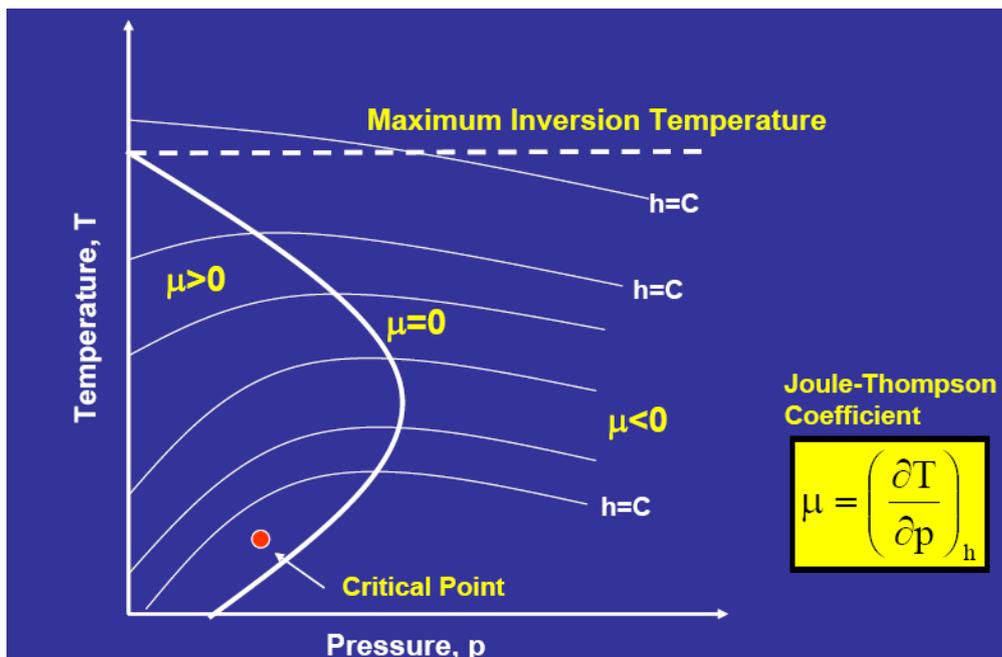


Figure 2.3: Joule Thomson expansion Curve. The value of u in T-P graph

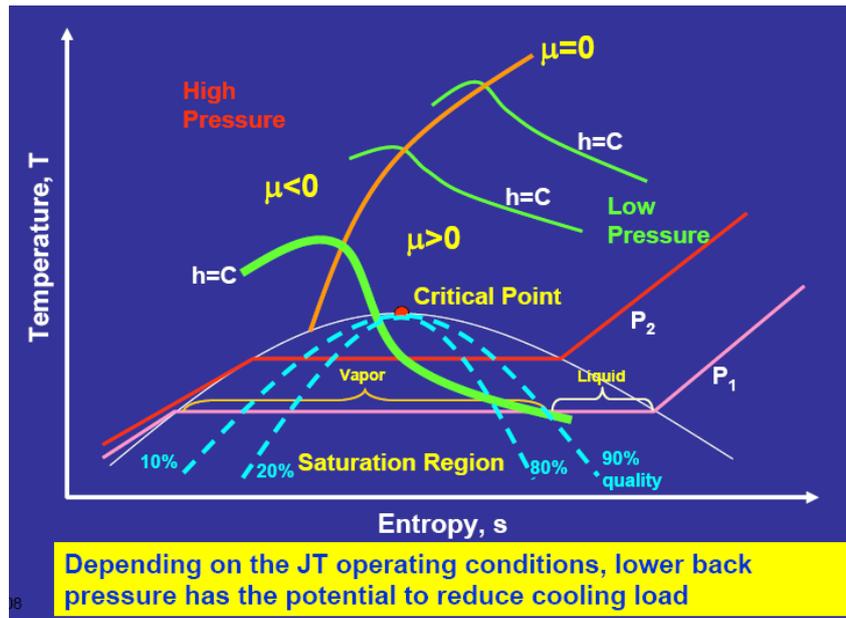


Figure 2.4 Joule Thomson expansions Curve. The value of μ in T-S graph

All real gases have an inversion point at which the value of μ_{JT} changes sign. The temperature of this point, the Joule–Thomson inversion temperature, depends on the pressure of the gas before expansion.

In a gas expansion the pressure decreases, so the sign of ∂P is always negative. With that in mind, the following table explains when the Joule–Thomson effect cools or warms a real gas:

If the gas temperature is	then μ_{JT} is	since ∂P is	thus ∂T must be	so the gas
below the inversion temperature	positive	always negative	negative	cools
above the inversion temperature	negative	always negative	positive	warms

For an ideal gas, μ_{JT} is always equal to zero: ideal gases neither warm nor cool upon being expanded at constant enthalpy. 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 a heat exchanger.

2.4 Joule Thomson Control Valve

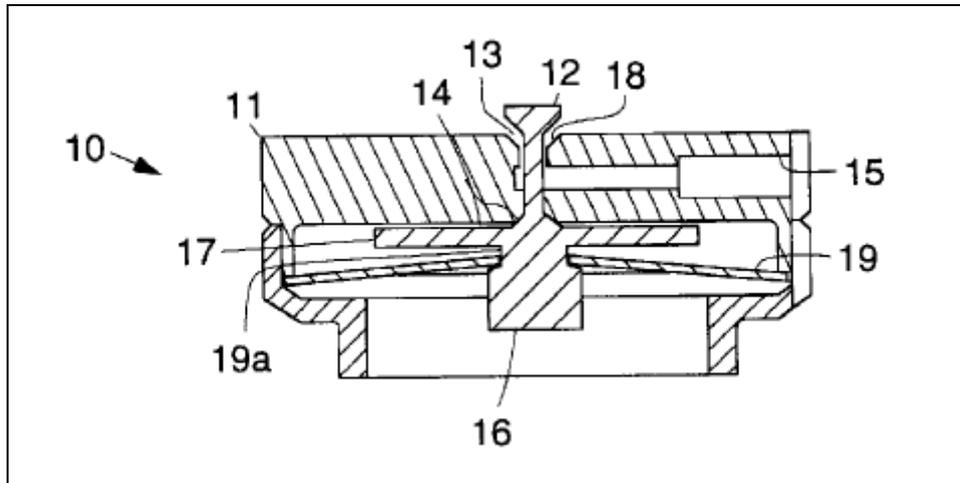


Figure 2.5 Structure of a Joule Thomson Valve Controller

Figure above shows an in-line valve flow controller for a Joule-Thomson cryostat. The controller has an in-line valve stem (12) that is part of, and is collinear with, an actuation stem (16) of the cryostat. Both the in-line valve stem and actuation stem sit in an orifice (13) of the Joule-Thomson cryostat. This arrangement automatically positions the valve stem over its valve seat (18). The in-line valve flow controller integrates with a temperature dependent snap disk (19) that is used to close the valve stem against the valve seat. Initial flow rate is determined only by the diameter of the orifice of the Joule-Thomson cryostat, and not by valve position. Bypass flow is also set by the diameter of the orifice, which is not subject wear, and the valve stem prevents contaminants from clogging the orifice

Joule Thomson Valve is a throttling valve or steady flow engineering device used to produce a significant pressure drop along with the large drop in temperature. In this valve,

- enthalpy remain constant
- No work device -mechanical or other forms
- Heat transfer almost always negligible
- PE and KE changes usually negligible

The Joule Thomson valve can be represented by 2 types of valves in figure 2.6 below. Joule Thomson valve can be a pipeline with orifice plate in the middle (right figure) or pipeline with a J-T valve controller.

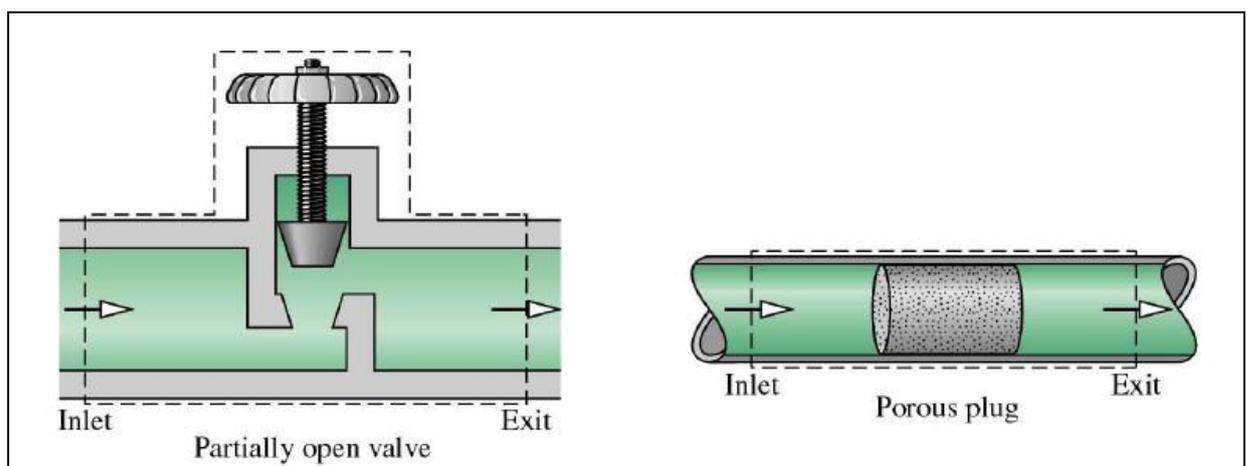


Figure 2.6 Internal structure of a Joule Thomson Valve and throttling device

Figure 2.7 below shows the process flow for Gas dehydration process using Joule Thomson Valve. Joule Thomson is usually used as a water extractor to remove water vapor from natural gas in a separation system.

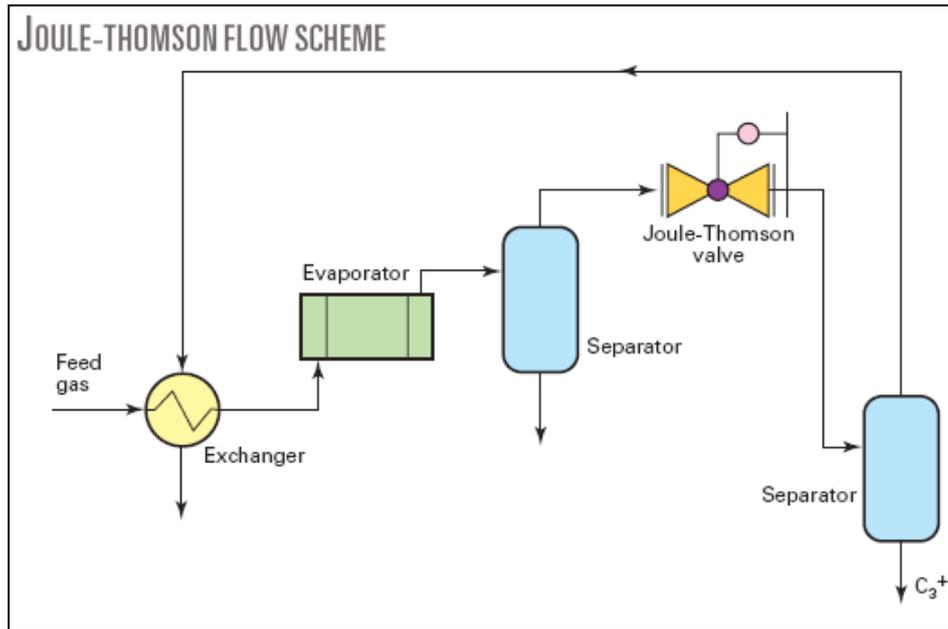


Figure 2.7 Flow Scheme for Joule Thomson Separation

2.5 Ideal Gas EOS

In this project, ideal gas equation of state is used to calculate the velocity of the gas flow under pipeline condition, given gas flow rate under standard condition. The Gas Density and Specific Volume Calculator calculate the density and specific volume of gas based on a modified version of the **Ideal Gas Law**:

$$PV = nRT$$

where:

P is the absolute pressure of the gas,

V is the volume of the gas,

n is the number of moles of gas,

T is the absolute temperature of the gas,

R is the universal gas constant

The Ideal Gas Law assumes the existence of a gas with no volume and no interactions with other molecules. Therefore, the Compressibility Factor (Z) can be used for a slight alteration to the ideal gas law to account for real gas behavior. Therefore the equation used for these calculations is:

$$PV = nZRT$$

where:

P is the absolute pressure of the gas,

V is the volume of the gas,

n is the number of moles of gas,

T is the absolute temperature of the gas,

R is the universal gas constant

Z is the gas compressibility factor

Any equation that relates the pressure, temperature, and specific volume of a substance is called the equation of state. The following equation is the ideal-gas equation of state.

A gas that obeys this relation is called an ideal gas

$$Pv = RT$$

R is the gas constant, which is determined from

$$R = R_u/M$$

where

R_u = universal gas constant, 8.314 kJ/(kmol-K)

M = molar mass, the mass of one mole of a
substance in grams

2.6 Mach number

Mach number (Ma or M) is the speed of an object moving through air, or any fluid substance, divided by the speed of sound as it is in that substance. It is commonly used to multiples of) the speed of sound.

$$M = \frac{v_s}{u}$$

where

M is the Mach number

v_s is the velocity of the source (the object relative to the medium)

u is the velocity of sound in the medium

The Mach number is commonly used both with objects travelling at high speed in a fluid, and with high-speed fluid flows inside channels such as nozzles, diffusers or wind tunnels. As it is defined as a ratio of two speeds, it is a dimensionless number. At a temperature of 15 degrees Celsius and at sea level, the speed of sound is 340.3 m/s (1225 km/h, or 761.2 mph, or 1116 ft/s) in the Earth's atmosphere. The speed represented by Mach 1 is not a constant; for example, it is dependent on temperature and atmospheric composition. In the stratosphere it remains constant irrespective of altitude even though the air pressure varies with altitude.

Since the speed of sound increases as the temperature increases, the actual speed of an object travelling at Mach 1 will depend on the fluid temperature around it. Mach number is useful because the fluid behaves in a similar way at the same Mach number.

So, an aircraft travelling at Mach 1 at sea level (340.3 m/s, 761.2 mph, 1,225 km/h) will experience shock waves in much the same manner as when it is travelling at Mach 1 at 11,000 m (36,000 ft), even though it is travelling at 295 m/s (654.6 mph, 1,062 km/h, 86% of its speed at sea level).

In order to accelerate a fluid flow to supersonic in a pipeline, it needs a convergent-divergent nozzle, where the converging section accelerates the flow to $M=1$, sonic speeds, and the diverging section continues the acceleration. Such nozzles are called de Laval nozzles and in extreme cases they are able to reach incredible, hypersonic velocities (Mach 13 at sea level).

2.7 Super Sonic Gas Separation Technique

3S Supersonic Gas Separation technique .is a new technology which is most exciting for everyone concerned with gas processing in the petro-chemical industry. 3S technology makes Gas Conditioning and Gas Separation more efficient, while at the same time giving equipment a smaller footprint, less weight and making process schemes simpler. In this project, this technique is used for separation of water from the gas in the pipeline.

The mixed Hydrocarbon Stream enters the 3S unit as pictured from the left. Flowing through a static arrangement of blades, the stream attains a high velocity swirl, as shown in **Appendix C**.

The stream continues through a nozzle, where it is accelerated to high sub-sonic or to supersonic speeds. Due to the rapid expansion at the exit of the nozzle - the working section - the desired condensates will form as a mist. The centrifugal force of the swirl moves those liquids as a film to the wall where they run off through a suitable constructive arrangement and are diverted together with some slip gas.

The gas stream - now dry - continues through an anti-swirling arrangement and through diffusers. Here the stream is slowed down and the kinetic energy converts back into pressure, regaining about 75-80% of the inlet pressure.

This technology is suitable for on-shore plants, particularly useful for off-shore plants due to the small footprint and reduced weight and has a great future for subsea installations.

Some of the advantages of 3S supersonic gas separation are shown below:

- Small footprint
- Weight Savings
- Portability and lower Installation Cost
- Lower Capex, lower Opex
- No moving parts - no maintenance
- Conservation of reservoir energy
- Higher efficiency than today's cryogenic technology

2.8 Twister Super Sonic Separator

The Twister Supersonic Separator is a unique combination of physical processes producing a completely revolutionary gas conditioning system. Condensation and separation at supersonic velocity is the key to achieving a significant reduction in both capital and operating costs.

Twister can be used to condense and separate water and heavy hydrocarbons from natural gas. Current applications include any combination of the following:

- Water Dewpointing (Dehydration)
- Hydrocarbon Dewpointing
- Natural Gas Liquids extraction (NGL/LPG)

These applications can be applied in the following market areas:

- Underground gas storage
- NGL recovery

New applications under study include bulk H²S removal upstream sweetening plants, landfill gas treatment and sub-sea gas processing. 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. Twister BV is currently working on a joint technology development project with Petrobras in Brazil for sub-sea gas processing using Twister technology.

In addition, the compact and low weight Twister system design enables de-bottlenecking of existing space and weight constrained platforms. The picture of twister supersonic separator is shown in Appendix C.

2.9 Centrifugation Force

Here, there are a few formula used to determine the centrifugation force.

1. Centrifugal Force in term of velocity

$$a_e = r\omega^2$$

a_e = acceleration from a centrifugal force (m/s²)

r = radial distance from centre

ω = angular velocity in rad/s

$$F_c = ma_e = mr\omega^2$$

$$\omega = \frac{v}{r}$$

$$F_c = \frac{mv^2}{r}$$

2. Centrifugal Force in term of rotational speed N rev/min (further derivation from 1)

$$\omega = \frac{2\pi N}{60} \quad N = \frac{60v}{2\pi r}$$
$$F_c = mr \left(\frac{2\pi N}{60} \right)^2 = 0.000341mrN^2$$

3. Centrifugation force in G

Centrifugation Force in angular velocity

$$F_c = ma_e = mr\omega^2$$

Gravitational Force,

$$F_g = mg$$

Centrifugal force in terms of gravitational force

$$\frac{F_c}{F_g} = \frac{r\omega^2}{g} = \frac{v^2}{rg} = \frac{r}{g} \left(\frac{2\pi N}{60} \right)^2 = 0.001118rN^2$$

The Twister™ Supersonic Separator has thermodynamics similar to a turbo-expander, combining the following process steps in a compact, tubular device:

- expansion
- cyclonic gas/liquid separation
- re-compression

Whereas a turbo-expander transforms pressure to shaft power, Twister achieves a similar temperature drop by transforming pressure to kinetic energy (i.e. supersonic velocity) . 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.

2.9.1 Application of Centrifugation Force

Centrifugation force is very useful and powerful technology. It had been modified and applied in many areas. Below are some of the application of centrifugation:

- A centrifugal governor regulates the speed of an engine by using spinning masses that move radially, adjusting the throttle, as the engine changes speed. In the reference frame of the spinning masses, centrifugal force causes the radial movement.
- A centrifugal clutch is used in small engine-powered devices such as chain saws, go-karts and model helicopters. It allows the engine to start and idle without driving the device but automatically and smoothly engages the drive as the engine speed rises. Inertial drum brake ascenders used in rock climbing and the inertia reels used in many automobile seat belts operate on the same principle.

- Centrifugal forces can be used to generate artificial gravity, as in proposed designs for rotating space stations. The Mars Gravity Biosatellite will study the effects of Mars-level gravity on mice with gravity simulated in this way.
- Spin casting and centrifugal casting are production methods that use centrifugal force to disperse liquid metal or plastic throughout the negative space of a mold.
- Centrifuges are used in science and industry to separate substances. In the reference frame spinning with the centrifuge, the centrifugal force induces a hydrostatic pressure gradient in fluid-filled tubes oriented perpendicular to the axis of rotation, giving rise to large buoyant forces which push low-density particles inward. Elements or particles denser than the fluid move outward under the influence of the centrifugal force.
- Some amusement park rides make use of centrifugal forces. For instance, a Gravitron's spin forces riders against a wall and allows riders to be elevated above the machine's floor in defiance of Earth's gravity.

2.10 Super Sonic Flow

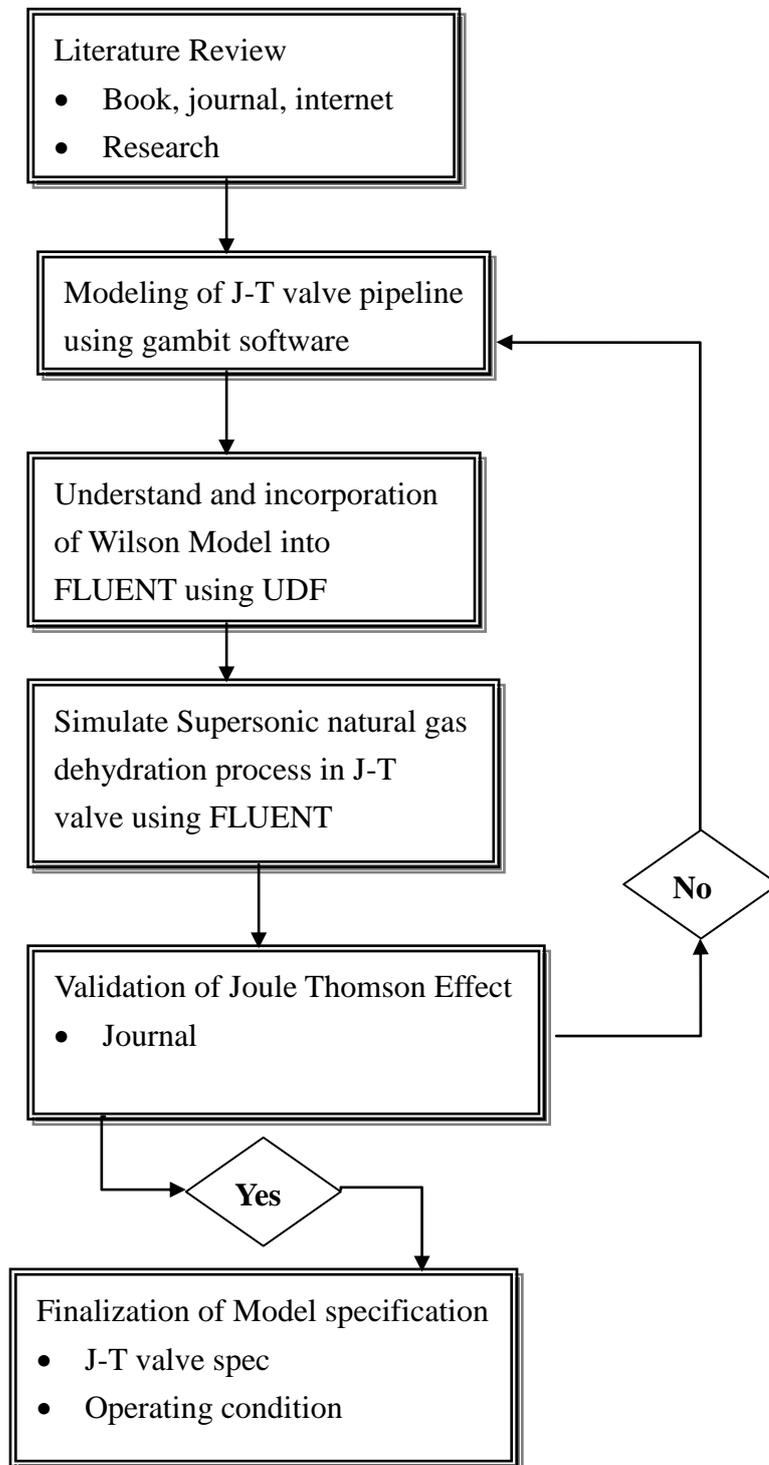
The term supersonic is used to define a speed that is over the speed of sound (Mach 1). At a typical temperature like 21 °C (70 °F), the threshold value required for an object to be traveling at a supersonic speed is approximately 344 m/s, (1,129 ft/s, 761 mph or 1,238 km/h). Speeds greater than 5 times the speed of sound are often referred to as hypersonic. Speeds where only some parts of the air around an object (such as the ends of rotor blades) reach supersonic speeds are labeled transonic (typically somewhere between Mach 0.8 and Mach 1.2)

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; (pressure has little effect). Since air temperature and composition varies significantly with altitude, Mach numbers for aircraft can change without airspeed varying. 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.

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. Therefore, since sound is in fact an infinitesimal pressure difference propagating through a fluid, the speed of sound in that fluid can be considered the fastest speed that "information" can travel in the flow. This difference most obviously manifests itself in the case of a fluid striking an object. In front of that object, the fluid builds up a stagnation pressure as impact with the object brings the moving fluid to rest. In fluid traveling at subsonic speed, this pressure disturbance can propagate upstream, changing the flow pattern ahead of the object and giving the impression that the fluid "knows" the object is there and is avoiding it. However, in a supersonic flow, the pressure disturbance cannot propagate upstream. Thus, when the fluid finally does strike the object, it is forced to change its properties -- temperature, density, pressure, and Mach number -- in an extremely violent and irreversible fashion called a shock wave. The presence of shock waves, along with the compressibility effects of high-velocity (see Reynolds number) fluids, is the central difference between supersonic and subsonic aerodynamics problems.

CHAPTER 3: METHODOLOGY

3.1 The Flow Chart of Methodology



3.2 Project Milestone

FYP 1

No.	Detail/ Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Selection of Project Topic														
2	Understand the topic and problem														
3	Job scope and preliminary report				X										
5	Learning Fluent and Gambit														
6	Learn simulation and Progress report								X						
7	Seminar and correction														
8	Oral Presentation													X	

X milestone

 Process

FYP2

No.	Detail/ Week	1	2	3	4	5	6	7	8	9	10	11	12	13	14
1	Review on FYP1 report and research														
2	Submission of Progress Report 1				X										
3	Research of Joule Thomson Model														
4	Submission of Progress Report 2								X						
5	Simulation of Joule Thomson Valve														
5	Simulation of various dimension of J-T valve														
6	Poster Exhibition												X		
7	Submission of Dissertation (soft bound)													X	
8	Proposal of best J-T valve specification														X
9	Submission of Project Dissertation (hard bound)														X

X milestone

 Process

3.3 Methodology

The objective of this project is to simulate the particle movement in the separation process using high gravitational concept. The methodology can be divided into two part. The first part is to draw the model by using *Gambit* software as a platform for simulation. The second part is to perform simulation process by using *fluent* software.

How to draw the geometry of the model by using *Gambit*

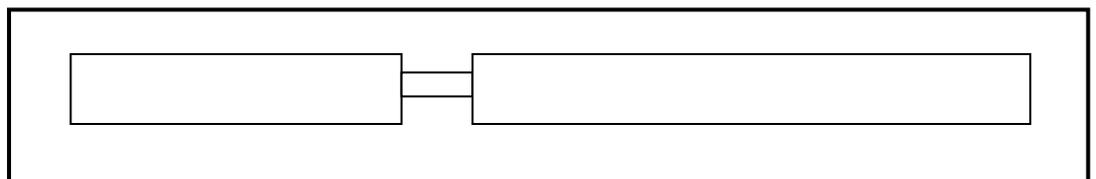
1. Go to *vertex* and choose click on *create real vertex*. Set the center point to be zero at x, y, and z direction and click apply.
2. Draw the vertex of the geometry, and then connect the vertex together by using *edge*. After that construct a face by combine the edges.

Geometry: A rectangular with concave in the middle

(Different size of J-T valve are drew to make comparison)

3. Go to *Geometry* → *Volume* → *revolve face*

Select the face , set the angle to be 360 degree and set the axis to be the edge to be revolved.



4. Select *Mesh* then *edge* to mesh the edge of the pipeline. Determine the number of interval to define the quality. Select *face* to mesh the faces followed by meshing the volume of the geometry.



5. Select *zones* and define type of boundary for each faces.
(Specify wall, velocity inlet and outlet)
6. Save and export the file as mesh file.

How to perform simulation for 3D model

1. Open the file exported from *Gambit*. (Go to file → read → case)
2. Define the model, material, boundary condition and operating condition
At material, add methane gas into the component
Set the inlet boundary as velocity 11 m/s
3. Go to *solve* to initialize then choose *iterate* to simulate the process. Iterate the process until the value converge to 0.0001
4. Display the simulation result (can display in grid, contour, vector, path line or particles track).

3.4 Software required

1. Microsoft office

Including words, excel, project and power point

2. Bloodshed Dec-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. Microsoft Visual Studio 6.0

The C code needs to be compiled by Microsoft Visual Studio 6.0 into a macro before being incorporated into FLUENT.

4. Gambit

This software is used to draw the J-T valve and pipeline designs. Functions include meshing and defining faces such as inlet, outlet and wall. Version 2.2.30 is used in the project.

5. FLUENT

This software is used to draw the pipe designs. Functions include meshing and defining faces such as inlet, outlet and wall. Version 2.2.30 is used in the project.

CHAPTER 4 RESULT AND DISCUSSION

4.1 Calculation Velocity for Gas Flow under Pipeline condition

Given (industrial standard condition),

Volume Flow rate = 2 mmscf /day

Outer diameter = 2 inch

$$\begin{aligned}\text{Area} &= \pi \times (1 \text{ inch} \times 0.0254 \text{ m/inch})^2 \\ &= 2.0268 \times 10^{-3} \text{ m}^2\end{aligned}$$

Volumetric = 2 MMSCF/day

$$\begin{aligned}\text{Flow rate} &= 2 \times 10^6 \text{ ft}^3/\text{day} \times 1 \text{ day} / (24 \times 60 \times 60) \text{ s} \times (1 \text{ m})^3 / (3.2808 \text{ ft})^3 \\ &= 0.6555 \text{ m}^3/\text{s}\end{aligned}$$

$$\begin{aligned}\text{Velocity} &= V/A \\ &= 0.6555 / 2.0268 \times 10^{-3} \\ &= 323.41 \text{ m/s (Standard condition, not pipeline condition!)}\end{aligned}$$

The velocity of 323m/s is under standard condition. The velocity of gas flow under pipeline operating condition need to be calculated through ideal gas equation.

$$\frac{PV}{ZNRT} \text{ at standard condition} = \frac{PV}{ZNRT} \text{ at pipeline condition}$$

$$\frac{PV}{ZT} \text{ at standard condition} = \frac{PV}{ZT} \text{ at pipeline condition}$$

Assumption

1. N and R at standard and pipeline condition are the same.
2. N and R value are cancelled out at standard and pipeline condition
3. The gas involved is 100% methane

At standard condition,

$$P = 1 \text{ atm} = 14.7 \text{ psia}$$

$$T = 25^\circ\text{C} = 536.67^\circ\text{R}$$

$$V = 0.6555 \text{ m}^3/\text{s}$$

At pipeline Condition

$$P = 40 \text{ bar} = 580.151 \text{ psia}$$

$$T = 400\text{K} = 720^\circ\text{R}$$

$$V = ?$$

To find the value of Z for both condition:

Given the critical value of methane

$$T_{\text{critical}} = -82.7^\circ\text{C} = 344.07^\circ\text{R}$$

$$P_{\text{critical}} = 45 \text{ bar} = 652.7 \text{ psia}$$

For standard condition,

$$T_r = \frac{T}{T_c} = \frac{536.67}{344.07} = 1.56$$

$$P_r = \frac{P}{P_c} = \frac{14.7}{652.7} = 0.0225$$

From figure below, **Z value is 1** under standard condition.

For pipeline condition,

$$T_r = \frac{T}{T_c} = \frac{720}{344.07} = 2.09$$

$$P_r = \frac{P}{P_c} = \frac{580.151}{652.7} = 0.88$$

From figure below, **Z value is 0.97** under pipeline condition.

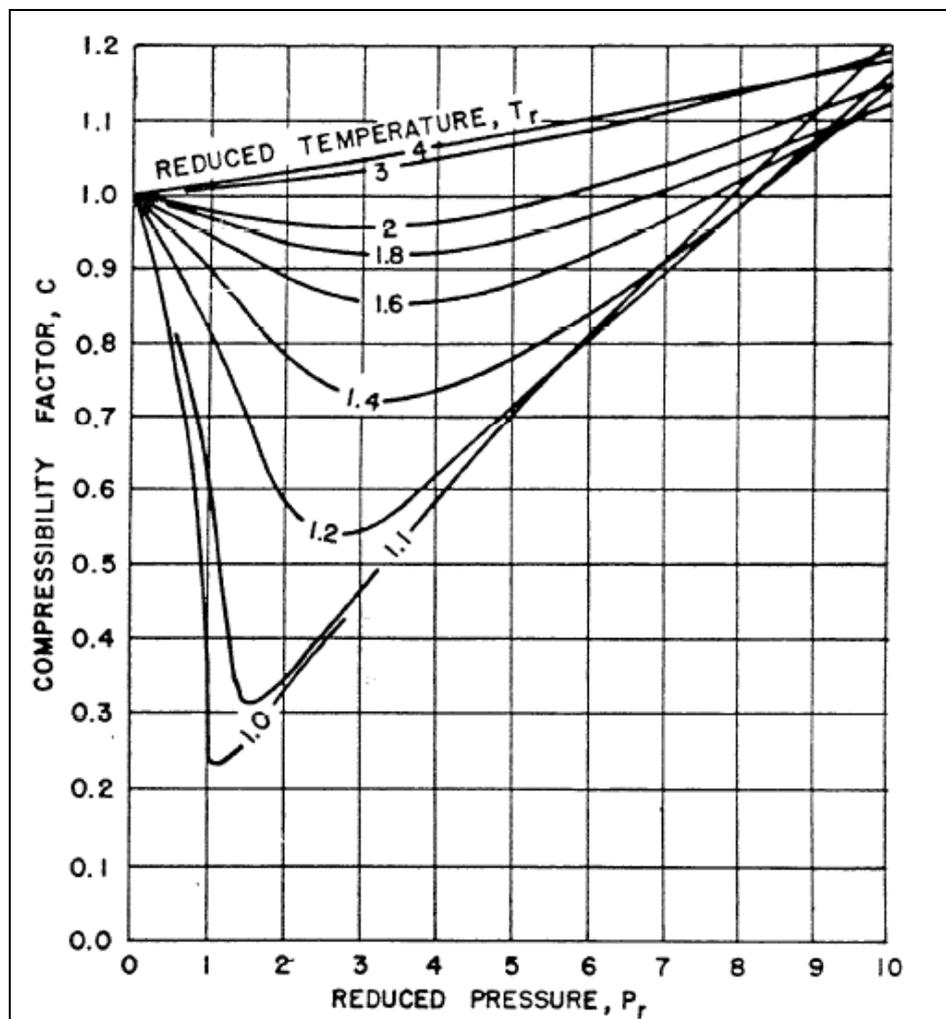


Figure 4.1 Compressibility Chart for Methane Gas

$$\frac{101.325 \times 0.6555}{1 \times 298} \text{ at std condition} = \frac{4000V}{0.97 \times 400} \text{ at pipeline condition}$$

$$V_{\text{pipeline}} = 0.0216 \text{ m}^3/\text{s}$$

$$\text{Velocity} = V/A$$

$$= 0.0216 \text{ m}^3/\text{s} / 2.0268 \times 10^{-3} \text{ m}^2$$

$$= \mathbf{10.67 \text{ m/s}}$$
 (pipeline operating condition)

$$\text{Mass Flow} = 0.0216 \text{ m}^3/\text{s} \times 0.717 \text{ kg/m}^3$$

$$= 0.0155 \text{ kg/s}$$

Thus, the operating condition in the inlet pipeline is **10.67 m/s**. According to the rule of thumb in industry, the inlet flow rate to a pipeline should not exceed 20m/s to avoid sudden backflow.

From the ideal gas equation of state, the velocity of gas flow is reduced from 323m/s under standard condition to 10.67 m/s under pipeline operating condition.

The speed of sound is 340.15m/s at 15m above sea level. Gas flow at the inlet is only 10.67 under pipeline condition but it is believed to increase to achieve the speed of sound (Mach = 1), 340.15m/s at the throttling part of the pipeline.

4.2 Geometry of J-T valve model

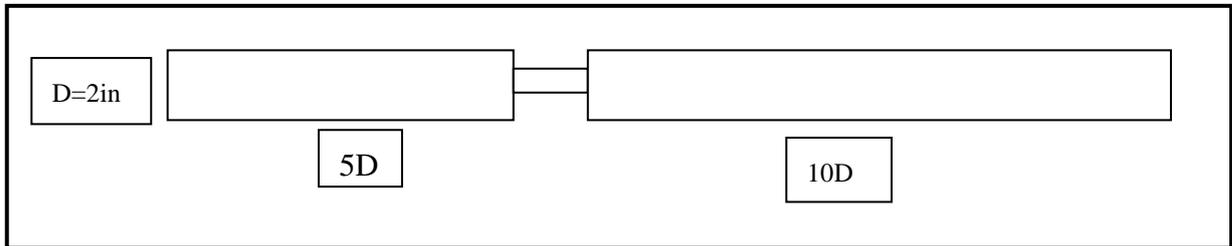


Figure 4.2 Dimension of J-T Model

Table 4.1 Dimension of J-T valve for simulation

Parts	Rule of Thumb	Dimension
Pipe Diameter	2 inch	2 inch
Length before throat	5 Diameter	10 inch
Length after throat	10 diameter	20 inch
Diameter of throat	none	1 inch @ 0.6 inch
Length of the throat	None	1 inch @ 2 inch

4.3 Basis for Simulation

Table 4.2 Dimension of J-T valve for different cases

Throttle diameter/ Throttle length	long diameter (D=1 inch)	Small diameter (D=0.6 inch)
Small length (L= 1 inch)	A1	A2
Long length (L=3 inch)	A3	A4

Table 4.3 Operating Condition and Components of Natural Gas

Operating Condition	value
Temperature	400K
Pressure	40 Bar
Velocity	11 m/s
Mass Flow Rate	00.0155 kg/s
Components	Mole Fraction
Methane	0.9
CO2	0.02
H2S	0.02
H2O Vapor	0.04

4.4 Simulation Result for Different Cases

4.4.1 Simulation Result of Case A 1

Table 4.4: Dimension for Case A1 J-T Valve

Criteria	Value
Length	1 inch (small)
Diameter	1 inch (long)

Table 4.5: Simulation Result For Case A1

Criteria	Value at inlet	Value at Throttle (max)	Change
Relative Pressure , bar	9.91	-8.75	-18.66 bar
Mach number	-	1	+1
Temperature ,K	400	380	-20
Velocity , m/s	12	342	+ 330
Molar concentration ,Kmol/m ³	82.7	55	-27.7

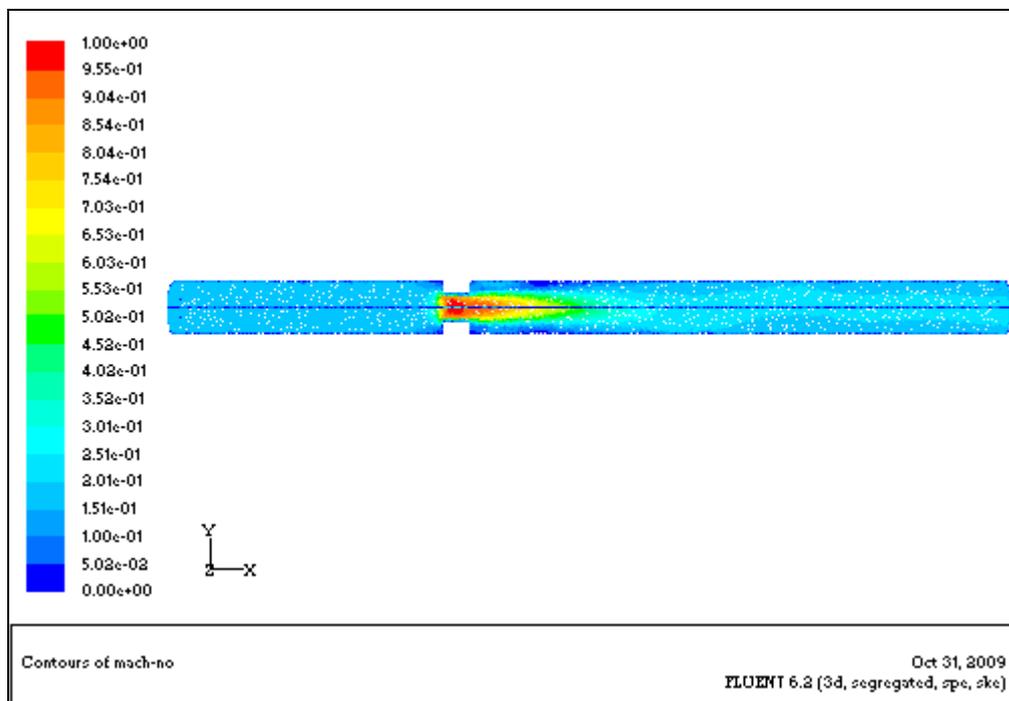


Figure 4.2: Contour of Mach number For Case A1

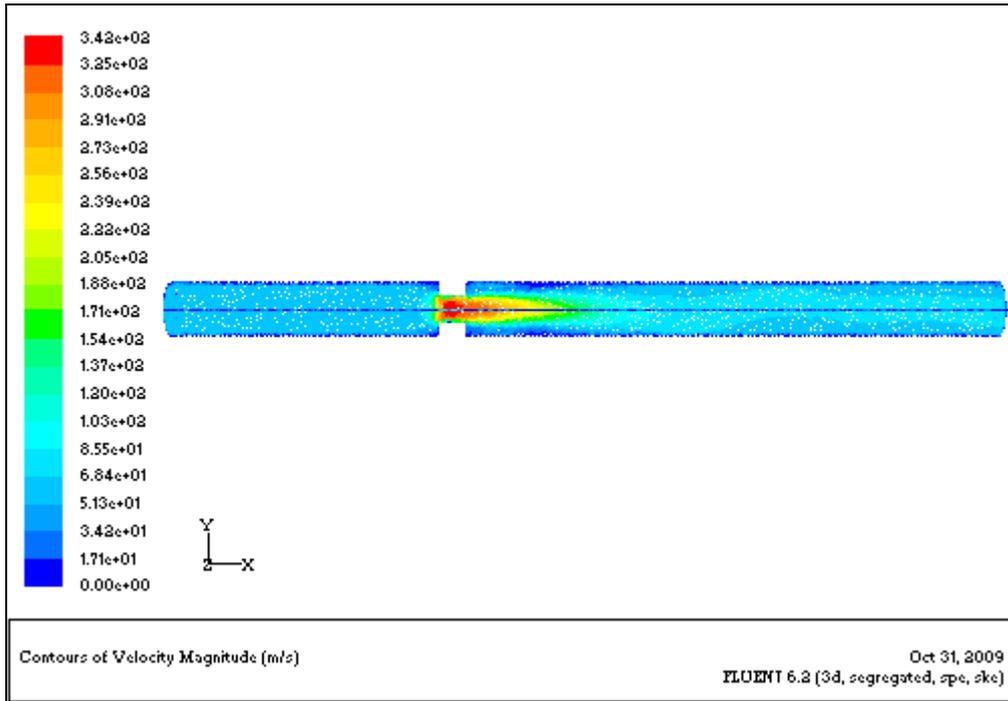


Figure 4.3: Contour of Velocity Magnitude For Case A1

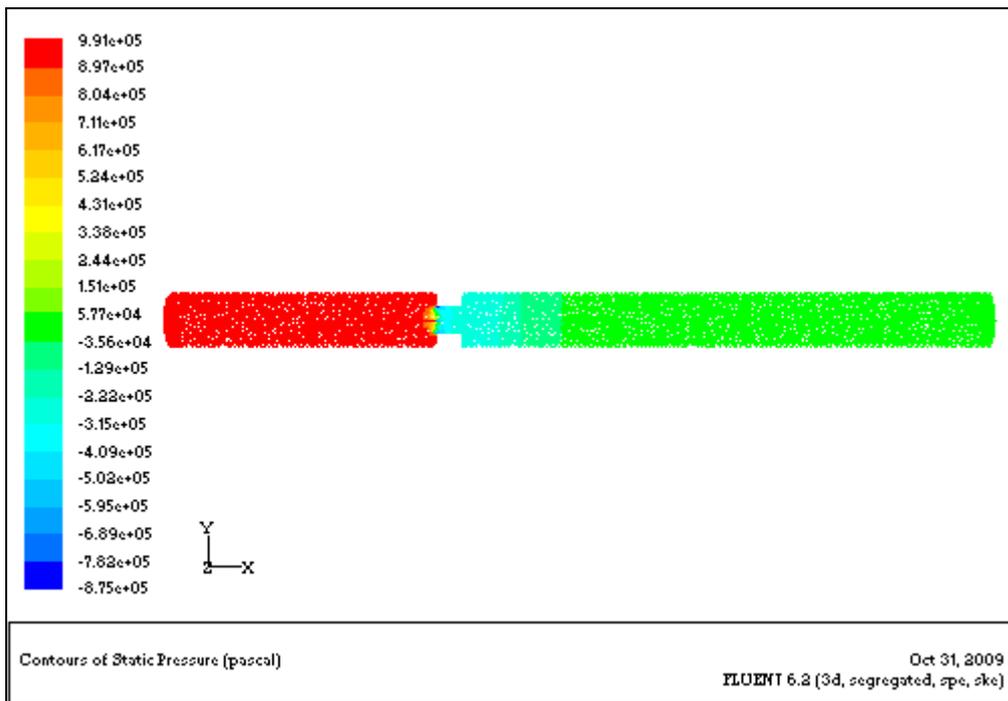


Figure 4.4: Contour of Static Pressure for Case A1

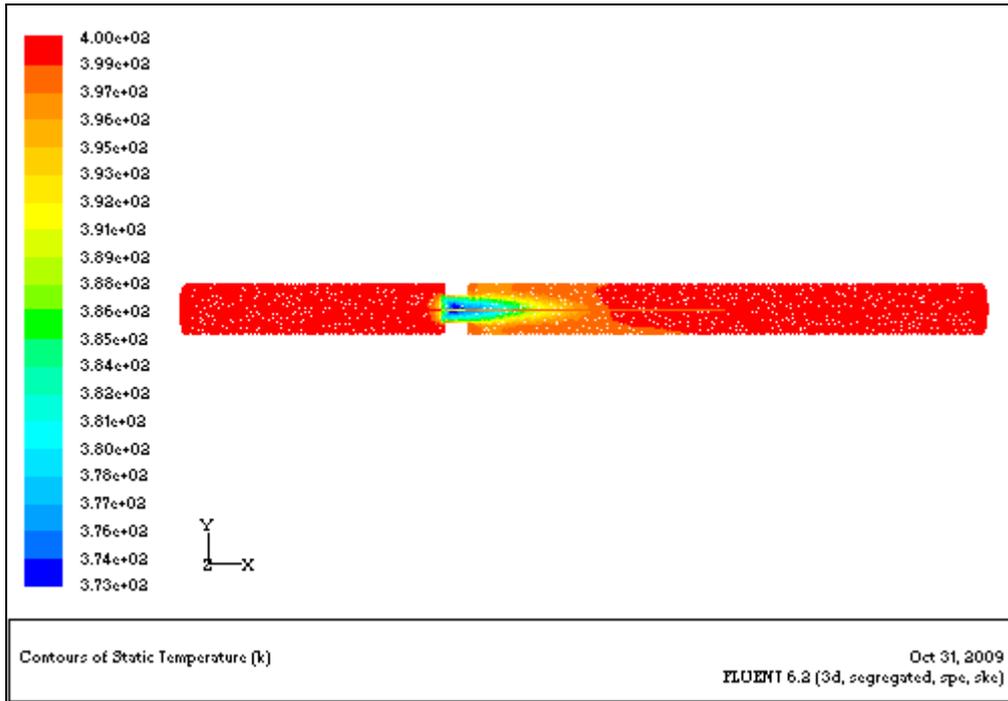


Figure 4.5: Contour of Static Temperature for Case A1

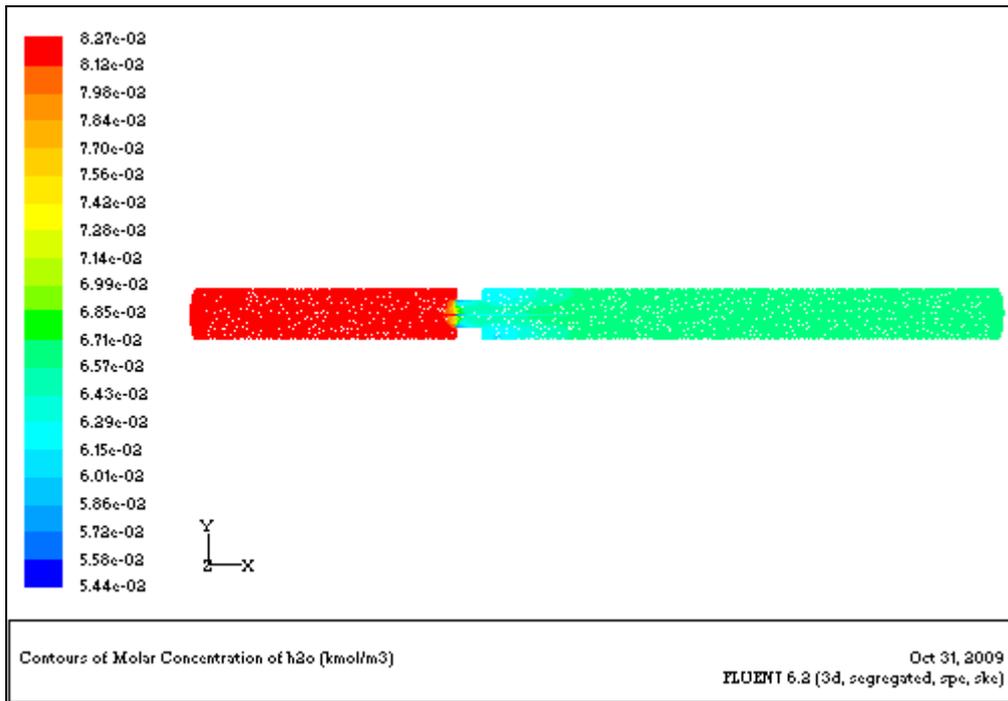


Figure 4.6 : Contour of H2O Molar Concentration For Case A1

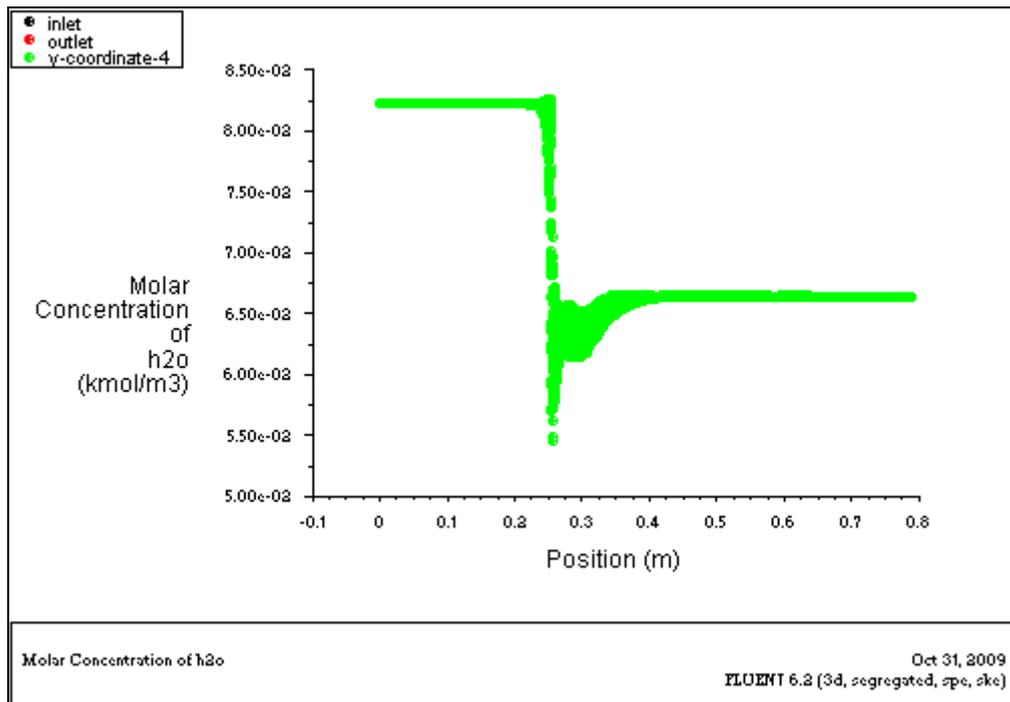


Figure 4.7 : H2O Molar Concentration For Case A1

4.4.2 Simulation Result of Case A 2

Table 4.6: Dimension for Case A2 J-T Valve

Criteria	Value
Length	1 inch (small)
Diameter	0.6 inch (small)

Table 4.7: Simulation Result For Case A2

Criteria	Value at inlet	Value at Throttle (max)	Change
Relative Pressure , bar	24	-10.6	-34.6 bar
Mach number	-	1.29	+1.29
Temperature ,K	400	373	-27
Velocity , m/s	12	438	+ 436
Molar concentration ,Kmol/m ³	106	53.3	-52.7

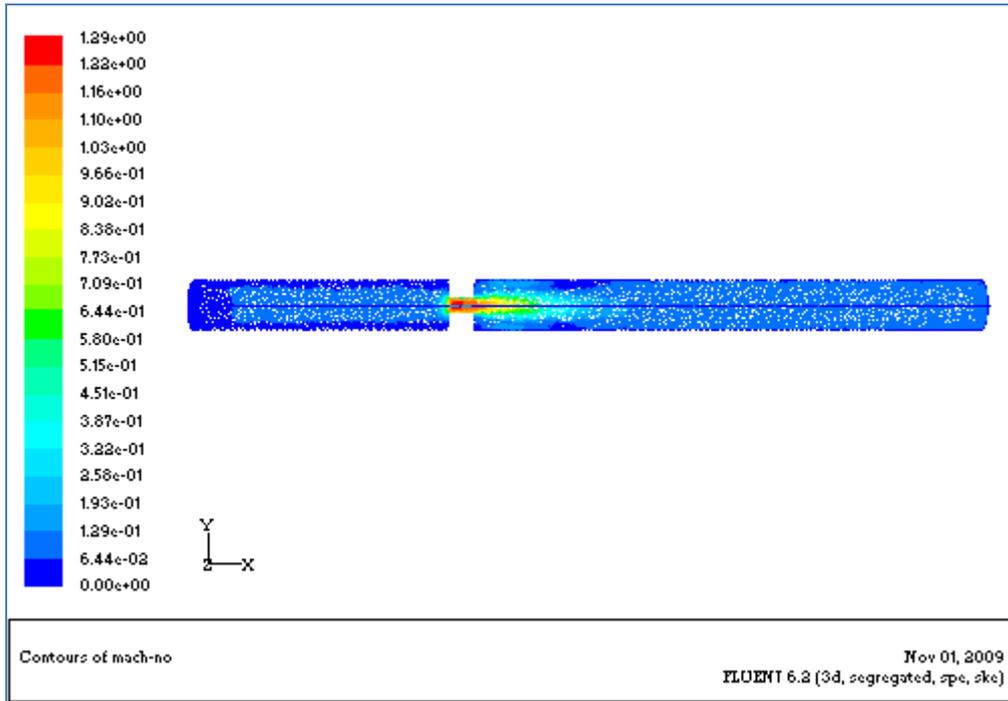


Figure 4.8: Contour of Mach Number For Case A2

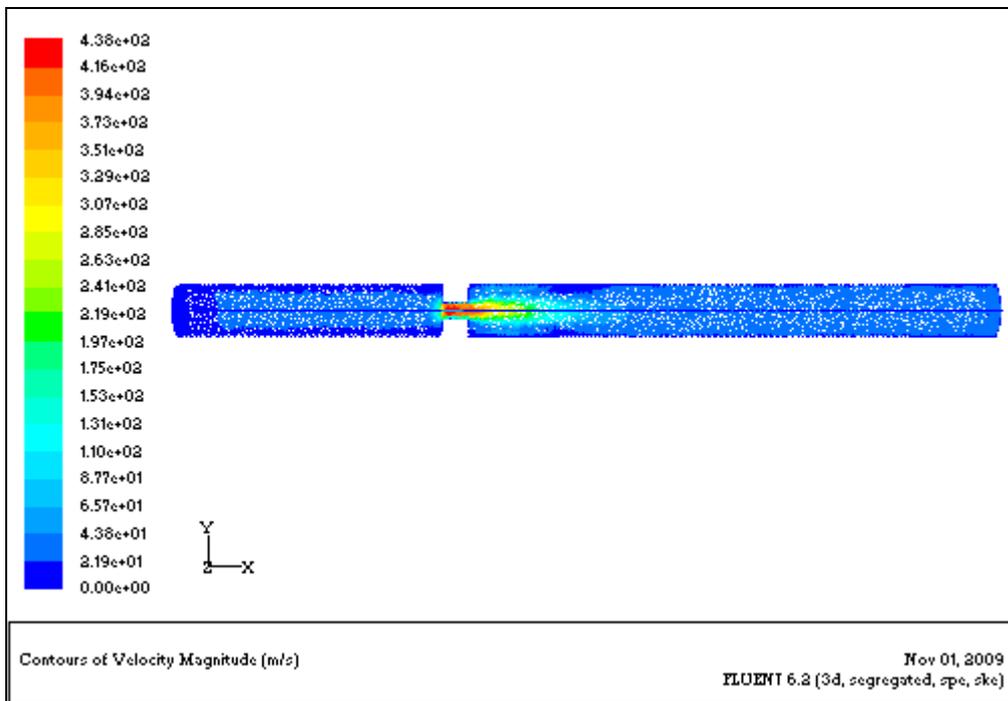


Figure 4.9: Contour of Velocity Magnitude For Case A2

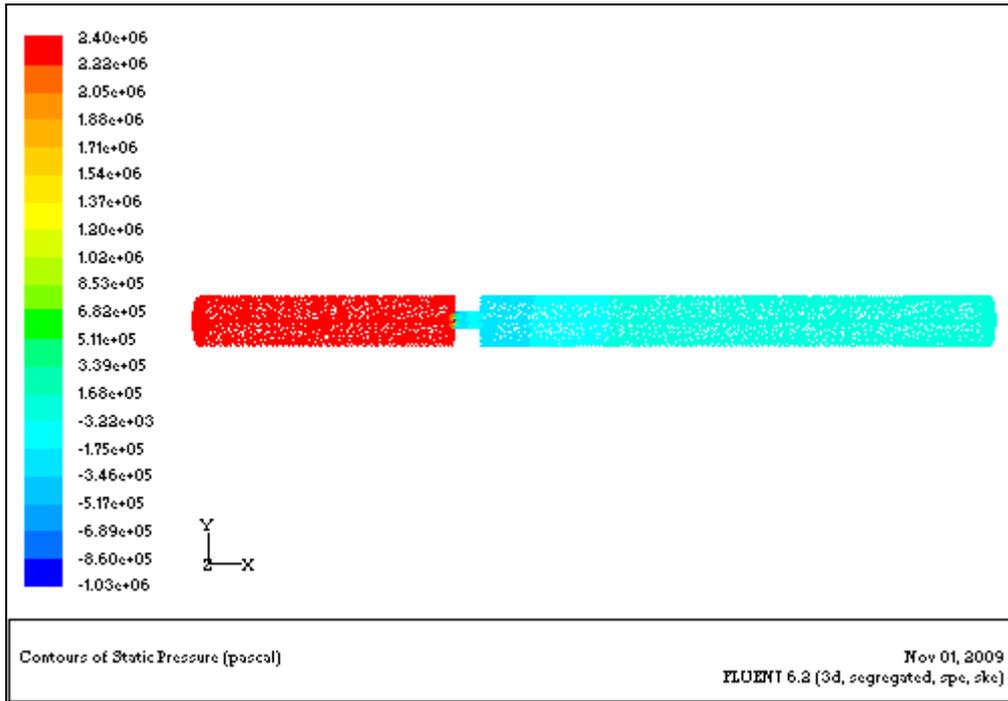


Figure 4.10 : Contour of Static Pressure For Case A2

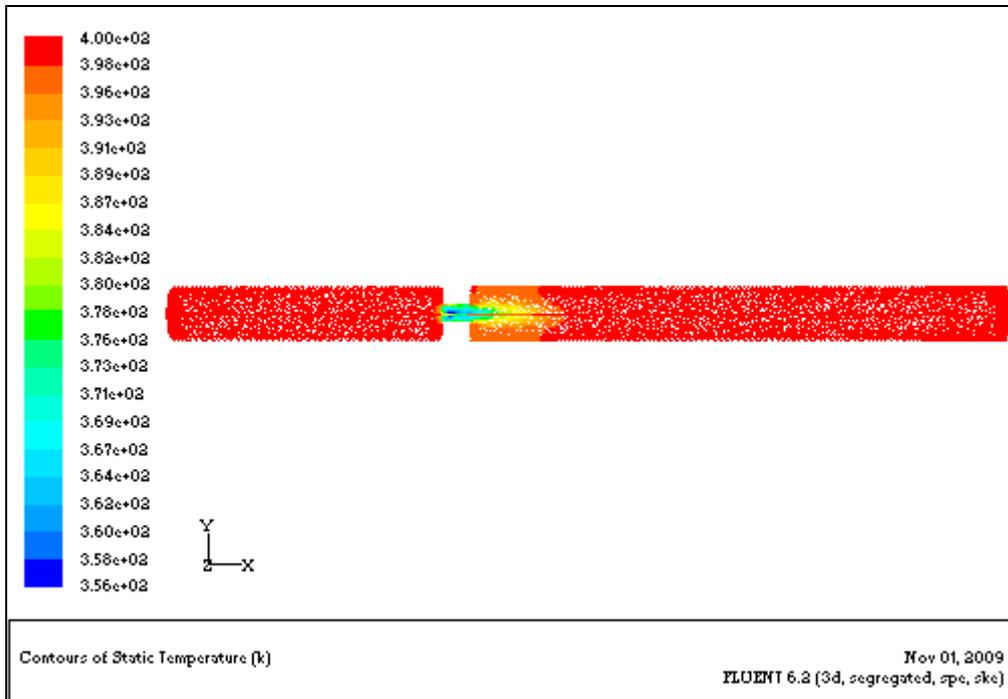


Figure 4.11: Contour of Static Temperature For Case A2

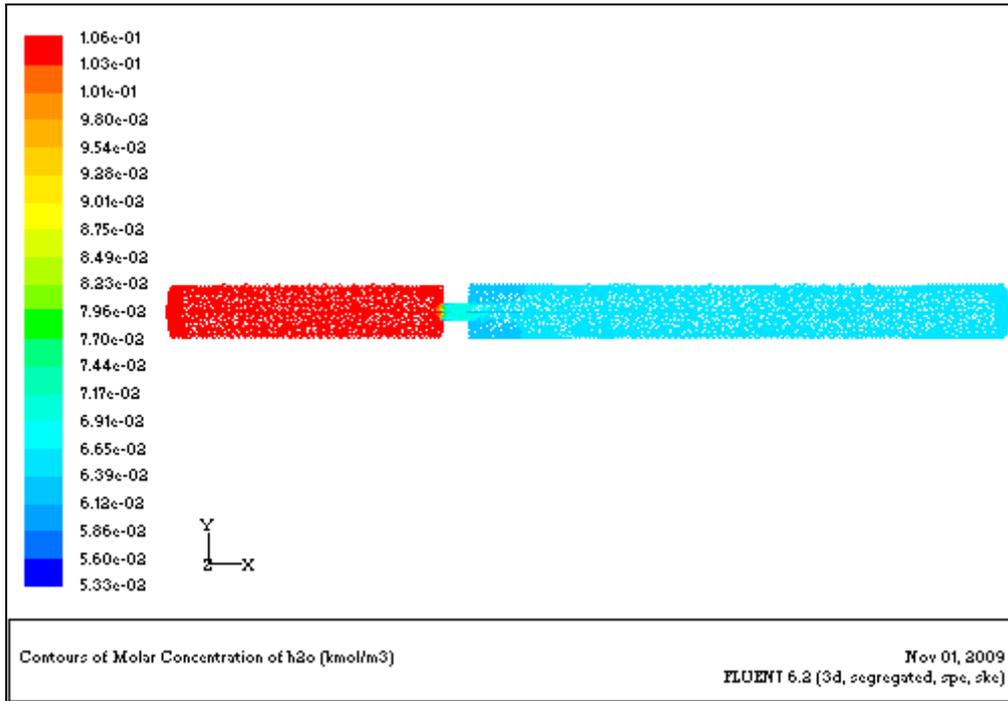


Figure 4.12: Contour of H2O Molar Concentration For Case A2

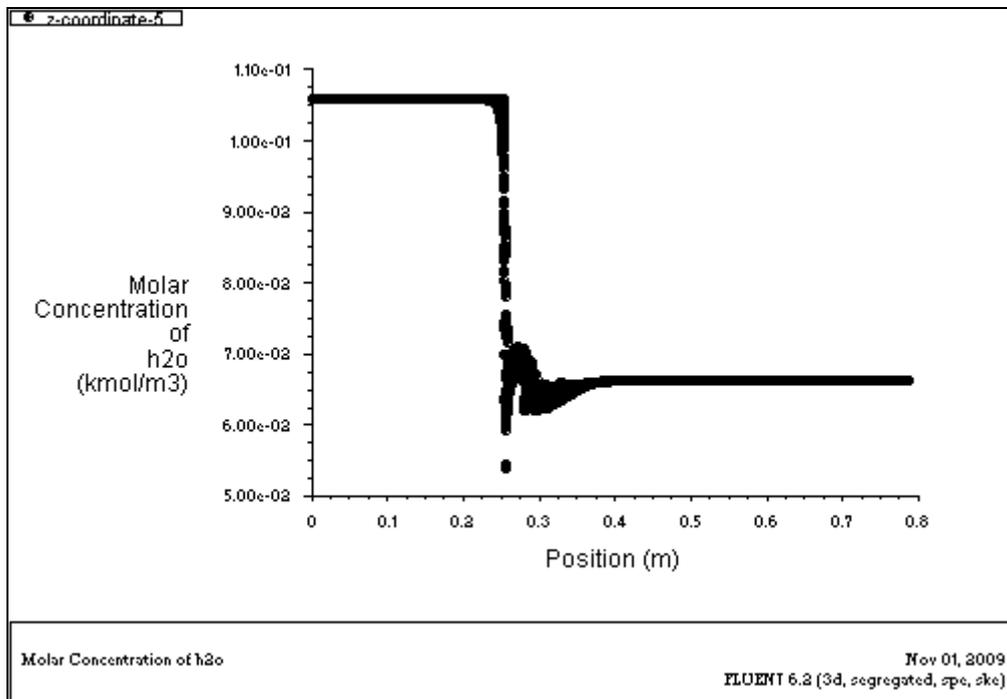


Figure 4.13: Molar Concentration of H2O For Case A2

4.4.3 Simulation Result of Case A 3

Table 4.8: Dimension for Case A3 J-T Valve

Criteria	Value
Length	3 inch (long)
Diameter	1 inch (long)

Table 4.9: Simulation Result For Case A3

Criteria	Value at inlet	Value at Throttle (max)	Change
Relative Pressure , bar	7.8	-4.12	-11.92 bar
Mach number	-	0.874	+0.874
Temperature ,K	400	385	-15
Velocity , m/s	12	297	+285
Molar concentration ,Kmol/m ³	75	55	-20

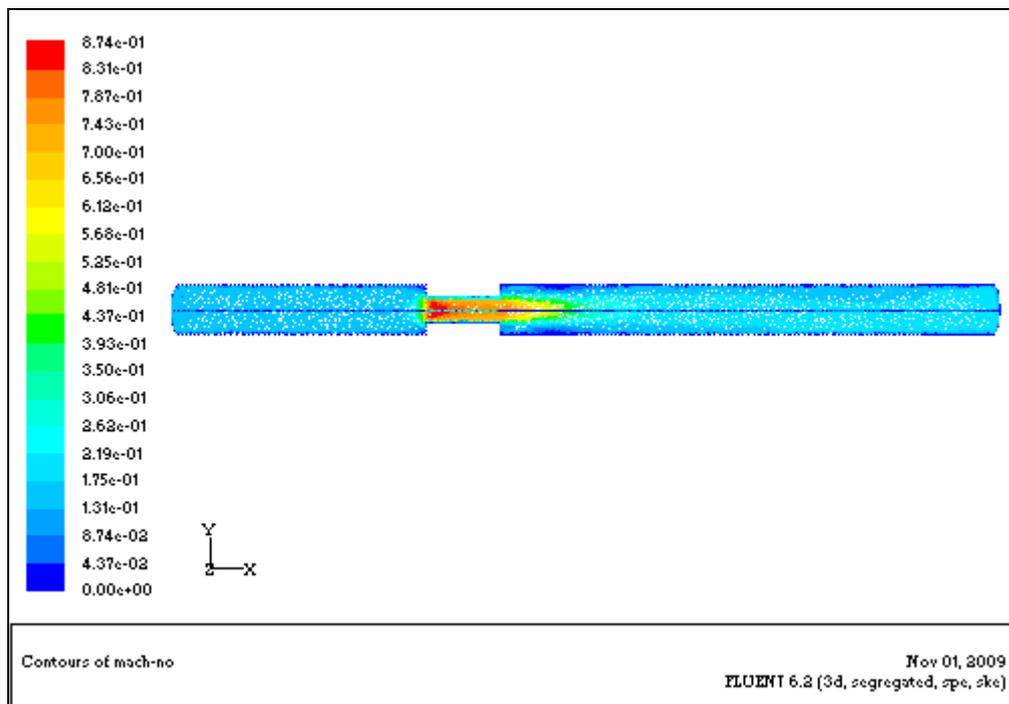


Figure 4.14: Contour of Mach number For Case A3

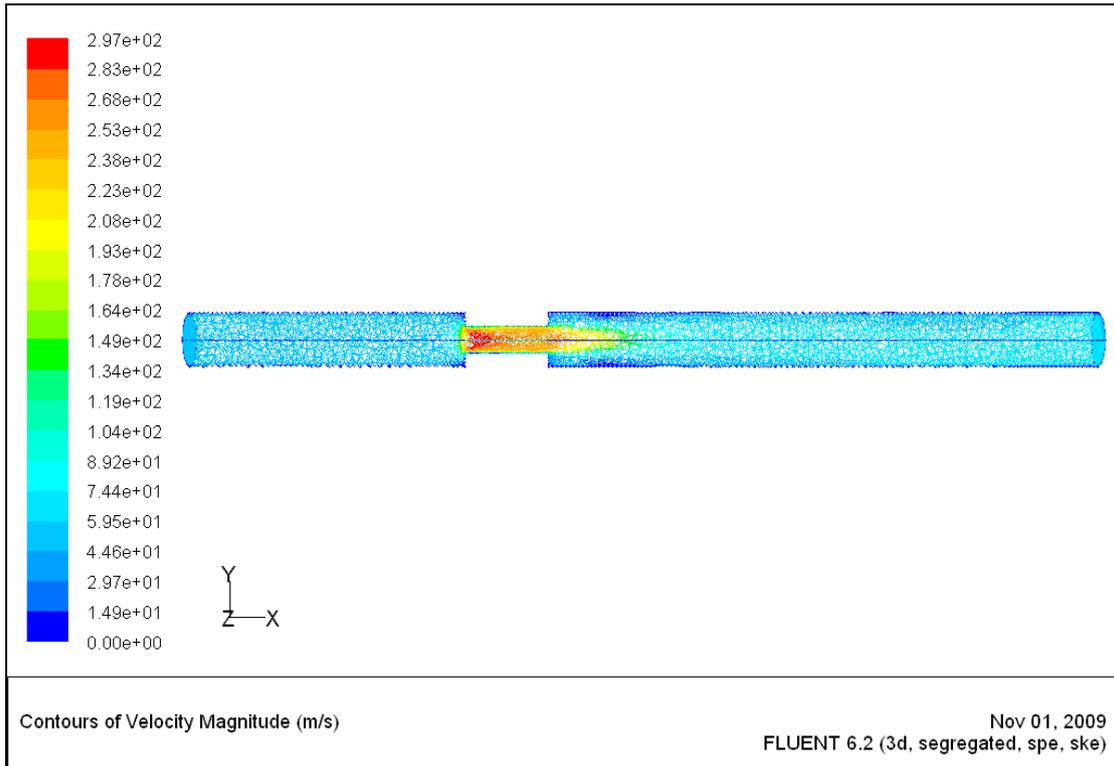


Figure 4.15: Contour of Velocity magnitude For Case A3

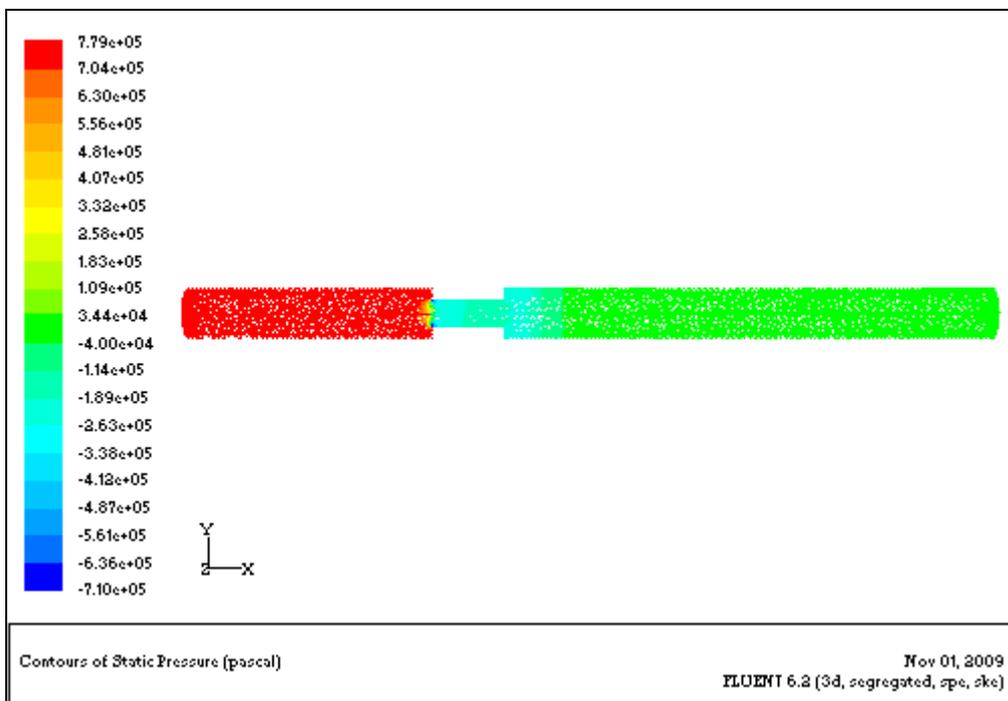


Figure 4.16: Contour of Static Pressure For Case A3

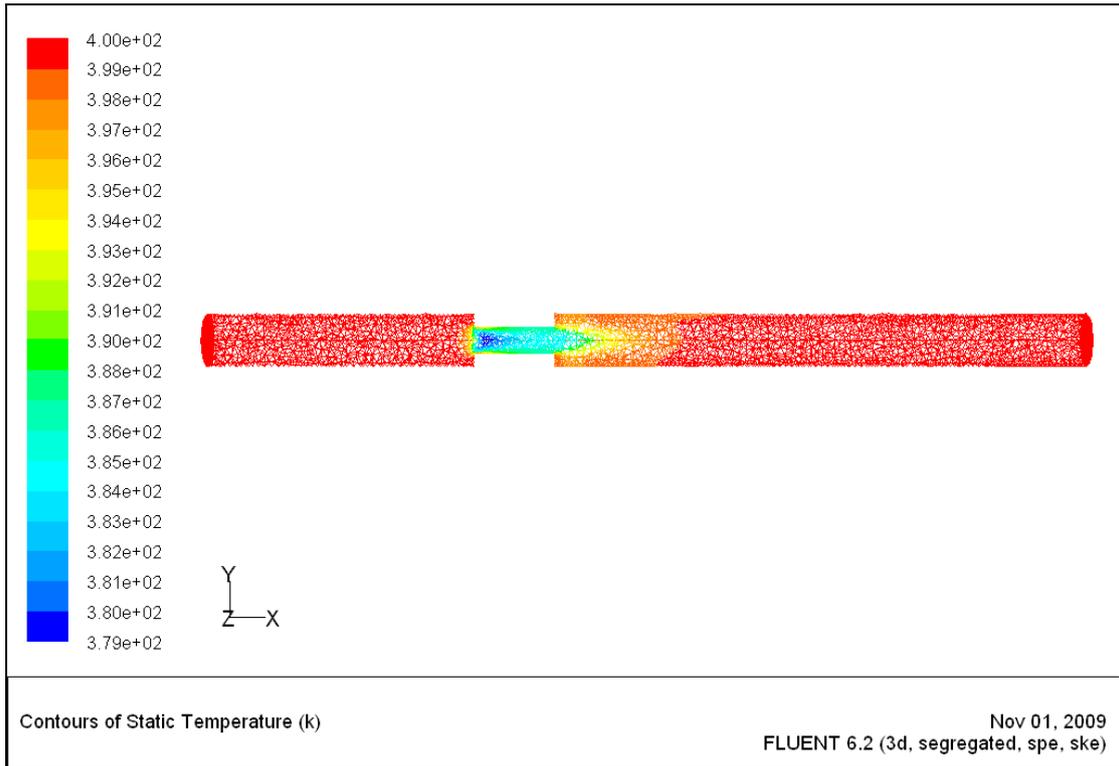


Figure 4.17: Contour of Static Temperature For Case A3

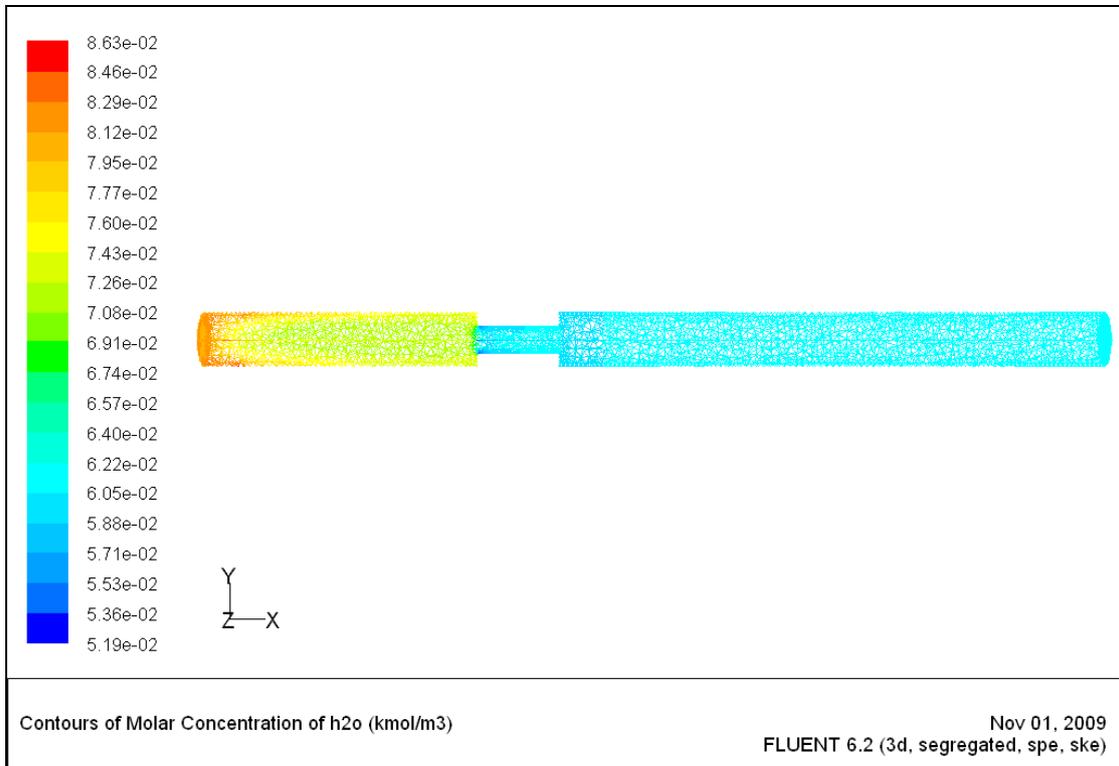


Figure 4.18: Contour of H2O Molar Concentration For Case A3

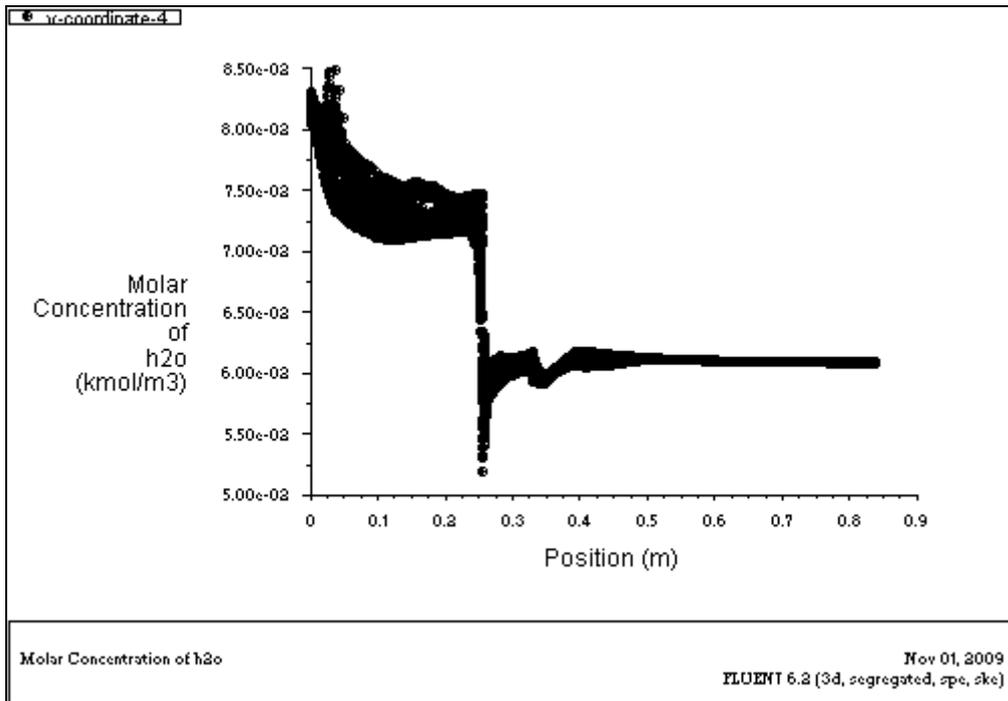


Figure 4.19: Graph of H₂) Concentration For Case A3

4.4.4 Simulation Result of Case A 4

Table 4.10: Dimension for Case A4 J-T Valve

Criteria	Value
Length	3 inch (long)
Diameter	0.6 inch (small)

Table 4.11: Simulation Result For Case A4

Criteria	Value at inlet	Value at Throttle (max)	Change
Pressure	28	-6	-34
Mach number	-	1.3	+1.3
Temperature	400	370	-30
Velocity	12	442	+430
Molar concentration	114	60	-44

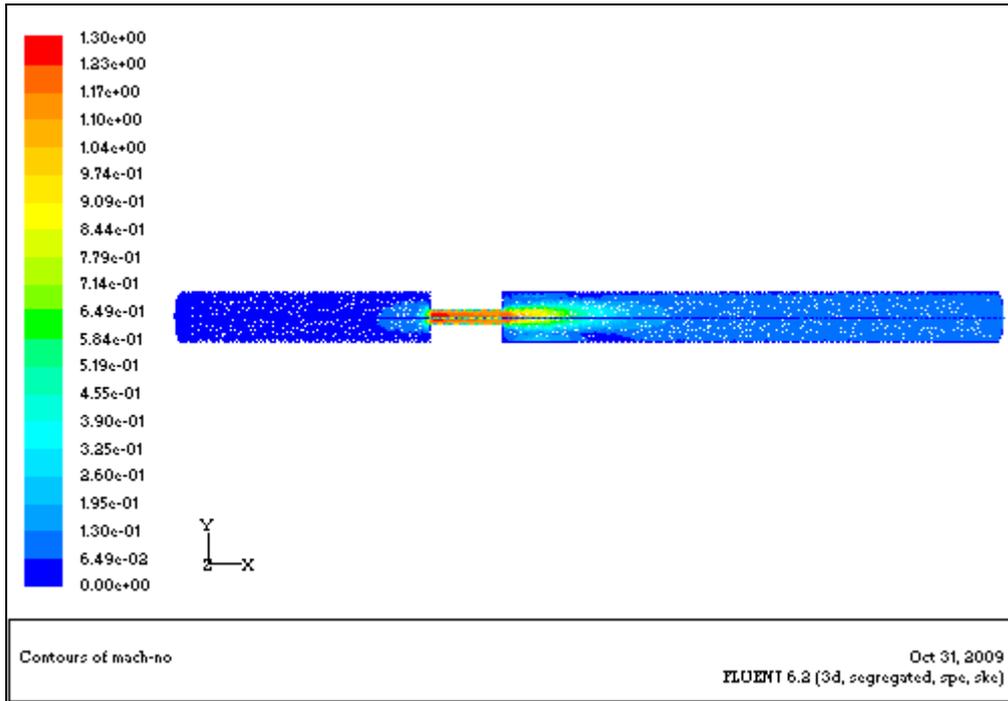


Figure 4.20: Contour of Mach Number For Case A4

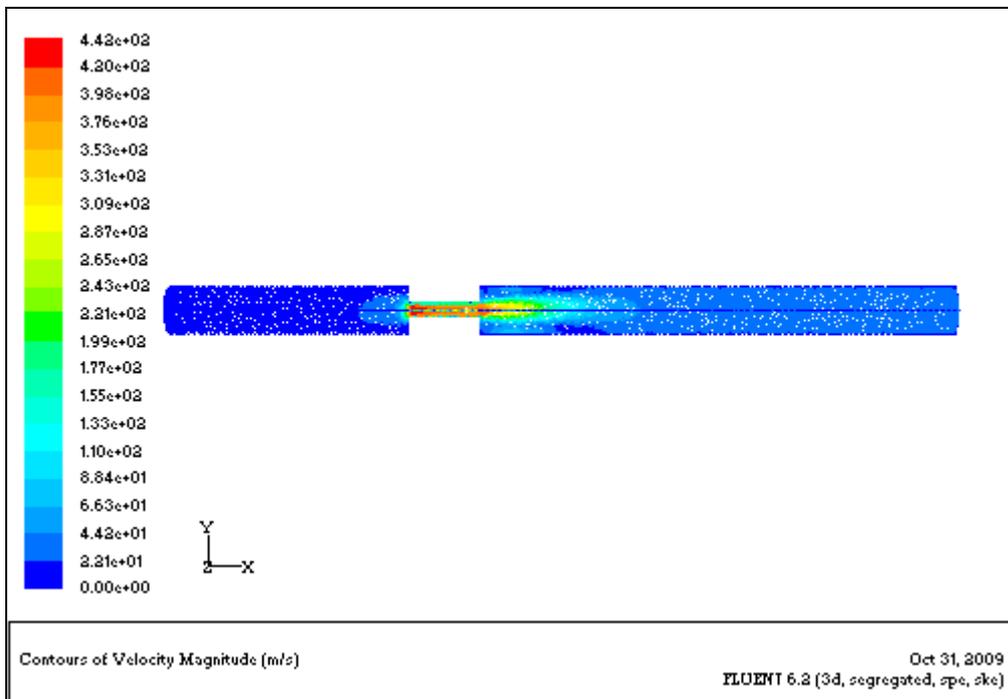


Figure 4.21 : Contour of Velocity Magnitude For Case A4

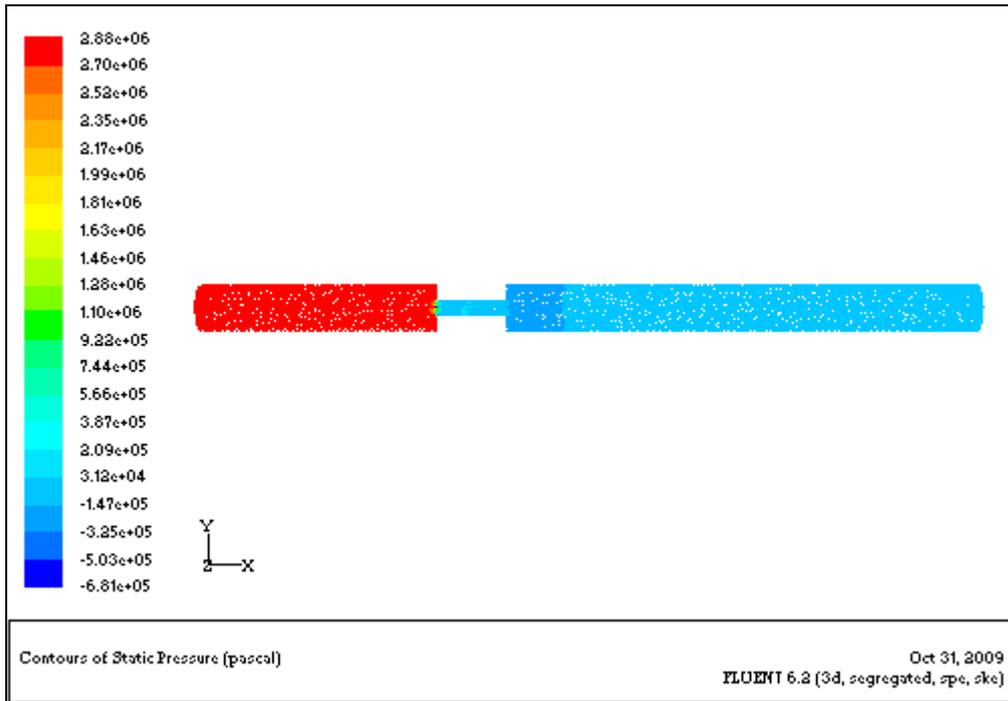


Figure 4.22: Contour of Static Pressure For Case A4

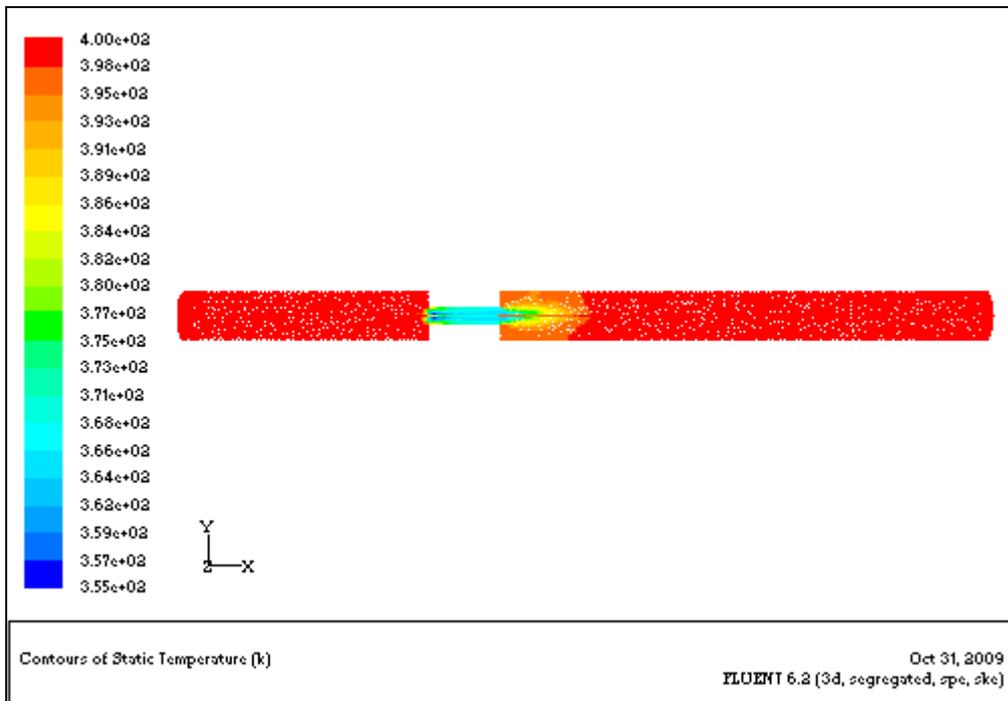


Figure 4.23 : Contour of Temperature For Case A4

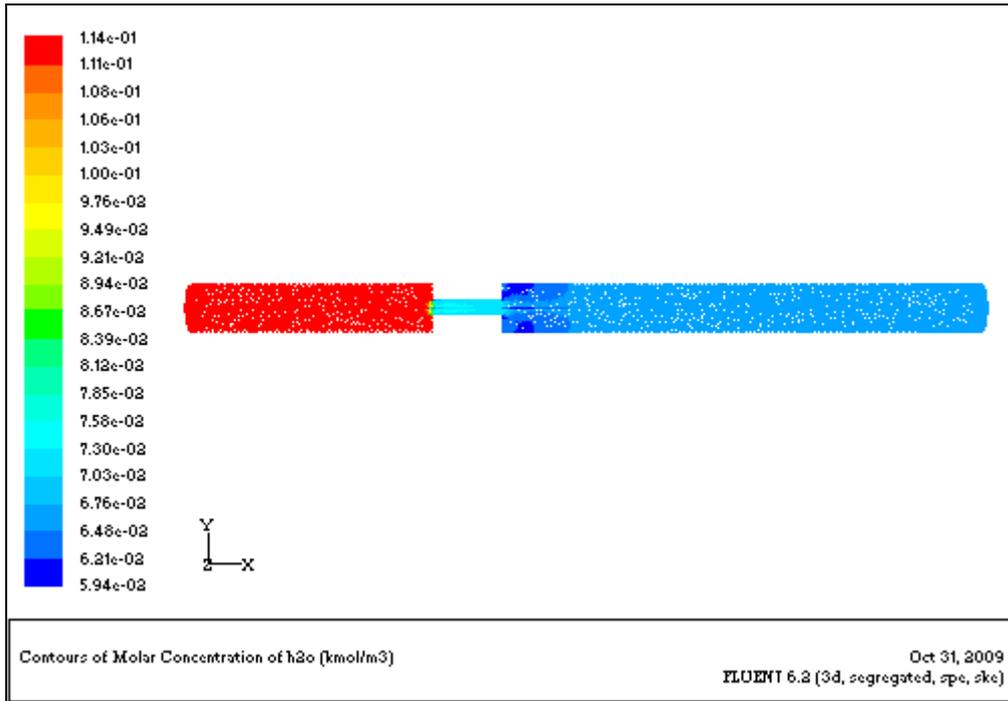


Figure 4.24: Contour of H2O Molar Concentration For Case A4

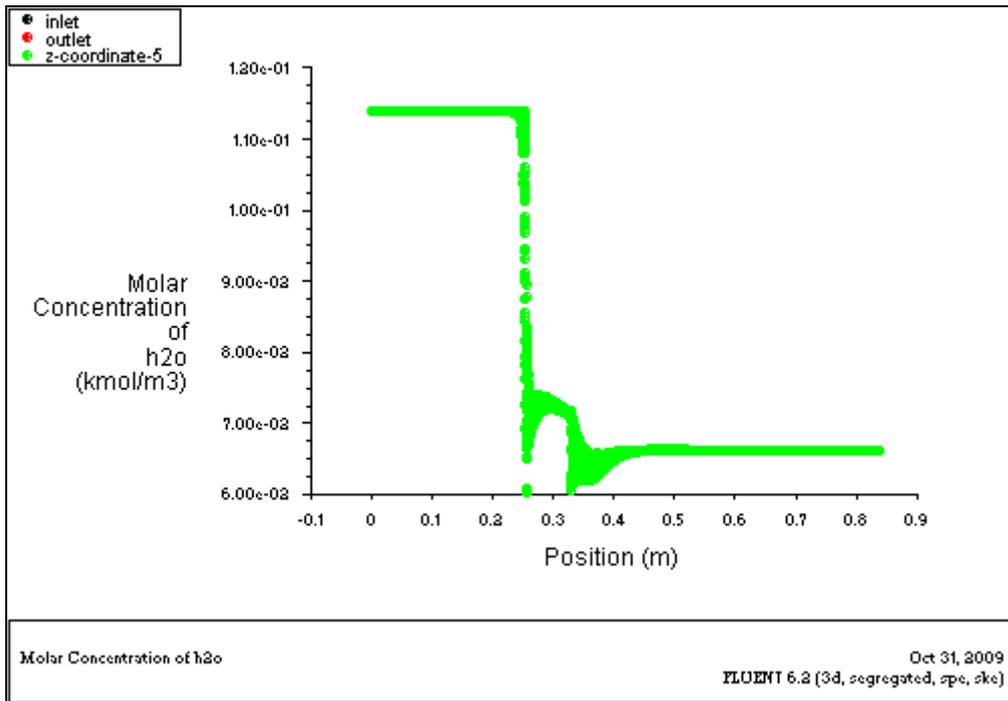


Figure 4.25: Graph of Molar Concentration For Case A4

4.5 Summary of Result

Table 4.12: Dimension of J-T valve for different cases

Throttle diameter/ Throttle length	long diameter (D=1 inch)	Small diameter (D=0.6 inch)
Small length (L= 1 inch)	A1	A2
Long length (L=3 inch)	A3	A4

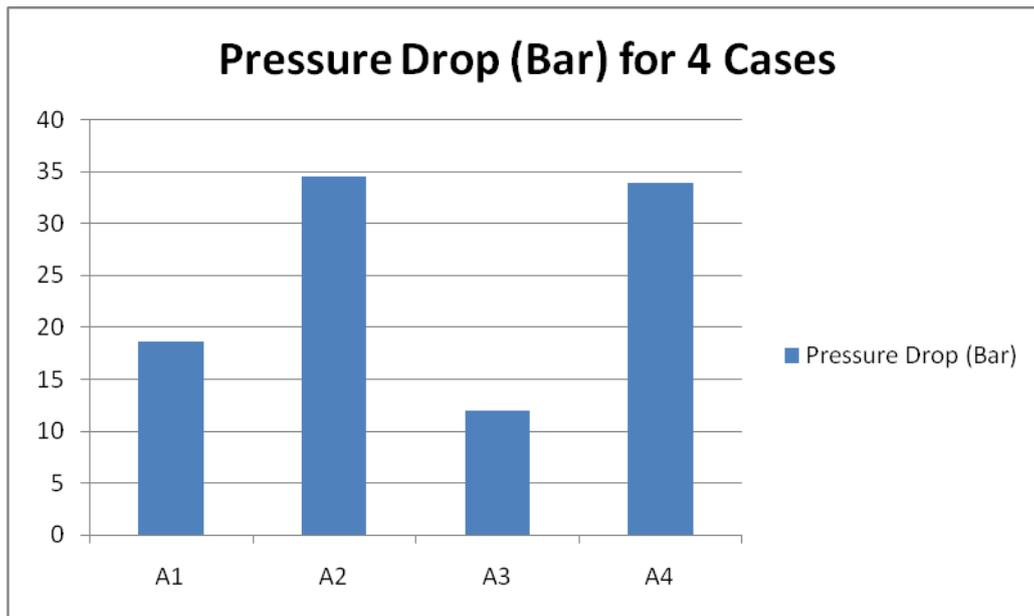


Figure 4.26 Pressure Drop Bar Chart for 4 Cases

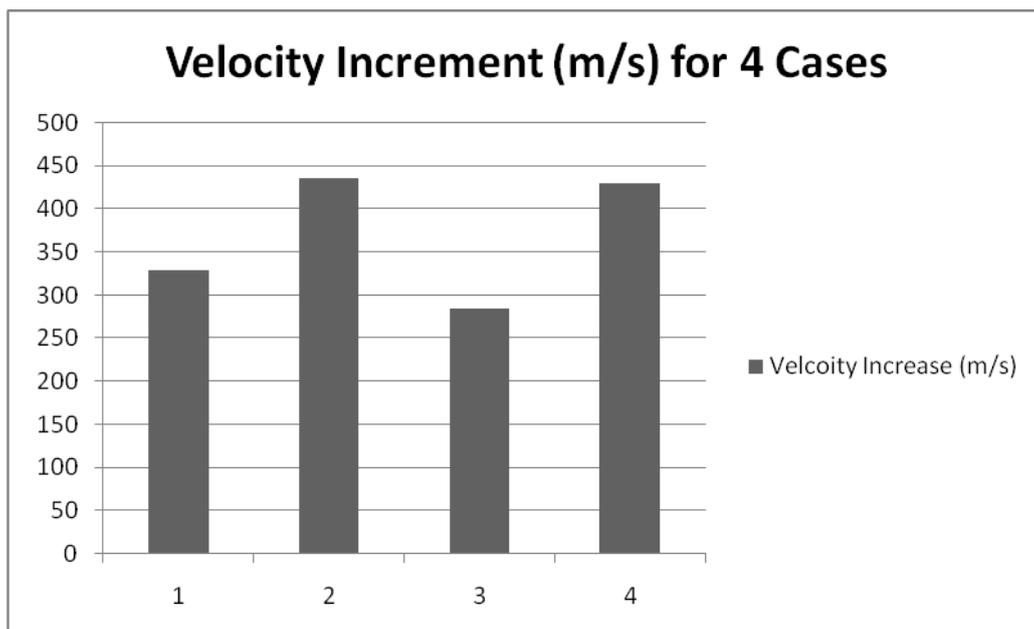


Figure 4.27 Velocity Increase Bar Chart for 4 Cases

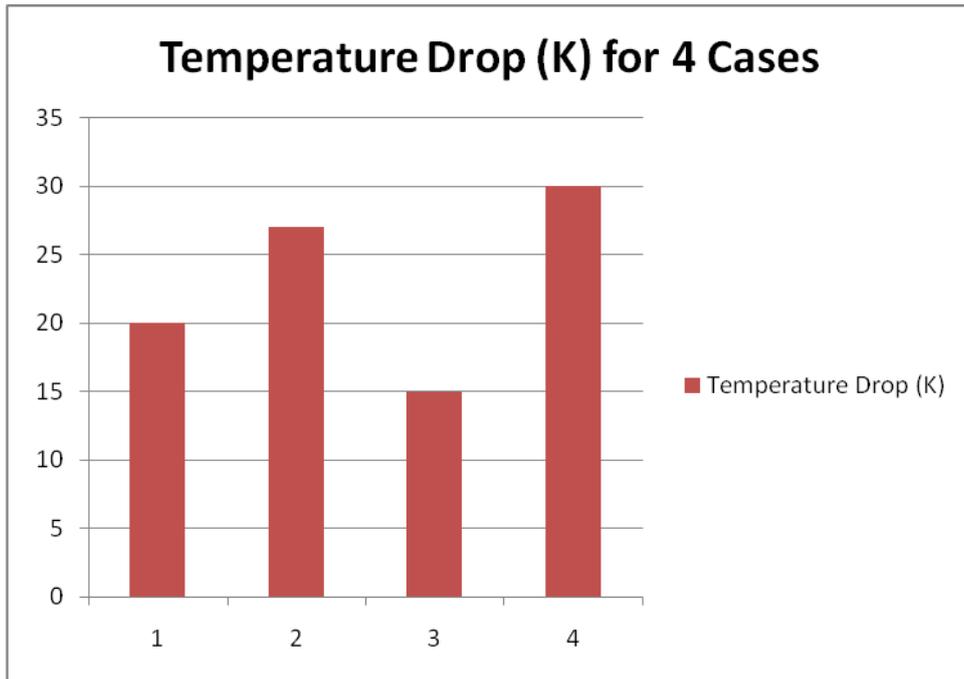


Figure 4.28 Temperature Drop Bar Chart for 4 Cases

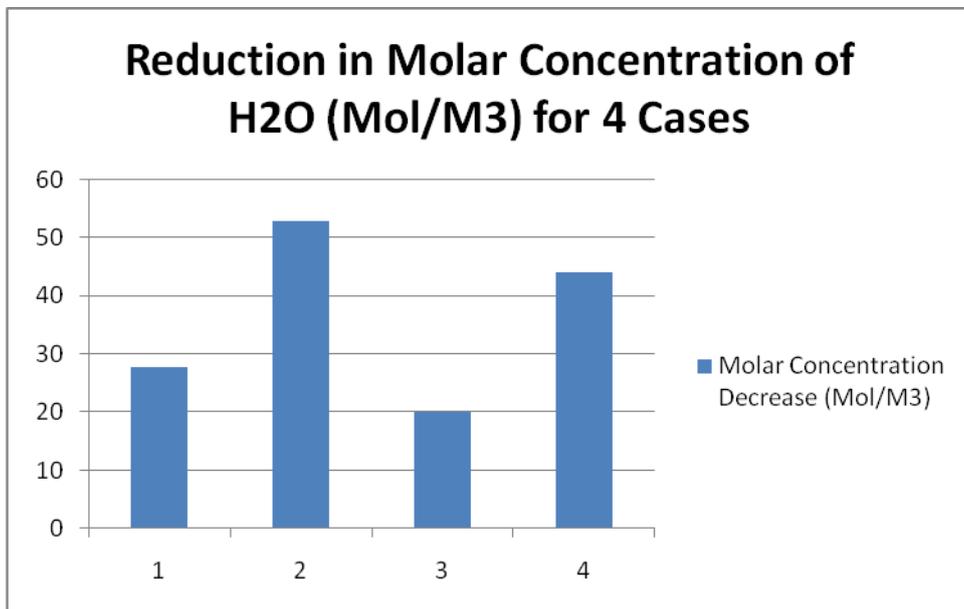


Figure 4.29 Molar Concentration Bar Chart for 4 Cases

4.6 Validation of Result

According to figure 2.2, the cooling curve of Joule Thomson Valve is plotted according to industrial experimental result. From the simulation Cases (A1, A2, A3, A4) , the graph of temperature drop Vs Pressure ratio is plotted and compared with the experimental result in figure 2.2. Both cooling curves are shown in Figure 4.30 below.

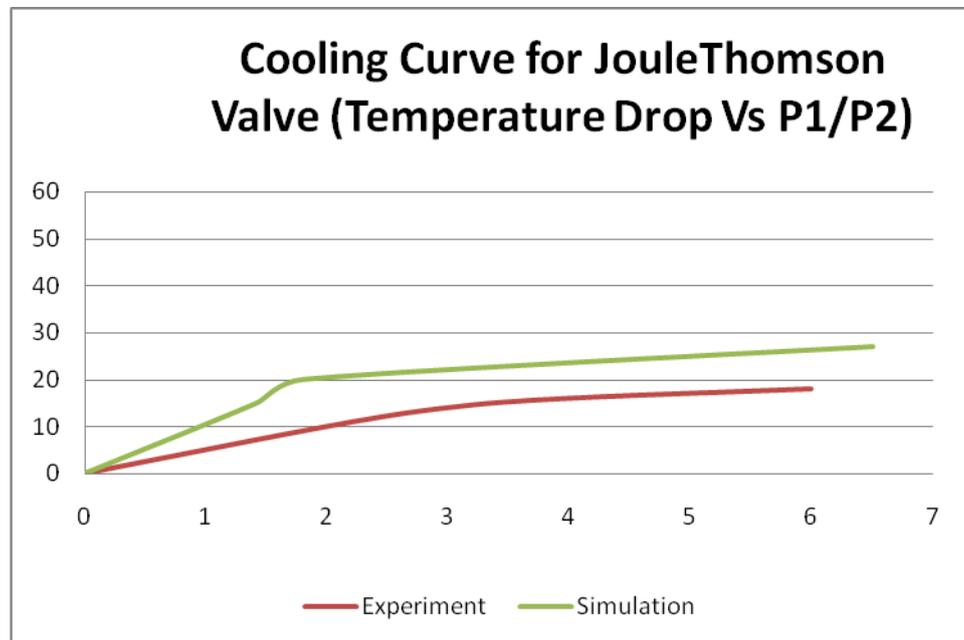


Figure 4.30 Joule Thomson Cooling Curve for experiment and simulation Result

4.7 Discussion

4.7.1 Joule Thomson Cooling Effect

According to the literature review and the research found, the concept of liquid vapor separation using Joule Thomson Cooling effect is feasible. It is because when the natural gas enters the convergence section, the velocity of the flow will increase and supersonic flow will be created. The velocity will increase until it achieves the speed of sound, 343 m/s (Mach =1) at the throat , thereby achieves supersonic flow.

After that throat, it will flow through divergence part and the natural gas will undergo swelling effect which causes sudden temperature and pressure drop. This phenomenon is called Joule Thomson Cooling Principle. The water will condense 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 natural gas will continue to flow out from the separator at high speed.

In real industry, this J-T valve is proposed to be installed with the baffles along the pipe inlet to implement centrifugation force to increase the flow speed. The baffles will cause the gas flow to swirl to create cyclonic flow (just like cyclone or twister). It can achieve supersonic flow more efficiently.

From the result, it is clearly shown that the velocity will increase when it enter the throttle due to convergence effect. After the throttle, velocity will decrease due to sudden expansion of pipe (divergence part). At throttle, the targeted velocity to be achieved is the speed of sound, 343m/s (Mach number =1) in order to achieve supersonic flow. Most of the case is able to achieve supersonic flow where Mach

number is equal to 1 at the throttle with only 11m/s flow at the pipe inlet.

When the flow enters the throttle, the pressure will decrease suddenly due to convergence of the pipeline. Huge pressure are “killed” at the throttle and after the throttle, pressure will increase due to expansion of the pipe. But it will not be as high as the inlet pressure. Hereby, the principle of joule Thomson cooling effect is applied. This pressure drop will help lower the dew point and enhance condensation process of water.

Just like pressure, temperature will decrease when the flow pass through the throttle. Decrease in temperature cause the water vapor to condense to become water liquid when the operating temperature reaches the condensation temperature of water. Due to high speed supersonic flow, the liquid droplet will be removed from the stream easily while the supersonic flow will continue to flow out of the pipe. After the throttle the temperature will increase back.

The pressure drop is proportional to the temperature drop. However, in J-T valve, large pressure drop is needed to cause small temperature drop. For example, in case A2, 34.6 Bar of pressure drop only cause 27 K temperature drop. The diagram below shows the relationship between P, T and velocity (Mach Number) in De-laval nozzle separator. The working principle of De-laval nozzle and J-T valve are similar.

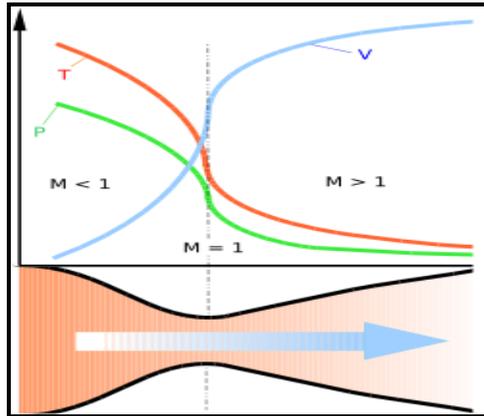


Figure 4.31: The relationship of P,T and velocity across De-Laval Nozzle.

The components involved in the natural gas are mainly methane, hydrogen sulfide, carbon dioxide and water vapor. At constant pressure (assume 1 atm), water has the highest boiling point, which means water will be condensed first when the temperature in the pipeline continue to decrease. Let's say at temperature 90 celcius (1 atm) , water will be in liquid stage while H₂S,CO₂ and H₂O will still remain as vapor. Thus, this technique is suitable to separate mainly water from natural gas since water has the highest boiling point. However, this separation technique might condense other components as well due to the large pressure drop and high operating pressure in the pipeline. Thus, pressure and temperature are important to determine the condensation point of these 4 components.

Table 4.13: Boiling Point For Components in Natural Gas

No	Components	Boiling Point, condensing point
1	Water	100
2	Methane	-164
3	Co ₂	-57
4	H ₂ S	-60.28

4.7.2 Different Dimension for Joule Thomson Valve

Different dimension in J-T valve will have different efficiency in separation. It will affect the changes in temperature, pressure, velocity, density and molar concentration of each component in the system. In industry, an optimum dimension and specification of J-T valve is very important for the benefit of the company. In second part of this project, different dimension of J-T valve are studied to determine their relationship and effect. The effect of the diameter and the length of the throttle are studied in case A1, A2, A3, A4.

Table 4.14: Dimension of J-T valve for different cases

Throttle diameter/ Throttle length	long diameter (D=1 inch)	Small diameter (D=0.6 inch)
Small length (L= 1 inch)	A1	A2
Long length (L=3 inch)	A3	A4

As summarize in section 4.5, the conclusion of the result is presented in Bar Chart. Form the result, it can be concluded that smaller diameter of throttle will be more efficient as it gives more cooling effect. It can be seen in cases A1 and A3 where they have higher velocity and temperature drop, which means more water will be separated out. However, the diameter of the throttle cannot be too small because it might cause backflow or eddy diffusion at the throttle inlet.

The length of the throttle has less significant impact to the separation process, compared to the diameter of the throttle. From the simulation result, shorter length of throttle will give slightly better cooling effect.

4.7.3 Validation of Simulation Result

From Figure 4.30, the cooling curve for simulation is compared with industrial experimental result, taken from gas processing journal. It is clearly shown that the temperature drop of simulation cases in this project is higher than temperature drop achieved in experiment result, which more efficient and ideal. The temperature of simulation cases is slightly higher, roughly 10 K because fluent simulator does not take into consideration of heat of condensation. When water vapor is condensed into water liquid, heat will be absorbed into the condensation process and the actually temperature drop will be lower than it should be ideally. The simulation process using fluent software in this Final Year Project does not consider energy balance equation because it is a very complex work.

CHAPTER 5 CONCLUSION

5.1 Conclusion

The concept of supersonic separator is integrated into the pipeline to create a nozzle-expander pattern, called J-T valve. When the stream passes through the nozzle, the flow will become supersonic. Straight after it, the flow will pass through expander and experience swelling effect, which causes pressure and temperature drop. The water vapor will condense and separated out when the temperature decreases. The heavier water droplet will fall onto the wall surface and channeled out through a small pipe.

In conclusion, this project is feasible technically and economically. This separation technique only requires low CAPEX, OPEX and maintenance work, compared to membrane and absorption separation technique. It does not require any chemical to operate. Technically, this technique had been proven by 3S and twister BV company that it is feasible. However, it is not commercialize yet, due to complex specification and dimension for this separator. Each J-T valve designed can only be specially used for one scenario due to different components and operating condition required.

The objective of this project is to determine the feasibility, efficiency and best design of this technology using *gambit and fluent* simulation software. From the simulation and studies of various dimension of J-T valve, the separation concept is technically proven. It is proposed also to build the throttle with smaller diameter to enhance Joule Thomson cooling effect. The diameter of the throttle cannot be too smaller to avoid backflow or eddy diffusion.

5.1 Recommendation

Due to time and budget constrain, this project can only be studied by using simulation.

There are a lot of recommendations to be further implement to develop this project:

1. The coding of energy balance equation should be written in UFD , user defined function to take into the consideration of heat of condensation to obtain the actual temperature drop.
2. The cyclonic blade can be installed at the inlet of the pipeline to create cyclonic effect to enhance centrifugal supersonic flow.
3. This project should be done experimentally as well to compare the result with the simulation result. Small prototype of J-T valve can be build to study its feasibility and efficiency.
4. Besides water, other components are being separated as well out in the system. The operating pressure and temperature in the pipe need to be control accurately, according to the dew point of each component.

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APPENDICES

Appendix A

Derivation of the Joule–Thomson (Kelvin) coefficient

A derivation of the formula for the Joule–Thomson (Kelvin) coefficient.

$$\mu_{JT} \equiv \left(\frac{\partial T}{\partial P} \right)_H = \frac{V}{C_p} (\alpha T - 1)$$

The partial derivative of T with respect to P at constant H can be computed by expressing the differential of the enthalpy dH in terms of dT and dP, and equating the resulting expression to zero and solving for the ratio of dT and dP.

It follows from the **fundamental thermodynamic relation** that the differential of the enthalpy is given by:

$$dH = TdS + VdP \text{ (here, } S \text{ is the } \mathbf{entropy} \text{ of the gas).}$$

Expressing dS in terms of dT and dP gives:

$$dH = T \left(\frac{\partial S}{\partial T} \right)_P dT + \left[V + T \left(\frac{\partial S}{\partial P} \right)_T \right] dP$$

Using

$$C_p = T \left(\frac{\partial S}{\partial T} \right)_P$$

$$dH = C_p dT + \left[V + T \left(\frac{\partial S}{\partial P} \right)_T \right] dP$$

The remaining partial derivative of S can be expressed in terms of the coefficient of thermal expansion via a **Maxwell relation** as follows. From the fundamental thermodynamic relation, it follows that the differential of the **Gibbs energy** is given by:

$$dG = -SdT + VdP$$

The **symmetry of partial derivatives** of G with respect to T and P implies that:

$$\left(\frac{\partial S}{\partial P} \right)_T = - \left(\frac{\partial V}{\partial T} \right)_P = -V\alpha$$

where α is the coefficient of thermal expansion. Using this relation, the differential of H can be expressed as

$$dH = C_p dT + V(1 - T\alpha) dP$$

Equating dH to zero and solving for dT/dP then gives:

$$\left(\frac{\partial T}{\partial P} \right)_H = \frac{V}{C_p} (\alpha T - 1)$$

Appendix B

Mach Number Equation

Assuming air to be an **ideal gas**, the formula to compute Mach number in a subsonic compressible flow is derived from Bernoulli's equation for $M < 1$:^[3]

$$M = \sqrt{\frac{2}{\gamma - 1} \left[\left(\frac{q_c}{P} + 1 \right)^{\frac{\gamma - 1}{\gamma}} - 1 \right]}$$

where:

M is Mach number

q_c is impact pressure and

P is static pressure

γ is the ratio of specific heats

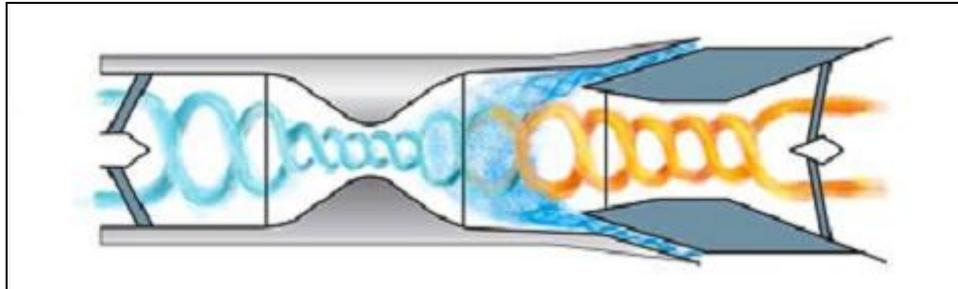
The formula to compute Mach number in a supersonic compressible flow is derived from the Rayleigh Supersonic Pitot equation:

$$M = 0.88128485 \sqrt{\left[\left(\frac{q_c}{P} + 1 \right) \left(1 - \frac{1}{7M^2} \right)^{2.5} \right]}$$

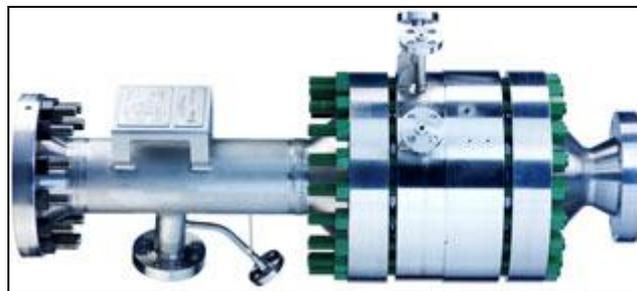
q_c is now impact pressure measured behind a normal shock

Appendix C

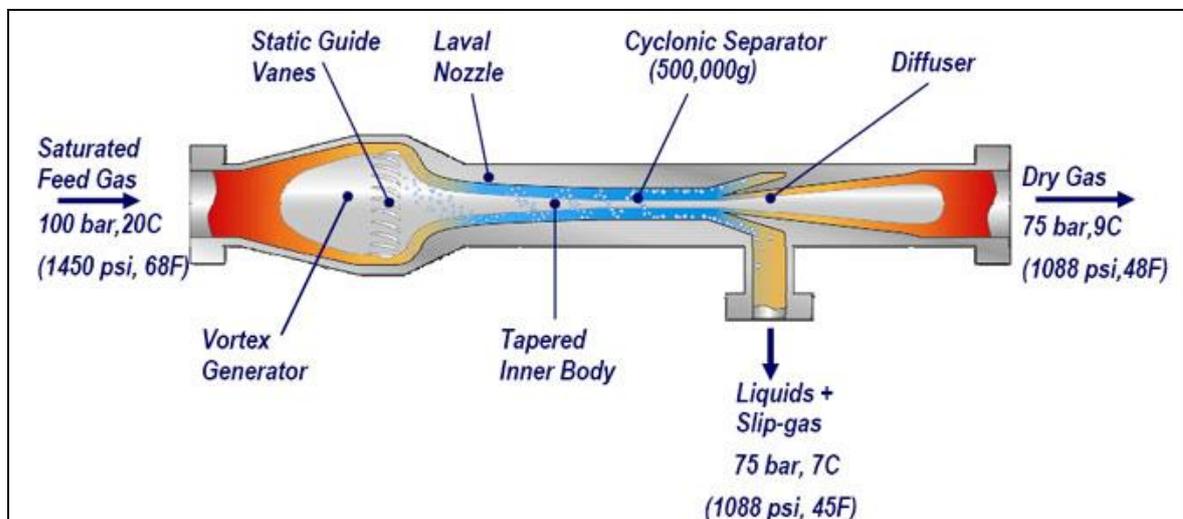
Equipment For Supersonic Gas Separation Concept



3S Super Sonic Gas Separation Concept



Twister Supersonic Separator



Cross-section of a Twister tube with typical process conditions.

Appendix D

Incompressible flow through an orifice

By assuming steady-state, incompressible (constant fluid density), inviscid, laminar flow in a horizontal pipe (no change in elevation) with negligible frictional losses, Bernoulli's equation reduces to an equation relating the conservation of energy between two points on the same streamline:

$$P_1 + \frac{1}{2} \cdot \rho \cdot V_1^2 = P_2 + \frac{1}{2} \cdot \rho \cdot V_2^2 \text{ or:}$$
$$P_1 - P_2 = \frac{1}{2} \cdot \rho \cdot V_2^2 - \frac{1}{2} \cdot \rho \cdot V_1^2$$

By continuity equation:

$$Q = A_1 \cdot V_1 = A_2 \cdot V_2 \text{ or } V_1 = Q / A_1 \text{ and } V_2 = Q / A_2 :$$
$$P_1 - P_2 = \frac{1}{2} \cdot \rho \cdot \left(\frac{Q}{A_2}\right)^2 - \frac{1}{2} \cdot \rho \cdot \left(\frac{Q}{A_1}\right)^2$$

Solving for Q :

$$Q = A_2 \sqrt{\frac{2 (P_1 - P_2) / \rho}{1 - (A_2 / A_1)^2}}$$

and:

$$Q = A_2 \sqrt{\frac{1}{1 - (d_2 / d_1)^4}} \sqrt{2 (P_1 - P_2) / \rho}$$

The above expression for Q gives the theoretical volume flow rate. Introducing the beta factor $\beta = d_2 / d_1$ as well as the coefficient of discharge C_d :

$$Q = C_d A_2 \sqrt{\frac{1}{1 - \beta^4}} \sqrt{2 (P_1 - P_2) / \rho}$$

And finally introducing the meter coefficient C which is defined as

$$C = \frac{C_d}{\sqrt{1 - \beta^4}}$$

to obtain the final equation for the volumetric flow of the fluid through the orifice:

$$(1) \quad Q = C A_2 \sqrt{2 (P_1 - P_2) / \rho}$$

Multiplying by the density of the fluid to obtain the equation for the mass flow rate at any section in the pipe:

$$(2) \quad \dot{m} = \rho Q = C A_2 \sqrt{2 \rho (P_1 - P_2)}$$

where:

Q = volumetric flow rate (at any cross-section), m³/s

\dot{m} = mass flow rate (at any cross-section), kg/s

C_d = coefficient of discharge, dimensionless

C = orifice flow coefficient, dimensionless

A_1 = cross-sectional area of the pipe, m²

A_2 = cross-sectional area of the orifice hole, m²

d_1 = diameter of the pipe, m

d_2 = diameter of the orifice hole, m

β = ratio of orifice hole diameter to pipe diameter, dimensionless

V_1 = upstream fluid velocity, m/s

V_2 = fluid velocity through the orifice hole, m/s

P_1 = fluid upstream pressure, Pa with dimensions of kg/(m·s²)

P_2 = fluid downstream pressure, Pa with dimensions of kg/(m·s²)

ρ = fluid density, kg/m³

Deriving the above equations used the cross-section of the orifice opening and is not as realistic as using the minimum cross-section at the vena contracta. In addition, frictional losses may not be negligible and viscosity and turbulence effects may be present. For that reason, the coefficient of discharge C_d is introduced. Methods exist for determining the coefficient of discharge as a function of the Reynolds number.

The parameter $\sqrt{1 - \beta^4}$ is often referred to as the *velocity of approach factor*^[11] and dividing the coefficient of discharge by that parameter (as was done above) produces the flow coefficient C . Methods also exist for determining the flow coefficient as a function of the beta function β and the location of the downstream pressure sensing tap. For rough approximations, the flow coefficient may be assumed to be between 0.60 and 0.75. For a first approximation, a flow coefficient of 0.62 can be used as this approximates to fully developed flow.

An orifice only works well when supplied with a fully developed flow profile. This is achieved by a long upstream length (20 to 40 pipe diameters, depending on Reynolds number) or the use of a flow conditioner. Orifice plates are small and inexpensive but do not recover the pressure drop as well as a venturi nozzle does. If space permits, a venturi meter is more efficient than a flowmeter.

Flow of gases through an orifice

In general, equation (2) is applicable only for incompressible flows. It can be modified by introducing the expansion factor Y to account for the compressibility of gases.

$$(3) \quad \dot{m} = \rho_1 Q = C Y A_2 \sqrt{2 \rho_1 (P_1 - P_2)}$$

Y is 1.0 for incompressible fluids and it can be calculated for compressible gases.

Calculation of expansion factor

The expansion factor Y , which allows for the change in the density of an ideal gas as it expands isentropically, is given by

$$Y = \sqrt{r^{2/k} \left(\frac{k}{k-1} \right) \left(\frac{1 - r^{(k-1)/k}}{1 - r} \right) \left(\frac{1 - \beta^4}{1 - \beta^4 r^{2/k}} \right)}$$

For values of β less than 0.25, β^4 approaches 0 and the last bracketed term in the above equation approaches 1. Thus, for the large majority of orifice plate installations:

$$(4) \quad Y = \sqrt{r^{2/k} \left(\frac{k}{k-1} \right) \left(\frac{1 - r^{(k-1)/k}}{1 - r} \right)}$$

where:

Y = Expansion factor, dimensionless

r = P_2 / P_1

k = specific heat ratio (c_p / c_v), dimensionless

Substituting equation (4) into the mass flow rate equation (3):

$$\dot{m} = C A_2 \sqrt{2 \rho_1 \left(\frac{k}{k-1} \right) \left[\frac{(P_2/P_1)^{2/k} - (P_2/P_1)^{(k+1)/k}}{1 - P_2/P_1} \right] (P_1 - P_2)}$$

and:

$$\dot{m} = C A_2 \sqrt{2 \rho_1 \left(\frac{k}{k-1} \right) \left[\frac{(P_2/P_1)^{2/k} - (P_2/P_1)^{(k+1)/k}}{(P_1 - P_2)/P_1} \right] (P_1 - P_2)}$$

and thus, the final equation for the non-choked (i.e., sub-sonic) flow of ideal gases through an orifice for values of β less than 0.25:

$$(5) \quad \dot{m} = C A_2 \sqrt{2 \rho_1 P_1 \left(\frac{k}{k-1} \right) \left[(P_2/P_1)^{2/k} - (P_2/P_1)^{(k+1)/k} \right]}$$

Using the ideal gas law and the compressibility factor (which corrects for non-ideal gases), a practical equation is obtained for the non-choked flow of real gases through an orifice for values of β less than 0.25:

$$(6) \quad \dot{m} = C A_2 P_1 \sqrt{\frac{2 M}{Z R T_1} \left(\frac{k}{k-1} \right) \left[(P_2/P_1)^{2/k} - (P_2/P_1)^{(k+1)/k} \right]}$$

where:

k = specific heat ratio (c_p / c_v), dimensionless

\dot{m} = mass flow rate at any section, kg/s

C = orifice flow coefficient, dimensionless

A_2 = cross-sectional area of the orifice hole, m²

ρ_1 = upstream real gas density, kg/m³

P_1 = upstream gas pressure, Pa with dimensions of kg/(m·s²)

P_2 = downstream pressure, Pa with dimensions of kg/(m·s²)

- M** = the gas molecular mass, kg/mol (also known as the molecular weight)
R = the Universal Gas Law Constant = 8.3145 J/(mol·K)
T₁ = absolute upstream gas temperature, K
Z = the gas compressibility factor at P_1 and T_1 , dimensionless

A detailed explanation of choked and non-choked flow of gases, as well as the equation for the choked flow of gases through restriction orifices, is available at [Choked flow](#).

The flow of real gases through thin-plate orifices never becomes fully choked. The mass flow rate through the orifice continues to increase as the downstream pressure is lowered to a perfect vacuum, though the mass flow rate increases slowly as the downstream pressure is reduced below the critical pressure.^[6] "Cunningham (1951) first drew attention to the fact that choked flow will not occur across a standard, thin, square-edged orifice."

Permanent pressure drop for incompressible fluids

For a square-edge orifice plate with flange taps^[8]:

$$\frac{\Delta P_p}{\Delta P_i} = 1 - 0.24\beta - 0.52\beta^2 - 0.16\beta^3$$

where:

ΔP_p = permanent pressure drop

ΔP_i = indicated pressure drop at the flange taps

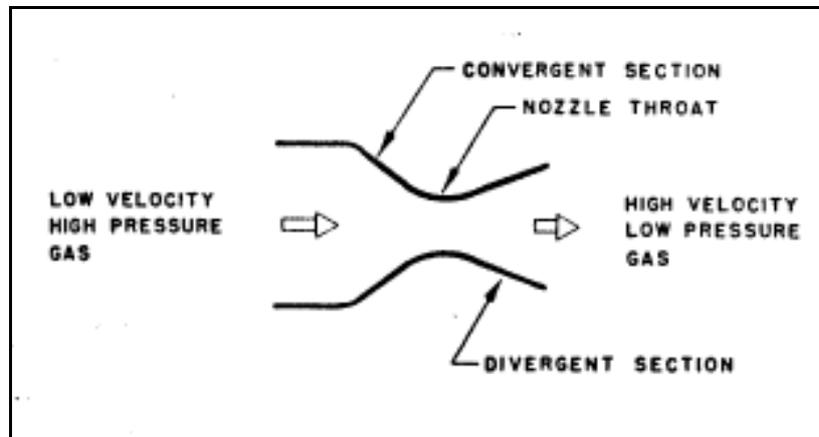
$\beta = d_2 / d_1$

And rearranging the formula near the top of this article:

$$\Delta P_i = P_1 - P_2 = \frac{Q^2 \rho (1 - \beta^4)}{2 C_d^2 A_2^2} = \frac{Q^2 \rho (1 - \beta^4)}{2 C_d^2 A_1^2 \beta^4}$$

Appendix E

De Laval Nozzle



De Laval nozzle Figure

The nozzle was developed by Swedish inventor Gustaf de Laval in 1897 for use on an impulse steam turbine. This principle was used in a rocket engine by Robert Goddard, and very nearly all modern rocket engines that employ hot gas combustion use de Laval nozzles.

A de Laval nozzle (or convergent-divergent nozzle, CD nozzle or con-di nozzle) is a tube that is pinched in the middle, making an hourglass-shape. It is used as a means of accelerating the flow of a gas passing through it to a supersonic speed. It is widely used in some types of steam turbine and is an essential part of the modern rocket engine and supersonic jet engines.

De laval nozzle is device, designed by Gustav de Laval, for efficiently converting the energy of a hot gas to kinetic energy (energy of motion). It was originally used in some steam turbines, it is now used as the nozzle design in practically all rockets. By constricting the outflow of the gas until it reaches the velocity of sound and then letting it expand again, an extremely fast jet is produced.

The diagram shows the result of velocity, temperature and pressure proportion with the flow throughout de Laval nozzle. Sudden expansion after the throat causes the temperature and pressure to drop significantly which causes condensation of water

vapor. The velocity of the supersonic flow will increase after passes through the throat. Mach number at the throat is ideally equal to 1 while the Mach number after the throat will be larger than 1.

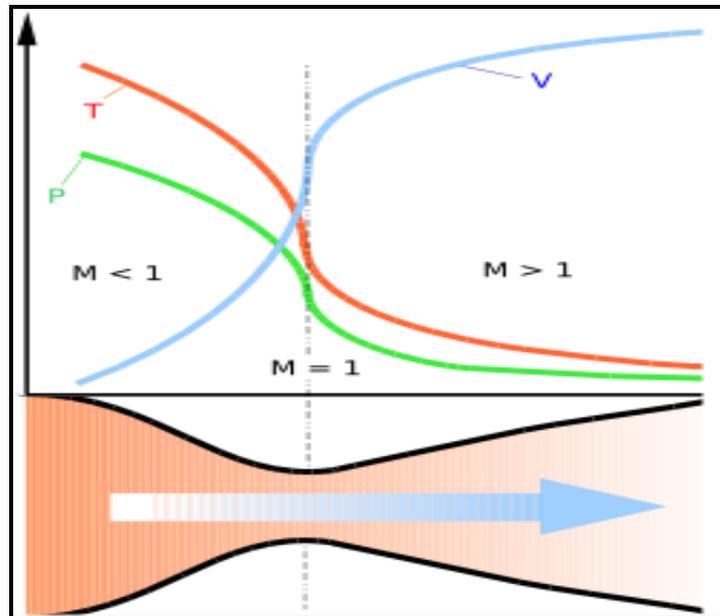


Diagram of a de Laval nozzle: Graph of flow velocity, temperature and pressure proportional with the flow across nozzle.

The analysis of gas flow through de Laval nozzles involves a number of concepts and assumptions:

- For simplicity, the gas is assumed to be an ideal gas.
- The gas flow is isentropic (i.e., at constant entropy). As a result the flow is reversible (frictionless and no dissipative losses), and adiabatic (i.e., there is no heat gained or lost).
- The gas flow is constant (i.e., steady) during the period of the propellant burn.
- The gas flow is along a straight line from gas inlet to exhaust gas exit (i.e., along the nozzle's axis of symmetry)
- The gas flow behavior is compressible since the flow is at very high velocities.

Operation

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. 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).

A 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.

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. In practice ambient pressure must be no higher than roughly 2-3 times the pressure in the supersonic gas at the exit for supersonic flow to leave the nozzle.

Exhaust Velocity

As the gas enters a nozzle, it is traveling at subsonic velocities. As the throat contracts down the gas is forced to accelerate until at the nozzle throat, where the cross-sectional area is the smallest, the linear velocity becomes sonic. From the throat the cross-sectional area then increases, the gas expands and the linear velocity becomes progressively more supersonic.

V_e is sometimes referred to as the *ideal exhaust gas velocity* because it is based on the assumption that the exhaust gas behaves as an ideal gas.

The linear velocity of the exiting exhaust gases can be calculated using the following equation

$$V_e = \sqrt{\frac{T R}{M} \cdot \frac{2 k}{k - 1} \cdot \left[1 - (P_e/P)^{(k-1)/k} \right]}$$

where:

V_e = Exhaust velocity at nozzle exit, m/s

T = absolute temperature of inlet gas, K

R = Universal gas law constant = 8314.5 J/(kmol·K)

M = the gas molecular mass, kg/kmol (also known as the molecular weight)

k = c_p/c_v = isentropic expansion factor

c_p = specific heat of the gas at constant pressure

c_v = specific heat of the gas at constant volume

P_e = absolute pressure of exhaust gas at nozzle exit, Pa

P = absolute pressure of inlet gas, Pa

Appendix F

Wilson Model Source Code For EOS Calculation (implemented as UDF in fluent)

```
#include <stdio.h>
#include <conio.h>
#include <math.h>
#include <udf.h>
//component user input
struct comp_parameters {
    float omega;
    float critP;
    float critT;
} UserInput [10];
char* name[10];

//for initial K calculation
struct comp_variables {
    float mol, massvap;
    float zi; // mol fraction
    float kvalue;
    float liqfrac, vapfrac, massvapfrac;
} Calculated[10];

float Total_mol, Total_mass;
float Nv, Nl; //vapour and liquid fraction respectively
float Dx, fnv, fPnv; //Newton-Raphson functions
//float A, B;
//General

float T, P;
int i, n; //for iteration purposes
int Ncomponent=4, Nmax=100;
float epsilon = 0.00001; //degree of accuracy
```

```

DEFINE_EXECUTE_AT_END(thermo2)
{
Domain *d;
Thread *t;
cell_t c;
FILE *fp1;
/**Creating new structured C data**/
fp1 = fopen("output.c","a");

// component constant parameters where P in psia and T in Rankine
    i = 1;
    name[i] = "C1";
    UserInput[i].omega=0.0104;
    UserInput[i].critP=666.4;
    UserInput[i].critT=343.33;

    i = 2;
    name[i] = "H2S";
    UserInput[i].omega=0.094;
    UserInput[i].critP=1300.65;
    UserInput[i].critT=672.3;

    i = 3;
    name[i] = "CO2";
    UserInput[i].omega=0.224;
    UserInput[i].critP=1071.37;
    UserInput[i].critT=547.56;

    i = 4;
    name[i] = "H2O";
    UserInput[i].omega=0.345;
    UserInput[i].critP=3200;
    UserInput[i].critT=1164.78;

d = Get_Domain(1);

```

```

thread_loop_c (t,d)

{
begin_c_loop (c,t)

// *****OBTAIN MASS FRACTION FROM FLUENT
AND CONVERT TO MOL FRACTION*****
// assume arbitrary 1g of mixture. Mol = (mass fraction*1g)/MW
i=1; //for methane
Calculated[1].mol = C_YI(c,t,0)/16.05;
i=2; //for H2S
Calculated[2].mol = C_YI(c,t,1)/34.07;
i=3; //for CO2
Calculated[3].mol = C_YI(c,t,2)/44.01;
i=4; //for H2O
Calculated[4].mol = C_YI(c,t,3)/18.02;

Total_mol = 0; //initial total mol = 0
for (i=1;i<=Ncomponent;i++)
{
    Total_mol = Total_mol + Calculated[i].mol;
}
i=1; //for methane
Calculated[1].zi = Calculated[1].mol/Total_mol;
i=2; //for H2S
Calculated[2].zi = Calculated[2].mol/Total_mol;
i=3; //for CO2
Calculated[3].zi = Calculated[3].mol/Total_mol;
i=4; //for H2O
Calculated[4].zi = Calculated[4].mol/Total_mol;

// *****OUTLET SEPARATOR
CONDITION*****

T = (C_T(c,t))*1.8; //obtain SI temperature (deg C) value from FLUENT and change
to Rankine
P = ((8001325+C_P(c,t))/101325)*14.7; //obtain SI pressure (Pa) value from
FLUENT and change to Psia

```

```

// *****CALCULATION OF EQUILIBRIUM RATIO,
// K-VALUE FOR EACH COMPONENT*****

for (i=1;i<=Ncomponent;i++)
    {
        Calculated[i].kvalue =
        (UserInput[i].critP/P)*exp(5.37*(1+UserInput[i].omega)*(1-(UserInput[i].critT/T)));
    }

// *****FLASH CALCULATION WITH THE
// CALCULATED K-VALUES*****

    Nv = 1; //initial vapour fraction to start with
    n = 0; //initial no. of iteration
    do
    {
        fnv = 0; //reset Newton_Raphson to begin calculation with new Nv value if
condition not met
        fPnv = 0; //reset Newton_Raphson to begin calculation with new Nv value
if condition not met
        for (i=1;i<=Ncomponent;i++) //to get equilibrium vapour fraction, Nv
using Newton-Raphson method
        {
            fnv = fnv +
Calculated[i].zi*(Calculated[i].kvalue-1)/(Nv*(Calculated[i].kvalue-1)+1);
            fPnv = fPnv +
Calculated[i].zi*(pow(Calculated[i].kvalue-1,2))/(pow((Nv*(Calculated[i].kvalue-1)+
1),2));
        }
        fPnv = -fPnv;
        Dx = fnv / fPnv;
        Nv = Nv-Dx; //this new Nv will be used to recalculated if conditions not met
        Nl = 1 - Nv;
        n++;
    }while((fabs(fnv))>epsilon && n<Nmax);

    if(Nv >1) //if vapour fraction calculated more than 1
    {
        Nv = 1;
    }

```

```

        Nl = 1-Nv;    }

if(Nv <0) //if vapour fraction calculated is a negative value
{
    Nv = 0;
    Nl = 1-Nv;
}

// *****THIS MACRO TO RETURN Nv, Nl, and
COMPONENT PHASE FRACTION*****
    for (i=1;i<=Ncomponent;i++) //to calculate component phase fraction using
latest Nv and Nl values
    {
        Calculated[i].liqfrac = Calculated[i].zi / (Nl+(Nv*Calculated[i].kvalue));
        Calculated[i].vapfrac = Calculated[i].liqfrac*Calculated[i].kvalue;
    }

// *****CONVERTING VAPOUR MOL FRACTION TO VAPOUR
MASS FRACTION*****

// assume arbitrary 1 mol of mixture. mass = (mol fraction*1 mol)*MW
i=1; //for methane
Calculated[1].massvap = Calculated[1].vapfrac*16.05;
i=2; //for H2S
Calculated[2].massvap = Calculated[2].vapfrac*34.07;
i=3; //for CO2
Calculated[3].massvap = Calculated[3].vapfrac*44.01;
i=4; //for H2O
Calculated[4].massvap = Calculated[4].vapfrac*18.02;

Total_mass = 0; //initial total mass = 0
    for (i=1;i<=Ncomponent;i++)
    {
        Total_mass = Total_mass + Calculated[i].massvap;
    }
i=1; //for methane
Calculated[1].massvapfrac = Calculated[1].massvap/Total_mass;
i=2; //for H2S

```

```

Calculated[2].massvapfrac = Calculated[2].massvap/Total_mass;

i=3; //for CO2
Calculated[3].massvapfrac = Calculated[3].massvap/Total_mass;
i=4; //for H2O
Calculated[4].massvapfrac = Calculated[4].massvap/Total_mass;

//fprintf(fp1,"%f %f %f %f %f\n", Calculated[1].vapfrac, Calculated[2].vapfrac,
Calculated[3].vapfrac, T, P);
C_YI(c,t,0)= Calculated[1].massvapfrac;
C_YI(c,t,1)= Calculated[2].massvapfrac;
C_YI(c,t,2)= Calculated[3].massvapfrac;
C_YI(c,t,3)= 1-(Calculated[1].massvapfrac + Calculated[2].massvapfrac +
Calculated[3].massvapfrac);
//fprintf(fp1,"%f \n",
C_U(c,t));//F_FLUX(C_FACE(c,t,i),C_FACE_THREAD(c,t,i));
end_c_loop (c,t)
} //fclose(fp1);
}
DEFINE_SOURCE(liquidfrac, c, t, dS, eqn)
{
real massvap;
//real A[ND_ND];
//real area = 0.0;
face_t f;
massvap = 0.5*F_FLUX(f,t)/C_VOLUME(c,t);
//area*Nv/C_VOLUME(c,t);
//F_AREA(A, C_FACE(c,t,i), C_FACE_THREAD(c,t,i));area += NV_MAG(A);
return massvap;
}

```