Study of Joule-Thomson cooling effect due to leakage in compressed gas pressure vessels

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STUDY OF JOULE-THOMSON COOLING EFFECT DUE TO LEAKAGE IN COMPRESSED GAS PRESSURE VESSELS

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ABSTRACT

The reliability of pressure vessels in Compressed Natural Gas (CNG) ship is very important because there is very high pressure inside the CNG container (up to 250 bar). A key way to maintaining the integrity of pressure vessels is the principle of Leak-Before-Failure (LBF). However, the temperature of leaking CNG will drop due to Joule-Thomson cooling effect when CNG passes through the crack. The localized cooling effect on the steel plates may affect the ductile to brittle transition failure. Hitherto, the LBF is applied to piping system without considering the temperature change of steel material caused by Joule-Thomson cooling effect. Simulation and experiments thus are desirable to verify the effect in a narrow leaking crack on pressure vessel. By this means, the application of LBF may need to be corrected.

The narrow leaking crack can be considered to comprise many short and equivalent parts along the through-wall direction. Each part can be considered as a small throttling type nozzle. An iterative calculation program in MATLAB has been developed in this thesis. Due to the similarity on Joule-Thomson effect, argon is chosen as a substitute for CNG with safety in mind. The program is developed to calculate the pressure, velocity, density, temperature, viscosity, thermal conductivity and heat transfer coefficient of leaking argon through the crack by considering the Joule-Thomson effect. The calculated results of temperature, pressure and heat transfer coefficient of argon along the crack depth are used as boundary conditions in COMSOL FEA program for the heat transfer and thermal stress simulation.

In MATLAB iterative calculations, the initial argon pressure inside the pressure vessel is the maximum pressure of 91 bar during test. The initial temperature is room temperature of 30 °C. Solutions of pressure, velocity and density of leaking argon of each small space inside the crack are firstly obtained after inputting the crack dimensions and roughness parameters. The pressure of leaking Argon drops from 91 bar at the entrance of the crack to 9.5 bar at the exit of the crack. The velocity of leaking Argon through the crack does not change much. The density of leaking Argon drops from 150.7 kg/m³ at the entrance of the crack to 16.8 kg/m³ at the exit of the crack. Then the temperature of leaking argon inside the crack is calculated. The temperature of leaking Argon decreases from 30 °C at the entrance of the crack to -0.04 °C at the exit of the crack. With

the pressure and temperature data, the viscosity, thermal conductivity and heat transfer coefficient of leaking argon in crack are obtained.

Having obtained the properties of leaking argon in the crack from MATLAB, the heat transfer and thermal stress simulation is implemented to predict the temperature and stress distribution of the pressure vessel wall around the crack. A three-dimensional quarter model of mild steel plate is created by utilizing the COMSOL Multiphysics program. The heat transfer of metal and gas is treated as a one-way coupling problem due to rapid expansion of gas during leaking through the crack. Calculated argon properties are input into COMSOL as boundary conditions on the crack surface. The simulated lowest temperature of steel agrees well with the experimental result. The maximum Von Mises stress value near the crack tip is 3.3 GPa. The value is much higher than the yield stress (0.22 GPa) of mild steel in this research.

Experiments are carried out by a designed and machined J-T rig to verify the J-T effect in the crack. An artificial through-thickness crack in the center of a round test plate is fabricated using the liquefied Nitrogen cracking method. The crack width and roughness are measured by a feeler gauge and TalyScan 150, respectively. These values are used as input parameters in the MATLAB iterative calculations. The test plate as a cover of pressure vessel is assembled with the pressure vessel to perform the Joule-Thomson experiment. A web-camera connected to a computer is used to monitor and record the display of the pressure gauge. The thermocouples are connected to a TDS-302 data logger from which temperature data can be recorded and printed. During the Argon test, the highest pressure in the pressure vessel is 91 bar. It is found that the lowest temperature near the crack caused by the Joule-Thomson effect is 12.5 °C. Good agreement of the lowest steel temperature is found between the simulation and experimental test result.

Keywords: compressed natural gas (CNG), marine transportation, crack, Leak-before-Failure (LBF), Joule-Thomson cooling effect, heat transfer.

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NOMENCLATURE USED IN ASME BOILER AND PRESSURE VESSEL CODE SECTION VIII DIVISION 1

Symbol	Description	Unit
A	outside diameter of flange	in.
A_1	area available in vessel wall	sq in.
A_2	area available in nozzle wall	sq in.
A_b	total actual bolt area	sq in.
A_m	total required cross-sectional area of bolts	sq in.
A_{m1}	total cross-sectional area of bolts at root of thread or section of last diameter under stress, required for the operating conditions	sq in.
A_{m2}	total cross-sectional area of bolts at root of thread or section of last diameter under stress, required for gasket seating	sq in.
A_r	total cross-sectional area of reinforcement required in the plane under consideration	sq in.
B	flange I.D.	in.
b	effective gasket seating width	in.
b_0	basic gasket seating width	in.
C	a factor depending upon the method of attachment of head, shell dimensions, and other items as listed in (d) of ug-34 ^[1]	—
$c.a.$	corrosion allowance	in.
C_b	bolt-circle diameter	in.
d	diameter, or short span, measured as indicated in fig. ug-34 ^[1]	in.
E	joint efficiency	—
F	correction factor to obtain minimum required thickness of the shell on the plane being examined	—
f_{r1}	ratio of nozzle neck allowable stress to vessel wall allowable stress	—
G	diameter at location of gasket load reaction	in.
H	total hydrostatic end force	lb

Symbol	Description	Unit
h_G	gasket moment arm	in.
H_p	total joint-contact surface compression load	lb
K_I	spherical radius factor	
L	inside spherical or crown radius	in.
m	gasket factor	—
N	width, in., used to determine the basic gasket seating width b_0 , based upon the possible contact width of the gasket	in.
N_{min}	gasket crushout width	
P	internal design pressure	psi
R	inside radius of the shell course under consideration	in.
R_m	Minimum Radial Distance	in.
S	maximum allowable stress value	psi
S_a	allowable bolt stress at atmosphere temperature	psi
S_b	allowable bolt stress at design temperature	psi
t_{min}	the smaller of $\frac{3}{4}$ in. or the thickness of the thinner of the parts joined by a fillet, single-bevel, or single-J weld	in.
t_c	not less than the smaller of $\frac{1}{4}$ in. or $0.7 t_{min}$	in.
t_f	minimum required thickness of circular flat plate or blind flange	in.
t_{fc}	minimum required thickness of flat unstayed circular heads and covers	in.
t_h	minimum required thickness of hemispherical head after forming	in.
t_n	minimum required thickness of nozzle	in.
t_r	minimum required thickness	
t_s	minimum required thickness of cylindrical shell	in.
W	flange design bolt load, for the operating conditions or gasket seating, as may apply	lb
W_{m1}	minimum required bolt load for the operating conditions	lb
W_{m2}	minimum required bolt load for gasket seating	lb
y_I	minimum design seating stress	psi

NOMENCLATURE

Symbol	Description	Unit
μ_{JT}	Joule-Thomson effect	K/Pa or °C/bar
T	temperature	K or °C
p	pressure	Pa or bar
α	crack surface angle relative to the crack direction through wall	rad
θ	average flow direction relative to the crack direction through-wall	rad
W_{ceff}	effective crack width perpendicular to the average flow direction	m or mm
W_c	crack opening displacement (or crack width) perpendicular to the through-wall direction	m or mm
t	crack through-wall thickness (or crack depth)	m or mm
t_{eff}	effective crack through-wall thickness	m or mm
R_{local}	local roughness	m or μm
R_{global}	global roughness	m or μm
R_{glamp}	peak-to-trough amplitude of the global roughness contours for a sawtooth geometry, equal to four times the global roughness R_{global}	m or μm
R_{eff}	effective roughness	m or μm
c	linear interpolant	—
r_1	upper limit of the narrow crack regime	—
r_2	lower limit of the wide crack regime	—
Δp	pressure loss	Pa or bar
Δp_{fric}	frictional term of pressure loss during fluid flowing through a crack	Pa or bar
Δp_{inert}	inertial term of pressure loss during fluid flowing through a crack	Pa or bar

Symbol	Description	Unit
Δp_{recirc}	recirculation term of pressure loss during fluid flowing through a crack	Pa or bar
ρ	fluid density	kg/m ³
v	mean leak velocity of the fluid through crack	m/s
f	friction factor of a crack	–
N	actual number of turns in a crack	–
Q	mass flow rate	kg/s
L	crack length	m or mm
C_D	discharge coefficient	–
F	sum of normalized pressure loss terms due to fictional, inertial, and recirculation effects	–
F_{fric}	fictional term of normalized pressure loss	–
F_{inert}	inertial term of normalized pressure loss	–
F_{recirc}	recirculation term of normalized pressure loss	–
A	cross-section area of a crack	m ²
p_0	Maximum pressure of Argon inside pressure vessel	Pa or bar
T_0	Initial temperature of Argon inside pressure vessel	K or °C
R	specific gas constant	J/(kg·K)
R_0	universal gas constant; $R_0 = 8.31 \text{ J/(K·mol)}$	J/(K·mol)
T_c	critical temperature	K or °C
p_c	critical pressure	Pa or bar
V_c	critical volume	cm ³ /mol
ρ_c	critical density	kg/m ³
t	length of one increment along the crack depth	m or mm
$\dot{v}$	specific volume (which is the reciprocal of density)	m ³ /kg
a' and b'	constants of R-K gas state equation	–
M	molar mass	g/mol
h	specific enthalpy	J/kg

Symbol	Description	Unit
C_p	isobaric heat capacity	J/(kg·K)
C_v	isochoric heat capacity	J/(kg·K)
$a_0, a_1, a_2,$ and a_3	empirical constants of gas property dependent	—
AAD	average absolute deviations	—
η	viscosity	$\mu\text{Pa}\cdot\text{s}$
η^0	dilute gas viscosity	$\mu\text{Pa}\cdot\text{s}$
η^r	residual fluid viscosity	$\mu\text{Pa}\cdot\text{s}$
σ	Lennard-Jones size parameter	nm
$\Omega(T^*)$	collision integral	—
T^*	a parameter in viscosity formula, $T^* = \frac{T}{\varepsilon/k}$	—
ε/k	Lennard-Jones energy parameter	K
b_i	coefficients of the collision integral equation	—
τ	a parameter of viscosity equations, $\tau = T_c / T$	—
δ	a parameter of viscosity and thermal conductivity equations; $\delta = \rho / \rho_c$	—
γ, l_i	parameters of viscosity and thermal conductivity equations; γ_i is zero when l_i is zero and one when l_i is not zero	—
N_i, t_i, d_i, l_i	coefficients and exponents of the residual fluid viscosity equations and residual fluid thermal conductivity equations	—
λ	thermal conductivity	$\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
λ^0	dilute gas thermal conductivity	$\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
λ^r	residual fluid thermal conductivity	$\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
λ^c	thermal conductivity critical enhancement	$\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
k	Boltzmann's constant	$\text{J}\cdot\text{K}^{-1}$
ξ	correlation length	nm
T_{ref}	reference temperature	K
$\tilde{\chi}(T, \rho)$	a parameter of correlation length equation	—

Symbol	Description	Unit
ξ_0, q_D	fluid-specific (fitted) terms	nm
Γ	fluid-specific (fitted) term	—
ν, γ, R_x	theoretical based constants	—
$\tilde{\Omega}, \tilde{\Omega}_0$	parameters of thermal conductivity critical enhancement equation	—
N_u	Nusselt number	—
h	heat transfer coefficient	W/(m ² ·K)
f	friction factor	—
Re	Reynolds number	—
L	characteristic length	m
Pr	Prandtl number	—
D_e	equivalent diameter	m
P	wetting perimeter	m
Nu_{Gn}	Gnielinski modified Nusselt number	—
D	diameter of microchannels	m
K	stress intensity factor	Pa·m ^{1/2}
K_{IC}	fracture toughness	Pa·m ^{1/2}
K_0	opening mode stress intensity factor for an isolated (plate width = ∞) crack	Pa·m ^{1/2}
σ_c	maximum tensile stress which occurs in the center of the surface of the plate in the absence of the crack	Pa

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CHAPTER 1 INTRODUCTION

The relationship between mankind and the earth is a fragile one. With the worldwide concerns of pollution, ozone layer depletion and global warming, we need to reconsider our use of conventional fuels such as gasoline, diesel and coal. In addition, the sharp decline of fossil-fuel supplies and uncertainty of nuclear power's future have increased interest in renewable natural-energy sources. However, as their use is still questionable, none of them is expected to take up the role of oil and natural gas in the near future. Neither solar nor wind energy can provide electricity 24 hours a day every day. Solar and wind systems provide energy only intermittently, requiring gas turbines for back-up when the sun is not shining or the wind is not blowing.

With improvements in extracting technology, natural gas is playing a more and more important strategic role in energy supply with global energy demand rises. Unlike other fossil fuels, natural gas plays a major role in most sectors of the modern economy — power generation, industrial, commercial and residential. It is clean and flexible. The price and environmental advantages render natural gas as one of the most acceptable forms of energy. Consequently, natural gas is described as the bridge to a renewable future.^[2-5]

However, it is more difficult to transport and store natural gas than oil and therefore it lagged behind oil for a considerable period.^[2-4] Transportation of natural gas from production sites to consumption markets remains a challenge. With the substantial new demand and with new robust market opportunities expected to arise, the ways of transporting the gas from offshore reserves and overseas sources have generated considerable and renewed interest and a flurry of activities in the development of new technologies to deliver these valuable hydrocarbons to market have being created.^[6-9] Several transportation technologies of natural gas are introduced here.

1.1 Pipelined natural gas (PNG)

Large diameter pipelines are the oldest and most common method to transport natural gas underground or on the ground. Transporting the natural gas by pipelines is generally convenient and economically attractive and is the preferred choice whenever feasible, such as for onshore

transport. Up to now, pipeline transmission of natural gas between countries or continents has largely dominated the international natural gas trade. However, large diameter and long distance pipelines need very high capital investment and capital charges typically make up at least 90% of the total cost of gas transmission pipelines. So the PNG technique requires large and high-value markets and substantial proven reserves to be economically viable. For the offshore transport of natural gas, subsea pipelines become challenging due to the sea depth, the transporting distance and the traversed terrain restrictions. Therefore, in some cases especially for transportation of stranded gases the PNG technology is not viable.^[6, 8, 10, 11]

1.2 Liquefied natural gas (LNG)

Whenever the PNG technology is not economically viable, LNG is often considered as the alternative. LNG, an effective way of transporting natural gas for long distances across the oceans, constitutes 25% of the world natural gas movement. LNG provides an appropriate way of transporting natural gas from offshore.^[6] Natural gas is liquefied under atmospheric pressure and a temperature around 113K. Converting natural gas to LNG reduces the gas to one six-hundredth of its volume allowing transportation by specialized LNG tanker vessels over long distances. The production and storage of LNG is usually proceeded in ashore facilities.^[10]

While LNG carriers can be efficient for shipping large volumes of gas over long distances (2500 miles and beyond), huge upfront investment and complicated construction process of the liquefaction and regasification plant and associated facilities make LNG unattractive for developing medium to small sized resource bases and targeting small market demand, especially where there is a degree of recourse size or political risk. Therefore, LNG requires large reserves of natural gas near the facilities to support a LNG project and obtain acceptable returns of capital investment.^[6, 10-12]

1.3 Compressed natural gas (CNG)

The natural gas resources are to a great degree located far from their markets. Some 30% of the discovered gas is considered “stranded” throughout the world. “Stranded” is defined as gas reservoir fractions that prevent their development or optimal production from an oil or gas field as a result of their distance from the market, lack of transport economy or conversion technology.

PNG technology is often defeated by small reserves, long marine distances, or difficult marine environments (deepwater, ice scour, or environmental concerns such as fisheries). LNG technology generally requires a fairly large volume ashore LNG plant and making it difficult to commercially serve offshore small market reserves. Therefore, neither PNG nor LNG transportation techniques can economically exploit these stranded gas reserves. In order to meet the future demands for natural gas energy, new cost effective solutions for transporting natural gas from the production points to the consumers need to be developed. Nautical compressed natural gas (CNG) technology proposed in recent years provides an alternate gas transportation system that economically fits between PNG and LNG. The basic idea of CNG is to compress the natural gas at pressures ranging between 100 and 250 bar, and sometimes chill it to lower temperatures (up to -40°C). The CNG technology is relatively simple and can be easily introduced into commercial applications. The first attempt to build up a CNG transportation vessel brought to commissioning a rudimentary cargo vessel with CNG capacity of 1,300 Mcf in 1969, but the overwhelming required investment (compared to the scarce profit achievable in those years with quite low natural gas prices) made the application and diffusion of this technology unworkable.^[13] In the last decade, the development of several innovative vessel concepts is finally promising to make CNG marine transportation attractive.

Exploiting small reserves and satisfying small demand markets are the two main aims that CNG schemes are intended to pursue. CNG technology can also be employed in the start-up phase of a PNG or a LNG project development and will enable an early gas transportation start-up, which will facilitate a gradual build-up of the output quantity without waiting for the large investment necessary for a fully developed output train. Therefore, CNG transportation can be considered as a niche that will supplement both PNG and LNG technologies for the exploitation of stranded gas.^[14] This would supply an effective way to exploit reserves which otherwise would remain stranded, and would unfold many small markets that could not be economically justified via PNG or LNG.

Due to high pressure inside CNG containers, however, the safety of CNG system is the first important factor to be considered. Leak-Before-Failure (LBF) is an important methodology of maintaining the integrity of pressure vessels, which means that partial failures which happen by sub-critical mechanisms (fatigue crack growth, stress corrosion cracking, etc.) are detected by

loss of pressure in the cylinder before final disastrous fracture occurs. This requires a crack to grow in a stable manner through the wall of the component and cause a detectable leak and consequent loss of pressure. This indication of a partial failure allows the plant to be shut down in a controlled manner and repairs/replacement carried out.^[15] The LBF technology in nuclear industry can be adapted into CNG systems, although there are significant differences. Besides the dimensional differences, the materials and the fluids used in nuclear industry are stainless steels and steam/water whereas they are low carbon steels (mainly X70 and X80 pipeline steel) and natural gas in CNG systems.

1.4 Motivation of the work

On account of high pressure inside CNG containers, the most critical characteristic expected in CNG systems with leakage is the Joule-Thomson (JT) effect. In thermodynamics, the Joule-Thomson effect describes the temperature change of a gas or liquid when it is forced through a valve or porous plug while kept insulated so that no heat is exchanged with the environment. This procedure is called a Joule-Thomson process or throttling process. At room temperature, all gases except hydrogen, helium and neon cool upon expansion by the Joule-Thomson process.^[16-21] The ultimate purpose of the project is to study the impact of the materials' temperature change caused by the J-T effect during leakage on the fracture toughness of materials and then to establish recommendations for material fracture toughness and other criteria for the purposes of LBF design. Fracture toughness is a property which describes the ability of a material containing a crack to resist fracture. It is an inherent property of the material and is independent of the geometry of material. In general, the fracture toughness of most steels decrease with the lowering of the temperature.^[22, 23]

For CNG system with leakage on the container wall, the temperature of leaking CNG gas will drop due to Joule-Thomson cooling effect when CNG gas passes through the crack, thus chilling the vessel wall in the vicinity of crack and reducing fracture toughness of the wall. This may push the transition of previously stable crack propagation to become critical leading to its rapid growth. As shown in Figure 1-1, the initial defect continues to propagate till it penetrates the wall thickness which results in a leak. According to Paris crack growth law, during this initial phase of subcritical crack growth, each advance of the crack front corresponds to

loading/unloading cycles of pressurization. Two interruptions to this steady progress can occur. Firstly, the possibility of rapid unstable crack growth which occurs when the stress intensity exceeds the fracture toughness of the material, the crack will penetrate the wall thickness in an instant. Secondly, the remaining ligament of material beyond the crack front is subjected to a high tensile stress, leading to tensile yielding or plastic instability and instantaneous rupture of the ligament. Failure of the ligament can therefore occur by either fracture or plastic instability. Beyond this stage, a through-wall thickness crack is created with resulting leakage of the gas. However, the small leak at this point may be too small to be detectable. The crack continues to grow in a stable mode ($2C_s$) provided its length is less than the critical crack length ($2C_g$). The internal ($2C_d$) and external crack lengths ($2C_l$) are enlarged and leakage flow rate increases to the point where it is now detectable. The main characteristic of safe LBF technology is the development of a small stable leak, which can be safely detected well before instability. The crack continues to grow outward, from $2C_d$ and approaches the critical length of $2C_g$. On reaching the critical length, unstable and rapid growth will occur causing the pipe will burst open longitudinally. However, JT cooling intervenes to reduce the temperature of the metal and its fracture toughness K_{Ic} as well as the plastic yield strength. The reduction in properties reduces the critical crack length to $2C_{JT}$ which will be shorter than the critical crack length $2C_g$ without JT cooling. Hence JT cooling effect reduces the time to respond to leakage and the margin to failure. Therefore, prior to applying LBF, it is necessary to evaluate the temperature drop of CNG gas leaking through a crack due to Joule-Thomson (JT) effect and then temperature change of the vessel wall around a crack due to heat transfer, and the effect on fracture toughness of surrounding metal.

Figure 1-1: Illustration of axial defect growth subjected to mainly cyclic internal pressurization and associated JT cooling

1.5 Original contributions expected in this thesis

Original contributions expected in this thesis include the following aspects:

- (1) Development of a new mathematical calculation model to apply the Joule-Thomson cooling effect into a gas flowing through a leaking crack;
- (2) Integration of the JT effect parameters to heat transfer analysis to determine the localized cooling of the steel plate in the vicinity of the leaking crack;

- (3) Design and fabrication of a novel pressure vessel test system for measuring the temperature drop of the gas and steel in the vicinity of the crack caused by the Joule-Thomson cooling effect.

1.6 Objectives and scope of the thesis

1.6.1 Objectives of the thesis

This project is motivated by an industry concern for the safe design of the Compressed Natural Gas (CNG) pressure vessels. The project suggests that Leak-before-Failure (LBF) procedures should take into account the JT cooling effect of a leaking gas flow through a crack. The objectives of this project are as follows:

- (1) Modelling and numerical simulation of Joule-Thomson (JT) cooling effect of the gas flowing through the leaking zig-zag (rough surface) crack and the integration of the JT effect parameters to the heat transfer analysis in order to determine the temperature and stress distribution of the metal/steel plate in the vicinity of the leaking crack;
- (2) Experimental study of the JT cooling effect from a gas flowing through a leaking crack in order to identify its impact on the localized cooling of the steel plates/walls of the pressure vessel by testing the temperature distribution around a leaking crack;
- (3) Comparison of the lowest temperature results obtained from simulation and experiment and appropriate calibration of computational model.

1.6.2 Scope of the thesis

The scope of this project is outlined below:

- (1) Numerical modeling of the JT cooling effect from a gas flowing through a leaking crack:
 - a) Development of a mathematical calculation model to apply the Joule-Thomson cooling effect into a gas flowing through a leaking crack;
 - b) Selection of an appropriate gas to substitute the flammable natural gas;
 - c) Evaluation of the properties of Argon flowing through a leaking crack, such as JT

coefficient, temperature, density, viscosity, thermal conductivity and heat transfer coefficient;

- (2) Numerical simulation of heat transfer between the leaking gas and the crack surfaces by employing the COMSOL Multiphysics program;
- (3) Experimental study of the localized cooling on the cracked steel plate of the pressure vessel caused by the JT cooling effect of the leaking gas:
 - a) Design and fabrication of a pressure vessel test system;
 - b) Fabrication of a test plate with an artificial through-thickness crack.
- (4) Comparison between the experimental and simulation result at the lowest temperature and the calibration of the established model

CHAPTER 2 LITERATURE REVIEW

2.1 Introduction

Joule-Thomson cooling effect during a gas leaking through a crack has a negative impact on the evaluation of Leak-Before-Failure principle. As introduced in Chapter 1, for a CNG container with leakage on the wall, the temperature of leaking gas will significantly drop due to Joule-Thomson cooling effect when the leaking gas passes through the crack, thus chilling the vessel wall in the vicinity of the crack and lowering the fracture toughness of the pressure vessel wall. This may push the transition of previously steady crack propagation to reach a critical length leading to its rapid growth. A literature review is carried out on the integrity assessment of the CNG container, Leak-Before-Failure principle and Joule-Thomson effect.

The literature review includes six sections. In section 2.2, the CNG transportation technologies are reviewed including CoselleTM and VORTANSTM. The benefit of CNG transportation for shorter distances is summarized in this part. It works as a foreshadowing for the introduction of integrity assessment of the CNG container. In section 2.3, the integrity assessment of CNG container is reviewed, which provides some references for the experiment in this project. In sections 2.4 and 2.5, the background knowledge of Leak-Before-Fracture methodology and Joule-Thomson effect are briefly introduced. In section 2.6, the evaluation of gas properties is reviewed. The gas properties include density, Joule-Thomson coefficient, viscosity, thermal conductivity and heat transfer coefficient. In the last section 2.7, the gas flowing through the crack is discussed. Sections 2.6 and 2.7 offer some hints for the implementation of modelling in this work.

2.2 CNG transportation technologies

Natural gas is transported with two known technologies: 70 percent by pipeline, 30 percent by liquefied natural gas (LNG). About offshore transportation, the pipeline has a distance limit and terrain restrictions. LNG technology is applicable for long sea distances and large gas volumes, because the facilities at both ends are expensive to construct and the entire process is

complicated, costly, and energy wasteful. However, compressed natural gas (CNG) transportation by boat is an alternative for shorter distances and smaller markets that are not connected to large pipelines or base load LNG accepting facilities. Although this approach has been proposed for years, it has not yet materialized into a sizeable project.^[24]

The scalability of the CNG sea-going transport system and the reusability of its major assets (the carrier vessels) make this technology even more attractive. Figure 2-1 illustrates the range of application for the today's known or contemplated technologies suitable to monetize natural gas.

Figure 2-1: Production volume versus distance to market framework for various gas technologies^[11]

The marine transport of compressed natural gas (CNG) represents a different means to the challenge of natural gas delivery. Recently, breakthroughs in the technology have suggested that CNG has the potential to effectively ship much larger volumes of gas over much greater distances. Thus, CNG technology is expected to help economically access moderately sized reserves (typically 1-5 Tcf) with greater scalability and flexibility while lowering overall investment.^[7] Wang, Xiuli et al.^[24] show that for shorter distances (e.g., 1,000 km) and especially for the far lower natural gas prices that have emerged since the 2008 economic crisis, LNG simply cannot compete with CNG. Even at longer distances (e.g., 2,000 km) CNG is still more attractive, assuming that offshore pipelines are not feasible. For smaller volumes, such as 1 to 2 billion cubic meters per year (Bcm/yr) or even less, CNG is the only solution to bring this energy

source to many markets. That is to say, smaller and smaller markets are suitable for CNG transportation. Many parts of the world (such as many markets in the entire Mediterranean basin, near Sakhalin Island, in South-East Asia and the Caribbean) would be better served by CNG even if LNG projects have already been approved and under construction near them.

Technically, compressed natural gas (CNG) is easy to deploy with higher flexibility of infrastructure and facilities. One could visualize the CNG solution comparable to a floating pipeline, with much less basic facilities required for exploitation of the natural gas reserve.^[25] Modern efforts to commercialize stranded natural gas by CNG technology include the construction of an actual gas carrier by Columbia Gas in the late 1960's. The design used high cost alloy steel and the project was deemed to be sub-economic and was decommissioned after a few transits.^[7] As the desire to exploit gas from more isolated and challenging sources increased towards the end of the 1990's, interest in CNG project re-emerged. Subsequently, “Coselle” and “VOTRANS” technologies were brought about, which are two close-at-hand commercial high-pressure gas storage and transport technologies for CNG.^[6]

2.2.1 Coselle™

In the early 1990s, the well known concept “Coselle™” was originally proposed by Cran & Stenning Technology Inc. of Calgary, Alberta, Canada, one of the proponents of the CNG technology. The conception of the “Coselle” pressure vessel and the development of the Coselle Compressed Natural Gas (CNG) Carrier promise to improve the economics of natural gas transportation over short marine routes and from modest reserves by reducing the manufacturing cost of the gas containment system by spooling small diameter (6 inch or so) coiled tubing into large carousels.^[7, 12] To put it more specifically, the Coselle is a high-pressure gas storage and transportation system based on a coil of relatively small-diameter pipe (6 to 8 inches, about 15 to 20 cm) sitting in a steel-girder carousel. Considering the natural gas pressured up to 3,000 psi at ambient temperature, a typical CNG carrier assembled with 108 carousels can offer up to 330 MMscf (about 10 MMscm) of capacity. Figure 2-2 shows this CNG vessel schematic.^[12] Similar methodology is used by others namely TransOcean Gas of Canadian and Knutsen O.A.S Shipping of Norway with varying characteristics of the containment system.^[6]

Figure 2-2: Coselle schematic of a CNG vessel, from Sea NG Corp.

2.2.2 VOTRANSTM

The Volume-Optimized Transport and Storage (VOTRANSTM) concept, another approach to CNG transportation, is developed by Enersea Transport LLC. The new CNG transport system has global applicability and allows a new perspective on remote offshore natural gas development. In the technology the natural gas is compressed and cooled to lower temperatures. This technology can achieve further reduction of the volume of the compressed natural gas compared to just compressing it at room temperatures. At the lower temperatures of 0 to -40°C , the process can work at lower pressures than at room temperatures.^[6, 26]

In the system, the natural gas is stored in a long and large-diameter cylinder in an insulated cold storage cargo package at moderate pressure. It is possible for the system to compress large amounts of gas into long tubular containers by chilling gas to a suitably low temperature (usually well below 0°C), so that the ratio of the weight of the gas stored to that of the container can be

optimized. The specific design examined by the American Bureau of Shipping (ABS) accommodates 700 to 800 million cubic feet of natural gas, depending on the specific gas composition. The cost of compression and that of the containers (and, therefore, the ships) can be greatly reduced by this method. Although these savings are somewhat offset by the costs of refrigeration and insulation, operational considerations and the sensitivity of cost effective ship design to the weight of CNG containers explicitly reveal the value of a lighter container. EnerSea intends to use the technology to support economic gas transportation services for applications with average supply rates ranging from 300 to 500 million cubic feet of gas per day (mmscfd) in markets from 200 up to 4,000 miles away. A range of ship designs is developed by EnerSea to offer transport for supply rates (or market needs) as low as 50 mmscfd to as much as 700mmscfd.^[26, 27]

This VOTRANS system is based on horizontal or vertical arrays of 36 meter (about 118 ft) long large diameters pipes (40 inches, about 1 m), segregated at 6 inches grid and manifolded into common pressure and flow system in groups of 24, called modules. These modules are then arranged in holds, whose sum determines the VOTRANS system carrier capacity; the largest model of such a VOTRANS system can offer up to 800 MMscf (about 22 MMscm) of capacity. Figure 2-3 shows this CNG vessel arrangement, Figure 2-4 shows the construction design of a CNG vessel, and Figure 2-5 illustrates the pipe tank modules of a CNG vessel.

Figure 2-3: Schematic of a CNG vessel, from EnerSea Transport LCC

Figure 2-4: Construction design of a CNG vessel, from EnerSea Transport LCC

Figure 2-5: Pipe tank modules of a CNG vessel, from EnerSea Transport LCC

2.3 The integrity assessment of CNG container

In CNG projects, the main capital expenditure is spent on building the ships which have very high pressure inside the CNG container (up to 250 bar), therefore the reliability of pressure

vessel and careful design of CNG transport fleets are very important. The CNG ships cost approximately \$230 million while for LNG the ships cost approximately \$160 million.^[6, 8, 10]

The key to the realization of the CNG concept is to use modern reliability calibrated limit state design codes that provide the same system safety, but with the use of smaller nominal safety factors on the structural design of the vessel cylinder. The underlying principle is that the CNG cylinders resemble modern pipelines designed against explicit failure modes caused by internal overpressure. A safe and yet optimal CNG tank design is in fact beyond the scope of traditional pressure vessel codes. Pressure vessel codes applying implicit acceptance criteria are considered adequate for vessels where the current failure modes are uncertain due to increased complexity, detrimental effect of nozzles, supports, and manual welding.

A crucial part of the verification of the safety of the CNG containers is to perform small scale or full scale experiments. Some experiments^[13, 28, 29] have been developed for the cylinder failure analysis. Erdelen-Peppler et al.^[29] have carried out experiments of small scale tests on strip and ring specimens for comparison. The test results lead to the conclusion that strip specimens sampled from the longitudinal weld may not be in all details representative of full scale specimens but they lead to conservative life predictions and may be employed to estimate the lower bound of the actual life time. They found that Ring fatigue tests could be considered a better alternative to substitute full scale experiments because they expose the complete and undeformed pipe circumference to fatigue loads.

Erdelen-Peppler et al.^[29] tested cylinders (2 Hifa[®] pipes and 1 conventional pipe) with a frequency of 90 s per cycle with inhibited water at room temperature. Failures were monitored by pressure drop due to water leakage after a crack propagated through the wall. The conventional pipe failed after 12,000 cycles by a fatigue crack in the longitudinal weld.

Figure 2-6: Fatigue test failures at girth welds

Figure 2-7: Fatigue failure at corrosion pitting in long seam

Figure 2-6 shows one Hifa[®] pipe fatigue test failure at girth welds after 31,000 cycles. Figure 2-7 shows that the other Hifa[®] pipes failed due to corrosion in the centre of the longitudinal weld after 41,000 cycles. The test results showed that the mean value of Hifa[®] pipes fatigue limit is

about 2-3 times higher than that of the conventional pipes. After testing, the welds were inspected with dye penetration testing and there were no signs of crack initiation along the weld. This means that the material of the Hifa[®] pipe has excellent toughness and sufficient ductility, and Leak-Before-Failure (LBF) had been demonstrated.

A researcher in DNV company^[30] calculated the expected temperature change of an area around a crack by a mathematical model. Due to the expansion of the gas through the crack the gas temperature drops from approximately +10 °C on the inside to -70 °C on the outside as shown in Figure 2-8 and Figure 2-9. It is noted that the low temperature in the crack tip area leads to a deterioration of the fracture toughness capacity. However, only a small area along the crack shows estimated temperatures below 0 °C. It can be seen that the temperature rise from -70 °C to -15 °C in a distance of only 25 mm. The significant benefit of the heavy wall of the solid steel is that it supplies a high heat capacity. Due to this heat capacity, a long time is necessary for the leaking gas to create a significant area of material at low temperatures. The high heat capacity of the heavy wall works as a large heat buffer during the time of the gas release. Stress analysis shows that temperature generated stresses are insignificant for the ship design.

Figure 2-8: Estimated temperature profile along crack tip^[31]

Figure 2-9: Temperature distribution in the cargo tank wall as a function of the distance from the crack^[31]

Several hydraulic full scale fatigue tests have been carried out successfully in accordance with the requirements in Det Norske Veritas rules for CNG carriers.^[31] The tank cylinders are manufactured out of large diameter pipes with the dimension of 42'' OD and a wall thickness of 33.5 mm. The pipe material grade is SAWL 555 and is equivalent to the API 5L X-80 grade. The natural gas is stored in the cylinders with a pressure of 250 bar at ambient temperature. Before performing a fatigue crack test, they machined a 5 mm depth axial notch (length 150 mm) on the outer surface of the cylinder as shown in Figure 2-10. The crack penetrated the inside surface after 6430 cycles. For measuring the temperature and strain beside the crack, the temperature and strain gauges were fixed on the outside surface close to the crack at six positions illustrated in Figure 2-11. In order to pressurize the pipe till 250 bar without leakage, the crack was sealed by a rubber padded steel bar pressed to the crack by using a hydraulic pipe which could be released by remote control. The test results in Figure 2-12 show the lowest temperature in the gas jet during the leak is -68 °C. The metal temperature at a distance of 20 mm from the crack is -24 °C. The author stated that the material reached a brittle state below the temperature of -35°C. From the microscopic investigation of the tested pipe segment containing the crack, the crack remained

stable during the test without experiencing any brittle crack growth. There are uncertainties related to the results as the shape of the leak affects the flow characteristics of the gas. The characteristic has a big impact on the pressure drop and consequently on the temperature.

Figure 2-10: Notch/crack appearance on the outside pipe surface^[31]

Figure 2-11: Schematic of the positioning of temperature and strain measurements on the vessel^[31]

Figure 2-12: Pressure-temperature over the time of the test^[31]

2.4 Leak-Before-Failure methodology

Leak-Before-Failure (LBF) is an important methodology of maintaining the integrity of pressure vessels, which means that partial failures which happen by sub-critical mechanisms (fatigue crack growth, stress corrosion cracking, etc.) are detected by loss of pressure in the cylinder before final disastrous fracture occurs. This requires a crack to grow in a stable manner through the wall of the vessel and cause a detectable leak and subsequent loss of pressure. This indication of a partial failure will allow the facilities to be shut down in a controlled approach and maintenance/replacement carried out. The concept of LBF aims at the application of fracture mechanics to demonstrate that it is impossible for sudden, disastrous failure to occur without prior signs of detectable leakage. The mechanism of LBF is widely used in the structural integrity design of pressurized components and vessels, such as missile casings, gas and oil pipelines, pressure containers, nuclear piping, etc.^[15]

In a pressure container part, such as a vessel, pipe, steam generator or pump casing, flaws are usually present, some of which could be detected during the manufacturing process itself. These flaws can develop due to one of several mechanisms, such as fatigue, corrosion and creep. The effects are very severe in the case of nuclear piping defects. In the nuclear industry, LBF has

been applied to piping for the reason of eliminating facilities that are used for restraining pipe whipping from a supposed pipe break.^[32] The concern in this application is with above-ground plant-piping systems where circumferential defects are historically more prevalent than axial defects. In this LBF method, it is desirable to identify small amounts of seepage at normal working situations in order that the seepage size (with some safety factor) would be steady at transient (typically seismic) stresses. For that reason, the defect orientation in these researches is circumferential, and pressure stresses as well as many other stress elements contribute to the LBF analysis. The stresses to be concerned are the normal working stresses for seepage detection, and transient stresses for fracture stability analysis. It is also necessary that there not be any subcritical crack growth mechanism that could cause a long surface defect to occur. Such long surface defects could lead to failure under the transient loads without any seepage warnings. If there were a mechanism that could cause long surface defects, then one would have to invoke an augmented examination procedure for LBF to work. For example, ultrasonic examination might be considered enough to making sure the defect lengths would be less than a preferred value.

Over recent years the concept of Leak-Before-Failure (LBF) has been considered as a more realistic design standard in establishing safety cases for piping mainly for the nuclear industry. The LBF approach is mainly applied to the design of nuclear power plants. Countries such as the USA, Japan, Italy, UK, Germany, France and Spain have changed or are in the route of changing the regulatory procedures to accommodate LBF in nuclear power plants design.^[32-49] B. Ghosh et al.^[48] suggested that the estimation of the crack opening area (COA) plays a nodal role in the demarcation of leakage size crack corresponding to the measurable leak flow rate from defective piping systems. The simple single-parameter models for COA due to Kastner et al.^[50], Wuthrich^[49] and Paris and Tada^[51] endure from one or other types of geometrical or physical restrictions in their applicability. In the study of B. Ghosh et al.^[48], COA has been estimated from more generalized two-parameter models based on thin shell theory.

An important part of the LBF analysis of nuclear piping is how to determine the related fracture toughness (or the J-resistance curve) for nonlinear fracture mechanics analysis. The practice to use fracture toughness from a standard C(T) sample is identified to usually offer conservative evaluations of toughness. To improve the accuracy of predicting piping failure, Nam-Su Huh et al.^[52] proposed a new method to determine fracture toughness employing a

nonstandard testing sample, curved wide-plate in tension. From the comparison between the J-resistance curves from the full-scale pipe test, the curve wide-plate test and C(T) specimen test, it is suggested that the J-resistance curve from the curved wide-plate tension test is analogous to, but that from the C(T) specimen is lower than, the J-resistance curve from the full-scale pipe experiment. It indicates that the use of toughness data from C(T) specimen is conservative.

For CNG systems, the temperature of the leaking CNG gas will drop due to the Joule-Thomson cooling effect when the gas passes through the crack, thus chilling the vessel wall in the vicinity of the crack and reducing fracture toughness of the localized metal.^[22, 23, 31] This may push the transition of a previously stable crack propagation to become critical, leading to its rapid growth. Therefore, prior to applying LBF technology, it is necessary to evaluate the temperature drop of CNG gas leaking through a crack due to the Joule-Thomson (JT) cooling effect and then the temperature change of the vessel wall around a crack due to heat transfer, and the effect on the fracture toughness of the metal.

2.5 Joule-Thomson effect

2.5.1 Background of Joule-Thomson effect

In thermodynamics, the Joule-Thomson effect or Joule-Kelvin effect explains the increase or decrease in the temperature of an actual gas (as differentiated from an ideal gas) when it is permitted to expand freely through a valve or other throttling apparatus while kept insulated so that no heat is transferred to or from the gas, and no external mechanical work is extracted from the gas.^[16-18, 53] This procedure is called a Joule-Thomson process or throttling process.^[21] The Joule-Thomson effect is named after James Prescott Joule and William Thomson, 1st Baron Kelvin who discovered it in 1852 following an earlier study by Joule on Joule expansion, in which a gas experiences free expansion in a vacuum.

The JT effect does not apply for ideal gases because there is no temperature variation when an ideal gas is permitted to expand through an insulated throttling device.

The adiabatic expansion of a gas may be performed in many ways. The alteration in temperature undergone by the gas during expansion relies not only on the initial and final

pressure, but also on the way in which the expansion is performed. If the expansion procedure is reversible, indicating that the gas is in thermodynamic equilibrium all the time, it is named an isentropic expansion. In this situation, the gas does positive work during the expansion, and its temperature drops. On the other hand, the gas does not work and absorbs no heat in a free expansion; therefore the internal energy remains constant. Expanded in this way, the temperature of an ideal gas would stay constant, but the temperature of a real gas may either increase or decrease, relying on the initial temperature and pressure.

The carbon dioxide fire extinguisher shown in Figure 2-13^[54], carbon dioxide gas is allowed to expand quickly from a fire extinguisher. If the gas is directed onto a piece of burlap or black cloth, the 'snow' will be visible and last for several minutes. The cold temperature doesn't really help put out the fire -- the carbon dioxide actually does the job by smothering the flames. Although CO₂ extinguishers primarily deprive a fire of oxygen, the low temperature of the gas probably has some kind of a secondary effect. It is not just the carbon dioxide that becomes cooler -- it quickly cools its surroundings as well.

Figure 2-13: CO₂ fire extinguisher: expanding gas freezes surrounding water vapor^[54]

2.5.2 Physical mechanism of JT effect

When a gas expands, the average distance between molecules grows. Due to intermolecular attractive forces, expansion causes an increase in the potential energy of the gas. If no external work is extracted and no heat is transferred, the whole energy of the gas remains constant due to the conservation of energy. The increase in potential energy thus indicates a decrease in kinetic energy and therefore in temperature.

A second mechanism is the converse effect. During gas molecules collision, kinetic energy is momentarily converted into potential energy. When the average intermolecular distance increases, there is a decrease in the number of collisions per time unit, which causes a drop in average potential energy. Furthermore, total energy keeps constant, thus this causes an increase in kinetic energy (temperature). Below the Joule-Thomson inversion temperature, the former effect (work done internally due to intermolecular attractive forces) governs, and free expansion leads to a drop in temperature. Above the inversion temperature, gas molecules move faster and so collide more frequently, and the latter effect (reduced collisions causing a drop in the average potential energy) governs: Joule–Thomson expansion causes a temperature increase.^[16, 17, 53]

Figure 2-14 demonstrates the test rig of the Joule-Thomson effect. The Joule-Thomson effect is an isenthalpic process, meaning that the enthalpy of the gas keeps constant during the procedure.^[21]

Figure 2-14: Schematic of the Joule-Thomson experimental equipment

In a Joule–Thomson process the enthalpy keeps constant. To verify this, the first step is to calculate the net work done by the gas that moves through the porous plug. Assume that the gas has a volume of V_1 in region 1 at pressure P_1 and a volume of V_2 when it comes to the region 2 at pressure P_2 . Then the work done on the gas by the remainder of the gas in region 1 is P_1V_1 . In region 2, the quantity of work done by the gas is P_2V_2 . Consequently, the whole work done by the gas is

$$P_1V_1 - P_2V_2 \quad (2-1)$$

By the first law of thermodynamics, The alteration in internal energy plus the work done by the gas is the total quantity of heat absorbed by the gas (here it is supposed that there is no alteration in kinetic energy). In the Joule-Thomson process the gas is kept insulated, thus no heat is absorbed. This means that

$$E_2 - E_1 + P_2V_2 - P_1V_1 = 0 \quad (2-2)$$

where E_1 and E_2 indicate the internal energy of the gas in regions 1 and 2, respectively. The above equation then implies that:

$$H_1 = H_2 \quad (2-3)$$

where H_1 and H_2 indicate the enthalpy of the gas in regions 1 and 2, respectively.

2.5.3 Joule-Thomson inversion temperature

Temperature alteration of either sign can happen during the Joule-Thomson process. A real gas (as differentiated from an ideal gas) expands through a throttling facility, the temperature may either increase or decrease, relying on the initial temperature and pressure. For any known pressure, real gases have a Joule-Thomson inversion temperature:^[17, 53] above which the JT expansion causes warming, and below which the JT expansion causes cooling. For most gases at atmospheric pressure, the inversion temperature is rather high (above room temperature), and hence most gases at those temperature and pressure circumstances are cooled by the JT expansion.

2.5.4 The Joule-Thomson (Kelvin) coefficient

The alteration of temperature with a drop of pressure in a Joule-Thomson process is the Joule-Thomson coefficient:^[16, 18, 53]

$$\mu_{JT} = \left(\frac{\partial T}{\partial p} \right)_H \quad (2-4)$$

where: μ_{JT} is in K/Pa or °C/bar.

For all real gases, it will equal zero at some points named the inversion points. As explained above, the Joule-Thomson inversion temperature is the temperature where the JT coefficient alters sign (i.e., where the JT coefficient equals zero). The JT inversion temperature relies on the pressure of the gas before expansion.

In a gas expansion the pressure reduces, hence the sign of ∂p is always negative. With that in mind, the following Table 2-1 gives details when the Joule-Thomson effect cools or warms a real gas:

Table 2-1: Joule-Thomson cooling or warming effect

Gas temperature	μ_{JT}	∂p	∂T	J-T effect
Below the inversion temperature	Positive	Always negative	Negative	Cooling
Above the inversion temperature	negative	Always negative	Positive	Warming

Hydrogen and helium are two gases whose Joule-Thomson inversion temperatures at one atmosphere pressure are very low (e.g., about 51 K (−222 °C) for helium). Therefore, hydrogen and helium will warm during a JT expansion at typical room temperatures. On the other hand, Nitrogen and oxygen have inversion temperature of 621 K (348 °C) and 764 K (491 °C), respectively: the two richest gases in air can be cooled by a JT expansion at typical room temperatures.^[16]

It should be noted that JT coefficient is always equal to zero for ideal gases. In other words, they will neither warm nor cool during an expansion through an insulated JT device.

2.5.5 Joule-Thomson effect for different gases

2.5.5.1 Natural gas

Ivan Marić et al.^[55] developed a numerical procedure to calculate the Joule-Thomson coefficient of a natural gas by using the AGA-8 extended virial-type characterization equation. Firstly, they derived the relation of the JT coefficient to the equation of state. Then the relation was adapted for the calculation of the JT coefficient of natural gas using the AGA-8 natural gas compression factor equation. Figure 2-15 and Figure 2-16 show the corresponding JT coefficients for methane and for a natural gas mixture calculated for the range of pressure from 0 to 60 MPa in 1 MPa steps and for six discrete temperatures in the range from 245 to 345 K. From these figures, it can be seen that for each temperature there exists a corresponding pressure (inversion point) at which the JT coefficient changes its sign.

Figure 2-15: Joule-Thomson coefficient μ_{JT} for methane for pressures from 0 to 60 MPa and temperatures from 245 to 345 K^[55]

Figure 2-16: Joule-Thomson coefficient μ_{JT} for a natural gas mixture and for pressures from 0 to 60 MPa and temperatures from 245 to 345 K^[55]

2.5.5.2 Argon

J. R. Roebuck et al.^[56] measured the Joule-Thomson effect in Argon. The Argon was of high purity except for 0.5 percent of Nitrogen. The values of the Joule-Thomson coefficient, μ_{JT} , over the field (-150 to 300 °C and 1 to 200 atm.) are calculated, tabulated and plotted as a function of temperature and pressure. The numerical values of μ_{JT} are obtained by taking the ratio of successive differences of temperature and of pressure for each run. These values of μ_{JT} are plotted against the average value of the pressures to give the set of isenthalpic curves as shown in Figure 2-17. The values of μ_{JT} for a series of selected values of pressure were picked off.

Figure 2-17: μ_T as function of pressure (p) at constant enthalpy^[56]

The values of μ_T and T are plotted in Figure 2-18 as isopiestic. μ_T goes up rapidly for the 1 and 20 atm. isopiestic such that the part of the diagram below -50°C has been cut off and shifted into the space above the main family of curves. The largest value of μ_T is almost 3°C per atm., and the observed maximum drop of temperature across the plug approaches 120°C .

Figure 2-18: μ_T as function of temperature (t) at constant pressure^[56]

2.5.5.3 Nitrogen

Roebuck et al.^[57] measured the Joule-Thomson effect in Nitrogen with the customary range of pressure (1 to 200 atm) and of temperature (-150 °C to 300 °C). The maximum observed drop in temperature across the experimental plug is 87 °C and the maximum value of μ_{JT} 2.32 °C/atm. These values are smaller than the corresponding values (120 °C and 3.0 °C/atm) for Argon. The relationship between μ_{JT} and temperature t are shown in Figure 2-19. The limit curve (long dashed line) enters at the lower left-hand edge of the diagram, bends upward so as to pass vertically through the critical point, and leaves at the point $\mu_{JT} = 2.20$. In the resulting limit curve, the upper branch, rising from the critical point, is associated with the steep isenthalps intersecting the vapor pressure curve from above. The lower branch, descending from the critical point, is associated with the flat isenthalps intersecting the vapor pressure curve from below.

Figure 2-19: μ_{JT} as a function of temperature (t) at constant pressure^[57]

2.6 Evaluation of gas properties

In heat transfer analysis, the heat transfer coefficient is one of most important parameters to be evaluated. As it is related to the gas physical properties in the crack, such as dynamic viscosity and thermal conductivity at high pressure, the first step of carrying out heat transfer analysis is to evaluate these physical properties of leaking gases in the crack.

2.6.1 Density and Joule-Thomson coefficient

Among different real gas state equations, RK (Redlich-Kwong) equation^[58-61] is adopted to evaluate the density and Joule-Thomson coefficient of gases in this work. The accuracy of RK equation to calculate the density and Joule-Thomson coefficient is demonstrated in the simulation chapter 3.

RK equation is given as,

$$p = \frac{RT}{\tilde{v}-b'} - \frac{a'}{\tilde{v}(\tilde{v}+b')T^{0.5}} \quad (2-5)$$

where R is the specific gas constant, J/(kg · K).

$\tilde{v}$ is the specific volume (which is the reciprocal of density), m³/kg.

a' and b' are constants,

$$a' = 0.4278 \frac{R_{con}^2 T_c^{2.5}}{p_c} \quad (2-6)$$

$$b' = 0.0867 \frac{R_{con} T_c}{p_c} \quad (2-7)$$

where T_c and p_c are critical temperature and pressure, respectively,

2.6.2 Viscosity and thermal conductivity of different gases

2.6.2.1 Viscosity of dilute methane

The transport properties of fluids at extremely low pressures may be quite different from those measured at “dilute” states. The dilute states of the gas are generally taken to be at a pressure of about one atmosphere, and most measurements of dilute gas transport properties are taken at this pressure. Chung, et al.^[62] have carried out some calculations for the dilute gas properties. Table 2-2 and Table 2-3 show the comparison between calculated and experimental low-pressure gas viscosity.

Table 2-2: Comparison between calculated and experimental low-pressure gas viscosity^[62]

Compound	$T, ^\circ\text{C}$	Experimental value, μP	Percent error		
			Chung et al., Eq. (9-4.10)	Lucas, Eq. (9-4.16)	Reichenberg, Eq. (9-4.21)
Methane	-13	98	-0.7	-0.5	—

Table 2-3: Comparison between calculated and experimental values of low-pressure gas viscosity^[63]

compound	data point	temp range, K	exptl ^a $\eta, \mu\text{P}$	deviation, %							
				this work		other methods ^a					
				AAD	MAX	Thodos et al.		Golubev		Reichenberg	
						AAD	MAX	AAD	MAX	AAD	MAX
I. Nonpolar Gases											
methane	5	293.2-773.2	109-227	0.28	0.7	0.38	0.7	---	---	---	---
ethane	4	293.2-523.2	90.1-153	1.50	-2.0	1.92	2.4	9.12	23.0	2.17	-2.4
propane	5	293.2-548.2	80.6-142	1.48	-2.5	2.28	4.1	7.62	16.0	0.82	-1.7
1-butane	3	293.2-393.2	73.9-99.8	1.22	1.5	0.53	0.6	2.26	3.0	1.80	-2.8
1-pentane	4	398.2-573.2	91.7-130	0.59	0.7	0.60	0.7	3.07	4.8	1.22	-1.6
isobutane	3	293.2-393.2	74.4-99.5	1.10	1.3	1.90	2.0	3.93	4.3	1.73	2.1
ethylene	4	273.2-523.2	94.5-168	0.31	0.5	1.15	-1.4	9.50	26.0	0.25	-0.4
propylene	4	293.2-523.2	84.3-147	1.54	-1.8	1.52	2.1	5.75	11.0	1.60	2.4
1-butene	3	293.2-393.2	76.1-99.8	1.63	-2.3	2.90	4.3	5.00	6.4	3.16	4.6
acetylene	3	303.2-473.2	102-155	0.60	0.6	0.63	-0.8	5.83	12.0	1.26	2.4
cyclohexane	5	308.2-573.2	72.3-129	1.46	2.3	1.54	3.5	4.08	5.4	3.20	-4.2
benzene	3	301.2-473.2	73.2-117	0.56	-1.0	1.96	3.3	4.66	6.9	2.66	4.4
toluene	3	333.2-523.2	78.9-123	4.10	5.0	3.43	-4.0	1.06	-1.8	2.53	-3.1
carbon dioxide	3	303.2-473.2	151-219	1.48	-2.9	2.96	4.8	9.80	10.0	---	---
carbon disulfide	3	303.2-473.2	94.6-151	4.62	-5.7	9.76	11.0	12.66	15.0	---	---
carbon tetrachloride	3	398.2-573.2	133-190	1.59	-2.4	3.13	4.2	5.23	6.1	2.03	-2.6
chlorine	3	293.2-473.2	133-209	3.32	-4.5	2.00	2.9	4.40	5.8	---	---
average error				1.6		2.2		8.0		1.9	

Compound	Data point	Temp range, K	Exptl value, μP	Deviation, %							
				This work		Thodos et al.		Golubev		Reichenberg	
				AAD	MAX	AAD	MAX	AAD	MAX	AAD	MAX
Methane	5	293.2- 773.2	109-227	0.28	0.7	0.38	0.7	...		...	

Note: “this work” represents Chung, et al. method. “AAD” denotes average absolute deviation, “MAX” denotes maximum deviation.

From Table 2-2 and Table 2-3, based on AAD and MAX, one can conclude that Chung, et al.’s method for the evaluation of low pressure viscosity of methane is a relatively accurate one compared to other researchers’ methods.

2.6.2.2 Viscosity of dense methane

As high pressure gas leaks through a narrow tortuous crack in a high pressure cylinder wall, the viscosity of the high pressure gas needs to be evaluated. Table 2-4, Figure 2-20 and Figure 2-21 show the comparison between experimental and calculated viscosities from the dilute gas state to the dense liquid at wide temperature and pressure ranges using Chung. et al.'s method. Table 2-4 lists the predicted results from Chung. et al. for the viscosity of different gases. Most viscosity values are predicted within about 3% deviation for paraffins and olefins, whereas the deviations are slightly higher for ring compounds with an average absolute deviation (AAD) of 4%. The AAD and maximum deviation for methane are 2.40% and -8.42%, respectively. The viscosity-density plot in Figure 2-21 shows that the viscosity increases drastically with density as the fluid becomes dense, which indicates that, for prediction of dense fluid viscosity, density is a very sensitive parameter. For this reason, the high accuracy region for the correlation generally corresponds to reduced temperatures (T/T_c) greater than about 0.4 and reduced densities (ρ/ρ_c) below about 2.5, although the correction yields reasonable results somewhat beyond this region.

Table 2-4: Comparison of calculated and experimental viscosities for pure fluid using Chung. et al. method ^[64]

fluid	data no.	temp range, K	pressure range, bar	deviation, %		ref ^a
				AAD	max	
methane	466	91-511	1-680	2.40	-8.42	1,2,3,4,5,6,7,8,39, ^b 40 ^b
ethane	60	311-444	4-544	1.90	-4.84	9,10, ^b 41 ^b
propane	136	173-411	7-544	2.18	8.67	2,9,39, ^b 40, ^b 41 ^b
<i>n</i> -butane	70	213-444	7-544	2.13	-9.67	9,10,11,40 ^b
<i>n</i> -pentane	85	173-470	1-204	2.57	-11.45	10,12,40 ^b
<i>n</i> -hexane	249	193-548	1-500	2.42	11.64	10,13,40 ^b
<i>n</i> -heptane	268	263-548	1-500	2.17	13.37	10,14,40 ^b
<i>n</i> -octane	232	283-569	1-500	2.12	-12.97	10,13,40 ^b
<i>n</i> -nonane	17	263-423	1	4.41	-7.42	10,14,40 ^b
<i>n</i> -decane	48	253-444	1-476	2.91	-9.92	10,15,40 ^b
<i>n</i> -undecane	23	263-474	1	7.11	-12.56	10,14
<i>n</i> -dodecane	41	273-408	1-3447	7.29	-16.92	10,13,16,40 ^b
<i>n</i> -tridecane	21	273-474	1	4.19	16.00	10,14,42 ^b
<i>n</i> -tetradecane	10	283-373	1	5.12	13.86	10,42 ^b
<i>n</i> -pentadecane	29	293-408	1-3447	4.68	-16.80	10,16
<i>n</i> -hexadecane	69	293-523	1-2731	3.91	-15.69	10,17,18,42 ^b
<i>n</i> -heptadecane	18	303-573	1	5.12	15.45	10,14 ^b
<i>n</i> -octadecane	24	303-408	1-1724	4.10	-10.28	10,16
<i>n</i> -eicosane	12	313-493	1	2.56	-4.84	10

				Deviation, %	
Fluid	Data no.	Temp range, K	pressure range, bar	AAD	MAX
Methane	466	91-511	1-680	2.40	-8.42

Figure 2-20: Comparison of calculated and experimental viscosity^[64] Figure 2-21: Comparison of calculated and experimental viscosity of methane^[64]

2.6.2.3 Thermal conductivity of dense methane

Table 2-5 and Figure 2-22 show the comparison of experimental and calculated thermal conductivities using Chung, et al.^[64] method for pure fluids at wide temperature and pressure ranges. In Table 2-5, the average absolute deviations (AAD) between the calculated and experimental values range between 1.9% and 5.1% for paraffins and 6.0% and 8.6% for aromatics. For polar and associating compounds such as chloroform, ammonia, and alcohols, the discrepancies vary between 3.3% and 8.3% AAD. The AAD and maximum deviation for methane are 2.90% and 24.11%, respectively. Chung, et al. suggested that the deviation in the predictions depends on the source of data. Because of the inherent difficulties involved in the measurement of thermal conductivity, it is quite common to have large discrepancies (5-15%) between data of different sources for the same fluid.

Table 2-5: Comparison of calculated and experimental thermal conductivities for pure fluids^[64]

fluid	data no.	temp range, K	pressure range, bar	deviation, %		ref ^a
				AAD	max	
methane	367	119-726	1-1247	2.90	24.11	1,2,3,14,19, ^b 20 ^b
ethane	196	199-800	1-1194	4.23	15.35	2,4,5,21 ^b
propane	152	112-444	1-674	4.30	-10.93	6,7,22 ^b
<i>n</i> -butane	76	277-444	1-345	4.12	-8.96	8,15, ^b 20 ^b
<i>n</i> -pentane	100	146-444	1-345	5.14	-10.93	9,10,15,16,22 ^b
<i>n</i> -hexane	171	273-633	1-500	4.92	11.59	10,16,22 ^b
<i>n</i> -heptane	175	192-633	1-500	3.85	-9.27	10,15,16,22, ^b 23 ^b
<i>n</i> -octane	171	273-633	1-500	2.41	-14.27	10,15,16,22, ^b 23 ^b
<i>n</i> -nonane	15	253-413	1	4.18	-7.20	10,16,22, ^b 23 ^b
<i>n</i> -decane	20	253-433	1	4.19	-6.51	10,16,22, ^b 23, ^b 24 ^b
<i>n</i> -dodecane	17	273-473	1	3.78	-13.64	10,16,25 ^b
<i>n</i> -tridecane	12	273-493	1	1.96	-6.16	10,26 ^b
<i>n</i> -tetradecane	12	293-513	1	3.79	-9.79	10,27, ^b 28 ^b
<i>n</i> -pentadecane	13	293-533	1	3.91	17.61	10,28 ^b
<i>n</i> -hexadecane	13	313-553	1	2.86	-8.55	10,29 ^b
<i>n</i> -heptadecane	14	313-573	1	3.16	-7.86	10,29 ^b
<i>n</i> -octadecane	14	313-573	1	3.67	6.02	10,29 ^b
<i>n</i> -eichosane	14	313-573	1	2.21	-6.10	10,30 ^b
isobutane	124	193-413	1-490	4.81	15.10	10,11 ^b
benzene	29	283-450	1-6	6.03	-13.85	10,16,23, ^b 31 ^b
toluene	13	193-373	1	8.58	-18.28	10,31 ^b
<i>o</i> -xylene	31	293-626	1-604	7.72	-13.61	10,31 ^b
<i>m</i> -xylene	64	293-615	1-600	8.06	-10.91	10,31 ^b
<i>p</i> -xylene	19	293-453	1-597	7.03	-9.52	10,16, ^b 23, ^b 31 ^b
nitrogen	60	298-348	6-1015	7.30	-16.20	3,17,18,32 ^b
oxygen	35	80-180	1-500	4.72	11.72	10,19 ^b

				Deviation, %	
Fluid	Data no.	Temp range, K	pressure range, bar	AAD	MAX
Methane	367	119-726	1-1247	2.90	24.11

Figure 2-22: Comparison of calculated and experimental thermal conductivity^[64]

2.6.2.4 Viscosity and thermal conductivity of Argon, Oxygen and Nitrogen

Several equations are currently available that calculate the transport properties of Argon, oxygen and Nitrogen. Viscosity and thermal conductivity correlations are available in the research of Stephan and Krauss^[65] for Nitrogen, Laesecke et al.^[66] for oxygen, Younglove and Hanley^[67] for Argon, and Younglove^[68] for all three fluids. However, Lemmon et al.^[69] provided a more accurate method to evaluate the transport property of gases. This method is a combination of theoretical models for the dilute gas and the thermal conductivity critical enhancement, and empirical equations for the residual contribution resulting from the interaction between molecules. Lemmon et al.'s equation for the dilute gas uses Chapman-Enskog theory with a collision integral fitted to experimental data. The critical enhancement uses the simplified crossover model of Olchowy and Sengers^[70]. The empirical equations for the residual contributions are similar to the terms used in typical Helmholtz energy equations of state^[71]. The number of terms was kept to a minimum to aid the extrapolation of the equations to low and high

temperatures and to high pressures and densities. The accuracy evaluation for Lemmon et al. correlations is presented in the simulation chapter 3.

2.6.2.5 Heat transfer coefficient

In heat transfer analysis between leaking Argon and surrounding metal around crack, the heat transfer coefficient is the key parameter to be evaluated. After a literature survey, Petukhov correlation was found to be suitable for the evaluation of the heat transfer in pipe. It is the one of the most accurate correlations for single-phase forced convection, which has a reported accuracy of ~ 5% and given by^[72]

$$\text{Nusselt number} \quad N_u = \frac{\left(\frac{f}{8}\right) Re Pr}{K + 12.7 \left(\frac{f}{8}\right)^{\frac{1}{2}} \left(Pr^{\frac{2}{3}} - 1\right)} \quad (2-8)$$

Figure 2-23 shows comparison between experimental and calculated heat transfer data using Petukhov correlation.

Figure 2-23: Comparison of Petukhov equation with experimental data on heat transfer to gases.

Nu_0 denotes values obtained from Petukhov equation, and Nu denotes experimental values

Note: o & ⊗: Nitrogen^[73], Δ & ▲: ammonia; ◇: air; □: air^[74], +: steam^[75], ∇: helium^[74].

Adams et al.^[76] have applied Petukhov correlation into microchannel after making some modifications. The microchannel in his paper means smaller diameter circular channels with diameters of 0.1–1.09 mm. In current research, the heat transfer occurred is in the crack, not in the pipe or circular channel. Therefore, some more modifications are given to try to apply Adams et al.'s theory to the crack.

2.7 Gas flowing through a crack

The crack tortuosity increases the distance or path length that the gas will have to travel. The natural cracked surface is rough leading to increase in friction. Both factors contribute to the effective friction in flow through the crack and results in loss of pressure. Chivers^[77] gave a model of gas flow through a crack based on a length and a friction factor. Bagshaw et al.^[78] and Rudland et al.^[79] have both recognized that the length of the flow path, incorporating the number of crack turns or deviations, are important factors. After comparison among different models^[77-81], Taggart et al.^[81] model is adopted in this research, which is a more physical model as more crack geometry parameters are considered and is supported by experimental data.

In general, the main uncertainty in the calculation of single phase flow (at least for a well-defined crack) seems to be the friction factor, and a large amount of the available references focus on this. For single phase flow, the program DAFTCAT is usually employed in the nuclear industry within the R6 framework. This program stands for flow through a crack of rectangular cross-section and applies approximations for diverging or converging crack.^[82, 83] For a totally rough flow, the friction factor presently applied was obtained from experiments employing rectangular slits with surfaces roughened by sand blasting by Button et al.^[84] and is given as a conventional friction factor

$$f = \left[2.25 \log_{10} \left(\frac{W_h}{R_a} \right) - 0.573 \right]^{-2} \quad (2-9)$$

where f is the conventional friction factor (four times the Fanning friction factor), W_h is the hydraulic radius (equal to half the hydraulic diameter or the full width of the crack), and R_a is the mean roughness (that is, mean deviation of the crack surface from its average level). Surface roughness is an important parameter affecting gas flow.^[85-87]

It was concluded for artificial flaws that the actual friction factor is usually determined by the relations due to Button et al.^[84] and Spence et al.^[88], depending on certain postulations about the relation between the surface roughness and the surface characteristics. The friction factor equation created by Spence et al. is

$$f = \left[1.82 \log_{10} \left(\frac{W_h}{R_a} \right) - 0.77 \right]^{-2} \quad (2-10)$$

The friction factor relations have not been confirmed for a very narrow crack (i.e. $f > 1$). It is considered that if $f > 1$, then f values of 1 and 4 should be applied to estimate uncertainties in flow rate, with a factor of uncertainty in the flow rates of up to 3.

The experiments on the water flow through an artificial macroscopic crack have been performed by Gardiner and Tyrrell^[89]. The derived friction factor was given by

$$f = \left[2.035 \log_{10} \left(\frac{W_h}{R_{glamp}} \right) + 0.568 \right]^{-2} \quad (2-11)$$

where R_{glamp} is the crack roughness (i.e., the peak-to-valley height of the roughness contours). Supposing $R_{glamp} = 4R_a$, the above equation can be also written as

$$f = \left[2.035 \log_{10} \left(\frac{W_h}{R_a} \right) - 0.657 \right]^{-2} \quad (2-12)$$

The experiments undertaken by Gardiner and Tyrrell were for incompressible flow; however, LBF cases in the nuclear industry usually involve compressible flow. Flow rates are calculated by Equation (2-12) are a little higher than the relation due to Spence et al. This implies that the relation due to Spence et al. (Equation (2-10)) is more conservative in the context of LBF.

Chivers et al.^[90] have studied the various friction factor relations, which are shown in Figure 2-24.^[90] The Von Karman version of Nikuradse's relation, obtained from experiments in artificially roughened pipes, which is similar to that of Button et al., and that due to scaled results from Gardiner and Tyrrell are also given.^[84, 89, 91] The relation applied for two phase flow in the program SQUIRT is also given for comparison, which gives a slightly lower friction factors (that is, higher values of $1/\sqrt{f}$) than the other relations.

Figure 2-24: $1/\sqrt{\lambda}$ versus $\log_{10}(W/R_a)$ for various friction factor relations

Note: In Figure 2-24, λ = friction factor (f), W = hydraulic radius (W_h)^[90]

Spence et al. have commented on the validity of the hydraulic diameter concept for crack, which may deserve further study for some cases, though its use could be valid.^[88] Clarke et al. found that the flow in a narrow crack does not match up to the predictions made on the same basis as those for a wider crack.^[78] They verified this point by carrying out experiments for crack less than about 50 μm in width. Rudland et al.^[92] also illustrated a crack morphology model, which explains the crack width in defining the flow pattern, and consequently, the friction factor, for turbulent two phase flow. They found that the required crack length for a known leakage rate changed by up to a factor of about 2, due to variations in the treatment of roughness.

A model is described by Chivers^[77] for leak rate through a crack based on a friction factor and a length. The factor was calculated from an empirical relationship obtained from experiments on roughened plates. Two flow regions (one laminar and one turbulent) were recognized and were explained using the friction factor. The crack tortuosity was accounted for

by changing its length. Bagshaw et al.^[78] and Rudland et al.^[79] have both found that the length of the flow path, including the number of turns or deviations, are main factors. This extra path length is auxiliary to conventional measurements of surface roughness and crack morphology.

CHAPTER 3 MODELLING AND SIMULATION

3.1 Introduction

This chapter introduces the modelling and simulation of heat transfer of high pressure gas leaking through a narrow tortuous crack considering the Joule-Thomson effect. The appropriate gas of Argon for the study of the Joule-Thomson effect during leaking in a pressure vessel is selected to substitute the principal composition of compressed natural gas (methane) for safety considerations. A reasonable crack model is built to calculate the pressure loss and flow rate of leaking gas through a narrow tortuous crack. A new method is provided to apply the theory of the Joule-Thomson effect into leaking gas flowing through a narrow crack. RK (Redlich-Kwong) equation with high accuracy is adopted to evaluate the density and temperature change during gas leaking through the crack. Lemmon et al.^[69] method is employed to evaluate the viscosity and thermal conductivity of Argon. In heat transfer analysis, the most important parameter, heat transfer coefficient, is calculated by employing a modified Petukhov^[72] correlation. The Petukhov correlation is modified by Adams et al.^[76] to accommodate the small diameters encountered in microchannels. In this research, more modifications are presented to apply the Petukhov correlation to a narrow crack. A MATLAB program is used to calculate the properties of leaking gas in crack as input parameters for the simulation. The temperature distribution of metal in the vicinity of crack is simulated using the COMSOL program.

3.2 Simulation methodology

- a) Methane is the principal composition of compressed natural gas (CNG). However, methane is a flammable gas and is not a safe gas for experimental work. Therefore, the first step is to find another gas with a similar Joule-Thomson effect to substitute methane;
- b) Build a crack model to perform the calculation of pressure loss and flow rate of leaking gas through the crack;
- c) The temperature and heat transfer coefficient of leaking gas through a narrow crack considering the Joule-Thomson cooling effect is calculated using a MATLAB

program to assist the heat transfer simulation between leaking gas and metal in the vicinity of the crack in the COMSOL program. Firstly, the physical properties and parameters of leaking gas through the crack are calculated using a MATLAB program. Secondly, based on the MATLAB calculation results, the metal temperature around the crack is simulated by employing the heat transfer module of the COMSOL program.

3.3 Gas selection

Methane is the principal composition of compressed natural gas (CNG). However, methane is a flammable gas. It is dangerous to perform Joule-Thomson experiments using methane. Therefore, it is necessary to find a substitution.

In thermodynamics, the Joule-Thomson effect describes the temperature change of a gas or liquid when it is forced through a porous plug when kept insulated. As a result, no heat is exchanged with the environment.^[16-18] This procedure is called a Joule-Thomson process or throttling process.^[21] The temperature change with the pressure drop in a Joule-Thomson process is the Joule-Thomson coefficient:^[16, 18, 53] The key to study Joule-Thomson effect is the Joule-Thomson coefficient given by

$$\mu_{JT} = \left(\frac{\partial T}{\partial P} \right)_H \quad (3-1)$$

where μ_{JT} is in K/Pa or °C/bar.

In Equation (3-1), the change of temperature (T) will become larger at the same decrease of pressure (p) when the Joule-Thomson coefficient μ_{JT} has a larger value. Table 3-1 shows the value of Joule-Thomson coefficient of different gases.

From Figure 3-1, it can be found that Argon has the maximum value of Joule-Thomson coefficient (about 0.29 °C/bar). As methane is a flammable gas, Argon is a suitable gas to be used in Joule-Thomson experiments to substitute methane for safety considerations. Both gases have similar values of the Joule-Thomson coefficient (Argon: 0.29 °C/bar, methane: 0.28 °C/bar), so the Joule-Thomson effect will be similar. Therefore, Argon is selected as the gas for simulation and experiment in this research.

Table 3-1: Joule-Thomson coefficient of different gases

Gases		μ_{JT} (°C/bar) (At temperature $T \approx 25$ °C, pressure $p \approx 100$ bar)
Carbon dioxide (CO ₂)		0.1005 ^[93] (Table VIII in Ref ^[93])
Argon (Ar)		0.29 ^[56] (Fig.3 in Ref ^[56])
Helium (He)		-0.06 ^[94] (Fig. 7 in Ref ^[94])
Air		0.152 ^[95] (Table II in Ref ^[95])
Methane (CH ₄) + Nitrogen (N ₂) ^[96]	100 percent CH ₄	0.28
	75 percent CH ₄ + 25 percent N ₂	0.25
	50 percent CH ₄ + 50 percent N ₂	0.21
	25 percent CH ₄ + 75 percent N ₂	0.17
	100 percent N ₂	0.14

Figure 3-1: Joule-Thomson coefficient of different gases

3.4 MATLAB calculation flow chart for the properties of leaking Argon through a crack

In order to determine the temperature and heat transfer coefficient of the gas at different depths into the crack, the crack is divided into many equivalent increments along the crack depth direction. As the calculation results in MATLAB are not sensitive to the number of increments, the crack surface is divided into 50 increments along the through-thickness direction. For each small increment, the gas properties inside the crack are evaluated according to the flow chart as shown in Figure 3-2. The detailed description of crack parameters is shown in section 3.6.1: Characterization of a crack. Repeating the calculation procedure, all gas properties along the crack can be obtained. The final step is to apply the calculated temperature and heat transfer coefficient to the FEA model to simulate the metal temperature around the crack. Table 3-2 shows the initial state parameters of Argon and crack geometry parameters. The MATLAB code is given in Appendix I.

Figure 3-2: Calculation Flow Chart in MATLAB Program (continued)

Figure 3-2: Calculation Flow Chart in MATLAB Program

Table 3-2: Initial state parameters of gas and crack geometry parameters

Input parameters	Description	Values (Refer to experiment data)
p_0	Initial gas pressure inside the vessel	91 bar
T_0	Initial gas temperature inside the vessel	30 °C
ρ_0	Initial gas density inside a vessel	149.93 kg/m ³
W_c	Crack width	0.25 mm
R_{global}	Global roughness	38.05 µm
α	Crack surface angle	$\pi/6$
t	Crack depth	18 mm

3.5 Modelling the J-T effect in a crack

In a real crack, the flow path often deviates from the plane surface and is three dimensional, this is known as tortuosity. Tortuosity increases the distance or path length that the gas will have to travel as illustrated in Figure 3-3. Beck et al.^[80] pointed out that the macroscopic tortuosity, as the crack path wanders (as shown in (a) and (c) of Figure 3-3), is much less significant than the microscopic tortuosity arising from the fracture process, provided that the crack faces remain coincident. Therefore, the planar crack model (b) is selected in this research.

Figure 3-3: Possible fracture surfaces where sawtooth peaks and valleys represented the roughness and tortuosity is represented by bends in the crack paths (a) with one bend, (b) planar without bends and (c) with multiple bends.

To apply Joule-Thomson theory into the above planar crack model, it is assumed that the crack can be divided into many short and equivalent parts along the through-wall direction as shown in Figure 3-4. Each part of the crack can be treated as a throttling device which can be solved by the Joule-Thomson theory.

Figure 3-4: A model of a crack divided into many equivalent parts

In addition, the Joule-Thomson expansion can be treated as an adiabatic process. An adiabatic process is any process occurring without input or output of heat within a system (i.e. the system is thermodynamically insulated during the process; there is no heat transfer with the surroundings). Many rapid chemical and physical processes are described or approximated in this way. Such processes are usually followed or preceded by events that do involve heat transfer (i.e. are non-adiabatic). Adiabatic processes can occur if the container of the system has thermally-insulated walls or the process happens in an extremely short time (e.g. Joule-Thomson expansion), so that there is no opportunity for significant heat exchange. No process is truly adiabatic, but a transformation of a thermodynamic system can be considered adiabatic when it is quick enough such that no significant heat is transferred between the system and the outside.^[97] In the Joule-Thomson expansion, the expansion of the high pressure gas is so rapid that the results can be approximated by describing this process as adiabatic, even though in fact heat is transferred between the environment and the gas as the gas warms up. For an adiabatic process, the amount of work done by the gas is equal to the change in its internal energy.

More specifically, molecules in the surrounding air and atoms of the metal of the pressure wall collide with molecules of the cold leaking gas, transferring energy to it and causing it to gradually warm up. The metal of the pressure vessel wall is an excellent conductor of heat, so it can rapidly transfer heat to the leaking gas. That means the metal is rapidly losing heat to the leaking gas. The leaking gas escapes quickly through the crack to outside the pressure vessel by carrying the heat absorbed from the surrounding metal. Then the new gas will come to the crack from the gas cylinder with same temperature. Gradually, the metal temperature around the crack will drop and approach the temperature of the cold leaking gas. That is to say, the metal will be cooled by the escaping gases in the crack due to the Joule-Thomson cooling effect only if there is enough high pressure gas supply in the cylinder. The continuous high pressure gas supply just acts as “cooling sources” to maintain the low temperature of the gas leaking through the crack.

The warming effect from the metal to the gas in the crack depends on the temperature difference between them. It will become negligible when the metal temperature approaches the gas temperature. However, the cooling effect from the gas to the surrounding metal will continue as long as there is enough supply of high pressure gas.

3.6 Evaluation of pressure drop and flow rate of leaking Argon through a crack

3.6.1 Characterization of a crack

Taggart et al.^[81] model is adopted in this research, which is a more physical model as more crack geometry parameters are considered and is supported by experimental data. In the crack model, turbulent flow is assumed as a default, where flow occurs from the pressurized vessel to the atmosphere. Three different flow patterns are proposed in the model, based on the ratio of the crack width relative to the roughness amplitude, that is, the mean overall height (peak-to-trough) of the contours of the crack.

A three dimensional diagram of a through-wall crack in a plate is shown in Figure 3-5. If a crack is very narrow, whose width is much less than the roughness amplitude, the overall flow tends to follow the global roughness curve. This is illustrated schematically in Figure 3-6 (a). For this flow pattern, the effective crack is the path following the roughness contours, and the effective roughness becomes the local roughness, which can be considered superimposed on the crack contours. For a wide crack, where the crack width is much greater than the roughness amplitude, the overall flow tends to bypass the global roughness contours and goes straight through the crack, as illustrated in Figure 3-6 (b). For this flow pattern, the effective roughness is equivalent to the global roughness. For a crack of intermediate width, the flow pattern tends to be intermediate between the flow patterns for narrow and wide crack. The effective roughness for this flow pattern lies between the local and global values.

The following accounts for the meaning of all parameters in Figure 3-6. α is the crack surface angle relative to the crack direction through wall, θ is the average flow direction relative to the crack direction through-wall, W_{ceff} is the effective crack width perpendicular to the average flow direction, W_c is the crack opening displacement (or crack width) perpendicular to the

through-wall direction, t is the crack through-wall thickness, t_{eff} is the effective crack through-wall thickness, R_{local} is the local roughness, R_{global} is the global roughness, and R_{glamp} is the peak-to-trough amplitude of the global roughness contours for a sawtooth geometry, equal to four times the global roughness R_{global} .

Figure 3-5: Diagram of a crack in a plate

Figure 3-6: (a) Schematic of flow around two crack turns: crack width much less than roughness amplitude ($W_c < R_{\text{glamp}}$).

Figure 3-6: (b) Schematic of flow around several crack turns: crack width much greater than roughness amplitude ($W_c > R_{glamp}$).

The effective roughness of the crack R_{eff} is given by

$$R_{eff} = R_{local} + c(R_{global} - R_{local}) \quad (3-2)$$

In Equation (3-2), c is a linear interpolant, given by the ratio of the crack width to the global roughness amplitude, relative to two constants, r_1 and r_2 , which denote the upper limit of the narrow crack regime and the lower limit of the wide crack regime respectively, as follows:

$$\frac{W_c}{R_{global}} < r_1, \quad c = 0.0 \quad (3-3)$$

$$r_1 < \frac{W_c}{R_{global}} < r_2, \quad c = \frac{\frac{W_c}{R_{global}} - r_1}{r_2 - r_1} \quad (3-4)$$

$$\frac{W_c}{R_{global}} > r_2, \quad c = 1.0 \quad (3-5)$$

The upper limit of the narrow crack regime (r_1) was assumed to be 0.1, based on a value used by Rudland et al.^[92] The lower limit of the wide crack regime (r_2) was assumed to be 2.0,

based on experiments performed by Bagshaw et al.^[98] In these experiments, the flow of air through narrow artificial crack was observed, and found to approach the flow pattern in Figure 3-6 (b) when the crack width was about twice the roughness amplitude.

A similar interpolation to that in Equation (3-2) is performed for the angle denoting the average direction of the flow:

$$\theta = \alpha(1 - 0.9c) \quad (3-6)$$

3.6.2 Calculation of pressure drop of leaking gas through a crack

Fluid is forced through a crack by a pressure gradient existing across the wall of a pressure vessel during leakage. The pressure dissipation through the crack depends on the flow geometry and effective roughness. The pressure is lost through the crack by three means^[80, 81]: friction with crack surface, inertia pressure and the recirculation of the gas, as shown in Equation (3-7):

$$\Delta p = \Delta p_{\text{fric}} + \Delta p_{\text{inert}} + \Delta p_{\text{recirc}} \quad (3-7)$$

where p_{fric} is the frictional term, which is calculated from the friction factor using

$$\Delta p_{\text{fric}} = \frac{\rho v^2}{2} \frac{f t_{\text{eff}}}{2W_{\text{ceff}}} \quad (3-8)$$

In Equation (3-8), ρ is the fluid density, v is mean leak velocity of the fluid through crack, f is the crack friction factor, t_{eff} is the effective crack through-wall thickness, W_{ceff} is the effective crack width perpendicular to the average flow direction. For the calculation of the crack friction factor f , the method of Spence et al.^[88] gave better agreement with measured results than the use of the relation due to Button et al.^[81] Therefore, the method of Spence et al.^[88] is adopted to calculate the crack friction factor f in the research and is given as

$$f = \left[1.82 \log_{10} \left(\frac{W_{\text{ceff}}}{R_{\text{eff}}} \right) - 0.77 \right]^{-2} \quad (3-9)$$

Forces act on the fluid bodies when the flow is undergoing accelerations. These forces are associated with a pressure gradient for which the difference is sometimes known as the inertia

pressure. In this case, the effect of inertia pressure loss within the idealized crack arises due to the fluid accelerating around the corners of the crack asperities. Equation (3-10) describes the inertia pressure loss.

$$\Delta p_{\text{inert}} = \frac{\rho v^2}{2} \frac{2N\theta W_{\text{ceff}}}{W_c} \quad (3-10)$$

In Equation (3-10), N is the actual number of turns in the crack, and θ is the average flow direction relative to the crack direction through-wall.

The tortuosity of the zig-zag crack profiles may result in flow separation from the surfaces of the crack. Vortices are created by some of the fluid flowing into the regions of low pressure created by this separation, and the fluid behavior become turbulent in these regions. The flow is at a lower pressure than in the main flow path in these regions. The flow is recirculated producing eddies. This effect can be estimated by the recirculation term in pressure loss, and is given by

$$\Delta p_{\text{recirc}} = \frac{\rho v^2}{2} \left(1 - \left(\frac{W_{\text{ceff}}}{W_c}\right)^2\right) \quad (3-11)$$

3.6.3 Flow rate evaluation of leaking gas through a crack

The mass flow rate can be expressed as

$$Q = C_D (p\rho)^{\frac{1}{2}} W_c L \quad (3-12)$$

where, p is the fluid pressure inside the vessel.

ρ is the fluid density inside the vessel

W_c is the mean width of a crack

L is the a crack length

C_D is the discharge coefficient, and given by

$$C_D = \frac{1}{1+\sqrt{F}} \quad (3-13)$$

where F is the sum of normalized pressure loss terms due to frictional, inertial, and recirculation effects, and is given by^[81]

$$F = F_{\text{fric}} + F_{\text{inert}} + F_{\text{recirc}} \quad (3-14)$$

where F_{fric} is the frictional term, F_{inert} is the inertial term, and F_{recirc} is the recirculation term, all of which are defined below.

$$F_{\text{fric}} = \frac{f t_{\text{eff}}}{2W_{\text{ceff}}} \quad (3-15)$$

$$F_{\text{inert}} = \frac{2N\theta W_{\text{ceff}}}{W_c} \quad (3-16)$$

$$F_{\text{recirc}} = 1 - \left(\frac{W_{\text{ceff}}}{W_c} \right)^2 \quad (3-17)$$

Then flow velocity can be obtained as follows

$$v = \frac{Q}{\rho A} \quad (3-18)$$

where ρ is the fluid density, kg/m³,

A is the cross-section area of a crack.

3.6.4 The results of evaluation for the pressure and velocity of leaking gas through a crack

The initial input values of the parameters in the MATLAB program for the calculation of the pressure and velocity of leaking Argon through the crack are shown in Table 3-3. The calculation results in MATLAB are not sensitive to the value of crack surface angle (α). Therefore, the value $\pi/6$ from Beck et al.^[80] is selected as the crack surface angle. Beck et al.^[80] concluded that comparison with experimental results indicates that in the absence of proper measurement, the value of $\pi/6$ for crack surface angle is reasonable.

Table 3-3: Initial input values of parameters in MATLAB program for the calculation of the pressure and velocity of leaking Argon through crack

Input parameters	Description	Values
P_0	Maximum pressure of Argon inside pressure vessel	91 bar
T_0	Initial temperature of Argon inside pressure vessel	30 °C
R	Gas constant of Argon	208 J/ kg·K
T_c	Critical temperature	150.86 K ^[62]
p_c	Critical pressure	48.98 bar ^[62]
t	Length of one increment along the crack depth in the experiment of this research (total increment: 50)	0.36 mm
W_c	Crack width in the experiment of this research	0.25 mm
R_{global}	Global roughness of crack surface in the experiment of this research	38.05 µm
α	Crack surface angle (refer to Beck et al. paper ^[80])	$\pi/6$

Figure 3-7 and Figure 3-8 present the pressure and velocity of leaking Argon through a crack, respectively. It is indicated that both the pressure and velocity of leaking Argon will decrease along the crack through-wall position from the inside to the outside pressure vessel. As is evident from Figure 3-7, the pressure of leaking Argon drops from 91 bar at the entrance of the crack to 9.5 bar at the exit of the crack. The pressure of 91 bar is the maximum value of the pressure reached inside pressure vessel during this experimental test. The total pressure drop of leaking Argon through the crack is 81.5 bar. As illustrated in Figure 3-8, the velocity of leaking Argon through the crack does not change much. The velocity of leaking Argon drops from 36.7 m/s at the entrance of the crack to 35.4 m/s at the exit of the crack. The average velocity of leaking Argon through the crack is 36 m/s.

Figure 3-7: The pressure of leaking Argon through a crack

Figure 3-8: The velocity of leaking Argon through a crack

3.7 Evaluation of the density and temperature drop of leaking Argon through a crack

3.7.1 Evaluation of the density of leaking gas through a crack

Among different real gas state equations, RK (Redlich-Kwong) equation^[58-61] with high accuracy is adopted and was given,

$$p = \frac{RT}{\tilde{v} - b'} - \frac{a'}{\tilde{v}(\tilde{v} + b')T^{0.5}} \quad (3-19)$$

where R is the specific gas constant, J/(kg · K).

$\tilde{v}$ is the specific volume (which is the reciprocal of density), m³/kg.

a' and b' are constants,

$$a' = 0.4278 \frac{R^2 T_c^{2.5}}{p_c} \quad (3-20)$$

$$b' = 0.0867 \frac{RT_c}{p_c} \quad (3-21)$$

where T_c and p_c are critical temperature and pressure, respectively,

Then the gas density can be solved as follows:

Equation (3-19) can be transformed into the standard form of the cubic equation

$$a\tilde{v}^3 + b\tilde{v}^2 + c\tilde{v} + d = 0$$

where $\tilde{v}$ is the specific volume (which is the reciprocal of density) in m³/kg

a , b , c and d are coefficients with the expressions:

$$a = pT^{0.5}$$

$$b = -RT^{1.5}$$

$$c = \frac{0.42748R^2T_c^{2.5}}{p_c} - pT^{0.5} \times \left(\frac{0.08664RT_c}{p_c} \right)^2 - \frac{0.08664R^2T^{1.5}T_c}{p_c}$$

$$d = - \frac{0.037R^3T_c^{3.5}}{p_c^2}$$

The specific volume $\bar{v}$ can be obtained after solving the cubic equation^[99]:

$$\bar{v} = -\frac{b}{3a} + \frac{1}{3a\sqrt[3]{2}} \left(-2b^3 + 9abc - 27a^2d + \sqrt{4(3ac - b^2)^3 + (-2b^3 + 9abc - 27a^2d)^2} \right)^{\frac{1}{3}}$$

$$- \frac{\sqrt[3]{2}(3ac - b^2)}{3a \left(-2b^3 + 9abc - 27a^2d + \sqrt{4(3ac - b^2)^3 + (-2b^3 + 9abc - 27a^2d)^2} \right)^{\frac{1}{3}}}$$

Then the density can be obtained:

$$\rho = \frac{1}{\bar{v}}$$

Figure 3-9 and Figure 3-10 show the accuracy of the method of calculating Argon density. AGA8 report (American Gas Association Report No. 8) is currently the industry standard to predict the density and compressibility factor of different gases with an acceptable accuracy.

It can be concluded that there is a good agreement between the calculated results of AGA8 report and R-K equation of state. Therefore, the R-K equation of state is selected to calculate the gas density in this research.

For Argon, specific gas constant, $R = 208 \text{ J/(kg}\cdot\text{K)}$; Molar mass, $M = 39.948 \text{ g/mol}$; Critical volume, $V_c = 74.57 \text{ cm}^3/\text{mol}$; Critical pressure, $p_c = 48.98 \text{ bar}$; Critical temperature, $T_c = 150.86 \text{ K}$.

Figure 3-9: Argon's density (ρ) vs. temperature (T)

Note: ★: calculated data using the R-K equation ^[58]; ■: calculated data using AGA8 state equation ^[100, 101]

Figure 3-10: Argon's density (ρ) vs. pressure (p)

★: calculated data using the R-K equation, refer to ^[58]; ■: calculated data using AGA8 state equation, refer to ^[100, 101]

3.7.2 Evaluation of the temperature drop of leaking gas through a crack

In thermodynamics, the differential equation of enthalpy is

$$dh = c_p dT + \left[v - T \left(\frac{\partial v}{\partial T} \right)_p \right] dp \quad (3-22)$$

as $dh = 0$, we can obtain

$$\mu_{JT} = \frac{dT}{dp} = \frac{1}{c_p} \left[T \left(\frac{\partial v}{\partial T} \right)_p - v \right] \quad (3-23)$$

then the expression of the J-T coefficient μ_{JT} can be obtained as follows

$$\mu_{JT} = \frac{1}{c_p} \left[\frac{T}{\rho^2} \left(\frac{\partial p}{\partial T} \right)_\rho - \frac{1}{\rho} \right] \quad (3-24)$$

Partial derivatives $\left(\frac{\partial p}{\partial T} \right)_\rho$ and $\left(\frac{\partial p}{\partial \rho} \right)_T$ in Equation (3-23) can be derived from the R-K equation, and then the expression of the J-T coefficient μ_{JT} can be obtained and given by:

$$\mu_{JT} = \frac{1}{c_p} \left[\frac{RT^2(v^2 + vb')^2(v-b') + 0.5a'T^{0.5}(v^2 + vb')(v-b')^2}{RT^2(v^2 + vb')^2 - a'T^{0.5}(2v + b')(v-b')^2} - v \right] \quad (3-25)$$

where

$$c_p = \frac{a_0 + a_1T + a_2T^2 + a_3T^3}{M} \quad (3-26)$$

a_0, a_1, a_2, a_3 are empirical constants of gas property dependence, and M is molar mass, g/mol.

Then the temperature drop of the gases can be obtained by employing numerical integrals (using the trapezoidal integration of the MATLAB program) after substituting the formula (3-25) into the definition formula of μ_{JT} , as follows:

$$\Delta T = \int_{p_1}^{p_2} \mu_{JT} dp \quad (3-27)$$

Figure 3-11 and Figure 3-12 show the accuracy of the calculation method of J-T coefficient of Argon:

Figure 3-11: Argon's Joule-Thomson coefficient (μ_{JT}) vs. temperature (T)

Note: ★: calculated data using the R-K equation, refer to^[58]; ■: experiment data of Roebuck's paper, refer to^[56]

Figure 3-12: Argon's Joule-Thomson coefficient (μ_{JT}) vs. pressure (p)

Note: ★: calculated data using the R-K equation, refer to^[58]; ■: experiment data of Roebuck's paper, refer to^[56]

3.7.3 The results of the evaluation for the density and temperature drops of leaking Argon through a crack

The initial input values of parameters of parameters in the MATLAB program for the calculation of the density and temperature drop of leaking Argon through crack are shown in Table 3-4.

Table 3-4: Initial input values of parameters in MATLAB program for the calculation of the density and temperature drop of leaking Argon through crack

Input parameters	Description	Values
p_0	Maximum pressure of Argon inside pressure vessel	91 bar
T_0	Initial temperature of Argon inside pressure vessel	30 °C
R	Gas constant of Argon	208 J/ kg·K
T_c	Critical temperature	150.86 K ^[62]
p_c	Critical pressure	48.98 bar ^[62]

The density and temperature drop of leaking Argon through a crack are illustrated in Figure 3-13 and Figure 3-14, respectively. It is noticed that both the density and temperature drop of leaking Argon will decrease along the crack through-wall position from the inside to the outside of the pressure vessel. As is evident from Figure 3-13, the density of leaking Argon drops from 150.7 kg/m³ at the entrance of the crack to 16.8 kg/m³ at the exit of the crack. The density of 150.7 kg/m³ is the density value corresponding to the initial room temperature and the maximum pressure (91 bar) reached inside the pressure vessel during this experimental test. The total density drop of leaking Argon through the crack is 133.9 kg/m³. As shown in Figure 3-14, the temperature of leaking Argon decreases from 30 °C at the entrance of the crack to -0.04 °C at the exit of the crack. The total temperature drop of leaking Argon through the crack is 30 °C.

Figure 3-13: The density of leaking Argon through a crack

Figure 3-14: The temperature of leaking Argon through a crack

3.8 The viscosity of Argon

3.8.1 Accuracy assessment of the viscosity formula for Argon

Lemmon et al.^[69] method is employed to evaluate Argon viscosity here. Table 3-5 shows the sources of experimental data, the temperature, pressure, and density ranges, the number of points, and the average absolute deviations (AAD) between the experimental data and calculated data using Lemmon et al.'s equations.

Table 3-5: Summary of experimental data of Argon viscosity and comparisons with the equations

Author	No. Points	Temperature range (K)	Pressure range (MPa)	Density range (mol · dm ⁻³)	AAD (%)
Yorizane et al. (1983) [285]	28	299–323	0.1–15	0.03–5.9	0.74
Zheng et al. (1984) [287]	18	298	0.1–15.6	0.04–6.11	0.87
Ziebland and Burton (1958) [289]	86	80.7–203	0.1–13.6	0.06–28.5	3.54
Ziebland and Marsh (1977) [290]	41	80–1400	0.1	Dilute Gas	0.85
Argon-viscosity					
Abachi et al. (1980) [27]	18	83.8–90	0.06–0.13	34.5–35.5	2.09
Baharudin et al. (1975) [34]	6	85.7–110	0.08–0.64	31.2–35.2	5.43
Bonilla et al. (1951) [38]	25	200–2500	0.1	Dilute Gas	4.84
Boon and Thomaes (1963) [39]	6	84–89	0.07–0.12	34.7–35.4	1.06
Boon et al. (1967) [40]	6	84–89	0.07–0.12	34.7–35.4	0.50
Clarke and Smith (1968) [52]	12	114–375	0.1	Dilute Gas	0.52
Clifford et al. (1975) [56]	9	321–1300	0.1	Dilute Gas	0.51
Dawe and Smith (1970) [58]	44	292–1530	0.1	Dilute Gas	0.66
de Bock et al. (1967) [59]	19	90	0.13–13.5	34.5–35.5	2.39
de Bock et al. (1967) [60]	72	88.5–140	0.39–19.6	24–36	4.71
De Rocco and Halford (1958) [63]	20	211–471	0.1	Dilute Gas	0.65
DiPippo and Kestin (1968) [66]	23	297–575	0.03–0.17	Dilute Gas	0.43
DiPippo et al. (1968) [68]	10	293–303	0.1–2.34	0.04–0.96	0.13
Evers et al. (2002) [71]	81	233–523	0.09–28.1	0.02–6.07	0.23
Filippova and Ishkin (1959) [73]	31	90.2–273	0.09–14.7	0.04–35.5	6.30
Filippova and Ishkin (1962) [74]	52	90.2–273	3.6–15.3	1.78–35.5	10.2
Flynn et al. (1963) [76]	27	195–373	2.92–18.8	1.2–17.4	0.23
Forster (1963) [77]	8	85.4–114	0.08–0.84	30.4–35.2	3.48
Michels et al. (1954) [189]	96	273–348	0.92–202	0.41–28.9	0.25

Note: The pressure and temperature range used in the experimental part of this research is covered by that of the highlighted data in the table.

From Table 3-5, it can be noticed that Lemmon et al. method is a relatively accurate one in evaluating the viscosity of Argon. Therefore, Lemmon et al. method is selected to evaluate Argon viscosity in this research.

3.8.2 Evaluation procedure of the viscosity

The viscosity of Argon using the equations of Lemmon et al. is expressed as,

$$\eta = \eta^0(T) + \eta^r(\tau, \delta) \quad (3-28)$$

where η is the viscosity in $\mu\text{Pa}\cdot\text{s}$,

η^0 is the dilute gas viscosity,

η^r is the residual fluid viscosity.

Figure 3-15 and Figure 3-16 show the comparison between the calculated viscosity of Argon using the equations of Lemmon and experimental data. The viscosity of Argon will increase with the rising pressure or temperature. It can be concluded that there is a good agreement between experimental data and the calculated viscosity of Argon using the equations of Lemmon. Therefore, Lemmon's equations are selected to calculate the gas viscosity in this research.

Figure 3-15: Argon viscosity (η) vs. pressure (p) at the temperature of 25 °C

Note: ★: calculated data using the equations in Lemmon's paper^[69]; ■: experiment data in Flynn's paper^[102]; ●: experiment data in Michels' paper^[103]

Figure 3-16: Argon viscosity (η) vs. temperature (T) at the pressure of 80 bar

Note: ★: calculated data using the equations in Lemmon's paper^[69]; ●: experiment data in Flynn's paper^[102]; ▲: experiment data in Michels' paper^[103]

3.8.2.1 Dilute gas viscosity

The dilute gas viscosity is given by

$$\eta^0(T) = \frac{0.0266958\sqrt{MT}}{\sigma^2\Omega(T^*)} \quad (3-29)$$

where M is the molar mass in g/mol

T is the gas temperature in K

σ is the Lennard-Jones size parameter

$\Omega(T^*)$ is the collision integral

$$T^* = \frac{T}{\varepsilon/k}$$

ε/k is the Lennard-Jones energy parameter (shown in Table 3-6).

The property values of Argon are shown in Table 3-6.

Table 3-6: Property values of Argon^[69, 104, 105]

Property values of Argon	Value
Specific gas constant, R	208 J/(kg·K)
Molar mass, M	39.948 g/mol
Critical volume, V_c	74.57 cm ³ /mol
Critical pressure, p_c	48.98 bar
Critical temperature, T_c	150.86 K
Critical density, ρ_c	531 kg/m ³
Lennard-Jones energy parameter, ε/k	143.2 K
Lennard-Jones size parameter, σ	0.335 nm

The collision integral $\Omega(T^*)$ is given by

$$\Omega(T^*) = \exp\left(\sum_{i=0}^4 b_i [\ln(T^*)]^i\right) \quad (3-30)$$

The coefficients b_i are given in Table 3-7.

Table 3-7: Coefficients of the Collision Integral Equation

i	b_i
0	0.431
1	-0.4623
2	0.08406
3	0.005341
4	-0.00331

Figure 3-17 shows the relationship between collision integral ($\Omega(T^*)$) and temperature (T). The collision integral ($\Omega(T^*)$) will decrease as the rising temperature.

Figure 3-17: Collision integral ($\Omega(T^*)$) vs. temperature (T)

Figure 3-18 shows the comparison between the calculated viscosity of dilute Argon using the equations of Lemmon and experimental data. The viscosity of dilute Argon will increase with the rising temperature. It can be concluded that there is a good agreement between experimental data and the calculated viscosity of dilute Argon using the equations of Lemmon.

Figure 3-18: Dilute Argon viscosity (η^0) vs. temperature (T)^[69, 106, 107]

Note: ★: calculated data using the equations in Lemmon's paper^[69]; ●: experiment data in De Rocco's paper^[106]; ▲: experiment data in Johnston's paper^[107]

3.8.2.2 Residual fluid viscosity

The residual fluid contribution to the viscosity is given (in $\mu\text{Pa}\cdot\text{s}$) by

$$\eta^r(\tau, \delta) = \sum_{i=1}^n N_i \tau^{t_i} \delta^{d_i} \exp(-\gamma_i \delta^{l_i}) \quad (3-31)$$

where $\tau = T_c/T$, $\delta = \rho/\rho_c$

T_c is the critical temperature

ρ_c is the critical density

γ_i is zero when l_i is zero and one when l_i is not zero

Table 3-8 shows the coefficients and exponents of the residual fluid viscosity equations (for Argon).

Table 3-8: Coefficients and exponents of the residual fluid viscosity equations (for Argon)

i	N_i	t_i	d_i	l_i
1	12.19	0.42	1	0
2	13.99	0.0	2	0
3	0.005027	0.95	10	0
4	-18.93	0.5	5	2
5	-6.698	0.9	1	4
6	-3.827	0.8	2	4

Figure 3-19 and Figure 3-20 show the relationship between the calculated residual fluid viscosity of Argon using the equations of Lemmon and pressure & temperature, respectively. The residual fluid viscosity of Argon will increase with the rising pressure, and it will decrease with the rising temperature.

Figure 3-19: Argon residual fluid viscosity (η^r) vs. pressure (p) at the temperature of 25 °C

Figure 3-20: Argon residual fluid viscosity (η^r) vs. temperature (T) at the pressure of 80 bar

3.8.3 The evaluation results for the viscosity of leaking Argon through crack

The initial input values of parameters in the MATLAB program for the calculation of the viscosity of leaking Argon through the crack are shown in Table 3-9.

Table 3-9: Initial input values of parameters in MATLAB program for the calculation of the viscosity of leaking Argon through crack

Input parameters	Description	Values
p_0	Maximum pressure of Argon inside pressure vessel	91 bar
T_0	Initial temperature of Argon inside pressure vessel	30 °C
R	Gas constant of Argon	208 J/ kg·K
T_c	Critical temperature	150.86 K ^[62]
p_c	Critical pressure	48.98 bar ^[62]
M	Molar mass	39.948 g/mol ^[69]
ρ_c	Critical density	531 kg/m ^{3[69]}
ε/k	Lennard-Jones energy parameter	143.2 K ^[69]
σ	Lennard-Jones size parameter	0.335 nm ^[69]

The viscosity of leaking Argon through a crack is presented in Figure 3-21. It is noticed that the viscosity of leaking Argon will decrease along the crack through-wall position from the inside to the outside of the pressure vessel. As indicated in Figure 3-21, the viscosity of leaking Argon decreases from 2.5×10^{-5} Pa·s at the entrance of the crack to 2.1×10^{-5} Pa·s at the exit of the crack. The viscosity of 2.5×10^{-5} Pa·s is the viscosity value corresponding to the initial room temperature and the maximum pressure (91 bar) reached inside pressure vessel during this experimental test. The total viscosity drop of leaking Argon through the crack is 0.4×10^{-5} Pa·s.

Figure 3-21: The viscosity of leaking Argon through a crack

3.9 The thermal conductivity of Argon

3.9.1 Accuracy assessment of the thermal conductivity formula for Argon

Lemmon et al. method is also employed to evaluate Argon thermal conductivity in this research. Table 3-10 shows the sources of experimental data, the temperature, pressure, and density ranges, the number of points, and the average absolute deviations (AAD) between the experimental data and calculated data using Lemmon et al.'s equations.

Table 3-10: Summary of experimental data of Argon thermal conductivity and comparisons with the equations

Author	No. Points	Temperature range (K)	Pressure range (MPa)	Density range (mol·dm ⁻³)	AAD (%)
Michels et al. (1963) [190]	110	274–348	0.1–246	0.03–30.4	0.76
Millat et al. (1987) [191]	77	308–428	0.58–10.9	0.22–3.7	0.65
Millat et al. (1989) [192]	61	174–309	0.36–9.68	0.20–8.3	0.66
Moszynski and Singh (1973) [196]	105	323–473	0.1–162	0.02–26.9	1.24
Patek and Klomfar (2002) [204]	170	299–426	0.15–15.7	0.04–6.45	1.11
Perkins et al. (1991) [5]	144	299–303	2.6–65.5	1.05–20.1	0.95
Perkins et al. (1991) [8]	84	103–324	0.19–11.4	0.20–4.87	0.68
Roder et al. (1988) [7]	1484	102–326	0.19–67.9	0.09–36	1.12
Roder et al. (2000) [9]	718	301–344	0.16–8.33	0.05–3.21	0.80

Note: The pressure and temperature range used in the experimental research of the project is covered by the highlighted data in the table.

From Table 3-10, it can be concluded that Lemmon et al. method is a more accurate one to evaluate the thermal conductivity of Argon. Therefore, Lemmon et al. method is selected to evaluate the thermal conductivity of Argon in this research.

3.9.2 Evaluation procedure of the thermal conductivity

Similar to the model for viscosity, the thermal conductivity of Argon is expressed as functions of temperature and density:

$$\lambda = \lambda^0(T) + \lambda^r(\tau, \delta) + \lambda^c(\tau, \delta) \quad (3-32)$$

where λ is the thermal conductivity in mW·m⁻¹·K⁻¹

λ^0 is the dilute gas thermal conductivity

λ^r is the residual fluid thermal conductivity

λ^c is the thermal conductivity critical enhancement

Figure 3-22 and Figure 3-23 show the comparison between the calculated thermal conductivity of Argon using the equations of Lemmon and experimental data. The thermal

conductivity of Argon will increase with the rising pressure or temperature. It can be concluded that there is a good agreement between experimental data and the calculated thermal conductivity of Argon using the equations of Lemmon. Therefore, Lemmon's equations are selected to calculate the gas thermal conductivity in this research.

Figure 3-22: Thermal conductivity of Argon (λ) vs. pressure (p) at the temperature of 25 °C

Note: ★: calculated data using the equations in Lemmon's paper^[69]; ■: experiment data in Perkins' paper^[108]; ●: experiment data in Bailey's paper^[109]; ▲: experiment data in Roder's paper^[110]

Figure 3-23: Thermal conductivity of Argon (λ) vs. temperature (T) at the pressure of 80 bar

Note: ★: calculated data using the equations in Lemmon's paper^[69]; ■: experiment data in Perkins' paper^[108]; ●: experiment data in Mardolcar's paper^[111]; ▲: experiment data in Roder's paper^[110]

3.9.2.1 Dilute gas thermal conductivity

The dilute gas thermal conductivity is given by

$$\lambda^0 = N_1 \left[\frac{\eta^0(T)}{1 \mu Pa \cdot s} \right] + N_2 \tau^{t_2} + N_3 \tau^{t_3} \quad (3-33)$$

where $\tau = T_c/T$, T_c is the critical temperature.

Figure 3-24 shows the comparison between the calculated thermal conductivity of dilute Argon using the equations of Lemmon and experimental data. The thermal conductivity of dilute Argon will increase with the rising temperature. It can be concluded that there is a good agreement between experimental data and the calculated thermal conductivity of dilute Argon using the equations of Lemmon.

Figure 3-24: Dilute Argon thermal conductivity (λ^0) vs. temperature (T)

Note: ★: calculated data using the equations in Lemmon's paper^[69]; ●: experiment data in Hammerschmidt's paper^[112]; ■: experiment data in Michels' paper^[113]; ▲: experiment data in Bailey's paper^[109]

3.9.2.2 Residual fluid thermal conductivity

The residual contribution to the thermal conductivity is given (in $\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$) by

$$\lambda^r = \sum_{i=4}^n N_i \tau^{t_i} \delta^{d_i} \exp(-\gamma_i \delta^{l_i}) \quad (3-34)$$

where γ_i is zero when l_i is zero and one when l_i is not zero.

The coefficients and exponents of the residual fluid thermal conductivity equations (for Argon) are shown in Table 3-11.

Table 3-11: Coefficients and exponents of the residual fluid thermal conductivity equations (for Argon)^[69]

i	N_i	t_i	d_i	l_i
1	0.8158			
2	-0.4320	-0.77		
3	0	-1.0		
4	13.73	0	1	0
5	10.07	0	2	0
6	0.7375	0	4	0
7	-33.96	0.8	5	2
8	20.47	1.2	6	2
9	-2.274	0.8	9	2
10	-3.973	0.5	1	4

Figure 3-25 and Figure 3-26 show the relationship between residual thermal conductivity of Argon (λ^r) and pressure (p) & temperature (T), respectively. The residual thermal conductivity of Argon (λ^r) will increase with the rising pressure, and it will decrease with the rising temperature. And it will keep constant at some ranges of temperature.

Figure 3-25: Residual thermal conductivity of Argon (λ^r) vs. pressure (p) at the temperature of 25 °C

Figure 3-26: Residual thermal conductivity of Argon (λ^r) vs. temperature (T) at the pressure of 80 bar

3.9.2.3 Thermal conductivity critical enhancement

The thermal conductivity critical enhancement model of Olchoway and Sengers^[114] was used to calculate the fluid properties in the critical region. The equations of Olchoway and Sengers are shown here:

$$\lambda^c = \rho C_p \frac{k R_x T}{6 \pi \xi \eta(T, \rho)} (\tilde{\Omega} - \tilde{\Omega}_0) \quad (3-35)$$

Figure 3-27 and Figure 3-28 show the relationship between thermal conductivity critical enhancement of Argon (λ^c) and pressure (p) & temperature (T), respectively. The thermal conductivity critical enhancement of Argon (λ^c) increases with the rising pressure (close to quadratic function) and it decreases with rising temperature.

Figure 3-27: Thermal conductivity critical enhancement of Argon (λ^c) vs. pressure (p) at the temperature of 25 °C

Figure 3-28: Thermal conductivity critical enhancement of Argon (λ^c) vs. temperature (T) at the pressure of 80 bar

Table 3-12: Parameters and coefficients in Equation (3-35)

Parameters	Expressions	Parameters in expressions
ρ is the density of the fluid in kg/m^3	ρ is calculated from Redlich–Kwong equation of state (i.e. RK equation): $p = \frac{RT}{\tilde{v} - b'} - \frac{a'}{\tilde{v}(\tilde{v} + b')T^{0.5}}$ $\rho = \frac{1}{\tilde{v}}$	p is the pressure in Pa
		R is the specific gas constant, For Argon, $R = 208 \text{ J/(kg}\cdot\text{K)}$
		T is the temperature in K
		a' and b' are constants, $a' = 0.4278 \frac{R^2 T_c^{2.5}}{p_c}$ $b' = 0.0867 \frac{RT_c}{p_c}$ where, T_c and p_c are critical temperature and pressure, respectively. For Argon, $T_c = 150.86 \text{ K}$, $p_c = 48.98 \text{ bar}$ ^[58]
C_p is the isobaric heat capacity in $\text{J/(kg}\cdot\text{K)}$	$C_p = \frac{2.5R_0}{M} \times 10^3$	$\tilde{v}$ is the specific volume in m^3/kg ; $\tilde{v}$ is the reciprocal of density.
		R_0 is the universal gas constant; $R_0 = 8.31 \text{ J/(K}\cdot\text{mol)}$ M is the molar mass in g/mol ; For Argon, $M = 39.948 \text{ g/mol}$
k is Boltzmann's constant in $\text{J}\cdot\text{K}^{-1}$	1.380658×10^{-23}	
ξ is the correlation length in nm ^[69]	$\xi = \xi_0 \left[\frac{\tilde{\chi}(T, \rho) - \tilde{\chi}(T_{ref}, \rho) \frac{T_{ref}}{T}}{\Gamma} \right]^{\frac{v}{\gamma}}$	$\tilde{\chi}(T, \rho) = \frac{p_c \rho}{\rho_c^2} \left(\frac{\partial \rho}{\partial p} \right)_T$ where p_c is the critical pressure, ρ_c is the critical density in kg/m^3 ; For Argon, $\rho_c = 531 \text{ kg/m}^3$ ^[69]
		T_{ref} is a reference temperature in K; $T_{ref} = 301.374 \text{ K}$ (for Argon) ^[69]
		ξ_0 and Γ are fluid-specific (fitted) terms. For Argon, $\xi_0 = 0.13 \text{ nm}$, $\Gamma = 0.055$ ^[69]
		v and γ are theoretical based constants, $v = 0.63$, $\gamma = 1.2415$ ^[69]
R_x is theoretical based constant	$R_x = 1.01$	Refer to Lemmon's paper ^[69]
$\tilde{\Omega}$ is a parameter ^[69]	$\tilde{\Omega} = \frac{2}{\pi} \left[\left(\frac{C_p - C_v}{C_p} \right) \tan^{-1} \left(\frac{\xi}{q_D} \right) + \frac{C_v}{C_p} \left(\frac{\xi}{q_D} \right) \right]$	q_D is fluid-specific (fitted) terms. For Argon, $q_D = 0.32 \text{ nm}$ ^[69]
		C_v is isochoric heat capacity, $C_v = C_p - R$
$\tilde{\Omega}_0$ is a parameter ^[69]	$\tilde{\Omega}_0 = \frac{2}{\pi} \left\{ 1 - \exp \left[\frac{-1}{\left(\frac{\xi}{q_D} \right)^{-1} + \frac{1}{3} \left(\frac{\xi}{q_D} \right)^2 \left(\frac{\rho_c}{\rho} \right)^2} \right] \right\}$	ξ is the correlation length in nm
		ρ_c is the critical density in kg/m^3
		ρ is the density of the fluid in kg/m^3

Figure 3-29 and Figure 3-30 show the relationship between the correlation length ξ (in thermal conductivity critical enhancement formula) of Argon and pressure (p) & temperature (T), respectively. The correlation length ξ will increase with the rising pressure (close to linear relationship) and will decrease with rising temperature.

Figure 3-29: The correlation length ξ (in thermal conductivity critical enhancement formula) for Argon vs. pressure (p) at the temperature of 25 °C

Figure 3-30: The correlation length ξ (in thermal conductivity critical enhancement formula) for Argon vs. temperature (T) at the pressure of 80 bar

Figure 3-31 and Figure 3-32 show the relationship between the parameter $\tilde{\Omega}$ (in thermal conductivity critical enhancement formula) of Argon and pressure (p) & temperature (T), respectively. The parameter $\tilde{\Omega}$ will increase with the rising pressure (close to linear relationship) and will decrease with rising temperature.

Figure 3-31: The parameter $\bar{\Omega}$ (in thermal conductivity critical enhancement formula) for Argon vs. pressure (p) at the temperature of 25 °C

Figure 3-32: The parameter $\bar{\Omega}$ (in thermal conductivity critical enhancement formula) for Argon vs. temperature (T) at the pressure of 80 bar

Figure 3-33 and Figure 3-34 show the relationship between the parameter $\tilde{\Omega}_0$ (in thermal conductivity critical enhancement formula) of Argon and pressure (p) & temperature (T), respectively. The parameter $\tilde{\Omega}_0$ will increase with the rising pressure (close to linear relationship) and will decrease with rising temperature.

Figure 3-33: The parameter $\tilde{\Omega}_0$ (in thermal conductivity critical enhancement formula) for Argon vs. pressure (p) at the temperature of 25 °C

Figure 3-34: The parameter $\tilde{\Omega}_0$ (in thermal conductivity critical enhancement formula) for Argon vs. temperature (T) at the pressure of 80 bar

3.9.3 The evaluation results for the thermal conductivity of leaking Argon through a crack

The initial input values of parameters in MATLAB program for the calculation of the thermal conductivity of leaking Argon through crack are the same as that of viscosity as shown in Table 3-9.

The thermal conductivity of leaking Argon through a crack is shown in Figure 3-35. As illustrated in Figure 3-35, the thermal conductivity of leaking Argon will decrease along the crack through-wall position from the inside to the outside of the pressure vessel. The thermal conductivity of leaking Argon decreases from 0.022 W/m·K at the entrance of the crack to 0.017 W/m·K at the exit of the crack. The thermal conductivity of 0.022 W/m·K is the thermal conductivity value corresponding to the initial room temperature and the maximum pressure (91 bar) reached inside the pressure vessel during this experimental test. The total thermal conductivity drop of leaking Argon through the crack is 0.005 W/m·K.

Figure 3-35: The thermal conductivity of Argon leaking through a crack

3.10 Evaluation of heat transfer coefficient of leaking Argon through crack

The heat transfer coefficient is the key parameter to be evaluated in heat transfer analysis. In this section, the accuracy assessment of correlations and evaluation procedure of the heat transfer coefficient are detailed.

3.10.1 Petukhov correlation

After a literature survey, it was found that Petukhov correlation with high accuracy is suitable for the evaluation of the heat transfer in the pipe. It is one of the most accurate correlations for a single-phase forced convection, which has a reported accuracy of $\sim 5\%$ and given by^[72, 76]

$$N_u = \frac{\left(\frac{f}{8}\right) R_e P_r}{K + 12.7 \left(\frac{f}{8}\right)^{\frac{1}{2}} \left(P_r^{\frac{2}{3}} - 1\right)} \quad (3-36)$$

From the definition formula of Nusselt number (N_u),

$$N_u = \frac{hL}{\lambda} \quad (3-37)$$

the heat transfer coefficient (h) can be obtained and given by

$$h = \frac{N_u \lambda}{L} \quad (3-38)$$

Meanings of symbols in Equation (2-8) and Equation (3-37) are shown in Table 3-13.

Table 3-13: Definition of symbols in Equation (2-8) and Equation (3-37)

Symbols	Definitions of symbols	Meanings of symbols in definitions
f is the friction factor	$f = [1.82 \lg(R_e) - 1.64]^{-2}$ Refer to Adams' paper ^[76]	R_e is Reynolds number
R_e is Reynolds number	$R_e = \frac{\rho v L}{\eta}$	ρ is the density of the fluid in kg/m ³
		v is gas velocity in m/s
		L is characteristic length in m
		η is dynamic viscosity in Pa s
P_r is Prandtl number	$P_r = \frac{\eta C_p}{\lambda}$	C_p is heat capacity at constant pressure in J/(kg K)
		λ is thermal conductivity in W/(m K)
K is a parameter	$K = 1.07 + \frac{900}{R_e} - \frac{0.63}{1 + 10P_r}$	R_e is Reynolds number
		P_r is Prandtl number
L is characteristic length in m	$L = D_e = \frac{4A}{P}$	D_e is the equivalent diameter in m
		A is the cross-section area in m ²
		P is the wetting perimeter in m
λ is thermal conductivity in W/(m K)	$\lambda = \lambda^0(T) + \lambda^r(\tau, \delta) + \lambda^c(\tau, \delta)$	$\lambda^0(T)$ is the dilute gas thermal conductivity
		$\lambda^r(\tau, \delta)$ is the residual fluid thermal conductivity
		$\lambda^c(\tau, \delta)$ is the thermal conductivity critical enhancement

Comparison between experimental and calculated heat transfer data using Petukhov correlation is shown in Figure 3-36.

Figure 3-36: Comparison of Petukhov equation with experimental data on heat transfer to gases. Nu_0 denotes values obtained from Petukhov equation, and Nu denotes experimental values^[72]

Note: o & ⊗: Nitrogen^[73]; Δ & ▲: ammonia; ◇: air^[115]; □: air^[74]; +: steam^[75]; ∇: helium^[74]

3.10.2 Extension of the application of Petukhov correlation to microchannels

3.10.2.1 Modification of characteristic length in heat transfer equation

The correlation of heat transfer can also be applied to non-circular cross-section (e.g. a crack) when the equivalent diameter is used as the characteristic length.^[116] The correlation of the equivalent diameter is,

$$L = D_e = \frac{4A}{P} \quad (3-39)$$

where L is characteristic length in m, D_e is the equivalent diameter in m, A is the cross-section area of a crack, m^2 ; P is the wetting perimeter, m. For a two dimensional crack, $A = l \times W_c$, $P = 2(l + W_c)$, where W_c is the crack opening displacement and $l \gg W_c$, then one can obtain that

$$L = D_e \approx 2W_c \quad (3-40)$$

3.10.2.2 Extension of the Reynolds number in heat transfer equation to a wider range

Gnielinski modified the Petukhov correlation to extend the Reynolds number range down to 2300.^[117] The Gnielinski correlation is given by

$$Nu_{Gn} = \frac{\frac{f}{8}(Re-1000)Pr}{1 + 12.7\left(\frac{f}{8}\right)^{\frac{1}{2}}\left(Pr^{\frac{2}{3}} - 1\right)} \quad (3-41)$$

where

$$f = (1.82 \log(Re) - 1.64)^{-2} \quad (3-42)$$

3.10.2.3 Modification of Gnielinski correlation to accommodate the small diameters encountered in microchannels

Adams et al.^[76] modified the Gnielinski correlation to accommodate the small diameters encountered in microchannels by using the following form:

$$Nu = Nu_{Gn}(1 + F) \quad (3-43)$$

where

$$F = CRe \left(1 - \left(\frac{D}{D_0}\right)^2\right) \quad (3-44)$$

In Equation (3-44), $C = 7.6 \times 10^{-5}$, $D_0 = 1.164 \text{ mm}$, D is the diameter of microchannels. In this research, D denotes the crack width (Wc).

3.10.3 The evaluation results for the heat transfer coefficient of leaking Argon through crack

The initial input values of parameters in the MATLAB program for the calculation of the heat transfer coefficient of leaking Argon through crack are shown in Table 3-14.

Table 3-14: Initial input values of parameters in MATLAB program for the calculation of the heat transfer coefficient of leaking Argon through crack

Input parameters	Description	Values
P_0	Maximum pressure of Argon inside pressure vessel	91 bar
T_0	Initial temperature of Argon inside pressure vessel	30 °C
R	Gas constant of Argon	208 J/ kg·K
T_c	Critical temperature	150.86 K ^[62]
p_c	Critical pressure	48.98 bar ^[62]
M	Molar mass	39.948 g/mol ^[69]
ρ_c	Critical density	531 kg/m ³ ^[69]
ε/k	Lennard-Jones energy parameter	143.2 K ^[69]
σ	Lennard-Jones size parameter	0.335 nm ^[69]
W_c	Crack width in the experiment of this research	0.25 mm
R_{global}	Global roughness of crack surface in the experiment of this research	38.05 μm
α	Crack surface angle (refer to Beck et al. paper ^[80])	$\pi/6$

The heat transfer coefficient of leaking Argon through a crack is shown in Figure 3-37. It is indicated that the heat transfer coefficient of leaking Argon will decrease along the crack through-wall position from the inside to the outside of the pressure vessel. The heat transfer coefficient of leaking Argon decreases from $6.7 \times 10^4 \text{ W}/(\text{m}^2 \cdot \text{K})$ at the entrance of the crack to $0.26 \times 10^4 \text{ W}/(\text{m}^2 \cdot \text{K})$ at the exit of the crack. $6.7 \times 10^4 \text{ W}/(\text{m}^2 \cdot \text{K})$ is the heat transfer coefficient value corresponding to the initial room temperature (30 °C) and the maximum pressure (91 bar) reached inside the pressure vessel during this experimental test.

Figure 3-37: The heat transfer coefficient of leaking Argon through a crack

3.11 Simulation of temperature and stress of test plate by COMSOL program

3.11.1 Description of simulation model

Side view of 2D geometry of test plate with a through-thickness crack spacing of 0.25 mm (crack depth: 18 mm) are shown in Figure 3-38 & Figure 3-39. Due to symmetry, only a 3D quarter model (radius: 0.1778 m) of the test plate is simulated as shown in Figure 3-40.

Figure 3-38: Diagram of the model of gas leaking through a crack

Figure 3-39: Schematic of simulation model

Figure 3-40: Quarter model of test plate

3.11.2 Mesh sensitivity

The calibration of mesh sensitivity is shown in Figure 3-41. It shows that the mesh becomes stable after mesh number **J**. Element number **L** (8122) is selected in the present research. The whole mesh and close-up mesh of the crack surface are shown in Figure 3-42 & Figure 3-43, respectively. The element used is a 3D tetrahedral mesh element. In heat transfer module, the type of element is linear Lagrange element with integration order 2. In structural mechanics module, the type of element is quadratic Lagrange element with integration order 4. The geometry body includes 8122 tetrahedral elements. Number of degrees of freedom is 41083. Number of mesh points is 1930. Geometry boundary includes 2140 triangular elements. Geometry edge includes 149 elements. Number of vertex elements is 8. Minimum element quality is 0.2898. Element volume ratio is 3.73E-7.

Figure 3-41: Calibration of mesh sensitivity

Figure 3-42: Mesh of test plate

Figure 3-43: Close-up of the mesh of the crack surface on test plate

3.11.3 Domain material property

The material used in this model is Steel AISI 4340 in COMSOL Materials/Coefficients library. The material properties are shown in Table 3-15.

Table 3-15: Properties of mild steel used in test plate

Parameter	Value
Heat capacity at constant pressure	475[J/(kg·K)]
Young's modulus	205e9[Pa]
Thermal expansion coefficient	12.3e-6[1/K]
Thermal conductivity	44.5[W/(m·K)]
Poisson's ratio	0.28
Density	7850[kg/m ³]

3.11.4 Boundary conditions

(1) Heat Transfer Module

- a) Arc-shaped boundary: temperature 30 °C (same as room temperature on the day of the experiment)

Figure 3-44: Arc-shaped boundary

- b) Crack surface boundary: heat transfer coefficient $h = 65291e^{-183z}$, external temperature $T_{inf} = -2 \times 10^6 z^3 + 144339z^2 - 3533.2z + 303.17$ (fitted results from the calculation of temperature and heat transfer coefficient of leaking argon flowing through a crack as shown in Table 3-16)

Figure 3-45: Crack surface boundary

Table 3-16: Temperature and heat transfer coefficient of leaking argon flowing through a crack

Crack through-wall position z ($\times 10^{-3}$, m)	Temperature T_{inf} ($^{\circ}\text{C}$) After fitting, $T_{inf} = -2 \times 10^6 z^3 + 144339z^2 - 3533.2z + 303.17$	Heat transfer coefficient h ($\text{W}/\text{m}^2 \text{ K}$) After fitting, $h = 65291e^{-183z}$
0	30	67239
0.36	28.7604	62855
0.72	27.5529	58746
1.08	26.3779	54894
1.44	25.2354	51287
1.8	24.1258	47910
2.16	23.0488	44750
2.52	22.0044	41794
2.88	20.9925	39030
3.24	20.0125	36447
3.6	19.0644	34032

Crack through-wall position z ($\times 10^{-3}$, m)	Temperature T_{inf} ($^{\circ}\text{C}$) After fitting, $T_{inf} = -2 \times 10^6 z^3 + 144339z^2 - 3533.2z + 303.17$	Heat transfer coefficient h ($\text{W/m}^2 \text{ K}$) After fitting, $h = 65291e^{-183z}$
3.96	18.1475	31778
4.32	17.2613	29672
4.68	16.4055	27706
5.04	15.5793	25872
5.4	14.7823	24160
5.76	14.0136	22563
6.12	13.2727	21074
6.48	12.5589	19685
6.84	11.8714	18390
7.2	11.2096	17183
7.56	10.5727	16057
7.92	9.9601	15008
8.28	9.3709	14031
8.64	8.8045	13119
9	8.2601	12270
9.36	7.7371	11478
9.72	7.2348	10741
10.08	6.7523	10053
10.44	6.2892	9412
10.8	5.8446	8815
11.16	5.4179	8257
11.52	5.0086	7738
11.88	4.6159	7254
12.24	4.2393	6802
12.6	3.8782	6381

Crack through-wall position z ($\times 10^{-3}$, m)	Temperature T_{inf} ($^{\circ}\text{C}$) After fitting, $T_{inf} = -2 \times 10^6 z^3 + 144339z^2 - 3533.2z + 303.17$	Heat transfer coefficient h ($\text{W/m}^2 \text{ K}$) After fitting, $h = 65291e^{-183z}$
12.96	3.532	5988
13.32	3.2	5621
13.68	2.8819	5278
14.04	2.577	4959
14.4	2.2848	4660
14.76	2.0049	4382
15.12	1.7367	4121
15.48	1.4799	3878
15.84	1.2338	3650
16.2	0.9982	3437
16.56	0.7726	3238
16.92	0.5566	3052
17.28	0.3497	2878
17.64	0.1517	2714
18	-0.0379	2561

- c) Inner surface boundary (inside the pressure vessel): heat transfer coefficient (selected from heat transfer coefficients library: external forced convection on a plate); external temperature 15°C (gas temperature inside pressure vessel during test)

Figure 3-46: Inner surface boundary (inside the pressure vessel)

- d) Outer surface boundary (outside the pressure vessel): heat transfer coefficient (selected from heat transfer coefficients library: external natural convection on a horizontal plate); external temperature 30 °C (same as room temperature on the day of the test)

Figure 3-47: Outer surface boundary (outside pressure vessel)

e) Symmetry boundaries

Figure 3-48: Symmetry boundaries

(2) Structural Mechanics Module

a) Arc-shaped surface boundary is shown in Figure 3-49: Fixed

Figure 3-49: Arc-shaped boundary (fixed)

b) Crack surface boundary is shown in Figure 3-50: Free

Figure 3-50: Crack surface boundary (Free)

$$\text{Load } F_x = p \times \sin(9.46) = 9 \times 10^6 \times e^{(-125.6 \times z)} \times \sin(9.46),$$

$$F_y = p \times \cos(9.46) = 9 \times 10^6 \times e^{(-125.6 \times z)} \times \cos(9.46)$$

where $p = 9 \times 10^6 \times e^{(-125.6 \times z)}$ is the fitted pressure results from the calculation of pressure distribution of leaking argon flowing through a crack shown in Table 3-17), where angle 9.46 is the crack slant angle shown in Figure 3-51.

Figure 3-51: Crack slant angle 9.46

Table 3-17: Pressure distribution of leaking argon flowing through a crack

Crack through-wall position $z (\times 10^{-3}, \text{ m})$	Pressure $p (\text{ bar})$ after fitting, $p = 9 \times 10^6 \times e^{(-125.6 * z)}$
0	91
0.36	86.976
0.72	83.13
1.08	79.454
1.44	75.94
1.8	72.582
2.16	69.373
2.52	66.305
2.88	63.373
3.24	60.571
3.6	57.892
3.96	55.332
4.32	52.885
4.68	50.547
5.04	48.311
5.4	46.175
5.76	44.133
6.12	42.182
6.48	40.316
6.84	38.534
7.2	36.83
7.56	35.201
7.92	33.644
8.28	32.157
8.64	30.735

Crack through-wall position $z (\times 10^{-3}, \text{m})$	Pressure $p (\text{bar})$ after fitting, $p = 9 \times 10^6 \times e^{(-125.6 \cdot z)}$
9	29.376
9.36	28.077
9.72	26.835
10.08	25.648
10.44	24.514
10.8	23.43
11.16	22.394
11.52	21.404
11.88	20.457
12.24	19.553
12.6	18.688
12.96	17.862
13.32	17.072
13.68	16.317
14.04	15.595
14.4	14.906
14.76	14.247
15.12	13.617
15.48	13.014
15.84	12.439
16.2	11.889
16.56	11.363
16.92	10.861
17.28	10.38
17.64	9.921
18	9.483

- c) Inner surface boundary is shown in Figure 3-52 (inside pressure vessel): Free;
Load $F_z=91$ bar (maximum pressure in pressure vessel during test)

Figure 3-52: Inner surface boundary (Free)

- d) Outer surface boundary is shown in Figure 3-53 (outside pressure vessel): Free

Figure 3-53: Outer surface boundary (Free)

e) Boundaries on other surfaces is shown in Figure 3-54: Symmetry

Figure 3-54: Symmetry boundaries

3.11.5 Modeling in COMSOL Multiphysics

A heat transfer application mode and a structural mechanics application mode are coupled to model thermal-structure interaction. Thermal-Structure Interaction predefined multiphysics coupling application mode is selected in COMSOL Multiphysics program. Then it can be modeled by configuring each application mode as usual. This includes subdomain setting such as the material, and boundary setting, such as loads and constraints for the structural mechanics application mode, or temperature and fluxes for the heat transfer application mode. Also, the reference temperature is defined for the thermal load on the structure. The analysis is a sequentially-coupled thermal-stress analysis, i.e. the thermal analysis is completed first, and then the temperatures are used as input to the structural analysis.

3.11.6 Results and discussion

3.11.6.1 Thermal analysis

Figure 3-55 shows the temperature distribution of the test plate with a central through-thickness crack. It is noticed that the highest and lowest temperatures on the test plate are 30 °C and 13.8 °C, respectively. The maximum temperature drop of the test plate is 16.2 °C.

Figure 3-55: Temperature distribution of test plate with a central through-thickness crack

3.11.6.2 Stress analysis

The Von Mises stress field surrounding the central through-thickness crack on the test plate considering the thermal effect is simulated and shown in Figure 3-56 and Figure 3-57. The maximum Von Mises stress value near the crack tip is 3.3 GPa. This value is higher than the yield stress (0.22 GPa) of mild steel in this research. Even considering the thermal effect, the yield stress of mild steel is the same in this experimental temperature range according to ASME Section II, Part D.^[118] It is noticed in Figure 3-57 that the high thermal stress part is concentrated at the inlet and outlet of the crack.

Figure 3-56: Von Mises stresses on the test plate

Figure 3-57: Von Mises stresses close to the crack surface on the test plate

The stress components (in X, Y, Z-directions) are shown in Figure 3-58 to Figure 3-60. The maximum thermal stresses in the X, Y, Z-directions experienced by the crack tip are 1.8 GPa, 2.6 GPa and 0.89 GPa, respectively.

Figure 3-58: Normal stress in X-direction around the crack

Figure 3-59: Normal stress in Y-direction around the crack

Figure 3-60: Normal stress in Z-direction around the crack

3.11.6.3 Strain analysis

The strain components (in X, Y, Z-direction) are shown in Figure 3-61 to Figure 3-63. The maximum strains in the X, Y, Z-direction experienced by the crack tip are 5.7 mm, 9.7 mm and 4.1 mm, respectively.

Figure 3-61: Normal strain in X-direction around the crack

Figure 3-62: Normal strain in Y-direction around the crack

Figure 3-63: Normal strain in Z-direction around the crack

3.12 Conclusions

The simulation adopts a two stage method. First stage is the properties evaluation of the leaking argon in a crack by using MATLAB program. Second stage is the temperature and stress evaluation of the localized metal in the vicinity of the crack by employing the heat transfer and structural mechanics models in the COMSOL Multiphysics program. For safety considerations, argon is selected as the research gas as its JT coefficient is close to methane. The planar crack model is adopted as the calculation model as the macroscopic tortuosity is much less significant than the microscopic tortuosity arising from the fracture process. The crack is divided into 50 equivalent increments along the crack depth direction in order to calculate the argon properties in each crack increment by using a MATLAB program.

The pressure of leaking Argon drops from 91 bar at the entrance of the crack to 9.5 bar at the exit of the crack. The total pressure drop of leaking Argon through the crack is 81.5 bar. The pressure of leaking Argon decreases along the crack through-wall position from the inside to the outside of the pressure vessel. The crack opening displacement, crack depth and crack surface roughness have significant influence on the pressure loss of leaking argon through the crack. The pressure loss is not sensitive to the value of crack surface angle. The temperature of the leaking

Argon decreases from 30 °C at the entrance of the crack to –0.04 °C at the exit of the crack. The total temperature drop of leaking Argon through the crack is about 30 °C. The maximum pressure reached inside the pressure vessel in this experiment is 91 bar. The pressure range in CNG container in the marine vessel is about 200 – 250 bar. According to the Joule-Thomson theory, a higher pressure inside the cylinder can cause a higher temperature loss during the leakage process. A lower temperature in the crack tip area leads to a deterioration of the fracture toughness capacity of the localized metal. Therefore, it is necessary to consider the negative impact of the J-T effect in the LBF methodology for the safer design of the pressure vessel.

The heat transfer and structural mechanics modules are selected to perform the thermal-structural coupling simulation. The lowest temperature of the test plate in the vicinity of the crack obtained from the simulation is 13.8 °C. The maximum temperature drop of the test plate due to the heat transfer of leaking Argon through a crack considering Joule-Thomson cooling effect is 16.2 °C. The lowest temperature of the test plate tested from the experiment is 12.5°C. The simulation result on the lowest temperature of the localized metal basically matches the experimental result. The two stage method in this modeling and simulation may cast light on the further study of the Joule-Thomson cooling effect of a high pressure gas leaking through a crack. Stress analysis shows the maximum Von Mises stress value near the crack tip is 3.3 GPa which is much higher than the yield stress (0.22 GPa) of mild steel used in the experiment.

CHAPTER 4 EXPERIMENTAL WORK

4.1 Introduction

In this chapter, the design of pressure retaining components of a J-T test rig according to ASME Boiler and Pressure Vessel Code is detailed. A test plate with an artificial through-thickness crack using a liquid Nitrogen cracking method is fabricated. The roughness of the crack surfaces is measured by the equipment of TalyScan 150 (Taylor Hobson Ltd, Leicester, England) using a scanning stylus contact method. The crack width on the test plate is tested by non-destructive ultrasonic testing (NDT technology) method and feeler gauge method. The thermocouple wires are inserted into the drilled holes on the test plate to collect temperature data around the crack. Gas tightness of the J-T test rig is examined by using the soap bubbles method. The data logger TDS-303 (Tokyo Sokki Kenkyujo Co., Ltd) is used to record the temperature data during the experiment. The Series 626 industrial pressure transmitter with led (Dwyer Instruments, Inc, Michigan, USA) is adopted to monitor the pressure inside the pressure vessel.

4.2 Experimental methodology

- (a) Design and fabricate a pressure vessel at a design pressure of 250 bar according to ASME Boiler and Pressure Vessel Code^[1, 118];
- (b) Fabricate a round steel plate with a central rectangular slot as the cover of the pressure vessel which is sandwiched between the upper and lower flanges of the pressure vessel, sealed by a pair of gaskets;
- (c) Fabricate an artificial through-thickness crack on a small piece of crack specimen which is the same size as the central slot on test plate by using a liquid Nitrogen cracking method;
- (d) Weld the small piece of crack specimen and the round steel plate to form a test plate
- (e) Conduct a Joule-Thomson experiment of high pressure leaking gas through the artificial crack on the test plate by pumping high pressure gas into the assembled test rig and collect temperature (around the artificial crack) and pressure (inside the pressure vessel) data using thermocouples and a pressure gauge, respectively.

4.3 Schematic of designed pressure vessel

The schematic of the designed pressure vessel (design pressure: 250 bar) is shown in Figure 4-1. The components of test rig include support, bolt, test plate, gaskets, cylindrical shell, hemispherical head, nozzles, pressure gauge, upper flange and lower flange.

Figure 4-1: Components of pressure vessel with manifold casing

4.4 Attempt of the fabrication of the crack specimen by using the X70 pipe line material

The material used in real cylinders on the CNG vessel is low carbon steels (mainly X70 or X80 pipeline steel). Therefore, it is necessary to carry out the experiment by using real X70 or

X80 pipeline steel. Some preliminary test work has been performed for the X70 pipeline steel and is shown as follows.

4.4.1 Acquisition of X70 pipeline steel material

The X70 pipeline steel segment acquired from a local company is shown in Figure 4-2 and Figure 4-3.

Figure 4-2: Larger X70 pipeline steel segments in a local company (pipe I.D.: 1054.1 mm, thickness 23 mm)

Figure 4-3: Smaller X70 pipeline steel segments sawn from the bigger one (each smaller segment dimensions: 710 × 235 × 23 mm)

4.4.2 Fatigue cracking of the X70 pipeline steel block

The finished fatigue cracking of the X70 pipeline steel block is shown in Figure 4-4. It is noticed that this fatigue sample cannot be used in Joule-Thomson experiment. The two crack surfaces cannot match well due to the ductility of material.

Figure 4-4: Finished fatigue cracking of X70 pipeline steel block (unbroken block dimensions: $120 \times 14 \times 10$ mm)

The procedure of fatigue cracking of X70 pipeline steel block is shown as follows.

(1) Tensile test of the X70 pipeline steel block

The results of tensile test of the X70 pipeline steel block are shown in and Figure 4-5.

Figure 4-5: Tensile test result of X70 pipeline steel block

From Figure 4-5, it can be noticed that the yield stress and the ultimate tensile stress of the X70 pipeline steel block are 526.96 MPa (= 76.4 ksi) and 585 MPa (= 84.85 ksi), respectively.

(2) Fatigue test of the X70 pipeline steel block

The fatigue test result of the X70 pipeline steel block during approaching ultimate failure is shown in Figure 4-6. The whole experiment is approximately one week long.

Figure 4-6: Fatigue test result of the X70 pipeline steel block during approaching ultimate failure (frequency: 1 Hz)

4.4.3 Liquefied Nitrogen cracking of X70 pipeline steel block

The procedure for the cracking of the X70 pipeline steel block is shown in Figure 4-7 to Figure 4-10. From Figure 4-10, it can be concluded that the liquefied Nitrogen cracking method is not suitable for Joule-Thomson experiment. The cracked surfaces cannot match well due to the ductility of material.

Figure 4-7: Liquefied Nitrogen poured into a little bucket

Figure 4-8: Position of X70 pipeline steel block under the hydraulic pump

Figure 4-9: Frozen and cracked X70 pipeline steel block

Figure 4-10: Cracked X70 pipeline steel block at room temperature

4.4.4 The possible reason for the infeasibility of fatigue and liquefied Nitrogen cracking of X70 pipeline steel block

Hardness is a measure of how resistant solid matter is to various kinds of permanent shape change when a force is applied. Hardness is dependent on ductility, elastic stiffness, plasticity, strain, strength, toughness, viscoelasticity, and viscosity. Indentation hardness measures the resistance of a sample to material deformation due to a constant compression load from a sharp object.^[119] The indentation hardness of X70 pipeline steel block is measured and the result is shown in Table 4-1.

Table 4-1: The indentation hardness (HRC) of X70 pipeline steel block

Times of measurement	1	2	3	4	5
HRC	10.3	10.9	11.4	10.4	13.1
Average value of HRC	11.22				

From above tested results, it is noticed that the indentation hardness of X70 pipeline steel block is smaller than that of commonly used steels (hardness (HRC): about 35-65 HRC). It indicates that the X70 pipeline steel has a good ductility. This is why it cannot be made into well matched brittle or fatigue crack surfaces. Although the X70 pipeline steel has a lower hardness, it has better toughness than commonly used steels.

4.5 Fabrication of test plate with an artificial through-thickness crack by using mild steel material

4.5.1 Flow chart of the fabrication of test plate with an artificial through-thickness crack

The illustration of the process of the fabrication of the test plate with an artificial through-thickness crack is shown in Figure 4-11. The steps A1 – A6 show the fabrication procedure of an artificial through-thickness crack on a small piece of crack specimen which has same size as the central slot on the test plate by using the liquid Nitrogen cracking method (brittle fracture) and

fatigue cracking method (ductile fracture). The steps B1 – B3 present the fabrication process of a round steel plate with a central rectangular slot as the cover of the pressure vessel which is sandwiched between the upper and lower flanges of the pressure vessel, sealed by a pair of gaskets.

Figure 4-11: Flow chart of the fabrication of test plate with an artificial through-thickness crack

4.5.2 CNC machining of rectangular mild steel plate

The following material is purchased for the fabrication of test plate:

(1) Rectangular mild steel plate: 340mm x 340mm x 25mm (Figure 4-12)	(Qty: 1)
(2) Small piece of mild steel block: 30mm x 65mm x 25mm (Figure 4-13)	(Qty: 1)

Figure 4-12: Rectangular mild steel plate

Figure 4-13: Small piece of mild steel block

The rectangular mild steel plate is sent to the CNC laboratory for machining and is cut into a rounded plate with diameter 330.2mm. At the same time, a rectangular slot is machined at the center of the test plate as shown in Figure 4-14 and Figure 4-15.

Figure 4-14: Engineering drawing of the machining of rectangular mild steel

Figure 4-15: Machining of rectangular mild steel to round plate with a central slot

4.5.3 Fabrication of artificial crack specimen

The steel block is broken into two separate blocks using the liquid Nitrogen cooling method. The following steps are taken.

Step 1: CNC machining of a notch of 5 mm depth on the middle of one surface of steel block

A 5mm depth notch is made by wire cutting process across the 65mm x 25mm face of the steel block as shown in Figure 4-16.

Figure 4-16: CNC Machining of a notch on one surface of steel block

Step 2: Freezing and cracking of steel block in liquid Nitrogen

The steel block is put into liquid Nitrogen for freezing as shown in Figure 4-17.

Figure 4-17: Freeze the steel piece in liquefied Nitrogen

Effervescence is observed as the steel block rapidly loses its temperature as shown in Figure 4-18.

Figure 4-18: Effervescence observed in liquid Nitrogen

The steel block is taken out when the effervescence disappears as presented in Figure 4-19.

Figure 4-19: Taking out the steel block when the effervescence disappeared

Upon removal of steel piece from the liquid Nitrogen, it is immediately placed onto the hydraulic press platform. (Note: cut side of steel block is faced downwards as shown in Figure 4-20.)

Figure 4-20: Placing the frozen steel block onto the hydraulic press platform

The pressure of the hydraulic pump is increased gradually until the steel block is broken. The broken steel block is shown in Figure 4-21.

Figure 4-21: A half of the broken steel block

A file is used to flatten the sharp edges of broken steel blocks as shown in Figure 4-22.

Figure 4-22: Removal of the sharp edges of broken steel blocks

The steel blocks are shaped into the same dimensions of 30 mm x 12 mm x 18 mm as shown in Figure 4-23 and Figure 4-24.

Figure 4-23: Shaping of steel blocks using milling machine

Figure 4-24: Finished steel block with an artificial crack

Step 3: Roughness measurement of the broken surfaces of steel block

Surface characteristics are vitally important with regard to friction and leakage in seals. Surface roughness, often shortened to roughness, is a measure of the texture of a surface. It is quantified by the vertical deviations of a real surface from its ideal form.^[120, 121] Surface roughness of the broken surfaces of steel block is measured by the equipment of TalyScan 150 (Taylor Hobson Ltd, Leicester, England). The contact method using a scanning stylus is selected to scan the broken surfaces of the steel block.

Figure 4-25: TalyScan 150

The scanning area on two broken surfaces is 1×1 mm. 3-D surface morphology of surface 1 and surface 2 are shown in Figure 4-26 and Figure 4-27. The value of root mean square R_q (RMS) in surface roughness parameters is selected to calculate surface roughness of broken surface due to the bumpiness of surface 1 and surface 2. The measured value of R_q for surface 1 and surface 2 are $46.27 \mu\text{m}$ and $29.83 \mu\text{m}$, respectively. Then the average roughness value of the two surfaces is $38.05 \mu\text{m}$. The average roughness value of $38.05 \mu\text{m}$ is taken as the global roughness of the broken surfaces.

Figure 4-26: 3-D surface morphology of surface 1 (Volume: $1 \times 1 \times 0.245$ mm)

Figure 4-27: 3-D surface morphology of surface 2 (Volume: $1 \times 1 \times 0.1529$ mm)

4.5.4 Welding of the steel block and the round steel plate

Some thin metal sheets are prepared as the supports for the welding of the steel block and round steel plate. The steel blocks are put into the slot of the round steel plate under the assistance of supports as shown in Figure 4-28. The supports are removed after finishing the welding on Side A and Side B. Then other sides except the central crack are welded as shown in Figure 4-29.

Figure 4-28: Supports used to position steel block on round steel plate

Figure 4-29: Welding of steel block and round steel plate

The test plate is sent to CNC laboratory to make two recesses at both its sides as shown in Figure 4-30 and Figure 4-31.

Figure 4-30: Engineering drawing of two recesses at both sides of the test plate

Figure 4-31: A recessed area at the center of the test plate

4.6 Measurement of crack width

After the crack specimen is welded, the crack width (or crack opening displacement) on the test plate is measured by two methods as follows:

- (1) Non-destructive ultrasonic testing (NDT technology);
- (2) Feeler gauge.

4.6.1 Non-destructive ultrasonic testing

4.6.1.1 Introduction of NDT technology

Non-destructive testing techniques are used to find material defects in many safety critical applications such as aircraft, nuclear reactors and bridges. Ultrasonic testing is one of these techniques and it is used to detect crack, voids or other discontinuities in metals, plastics or composites. It is used normally to detect defects which occur below the surface of a specimen although it also can detect surface opening defects.^[122-124]

4.6.1.2 Ultrasonic “A” scan testing

Ultrasonic scan inspection is carried out by placing a probe, connected to an ultrasonic instrument, on the specimen to be examined (Figure 4-32 (a)). Pulses of ultrasonic waves are generated by the probe and these travel into the specimen. A layer of liquid (“the couplant”) e.g. oil needs to be placed between the probe and the specimen surface because the ultrasound cannot travel through air. The ultrasonic waves are reflected by the cavity and the back of the specimen to produce the signals shown in Figure 4-32 (b).

Figure 4-32: Basic principle of ultrasonic testing with a compression wave probe:

(a) Set-up of a probe on a specimen

(b) Standard A-scan display on an ultrasonic cathode ray tube screen

The probe described above emits compression waves which travel normal to the surface of the specimen (termed a “0°” probe because the angle between the wave traveling into the specimen and the normal to the surface is 0°). In this case of a compression wave, the particle vibration direction is in the same direction as the energy propagation. Defects are often inclined to the inspection surface at a variety of angles and it is always desirable for the ultrasonic beam to strike a defect at right angles in order to return the maximum amount of energy back to the probe. Therefore shear wave probes are often used in ultrasonics to direct the energy into the specimen at an angle to the normal other than “0°” e.g. 60°. For shear waves the particle vibration is at right angles to the energy propagation direction. The waves leave the probe at the probe index point.

4.6.1.3 Crack sizing using USM 35 portable ultrasonic flaw detector

Figure 4-33 shows a picture of USM 35 portable ultrasonic flaw detector from GE's Inspection Technologies business.

Figure 4-33: GE inspection technologies USM 35

4.6.1.3.1 Calibrate ultrasonic instrument for shear wave testing

(1) Find the probe index position

The probe is positioned on the standard steel block until the maximum wave amplitude appears on the oscilloscope, and then one can find the accurate probe index position which can be marked using a marker on the probe as shown in Figure 4-34.

Figure 4-34: Find the accurate probe index position using a standard steel block

(2) Check the probe angle accuracy and probe sensitivity

The probe angle accuracy and probe sensitivity calibration are shown in Figure 4-35 and Figure 4-36.

Figure 4-35: Probe angle accuracy calibration (probe angle = 60°)

Figure 4-36: Probe sensitivity testing using the hole with a diameter of 3 mm on the standard steel block

(3) Calibration of oscilloscope reading scale

The ultrasonic beam is directed towards the 25 mm radius of the test block shown in Figure 4-37. Position “A” is a 25 mm radius with centre “O”. Position “B” is a 50 mm radius with centre “O”. Two peaks are observed. The first peak is from the reflection at point A (total travel distance 50 mm). The second peak is due to multiple reflection at points A, O, B, O and then finally back to A again (total travel distance = $50 + 100 + 50 = 200$ mm). The two peaks are positioned at the 25 and 100 mm positions respectively on the time base.

Figure 4-37: Miniature calibration block for shear waves

4.6.1.3.2 Sizing a crack using the maximum amplitude technique

The maximum amplitude technique is employed to size the crack width in this research. Shear wave probes are used to direct the energy into the specimen at an angle.

Experimental procedure is as follows:

(a) Magnetic particle inspection (MPI)

Before carrying out ultrasonic testing, Magnetic Particle Inspection (MPI) should be done first to check the presence of a surface or subsurface discontinuity in the material. Magnetic Particle Inspection (MPI) is a non-destructive testing (NDT) process for detecting surface and slightly subsurface discontinuities in ferromagnetic materials such as iron, nickel, cobalt, and some of their alloys. The process puts a magnetic field into the part. The piece can be magnetized by direct or indirect magnetization. This test procedure is as follows:

- (1) Clean the surface of the test plates using dye penetration inspection systems and spray some white paint of magnetic particle on the test plates as shown in Figure 4-38.

Figure 4-38: Clean the test plate surface using dye penetration inspection systems

- (2) Use the Castrol strip to test the workability of Poka-Yoke technology as shown in Figure 4-39 and Figure 4-40.

Figure 4-39: Castrol strip of Poka-Yoke technique

Figure 4-40: Using Poka-Yoke technology for early defect detection

- (b) Measure and mark the central thickness of the test plate as input parameter of ultrasonic instrument showed in Figure 4-41.

Figure 4-41: Measurement of central thickness of test plate using ultrasonic technique

- (c) Put one shear wave probe at the point A on one side of crack (shown in Figure 4-42), then the length value of “BC”, “AC” can be read on the display of ultrasonic instrument. A vernier caliper is used to measure the distance of “AO”. The lengths of “B’C” (equals to “BC”), “A’C” and “A’O” can also be measured by following same procedure on the opposite side of crack (point A’). Therefore, the crack width BB' equals to $AO + A'O - AC - A'C'$.
- (d) Follow the above procedures; different crack widths at different crack depths (different positions of the line of “BB’”) can be measured.

Figure 4-42: Sizing crack width using ultrasonic technology

4.6.1.4 Crack width test results (ultrasonic beam angle: 60°)

The crack width test results using ultrasonic wave NDT method are shown in Table 4-2. The tested results show a wide variation in crack width ranging from -1.98 to 1.83 mm. It can be concluded that the NDT method is not suitable to measure this type of narrow crack width due to the following system and accidental errors.

Table 4-2: Crack width test results using ultrasonic wave NDT method

Crack depth position (mm) (Total depth=18 mm)	Test data on one side of the crack (mm)		Test data on opposite side of the crack (mm)		Calculated crack width W_c (mm)
BC (B'C')	AC	AO	A'C'	A'O	$BB' = AO + A'O - AC - A'C'$
16.82	16.14	13.4	16.15	20	1.11
14.9	12.82	8.5	12.16	14.5	-1.98
12.67	8.95	7.9	8.92	9.9	-0.07
10.99	6.04	3.0	6.11	7.8	-1.35
8.69	2.05	2.0	2.12	3.9	1.73
7.68	0.3	-1.4	0.39	2.2	0.11
5.92	-2.73	-2.5	-2.6	-1.0	1.83
4.86	-4.57	-5	-4.48	-3.5	0.55

4.6.1.5 Error analysis of NDT ultrasonic method

(a) System error

The system error includes the following items:

- (1) Instrument calibration error
- (2) Marker line width error
- (3) Unstable ultrasonic wave display

(b) Accidental error

The accidental error includes the following items:

- (1) Reading error
- (2) Probe position cannot be fixed stably because of the lubricous couplant

4.6.2 Feeler gauge method

A feeler gauge is a simple tool used to measure gap widths. Feeler gauges are mostly used in engineering to measure the clearance between two parts. They consist of a number of small lengths of steel of different thicknesses with thickness values marked on each piece. They are flexible enough that, even if they are all on the same hinge, several can be stacked together to gauge intermediate values. The picture of feeler gauge is shown in Figure 4-43.

Figure 4-43: Feeler gauge

In the present research, the steel piece of 0.25 mm in the feeler gauge can go through the crack on the test plate. Therefore, the crack width should be around 0.25 mm. As the NDT

method is not suitable to measure the crack width, the measured value of 0.25 mm using feeler gauge method is regarded as the crack width.

4.7 Mounting and testing of thermocouple wires on test plate

4.7.1 Drilling of thermocouple holes on the outer surface of test plate

The test plate is sent to the CNC Laboratory for drilling 1 (diameter) $\times$ 4 (depth) mm holes for the insertion of thermocouple wires. Figure 4-44 to Figure 4-46 show engineering drawings to illustrate the positions of the thermocouples inserted. The fabricated round plate with thermocouple holes is shown in Figure 4-47.

Figure 4-44: Sectional view of test plate with thermocouple mounting holes

Figure 4-45: Position of thermocouple mounting holes along crack line

Figure 4-46: Position of thermocouple mounting holes at 45 ° direction

Figure 4-47: Fabricated round plate with thermocouple holes

4.7.2 Mounting method of thermocouple wires on test plate

4.7.2.1 Welding of thermocouple wires

As mentioned in the earlier part of this report, type K thermocouple is chosen for the experiment due to the match between the expected experiment temperature range and operating temperature range of the thermocouple wire. The single spool thermocouple wires are cut into thirty pieces, each with a length of two meters.

A thermocouple wire consists of a positive terminal (red-cable) and a negative terminal (white-cable) as shown in Figure 4-48.

Figure 4-48: A thermocouple wire

To use the thermocouple wire, it is required that the ends of two metallic cables of the thermocouple wire are welded together using thermocouple welder as shown in Figure 4-49. Figure 4-50 shows a welded thermocouple.

Figure 4-49: Thermocouple welder

Figure 4-50: A welded thermocouple wire

4.7.2.2 Insertion and fastening of thermocouple wires to the holes on test plate

In this process, the welded end of the thermocouple wire is inserted into the drilled holes on test plate. Firstly, a puncher is positioned next to the thermocouple hole and thermocouple wire inserted as illustrated in Figure 4-51.

Figure 4-51: A puncher next to the thermocouple hole and thermocouple wire inserted

As depicted in Figure 4-52, a hammer is used to knock the puncher so as to deform the surrounding area of the hole. The deformation will clamp the wire in position and prevent it from detaching from the round plate.

Figure 4-52: Deformation knocked at the hole surrounding area

Once the thermocouple wires are inserted to the corresponding holes on the round plate, the thermocouple wires are neatly arranged and labeled as shown in Figure 4-53.

Figure 4-53: Test plate with mounted and bundled thermocouple wires

4.7.3 Drilling of thermocouple holes on the inner surface of test plate

To measure the inner surface temperature of the test plate, thermocouples have to be inserted on the inner surface. Thus, 1mm diameter holes, similar to holes at the outer surface, are drilled on the inner surface. Twenty holes in the horizontal and vertical directions are drilled in the inner surface as shown in Figure 4-54.

Figure 4-54: Drilled holes on the inner surface of test plate

With the thermocouple wires on the inner surface of the test plate, a through-thickness hole has to be drilled so that these thermocouple wires can be guided through the test plate and subsequently the upper flange to connect with the data logger.

A through-thickness hole is drilled through the test plate with its tapered end at the inner surface of the test plate as shown in Figure 4-55.

Figure 4-55: Tapered through-thickness hole on test plate

The mounted thermocouple wires at the inner surface of test plate are guided out to the outer surface through the tapered hole. Thereafter, epoxy is used to seal the hole to prevent gas leakage during the experiment as illustrated in Figure 4-56.

Figure 4-56: Thermocouple wires guided through the tapered hole

4.7.4 Measuring method of the gas temperature at crack inlet and outlet by mounting thermocouple wires

In order to measure the gas temperature at the inlet and outlet of the crack, thermocouples are positioned at the respective position. One outside thermocouple wire is protruding out into the gas about 10 mm above the crack surface to measure the leaking gas temperature. And one inside thermocouple wire is also protruding out into the pressure vessel above metal surface. These two wires are not embedded into the metal to measure metal temperature. The thermocouples are positioned to measure the inlet and outlet gas temperature. The epoxy holds the thermocouples firmly in position to prevent leakage as shown in Figure 4-57 and Figure 4-58.

Figure 4-57: Thermocouple at the inlet of the crack

Figure 4-58: Thermocouple at the outlet of the crack

4.7.5 Testing of thermocouple function

Before conducting the Joule-Thomson experiment, it is important to carry out a thermocouple test in order to ensure that all the installed thermocouples are functioning properly. This is a critical test as a positive test outcome implies that the results obtained during the experiment are an accurate reflection of the temperature change due to the Joule-Thomson effect and not due to errors in the thermocouple wire.

To test the installed thermocouples, the round test plate is placed on top of a heater and all installed thermocouple wires are connected to the data logger. This is shown in Figure 4-59.

Figure 4-59: Testing set-up of thermocouple function

The heater is set to a temperature of 100°C. The temperature of the round test plate is measured and recorded at constant time intervals by the data logger. Subsequently, the measured temperature data is graphically plotted. For clearer viewing, the data are plotted into three separate graphs as depicted from Figure 4-60 to Figure 4-62.

Figure 4-60: Temperature vs time (for T1 to T9)

Figure 4-61: Temperature vs time (for T10 to T18)

Figure 4-62: Temperature vs time (for T19 to T27)

From Figure 4-60 to Figure 4-62, all the lines are close to each other. This means that at a specific time, all the thermocouple wires managed to capture the same changing temperature of the round test plate. Furthermore, all the thermocouple wires' initial and final measured temperature matched the room temperature and the set-temperature of the heater (i.e. 100 °C) respectively. Thus, it shows that the temperatures measured by all thermocouple wires are accurate.

As a result, it can be concluded from the graphical outcome of this test that all the thermocouple wires are functioning properly.

4.8 J-T experimental procedure and results

The temperature measurement on the surface of test plate around the central crack is performed to investigate the Joule-Thomson cooling effect during gas leaking. The test rig is fabricated by a local manufacturer and assembled in the laboratory.

4.8.1 Arrangement of experimental apparatus

Figure 4-63 shows the overall arrangement of the crack's Joule-Thomson (J-T) cooling effect testing facility with detailed location of pressure transducer and thermocouples. Argon gas with 99.9995 % purity and up to 200 bar is tapped from two gas tanks into the bottom nozzle (1/2" NPT) of the experimental pressure vessel and leaking from a crack in the test plate between two flanges. In the experimental pressure vessel, the high pressure Argon is expanded through the crack made by liquid Nitrogen cracking method where the J-T effect is produced by the rapidly expanding gas.

Figure 4-63: Overall arrangement of Joule-Thomson (J-T) cooling effect testing facility

The temperatures of test plate material around the crack and the pressures inside experimental pressure vessel are recorded and monitored by thermocouples and digital pressure gauge, respectively. Type K thermocouples with FEP insulated stainless steel sheathed probes are used to measure the temperature. The probe diameter of thermocouples is 0.32 mm. Thermocouples are calibrated to an accuracy of ± 1 °C. The thermocouples are connected to a TDS-302 data logger from which temperature data can be recorded and printed. The digital pressure gauge with a relative accuracy of 1% is connected to the side nozzle of pressure vessel to monitor and record the pressure inside the pressure vessel.

4.8.2 Experimental procedure

An assembled test rig is shown in Figure 4-64.

Figure 4-64: Assembled test rig

- (1) Pressure vessel is put into manifold casing; the lower flange and the lower gasket are positioned on the pressure vessel, respectively; a hydraulic hose is connected with the lower flange of the pressure vessel and gas cylinders;
- (2) The test plate with mounted thermocouple wires and the upper gasket are put onto the lower gasket;
- (3) The pressure vessel and the gas regulator are connected using a 6 meters long (for safety) hydraulic hose as shown in Figure 4-65;

Figure 4-65: Fitting of pressure vessel in one room and control in the adjacent room

- (4) Thermocouple wires are bundled to go through the central hole of upper flange under the assistance of the hydraulic lifter as illustrated in Figure 4-66;

Figure 4-66: Assembly of upper flange

- (5) Bolts are fastened by using a spanner;
- (6) Thermocouple wires are connected to data logger TDS-303 (Tokyo Sokki Kenkyujo Co., Ltd) as shown in Figure 4-67;

Figure 4-67: Thermocouple wires connected to data logger in the adjacent room

- (7) A webcam facing the digital pressure gauge display (Dwyer Instruments, Inc, Michigan, USA) is used to monitor the pressure change inside the pressure vessel and is powered by a 12 V power supply;
- (8) Gas cylinders are chained and regulators are installed and tightened with hydraulic hoses as shown in Figure 4-68;

Figure 4-68: Installation of gas cylinders and control valve

- (9) Leak detection of J-T test rig system

Prior to the J-T experiment, it is important to conduct a leak test on the equipment to ensure that the components are installed properly and that the only leakage that occurred during the experiment is through the artificial crack at the center of the round test plate. The soap bubbles method is used for the leak test. To conduct the leak test, the pressure vessel is attached to the compressed air supply which has a maximum pressure of 10 bar as shown in Figure 4-69.

Figure 4-69: Pressure vessel connected to air supply

The pressurized air supply is turned on. Then the soap solution is brushed onto all joints and welds between components of the test rig to see if soap bubbles form as depicted in Figure 4-70.

Figure 4-70: Soap solution brushed onto joints and welds

The produced bubbles during pressurization of pressure vessel by using air supply show the detected leakage as shown in Figure 4-71 & Figure 4-72.

Figure 4-71: Leakage detected around test plate

Figure 4-72: Leakage detected on lower nozzle

To resolve the leakage issue, more sealing tape is used and the connectors are further tightened. The leak test is repeated to determine if the leakage problem persists. After the

repeated leak test, it can be concluded that the test rig is properly installed and proven to be leak proof (at low pressure) since no more bubbles are observed.

To conduct a credible leak test, the test rig should be subjected to a pressure even higher than what the test rig is expected to experience during the actual experiment. However, due to limited resources, the leak test is conducted at a much lower pressure.

From the result of this leak test, it can at least prove that the test rig is leak proof at low pressure. If the leak test yields a negative result even at low pressure, it would show that the test rig is poorly installed and further corrective work should be taken to improve the test rig proofing ability.

(10) Implementation of J-T experiment

Prior to the experiment, a check is done to ensure all components, units and tubing are assembled properly according to the layout shown in Figure 4-73.

Figure 4-73: Schematic of experimental apparatus

Two cylinders of Argon with a pressure of 200 bar are used as gas source for this experiment. The initial temperature of the metal surrounding the artificial crack before leakage is measured by using the thermocouples and data logger.

The valves and regulators on the Argon gas cylinders are fully opened to pressurize the pressure vessel. At the same time, a computer is connected to the webcam to observe and record the pressure change inside pressure vessel. The temperature data are printed by data logger every few seconds.

Once the temperature stabilizes for a while, the vessel is depressurized by closing the valves of gas cylinders. The temperature and pressure data are collected until the metal temperature reaches room temperature.

4.8.3 Experimental results for Argon and Nitrogen

For obtaining results for different gases, Nitrogen is also tested in the experiment. In the experiment, the following parameters are recorded: t (test time), p (pressure inside pressure vessel), T (temperature of test points). Figure 4-74 shows the thermocouple mounting positions: horizontal (along the crack line, H1 – H10), vertical (perpendicular to crack line, V1 – V10), and diagonal (45 ° angle to crack line, D1 – D10). The labeled thermocouples are mounted on the inside and outside surface of the test plate around the crack in order to provide information on how cold adjacent materials would become in the event of gas release impinging directly onto them.

Figure 4-74: Notation of thermocouple mounting positions

4.8.3.1 Experimental results for Argon

In this experiment, the maximum Argon pressure reached in the pressure vessel is 91 bar. The temperature change on the outside surface of the test plate (in horizontal, diagonal direction to the crack line) is shown in Figure 4-75 and Figure 4-76, respectively. Figure 4-77 shows the temperature change on the inside surface of the test plate (in the horizontal direction to the crack line). From the three figures, it can be seen that the temperature changing trends are almost identical during the test.

In Figure 4-75, H1 is the point closest to the crack. H2 and H8 are the positions of broken thermocouple wires during the experiment. It is noticed that the lowest temperature of H1 point during the Joule-Thomson effect is 12.5 °C. The total temperature drop (due to the J-T effect) of this point from room temperature is 17.5 °C. In Figure 4-76, D1 is the point closest to the crack. D10 is the location above the crack to measure the temperature of the outlet gas. It is shown that the lowest temperature of the D1 point during the Joule-Thomson effect is 7.9 °C. The total temperature drop (due to the J-T effect) of this point from room temperature is 22.1 °C. In Figure 4-77, H1 is the point closest to the crack. H10 is the location on the inner surface of test plate to measure the gas temperature inside pressure vessel. It is indicated that the lowest temperature of the H1 point during the Joule-Thomson effect is 15.0 °C. The total temperature drop (due to the J-T effect) of this point from room temperature is 15.0 °C.

From Figure 4-75 to Figure 4-77, the temperature rise on the surface of test plate at the beginning of the experiment is caused by the temperature increase of the gas inside the pressure vessel. At the beginning of the experiment, high pressure gas is pumped into pressure vessel while the leakage is negligible at the beginning lower pressure. Sharp increase in the gas pressure inside the pressure vessel is the reason for the rise of gas temperature according to the first law of thermodynamics. The gas warming effect disappears when the gas pressure inside the pressure vessel tends to be stable. At the same time, the Joule-Thomson cooling effect of the gas through the crack begins to dominate to cool the leaking gas and then the test plate by heat transfer. During the stable stage (between 160 – 400 s), the temperature of the metal increases slightly because the pressure in the cylinders of gas supply drops gradually. When the gas supply is stopped, the metal temperature decreases abruptly as the sharp decreased gas pressure inside pressure vessel according to the first law of thermodynamics.

Figure 4-75: Temperature change on the outside surface of test plate (in horizontal direction H1 to H10)

Figure 4-76: Temperature change on the outside surface of test plate (in diagonal direction D1 to D10)

Figure 4-77: Temperature change on the inside surface of test plate (in horizontal direction H1 to H10)

The comparison between the experimental and simulation results for Argon at the lowest temperature is shown in Figure 4-78. The lowest temperature on the outside surface of the test plate (in the horizontal direction to the crack line) during the Joule-Thomson cooling period is 12.5 °C, and the lowest temperature in the simulation is 13.8 °C. It can be concluded that the simulation results basically match the experimental results.

Figure 4-78: Comparison between experimental and simulation result at the lowest temperature

The temperature results on the outside surface of the test plate (in the diagonal direction to the crack line) are lower than that of horizontal direction to the crack. However, there is a depression at the side of the crack which is caused by the insufficient weld metal deposition during welding as illustrated in Figure 4-79. The depression could affect the temperature results in the diagonal direction as the leaking gas impacts the depression directly. In addition, some temperature results in the diagonal direction are not stable as shown in Figure 4-76. There are no recesses or defects on the path of the horizontal direction to the crack. Therefore, the temperature

results on the outside surface of test plate (in the horizontal direction to the crack line) are selected to compare with the simulation results as shown in Figure 4-78.

Figure 4-79: A recess near the crack on the surface of test plate

4.8.3.2 Experimental results for Nitrogen

The experiment is conducted using nitrogen as an alternative gas. The maximum Nitrogen pressure reached in the pressure vessel is 70 bar. The temperature change on the outside surface of test plate (in the horizontal and diagonal directions to the crack line) is given in Figure 4-80 & Figure 4-81, respectively. Figure 4-82 shows the temperature change on the inside surface of the test plate (in the horizontal direction to the crack line). The disconnected lines in the figures are the data which are not recorded in the experiment due to failed thermocouple possibly caused by the excessive movement during the assembly of test rig. From the three figures, it can be concluded that the temperature changing trends are also almost identical during the test.

In Figure 4-80, H1 is the point closest to the crack. H2 and H4 are the positions of failed thermocouple wires during the experiment. It is noticed that the lowest temperature of the H1

point during the Joule-Thomson effect is 18.2 °C. The total temperature drop (due to the J-T effect) of this point from room temperature is 9.6 °C. In Figure 4-81, D1 is the point closest to the crack. D10 is the location above the crack to measure the temperature of outlet gas. It is shown that the lowest temperature of the D1 point during the Joule-Thomson effect is 15.5 °C. The total temperature drop (due to the J-T effect) of this point from room temperature is 11.8 °C. In Figure 4-82, H1 is the point closest to the crack. H10 is the location on the inner surface of test plate to measure the gas temperature inside the pressure vessel. It is indicated that the lowest temperature of the H1 point during the Joule-Thomson effect is 18.2 °C. The total temperature drop (due to the J-T effect) of this point from room temperature is 9.0 °C. (Note: in Figure 4-80 to Figure 4-82, the missed pressure data in initial stage are not recorded during the experiment.)

Figure 4-80: Temperature change on the outside surface of test plate (in horizontal direction)

Figure 4-81: Temperature change on the outside surface of test plate (in diagonal direction)

Figure 4-82: Temperature change on the inside surface of test plate (in horizontal direction)

4.9 Conclusions

A pressure vessel at a design pressure of 250 bar is designed and fabricated according to ASME Boiler and Pressure Vessel Code. A round steel plate with a central rectangular slot is machined as the cover of the pressure vessel. A round steel plate with a central through-thickness crack is machined as the cover of the pressure vessel. The crack specimens made from X70 steel cannot be used in the J-T experiment because the two crack surfaces produced cannot match well to form a natural-like crack due to the ductility of the X70 material. Therefore, commonly used mild steel is used to replace the X70 steel to fabricate the brittle crack specimen by using a liquid Nitrogen cracking method. The crack width (or crack opening displacement) on the test plate is measured by Non-Destructive Ultrasonic Testing (NDT) and feeler gauge. The crack width of 0.25 mm is measured by a feeler gauge. The NDT method is not suitable to measure this type of crack width due to the higher error. The roughness of the broken surfaces of steel block is measured by the equipment of TalyScan 150 (Taylor Hobson Ltd, Leicester, England) using scanning stylus contact method. The average roughness value of the two broken surfaces of the crack is 38.05 μm .

During the J-T experiment, the temperature of the localized material of the test plate around the crack and the pressure inside the pressure vessel are recorded by thermocouples and digital pressure gauge, respectively. For the experiment using Argon, the maximum pressure reached in the pressure vessel is 91 bar in the J-T experiment. The lowest temperature of the localized material in the vicinity of the crack caused by the Joule-Thomson effect is 12.5 °C. The total temperature drop of the localized metal is 17.5 °C. From the comparison between the experimental and simulation results (i.e. the lowest temperature of 13.8 °C) at the lowest temperature, it can be found that the simulation results basically match the experimental results. In order to test the Joule-Thomson for different gases, Nitrogen is also used in this study. For the experiment using Nitrogen, the maximum pressure reached in the pressure vessel is 70 bar. The lowest temperature of the localized material around the crack produced by the Joule-Thomson effect is 18.2 °C. The total temperature drop of the localized metal in the vicinity of the crack is 9.6 °C.

The new Joule-Thomson test system provided in this research may be a cost efficient and timesaving design providing a convenient method to perform the high pressure gas leakage experiment. Its advantage is the flexibility of making an artificial through-thickness crack. The brittle and fatigue cracks are easily fabricated on a small crack specimen compared to the difficult fabrication on the body of the pipe. Only the test plate is replaced for different types of cracks without changing the whole J-T test rig. The regular shape of the test plate with a central through-thickness crack greatly improves the efficiency of the simulation. In all, these benefits provide a significant investigation into the experiment and modelling and simulation of the J-T effect of the leaking gas in a crack and pave a way for further studies.

CHAPTER 5 CONCLUSIONS AND CONTRIBUTIONS

5.1 Introduction

Compressed natural gas (CNG) is an emerging marine transportation technology for natural gas. On account of the high pressure inside CNG containers, the most critical characteristic expected in CNG systems with leakage is the Joule-Thomson (JT) effect. Study on the JT effect occurring during a gas flowing through a crack is rare. The temperature and heat transfer coefficient of a gas leaking through a crack are affected by the pressure, leaking velocity, density, viscosity and thermal conductivity of the gas. For safety considerations, argon is selected as the research gas as its JT coefficient is close to methane. In this modeling and simulation, the planar crack model is adopted as the calculation model as the macroscopic tortuosity is much less significant than the microscopic tortuosity arising from the fracture process. The crack is divided into 50 equivalent increments along the crack depth direction in order to calculate the argon properties in each crack increment by using a MATLAB program. In this experiment, a pressure vessel at a design pressure of 250 bar is designed and fabricated according to ASME Boiler and Pressure Vessel Code. A round steel plate with a central through-thickness crack is machined as the cover of the pressure vessel. Both the simulation and experiment provide an efficient way to study the JT effect of the leaking gas in a crack.

5.1.1 Modeling and simulation conclusions

The simulation in this research adopts a two stage method. First stage is the properties evaluation of the leaking argon in a crack by using MATLAB program. Second stage is the temperature and stress evaluation of the localized metal in the vicinity of the crack by employing the heat transfer and structural mechanics models in the COMSOL Multiphysics program.

In the first stage, the leaking argon's properties in a crack are evaluated. The pressure of leaking argon through the crack is lost by three means: friction with the crack surface, inertia pressure and the recirculation of the gas. The pressure of leaking Argon drops from 91 bar at the

entrance of the crack to 9.5 bar at the exit of the crack. The total pressure drop of leaking Argon through the crack is 81.5 bar. The pressure of leaking Argon decreases along the crack through-wall position from the inside to the outside of the pressure vessel. The crack opening displacement, crack depth and crack surface roughness have significant influence on the pressure loss of leaking argon through the crack. The pressure loss is not sensitive to the value of crack surface angle. The RK (Redlich-Kwong) state equation is selected to calculate the density of the leaking argon through the crack. It is found that there is a good agreement between the calculated results of AGA8 (American Gas Association Report No. 8) report and the R-K equation of state. The density of leaking Argon drops from 150.7 kg/m^3 at the entrance of the crack to 16.8 kg/m^3 at the exit of the crack during the leaking process. The temperature of the leaking Argon decreases from $30 \text{ }^\circ\text{C}$ at the entrance of the crack to $-0.04 \text{ }^\circ\text{C}$ at the exit of the crack. The total temperature drop of leaking Argon through the crack is about $30 \text{ }^\circ\text{C}$. The maximum pressure reached inside the pressure vessel in this experiment is 91 bar. The pressure range in CNG container in the marine vessel is about 200 – 250 bar. According to the Joule-Thomson theory, a higher pressure inside the cylinder can cause a higher temperature loss during the leakage process. A lower temperature in the crack tip area leads to a deterioration of the fracture toughness capacity of the localized metal. Therefore, it is thus necessary to consider the negative impact of the J-T effect in the LBF methodology for the safer design of the pressure vessel.

In the second stage, the temperature and stress evaluation of the localized metal in the vicinity of the crack are evaluated. Firstly, the calculation results of temperature and heat transfer coefficient are fitted into correlations as the input parameters of the boundary conditions in the COMSOL Multiphysics program. The heat transfer and structural mechanics modules are selected to perform the thermal-structural coupling simulation. The lowest temperature of the test plate in the vicinity of the crack obtained from the simulation is $13.8 \text{ }^\circ\text{C}$. The maximum temperature drop of the test plate due to the heat transfer of leaking Argon through a crack considering Joule-Thomson cooling effect is $16.2 \text{ }^\circ\text{C}$. The lowest temperature of the test plate tested from the experiment is 12.5°C . There is a good agreement between the simulation and experiment at the lowest temperature in the test plate. Stress analysis shows the maximum Von Mises stress value near the crack tip is 3.3 GPa which is much higher than the yield stress (0.22 GPa) of mild steel used in the experiment.

The simulation result on the lowest temperature of the localized metal basically matches the experimental result. The two stage simulation method may shed a light on the study of the Joule-Thomson cooling effect of a high pressure gas leaking through a crack.

5.1.2 Experimental conclusions

In this study, the brittle and fatigue crack specimens are fabricated by using X70 pipeline steel material. However, these crack specimens cannot be used in the J-T experiment because the two crack surfaces produced cannot match well to form a natural-like crack due to the ductility of the X70 material. Therefore, commonly used mild steel is used to replace the X70 steel to fabricate the brittle crack specimen by using a liquid Nitrogen cracking method. The crack width (or crack opening displacement) on the test plate is measured by Non-Destructive Ultrasonic Testing (NDT) and feeler gauge. The crack width of 0.25 mm is measured by a feeler gauge. The NDT method is not suitable to measure this type of crack width due to the higher error. The roughness of the broken surfaces of steel block is measured by the equipment of TalyScan 150 (Taylor Hobson Ltd, Leicester, England) using scanning stylus contact method. The average roughness value of the two broken surfaces of the crack is 38.05 μm .

During the J-T experiment, the temperature of the localized material of the test plate around the crack and the pressure inside the pressure vessel are recorded by thermocouples and digital pressure gauge, respectively. For the experiment using Argon, the maximum pressure reached in the pressure vessel is 91 bar in the J-T experiment. The lowest temperature of the localized material in the vicinity of the crack caused by the Joule-Thomson effect is 12.5 °C. The total temperature drop of the localized metal is 17.5 °C. In order to test the Joule-Thomson for different gases, Nitrogen is also used in the study. For the experiment using Nitrogen, the maximum pressure reached in the pressure vessel is 70 bar. The lowest temperature of the localized material around the crack produced by the Joule-Thomson effect is 18.2 °C. The total temperature drop of the localized metal in the vicinity of the crack is 9.6 °C.

The Joule-Thomson test system in this research may be a cost efficient and timesaving design providing a convenient method to perform the high pressure gas leakage experiment. Its advantage is the flexibility of making an artificial through-thickness crack. The brittle and fatigue cracks are easily fabricated on a small crack specimen compared to the difficult

fabrication on the body of the pipe. Only the test plate is replaced for different types of cracks without changing the whole J-T test rig. The regular shape of the test plate with a central through-thickness crack greatly improves the efficiency of the simulation. In all, these benefits provide a significant investigation into the experiment and modelling and simulation of the J-T effect of the leaking gas in a crack and pave a way for further studies.

5.2 Contributions

- The new mathematical calculation model presented by dividing the crack route into multiple segments with equal length could help to apply the Joule-Thomson theory into a gas flowing through a leaking crack to solve more realistic problems, such as higher pressure inside the pressure vessel, different thicknesses of pressure vessel wall (namely, different crack depths), different crack opening displacements and crack surface roughness;
- The development of MATLAB calculation flow chart for gas properties in the crack improves our insight into the elementary aspects of a leakage process. Discussions on the underlying physics of the Joule-Thomson cooling effect from a gas flowing through a leaking crack may provide other researchers some ideas worthy of future work;
- The novel Joule-Thomson test system may provide a cost efficient and timesaving method for the study of the Joule-Thomson cooling effect from a gas flowing through a leaking crack on the localized cooling of the steel plates/walls of the pressure vessel. Moreover, the convenience and flexibility of the method of making a crack specimen in Joule-Thomson test system in this research may provide an alternative to the crack fabrication on the pipe for the research of the J-T effect;
- The Joule-Thomson effect is experimentally measured in a realistic crack. This experiment proves there is a significant temperature drop of the metal around crack. Under higher pressure, it may affect the LBF validity.

CHAPTER 6 FUTURE WORK

The dissertation describes the Joule-Thomson (J-T) cooling effect occurred when gas leaks through a narrow tortuous crack on the wall of the high pressure vessel and the effect on the vessel wall in the vicinity of the crack. Future work includes the following parts.

6.1 Using a larger gas supply

In the current experiment, the highest pressure reached in the pressure vessel is 91 bar. The maximum pressure of the supply gas is 200 bar. The pressure losses in the system are caused by the following aspects: 1) the pressure loss in the hydraulic hose (about 6 meters) connecting the gas supply cylinder and the pressure vessel; 2) the pressure loss as the supplied gas is filling the pressure vessel which has a larger volume (about I.D.: 7 in, height: 13 in); 3) the pressure loss due to the leakage of gas flowing through the crack on the wall of the pressure vessel. However, in a practical CNG vessel, the pressure in the gas cylinders is 200 – 250 bar. Therefore, the gas supply should be increased so that an experiment with a higher pressure can be carried out.

6.2 Alternative method of creating artificial crack surface for X70 pipe line material

Electric discharge machining (EDM) is a manufacturing process whereby a desired shape is obtained using electrical discharges (sparks). Material is removed from the workpiece by a series of rapidly recurring current discharges between two electrodes, separated by a dielectric liquid and subject to an electric voltage. The EDM machining method has two types: Die-sink EDM and Wire-cut EDM. Die-sink EDM, also called cavity type EDM or volume EDM, consists of an electrode and workpiece submerged in an insulating liquid such as, more typically oil or, less frequently, other dielectric fluids. The electrode and workpiece are connected to a suitable power supply. The power supply generates an electrical potential between the two parts. As the electrode approaches the workpiece, dielectric breakdown occurs in the fluid, forming a plasma channel and spark discharge which ejects materials.^[125]

The Die-sink EDM machining method can create a rougher or smoother finish on the workpiece. Therefore, this machining method can be applied to make rougher surfaces on the sawn pipeline steel blocks to simulate the real crack situation as shown from Figure 6-1 to Figure 6-4. The desired roughness can be controlled by adjusting the setup parameters of EDM machine as shown in Figure 6-3.

Figure 6-1: Machined surfaces of a pair of sawn X70 pipeline steel blocks using EDM method

(a) Crack surface fabricated by liquefied Nitrogen method (roughness: 38.05 μm)

(b) Crack surface made by EDM method (roughness: 31.67 μm)

Figure 6-2: Comparison between crack surfaces made by liquefied Nitrogen and EDM method

Figure 6-3: EDM crack surfaces with different roughness (from left to right: smooth to rough)

Figure 6-4: Insertion of X70 steel blocks into the central slot of mild steel round plate

However, the drawback of this method is that the crack faces cannot match like a real crack.

APPENDIX I MATLAB CODE

(1) Evaluation of gas density (step (7) in MATLAB flow chart)

```

1. Function [y] = density(p,T,R,Tc,pc)
   % Here, the function density(p,T,R,Tc,pc) is the gas density
   in kg/m3
   p is the pressure in Pa
   T is the temperature in °C
   R is the specific gas constant in J/(kg·K). For Argon, R=208
   J/(kg·K).

Tc is the critical temperature in K.
For Argon, Tc = 150.86 K.
   pc is the critical pressure in Pa.
   For Argon, pc = 48.98×105 Pa.

2. a1=0.42748*R^2*Tc^2.5/pc;
3. b1=0.08664*R*Tc/pc;
   % Here, a1 and b1 are the parameters in Redlich-Kwong
   equation of state.

4. a=p*T^0.5;
5. b=-R*T^1.5;
6. c=a1-p*b1^2*T^0.5-R*b1*T^1.5;
7. d=-a1*b1;
8. v̄=-b/(3*a)+(1/(3*2^(1/3)*a))*(-2*b^3+9*a*b*c-
   27*a^2*d+(4*(3*a*c-b^2)^3+(-2*b^3+9*a*b*c-
   27*a^2*d)^2)^0.5)^(1/3)-(2^(1/3)*(3*a*c-b^2))/(3*a*(-
   2*b^3+9*a*b*c-27*a^2*d+(4*(3*a*c-b^2)^3+(-2*b^3+9*a*b*c-
   27*a^2*d)^2)^0.5)^(1/3));
   % Here, v̄ is the gas specific volume in m3/kg.

9. y=1/v;
```

(2) Evaluation of fluid velocity (step (10) in MATLAB flow chart)

Figure App I-1: Detailed schematic of flow around several crack turns

1. `Function [y] = v(T,p,R,Tc,pc,Wc,alfa,Rglobal)`
`%Here, v(T,p,R,Tc,pc,Wc,alfa,Rglobal) is the flow velocity`
`of the fluid in m/s.`
`T is the temperature in °C`
`p is the pressure in Pa`
`R is the specific gas constant in J/(kg·K)`
`Tc is the critical temperature in K`
`pc is the critical pressure in Pa`
`Wc is the crack opening displacement (or crack width)`
`alfa is the crack surface angle relative to the crack`
`direction through wall`
`Rglobal is the global roughness of the crack`
2. `t=3.6e-3;`
`%Here, t is the crack through-wall thickness for every`
`increment. And this value is an empirical value.`

```

3. c1=1.0;
   %Here, c1 is a linear interpolant.
4. sita=alfa*(1-0.9*c1);
   %Here, sita is the average flow direction relative to the
   crack direction through-wall
5. Reff=Rglobal;
   %Here, Reff is the effective roughness
6. Rglamp=4*Rglobal;
   %Here, Rglamp is the peak-to-trough amplitude of the global
   roughness contours for a sawtooth geometry
7. N=t*tan(alfa)/(2*Rglamp);
   %Here, N is the actual number of turns in the crack
8. teff=t/cos(sita);
   %Here, teff is the effective crack through-wall thickness
9. l=Rglamp/tan(alfa);
10. W3=l*tan(sita);
11. W2=Rglamp-W3;
12. W1=Wc-W2;
13. Wceff=W1*cos(sita);
   % Here, Wceff is the effective crack width perpendicular to
   the average flow direction
14. f=(1.82*log10(Wc/Reff)-0.77)^-2;
   % Here, f is the friction factor in crack
15. F1=f*teff/(2*Wceff);
16. F2=2*N*sita*Wceff/Wc;
17. F3=1-(Wceff/Wc)^2;
18. F=F1+F2+F3;
   % Here, F is the sum of pressure loss terms due to
   frictional (F1), inertial (F2), and recirculation effects
   (F3).
19. Cd=1/(1+F^0.5);
   % Here, Cd is the discharge coefficient

```


20. $y = (C_d * (p * \text{density}(p, T, R, T_c, p_c))^{0.5}) / \text{density}(p, T, R, T_c, p_c);$

(3) Evaluation of pressure drop for every calculation step length of the crack through-wall thickness (step (2)-(3) in MATLAB flow chart)

```
1. Function [y] = pd(T,p,R,Tc,pc,t,Wc,alfa,Rglobal)
% Here, pd(T,p,R,Tc,pc,t,Wc,alfa,Rglobal) is the pressure drop
for every calculation step of the crack through-wall thickness
in Pa.

    t is the crack through-wall thickness for every increment.

2. Reff=Rglobal;
3. Rglamp=4*Rglobal;
4. N=t*tan(alfa)/(2*Rglamp);
5. c=1.0;
    % Here, c1 is a linear interpolant.

6. sita=alfa*(1-0.9*c);
7. teff=t/cos(sita);
8. l=Rglamp/tan(alfa);
9. W3=l*tan(sita);
10. W2=Rglamp-W3;
11. W1=Wc-W2;
12. Wceff=W1*cos(sita);
13. f=(1.82*log10(Wc/Reff)-0.77)^-2;
14. y=density(p,T,R,Tc,pc)*v(T,p,R,Tc,pc,Wc,alfa,Rglobal)^2/2*
    (f*teff/(2*Wceff)+2*N*sita*Wceff/Wc+1-(Wceff/Wc)^2);
```

(4) Evaluation of Joule-Thomson coefficient (step (4) in MATLAB flow chart)

```
1. function [y]=U(p,T,R,Tc,pc)
    % Here, U(p,T,R,Tc,pc) is the Joule-Thomson coefficient in K/Pa
```

```

2. v=1/density(p,T,R,Tc,pc);
   % Here, v is the specific volume in m3/kg.
3. R1=8.31;
   % Here, R1 is the universal gas constant in J / (K · mol)
4. M=39.948;
   % Here, M is the molar mass in g/mol
5. Cp=2.5*R1/M*103;
   % Here, Cp is the isobaric heat capacity in J/(K · kg)
6. a=0.42748*R2*Tc2.5/pc;
7. b=0.08664*R*Tc/pc;
   % Here, a and b are the parameters in Redlich-Kwong
   equation of state.
8. y= ((R*T2*(v2+v*b)2*(v-b)+0.5*a*T0.5*(v2+v*b)*(v-
   b)2)/(R*T2*(v2+v*b)2-a*T0.5*(2*v+b)*(v-b)2)-v)/Cp;

```

(5) Evaluation of temperature drop for every calculation step length of the crack through-wall thickness (step (4) in MATLAB flow chart)

```

1. Function [y] = integration(p2,p1,T,R,Tc,pc,N)
   % Here, integration(p2,p1,T,R,Tc,pc,N) is the temperature drop for
   every calculation step length of the crack through-wall thickness
2. y=0;
3. h=(p2-p1)/N;
   % Here, h is the integration step size. The more big the value of N, the more accurate the
   integration result will be. In this research, N = 10000.
4. for i=1:N
5. y=y+U(p1+(i-1)*h,T,R,Tc,pc)*h;
6. end;

```

(6) Evaluation of the parameter of the collision integral in gas viscosity formula (step (8) in MATLAB flow chart)

```

1. Function [y] = OMG(T,E)
% Here, OMG(T,E) is the collision integral.
% E is the Lennard-Jones energy parameter.
% For Argon, E=143.2.
2. Ta=T/E;
3. b0=0.431;
4. b1=-0.4623;
5. b2=0.08406;
6. b3=0.005341;
7. b4=-0.00331;
8. y=exp(b0+b1*log(Ta)+b2*(log(Ta))^2+b3*(log(Ta))^3+b4*(log(Ta))^4);

```

(7) Evaluation of the viscosity of dilute gas (step (8) in MATLAB flow chart)

```

1. Function [y] = N_L(T,M,E,XGM)
% Here, N_L(T,M,E,XGM) is the viscosity of dilute gas.
% M is molar mass in g/mol
% E is the Lennard-Jones energy parameter
% XGM is the Lennard-Jones size parameter in nm. For Argon,
% XGM=0.335 nm.
2. Ta=T/E;
3. b0=0.431;
4. b1=-0.4623;
5. b2=0.08406;
6. b3=0.005341;
7. b4=-0.00331;
8. OMG=exp(b0+b1*log(Ta)+b2*(log(Ta))^2+b3*(log(Ta))^3+b4*(log(Ta))^4);
% Here, OMG is the collision integral.
9. y=0.0266958*sqrt(M*T)/(XGM^2*OMG)*10^(-6);

```


(8) Evaluation of the residual fluid viscosity (step (8) in MATLAB flow chart)

```

1. Function [y] = Nr(T,p,R,Tc,pc,rhoc)
    % Here, Nr(T,p,R,Tc,pc,rhoc) is the residual fluid viscosity
    in Pa.s.

rhoc is the critical density in kg/m3.
For Argon, rhoc = 533kg/m3

2. N1=12.19;
3. N2=13.99;
4. N3=0.005027;
5. N4=-18.93;
6. N5=-6.698;
7. N6=-3.827;
8. tao=Tc/T;
9. t1=0.42;
10. t2=0;
11. t3=0.95;
12. t4=0.5;
13. t5=0.9;
14. t6=0.8;
15. delta=density(p,T,R,Tc,pc)/rhoc;
16. d1=1;
17. d2=2;
18. d3=10;
19. d4=5;
20. d5=1;
21. d6=2;
22. l4=2;
23. l5=4;
24. l6=4;

```

```

25. abc=N1*tao^t1*delta^d1+N2*tao^t2*delta^d2+N3*tao^t3*delta^
    d 3 + N 4 * t a o ^ t 4 * d e l t a ^ d 4 * e x p ( -
    d e l t a ^ l 4 ) + N 5 * t a o ^ t 5 * d e l t a ^ d 5 * e x p ( -
    d e l t a ^ l 5 ) + N 6 * t a o ^ t 6 * d e l t a ^ d 6 * e x p ( - d e l t a ^ l 6 ) ;
26. y=abc*10^(-6);

```

(9) Evaluation of fluid viscosity (step (8) in MATLAB flow chart)

```

1. Function [y] = N_H(T,p,R,M,E,XGM,Tc,pc,rhoc)
    % Here, N_H(T,p,R,M,E,XGM,Tc,pc,rhoc) is the fluid viscosity
    in Pa.s.
    rhoc is the critical density in kg/m3.
    For Argon, rhoc= 533kg/m3
2. N1=12.19;
3. N2=13.99;
4. N3=0.005027;
5. N4=-18.93;
6. N5=-6.698;
7. N6=-3.827;
8. tao=Tc/T;
9. t1=0.42;
10. t2=0;
11. t3=0.95;
12. t4=0.5;
13. t5=0.9;
14. t6=0.8;
15. delta=density(p,T,R,Tc,pc)/rhoc;
16. d1=1;
17. d2=2;
18. d3=10;
19. d4=5;

```

```

20. d5=1;
21. d6=2;
22. l4=2;
23. l5=4;
24. l6=4;
25. Nr=N1*tao^t1*delta^d1+N2*tao^t2*delta^d2+N3*tao^t3*delta^d
    3 + N 4 * t a o ^ t 4 * d e l t a ^ d 4 * e x p ( -
    d e l t a ^ l 4 ) + N 5 * t a o ^ t 5 * d e l t a ^ d 5 * e x p ( -
    d e l t a ^ l 5 ) + N 6 * t a o ^ t 6 * d e l t a ^ d 6 * e x p ( - d e l t a ^ l 6 ) ;
26. y=N_L(T,M,E,XGM)+Nr*10^(-6);

```

(10) Evaluation of the thermal conductivity of dilute gas (step (13) in MATLAB flow chart)

```

1. Function [y] = lamd_0(T,M,E,XGM,Tc)
    % Here, lamd_0(T,M,E,XGM,Tc) is the thermal conductivity of
    dilute gas.
    Tc is the critical temperature in K.
    For Argon, Tc = 150.86 K.
2. N1=0.8158;
3. N2=-0.4320;
4. N3=0;
5. tao=Tc/T;
6. t2=-0.77;
7. t3=-1;
8. y=(N1*N_L(T,M,E,XGM)*10^6+N2*tao^t2+N3*tao^t3)*10^-3;

```

(11) Evaluation of the residual fluid thermal conductivity (step (13) in MATLAB flow chart)

```

1. Function [y] = lamd_r(T,p,R,Tc,pc,rhoc)
    % Here, lamd_r(T,p,R,Tc,pc,rhoc) is the residual thermal
    conductivity in W·m-1·K-1

```

```

2. N4=13.73;
3. N5=10.07;
4. N6=0.7375;
5. N7=-33.96;
6. N8=20.47;
7. N9=-2.274;
8. N10=-3.973;
9. tao=Tc/T;
10. t4=0;
11. t5=0;
12. t6=0;
13. t7=0.8;
14. t8=1.2;
15. t9=0.8;
16. t10=0.5;
17. delta=density(p,T,R,Tc,pc)/rhoc;
18. d4=1;
19. d5=2;
20. d6=4;
21. d7=5;
22. d8=6;
23. d9=9;
24. d10=1;
25. l7=2;
26. l8=2;
27. l9=2;
28. l10=4;
29. lamd_r=N4*tao^t4*delta^d4+N5*tao^t5*delta^d5+N6*tao^t6*del
    ta ^ d 6 + N 7 * t a o ^ t 7 * d e l t a ^ d 7 * e x p ( -
    d e l t a ^ l 7 ) + N 8 * t a o ^ t 8 * d e l t a ^ d 8 * e x p ( -
    d e l t a ^ l 8 ) + N 9 * t a o ^ t 9 * d e l t a ^ d 9 * e x p ( -
    d e l t a ^ l 9 ) + N 1 0 * t a o ^ t 1 0 * d e l t a ^ d 1 0 * e x p ( - d e l t a ^ l 1 0 );

```

30. $y = \text{lamd_r} \cdot 10^{-3};$

(12) Evaluation of the correlation length in thermal conductivity critical enhancement formula (step (4) in MATLAB flow chart)

```
1. Function y = ksi(T,p,R,Tc,pc,rhoc)
    % Here, ksi(T,p,R,Tc,pc,rhoc) is the correlation length in
    nm.
2. niu=0.63;
3. gama=1.2415;
    % Here, the niu and gama are theoretically base constants.
4. Tref=2*Tc;
    % Here, Tref is the reference temperature that is
    significantly above the critical temperature (in this work,
    Tref was taken as twice the critical temperature.)
5. ksi0=0.13;
6. L=0.055;
    % Here, ksi0 and L are fluid-specific (fitted) terms.

7. % Here, the original formula for X is as follows:
```

$$X = \tilde{\chi}(T, \rho) = \frac{p_c \rho}{\rho_c^2} \left(\frac{\partial \rho}{\partial p} \right)_T$$

```
X=(pc*density(p,T,R,Tc,pc)/rhoc^2)*(-
1/(1/3*R*T/p+140737488355328/531954372264637/p/T^(1/2)*(2*R
^3*T^(9/2)-9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2+(4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2)-
```

```

9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2))^(1/3) -
1/3*(17022539912468385/4503599627370496*p*T^(1/2)*(10687/25
000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2)) -
5674179970822795/4503599627370496*R^2*T^3)/p/T^(1/2)/(2*R^3
*T^(9/2)-9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2+(4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2) -
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2))^(1/3))^2*(-1/3*R*T/p^2-
140737488355328/531954372264637/p^2/T^(1/2)*(2*R^3*T^(9/2) -
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2+(4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2) -
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2))^(1/3)+140737488355328/1595863116793
911/p/T^(1/2)/(2*R^3*T^(9/2) -
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-

```

```

1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2+(4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2) -
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2))^(2/3)*(-
9*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+10556001/156250000*p*T^(5/2)*
R^3*Tc^2/pc^2+312498567/312500000*T*R^3*Tc^(7/2)/pc^2+1/2/(
4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2) -
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2)*(12*(3*p*T^(1/2)*(10687/25000*R^2*Tc
^(5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-
R^2*T^3)^2*(3*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-
3518667/156250000*p*T*R^2*Tc^2/pc^2)+2*(2*R^3*T^(9/2) -
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)*(-9*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+10556001/156250000*p*T^(5/2)*

```

```

R^3*Tc^2/pc^2+312498567/312500000*T*R^3*Tc^(7/2)/pc^2))-
1/3*(17022539912468385/4503599627370496*T^(1/2)*(10687/2500
0*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))-
3993109963079026322853/1407374883553280000000000*p*T*R^2*Tc^
2/pc^2)/p/T^(1/2)/(2*R^3*T^(9/2)-
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2+(4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2)-
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2))^^(1/3)+1/3*(17022539912468385/450359
9627370496*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))-
5674179970822795/4503599627370496*R^2*T^3)/p^2/T^(1/2)/(2*R
^3*T^(9/2)-9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2+(4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2)-
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2))^^(1/3)+1/9*(17022539912468385/450359
9627370496*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-

```



```

1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2)) -
5674179970822795/4503599627370496*R^2*T^3)/p/T^(1/2)/(2*R^3
*T^(9/2)-9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2+(4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2)-
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2))^(4/3)*(-
9*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+10556001/156250000*p*T^(5/2)*
R^3*Tc^2/pc^2+312498567/312500000*T*R^3*Tc^(7/2)/pc^2+1/2/(
4*(3*p*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-R^2*T^3)^3+(2*R^3*T^(9/2)-
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)^2)^(1/2)*(12*(3*p*T^(1/2)*(10687/25000*R^2*Tc
^(5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-
R^2*T^3)^2*(3*T^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -
1083/12500*R^2*Tc/pc*T^(3/2))-
3518667/156250000*p*T*R^2*Tc^2/pc^2)+2*(2*R^3*T^(9/2)-
9*p*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2) -

```

```
1083/12500*R^2*Tc/pc*T^(3/2))+312498567/312500000*p*T*R^3*T
c^(7/2)/pc^2)*(-9*T^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*T^(1/2)-
1083/12500*R^2*Tc/pc*T^(3/2))+10556001/156250000*p*T^(5/2)*
R^3*Tc^2/pc^2+312498567/312500000*T*R^3*Tc^(7/2)/pc^2)))));
```

8.

% Here, the original formula for X1 is as follows:

$$X1 = \tilde{\chi}(T_{ref}, \rho) = \frac{p_c \rho}{\rho_c^2} \left(\frac{\partial \rho}{\partial p} \right)_T \quad (In X1, T = T_{ref})$$

```
X1=(pc*density(p,T,R,Tc,pc)/rhoc^2)*(-
1/(1/3*R*Tref/p+140737488355328/531954372264637/p/Tref^(1/2)
)*(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2+(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(
5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2))^(1/3)-
1/3*(17022539912468385/4503599627370496*p*Tref^(1/2)*(10687
/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
5674179970822795/4503599627370496*R^2*Tref^3)/p/Tref^(1/2)/
(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
```

```

1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2+(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(
5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2))^(1/3))^2*(-1/3*R*Tref/p^2-
140737488355328/531954372264637/p^2/Tref^(1/2)*(2*R^3*Tref^
(9/2)-9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2+(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(
5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2))^(1/3)+140737488355328/1595863
116793911/p/Tref^(1/2)/(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2+(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(
5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref

```

```

*R^3*Tc^(7/2)/pc^2)^2)^(1/2))^(2/3)*(-
9*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+10556001/156250000*p*Tref^
(5/2)*R^3*Tc^2/pc^2+312498567/312500000*Tref*R^3*Tc^(7/2)/p
c^2+1/2/(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2)*(12*(3*p*Tref^(1/2)*(10687/250
00*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^2*(3*Tref^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
3518667/156250000*p*Tref*R^2*Tc^2/pc^2)+2*(2*R^3*Tref^(9/2)
-9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)*(-
9*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+10556001/156250000*p*Tref^
(5/2)*R^3*Tc^2/pc^2+312498567/312500000*Tref*R^3*Tc^(7/2)/p
c^2)))-
1/3*(17022539912468385/4503599627370496*Tref^(1/2)*(10687/2
5000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-

```

```

1083/12500*R^2*Tc/pc*Tref^(3/2))-
3993109963079026322853/1407374883553280000000000*p*Tref*R^2*
Tc^2/pc^2)/p/Tref^(1/2)/(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2+(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(
5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2))^(1/3)+1/3*(17022539912468385/
4503599627370496*p*Tref^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
5674179970822795/4503599627370496*R^2*Tref^3)/p^2/Tref^(1/2
)/(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2+(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(
5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2)-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2))^(1/3)+1/9*(17022539912468385/
4503599627370496*p*Tref^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-

```

```

1083/12500*R^2*Tc/pc*Tref^(3/2))-
5674179970822795/4503599627370496*R^2*Tref^3)/p/Tref^(1/2)/
(2*R^3*Tref^(9/2))-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2+(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(
5/2)/pc-1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2))-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2))^(4/3)*(-
9*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+10556001/156250000*p*Tref^
(5/2)*R^3*Tc^2/pc^2+312498567/312500000*Tref*R^3*Tc^(7/2)/p
c^2+1/2/(4*(3*p*Tref^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^3+(2*R^3*Tref^(9/2))-
9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)^2)^(1/2)*(12*(3*p*Tref^(1/2)*(10687/250
00*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))-
R^2*Tref^3)^2*(3*Tref^(1/2)*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2))-
1083/12500*R^2*Tc/pc*Tref^(3/2))-

```

```

3518667/156250000*p*Tref*R^2*Tc^2/pc^2)+2*(2*R^3*Tref^(9/2)
-9*p*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+312498567/312500000*p*Tref
*R^3*Tc^(7/2)/pc^2)*(-
9*Tref^2*R*(10687/25000*R^2*Tc^(5/2)/pc-
1172889/156250000*p*R^2*Tc^2/pc^2*Tref^(1/2)-
1083/12500*R^2*Tc/pc*Tref^(3/2))+10556001/156250000*p*Tref^
(5/2)*R^3*Tc^2/pc^2+312498567/312500000*Tref*R^3*Tc^(7/2)/p
c^2)))));
9. y=ksi0*((X-X1*Tref/T)/L)^(niu/gama);

```

(13) Evaluation of the parameter $\tilde{\Omega}$ in thermal conductivity critical enhancement formula (step (13) in MATLAB flow chart)

```

1. Function y = OMG2(T,p,R,M,Tc,pc,rhoc)
    % Here, OMG2(T,p,R,M,Tc,pc,rhoc) is the parameter  $\tilde{\Omega}$  in
    thermal conductivity critical enhancement formula
2. qD=0.32;
    % Here, qD is fluid-specific (fitted) term.
3. Cv=Cp(M)-R;
    % Here, Cv is the isochoric heat capacity in J/(kg·K).
    R is the specific gas constant.
4. y=(2/pi)*((Cp(M)-
    Cv)/Cp(M))*atan(ksi(T,p,R,Tc,pc,rhoc)/qD)+(Cv/Cp(M))*ksi(T
    ,p,R,Tc,pc,rhoc)/qD);

```

(14) Evaluation of the parameter $\tilde{\Omega}_0$ in thermal conductivity critical enhancement formula (step (13) in MATLAB flow chart)

```
1. Function y = OMG2_0(T,p,R,M,Tc,pc,rhoc)
   % Here, OMG2_0(T,p,R,M,Tc,pc,rhoc) is the parameter  $\tilde{\Omega}_0$  in
   % thermal conductivity critical enhancement formula
2. qD=0.32;
3. Cv=Cp(M)-R;
4. y=(2/pi)*(1-exp((-1)/((ksi(T,p,R,Tc,pc,rhoc)/qD)^(-
   1)+(1/3)*(ksi(T,p,R,Tc,pc,rhoc)/qD)^2*(rhoc/density(p,T,R,T
   c,pc))^2))));
```

(15) Evaluation of the thermal conductivity critical enhancement (step (13) in MATLAB flow chart)

```
1. Function [y] = lamd_c(T,p,R,M,E,XGM,Tc,pc,rhoc)
   % Here, lamd_c(T,p,R,M,E,XGM,Tc,pc,rhoc) is the thermal
   % conductivity critical enhancement in  $W \cdot m^{-1} \cdot K^{-1}$ 
2. k=1.380658*10^-23;
   % Here, k is Boltzman's constant.
3. R0=1.01;
   % Here, R0 is theoretically based constant.
4. Cv=Cp(M)-R;
5. OMG=(2/pi)*((Cp(M)-
   Cv)/Cp(M))*atan(ksi/qD)+(Cv/Cp(M))*(ksi/qD);
6. OMG0=(2/pi)*(1-exp((-1)/((ksi/qD)^(-
   1)+(1/3)*(ksi/qD)^2*(rhoc/density(p,T,R,Tc,pc))^2)))));
7. lamd_c=density(p,T,R,Tc,pc)*Cp(M)*(k*R0*T)/(6*pi*ksi(T,p,R,
   Tc,pc,rhoc)*N_H(T,p,R,M,E,XGM,Tc,pc,rhoc))*(OMG-OMG0);
8. y=lamd_c*10^-3;
```

(16) Evaluation of the thermal conductivity (step (13) in MATLAB flow chart)

```
1. Function y = lamd(T,p,R,M,E,XGM,Tc,pc,rhoc)
```



```
% Here, lamd(T,p,R,M,E,XGM,Tc,pc,rhoc) is the thermal
conductivity in  $W \cdot m^{-1} \cdot K^{-1}$ 
2. y=(lamd_0(T,M,E,XGM,Tc)+lamd_r(T,p,R,Tc,pc,rhoc)+lamd_c(T,p
,R,M,E,XGM,Tc,pc,rhoc))*10^-3;
% Here, lamd_0(T,M,E,XGM,Tc) is the thermal conductivity of
dilute gas
lamd_r(T,p,R,Tc,pc,rhoc) is the residual fluid thermal
conductivity
lamd_c(T,p,R,M,E,XGM,Tc,pc,rhoc) is the thermal
conductivity critical enhancement.
```

(17) Evaluation of the Reynolds number (step (14) in MATLAB flow chart)

```
1. Function [y] = Re(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal)
% Here, Re(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal) is the
Reynolds number.
Wc is the crack opening displacement (or crack width)
alfa is the crack surface angle relative to the crack
direction through wall
Rglobal is global roughness
2. L=2*Wc;
% Here, L is the characteristic length in m
3. y=density(p,T,R,Tc,pc)*v(T,p,R,Tc,pc,Wc,alfa,Rglobal)*L/N_H
(T,p,R,M,E,XGM,Tc,pc,rhoc);
% Here, density(p,T,R,Tc,pc) is the density of fluid
v(T,p,R,Tc,pc,Wc,alfa,Rglobal) is the velocity of fluid
N_H(T,p,R,M,E,XGM,Tc,pc,rhoc) is the viscosity of fluid
```

(18) Evaluation of the Prandtl number (step (9) in MATLAB flow chart)

```
1. Function [y] = Pr(T,p,R,M,E,XGM,Tc,pc,rhoc)
% Here, Pr(T,p,R,M,E,XGM,Tc,pc,rhoc) is the Prandtl number.
```

```

2. R1=8.31;
3. Cp(M)=2.5*R1/M*10^3;
   % Here, R1 is the universal gas constant in J/(K.mol)
   Cp(M) is the isobaric heat capacity in J/(kg.K)
   M is the molar mass in g/mol
4. y=N_H(T,p,R,M,E,XGM,Tc,pc,rhoc)*Cp(M)/lamd(T,p,R,M,E,XGM,Tc,pc,rhoc);
   % Here, lamd(T,p,R,M,E,XGM,Tc,pc,rhoc) is the thermal conductivity.

```

(19) Evaluation of the Nusselt number (step (11) in MATLAB flow chart)

```

1. Function [y] = Nu(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal)
   % Here, Nu(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal) is the Nusselt number.
2. C=7.6*10^-5;
3. D0=1.164e-3;
4. F=C*Re(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal)*(1-(Wc/D0)^2);
5. f=(1.82*log10(Re(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal))-1.64)^-2;
   % Here, f is the friction factor.
6. NuGn=(f/8)*(Re(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal)-1000)*Pr(T,p,R,M,E,XGM,Tc,pc,rhoc)/(1+12.7*(f/8)^0.5*((Pr(T,p,R,M,E,XGM,Tc,pc,rhoc))^(2/3)-1));
   % Here, Re(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal) is the Reynolds number
   Pr(T,p,R,M,E,XGM,Tc,pc,rhoc) is the Prandtl number.
7. y=NuGn*(1+F);

```

(20) Evaluation of the heat transfer coefficient (step (7) in MATLAB flow chart)

1. `Function [y] = h(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal)`
 `% Here, h(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal) is the`
 `heat transfer coefficient in W/m2·K`
2. `L=2*Wc;`
 `% Here, L is characteristic length in m`
3. `y=Nu(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal)*lamd(T,p,R,M`
 `,E,XGM,Tc,pc,rhoc)/L;`
 `% Here, Nu(T,p,R,M,E,XGM,Tc,pc,rhoc,Wc,alfa,Rglobal) is the`
 `nusselt number`
 `lamd(T,p,R,M,E,XGM,Tc,pc,rhoc) is the thermal conductivity.`

APPENDIX II RISK ASSESSMENT REPORT OF THE EXPERIMENT

School of Mechanical & Aerospace Engineering

Updated 21 July 2010

RISK ASSESSMENT FORM									
Workplace/ location:		Thermal Spray Lab			Project Supervisor		A/P Ng Heong Wah		
Process / Equipment:		Test rig of Joule-Thomson effect / N4-B4a-02, the southernmost room			Conducted by: (Name, Designation, Signature & date)		Researcher/ Others		
Approved By: Division HOD		A/P Du Hejun Name/ Signature / Date: 15/3/11 Assoc Prof Du Hejun Head, Engineering Mechanics Division			Staff (Equipment IC)		Ai Gang, Lee Kim Hua		
Form No:		Revision No:			Lab PIC		Lab TIC		
Date conducted:		10 March 2011			Next Review Date:		10 March 2012		
1. Hazard Identification				2. Risk Evaluation (Using 5 x 5 matrix)				3. Risk Control	
1a.	1b.	1c.	1d.	2a.	2b.	2c.	2d.	3a.	3b.
S/N	Work Activity	Hazard	Possible accident / ill health to persons, fire or property loss	Existing Risk Control	Severity	Likelihood	Risk Level	Additional control measures	Follow up by (name & date)
1	Assemble the test rig of Joule-Thomson effect	Struck by falling object	Injury	Gloves & covered shoes	Marginal	Occasional	Low	NIL	Ay, 16 March, 2011 Ai Gang
2	Turn on the ventilation equipment	NIL	NIL	NIL	Negligible	Unlikely	Low	NIL	
3	Open the valves of nitrogen gas supply cylinders	NIL	NIL	NIL	Negligible	Unlikely	Low	NIL	

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4	Adjust the gas pressure to the desired level	High pressure	Pipe burst	Control gas pressure far below pipe allowable pressure	Marginal	Remote	Low	NIL	Ay, 16 March, 2011 Ai Gang.
5	Press data logger button to print data	NIL	NIL	NIL	Negligible	Unlikely	Low	NIL	
6	Turn off the valve of nitrogen gas supply cylinder after collecting enough data	NIL	NIL	NIL	Negligible	Unlikely	Low	NIL	
7	Turn off the ventilation equipment after 1 h	NIL	NIL	NIL	Negligible	Unlikely	Low	NIL	

**Record to be filed by Lab TIC/ DY for 3 years

Figure App II-1: Risk assessment report of the experiment

APPENDIX IIIa DESIGN OF PRESSURE VESSEL

The main part of Joule-Thomson test rig is the pressure vessel. The pressure retaining components of pressure vessel in this research include cylindrical shell, hemispherical head, nozzles and flanges. Each component is designed according to ASME Boiler and Pressure Vessel Code Section VIII, Division 1^[1] and Section II: Part D^[118].

Two distinct types of gasket material are given for comparison in calculation to select a suitable one in present research.

Table IIIa-1: Material specification of shell, hemispherical head, flange and nozzle

Nominal Composition	C
Spec. No.	SA-53
Type/Grade	S/A
Alloy Design. /UNS No.	K02504
Min. Tensile Stress (ksi)	48
Min. Yield Stress (ksi)	30
Max. Allowable Stress (ksi) at -20 to 100 °F	12.0

Table IIIa-2: Material specification of bolting

Nominal Composition	Spec. No.	Min. Tensile Stress (ksi)	Min. Yield Stress (ksi)	Max. Allowable Stress (ksi) at -20 to 100 °F
C	SA-325	105	81	20.2

Table IIIa-3: Material specification of gasket

Type	Gasket Material	Gasket Factor m	Min. Design Seating Stress y (psi)	Basic Gasket Seating width, b_0	Effective Gasket Seating Width, b
1	Elastomers without fabric or high percent of asbestos fiber, 75A or higher Shore Durometer	1.00	200	$N/2$ (where N is the possible contact width of the gasket)	$b = b_0$, when $b_0 \leq \frac{1}{4}$ in; $b = 0.5\sqrt{b_0}$, when $b_0 > \frac{1}{4}$ in; as shown in Figure IIIa-1.
2	Spiral-wound metal, asbestos filled, Stainless, Monel, and nickel-base alloys	3.00	10,000	$N/2$

Figure IIIa-1: Location of gasket load reaction

- **Hemispherical head of pressure vessel**

When the thickness of a hemispherical head does not exceed $0.356L$, or P does not exceed $0.665SE$, the following formulas shall apply^[1]:

$$t_h = \frac{PL}{2SE - 0.2P} \quad \text{or} \quad P = \frac{2SEt_h}{L + 0.2t_h}$$

where t_h = minimum required thickness of hemispherical head after forming, in

L = inside spherical or crown radius, in

p = internal design pressure, psi

S = maximum allowable stress value, psi

E = joint efficiency for, or the efficiency of, appropriate joint in cylindrical or spherical shells, or the efficiency of ligaments between openings, whichever is less.^[1]

The input values for the calculation of the thickness of hemispherical head of pressure vessel are as follows:

$$p = 3625.9436 \text{ psi (250 bar)}$$

$$L = 3.5005 \text{ in (I.D. = 7.001 in)}$$

$$S = 1.2 \times 10^4 \text{ psi}$$

$$E = 0.65$$

So the minimum required thickness of hemispherical head after forming is

$$t_h = \frac{PL}{2SE - 0.2P} = \frac{3625.9436 \times \frac{7.001}{2}}{2 \times 12 \times 1000 \times 0.65 - 0.2 \times 3625.9436} = 0.8533 \text{ in}$$

Nominal thickness used in present research is 0.875 in.^[126]

- **Cylindrical shell and nozzles of pressure vessel**

For longitudinal stress (circumferential joints) case in cylindrical shell and nozzles design of pressure vessel:

When the thickness of a cylindrical shell (or nozzle) does not exceed one-half of the inside radius, or P does not exceed $1.25SE$, the following formulas shall apply:

$$t_s = \frac{PR}{2SE + 0.4P} \quad \text{or} \quad P = \frac{2SEt_s}{R - 0.4t_s} \quad (6-1)$$

where t_s = minimum required thickness of cylindrical shell (or nozzle), in

p = internal design pressure, psi

R = inside radius of the shell (or nozzle) under consideration, in

S = maximum allowable stress value, psi

E = joint efficiency for, or the efficiency of, appropriate joint in cylindrical or spherical shells, or the efficiency of ligaments between openings, whichever is less.^[1]

Cylindrical shell

The input values for the calculation of the thickness of cylindrical shell of pressure vessel are as follows:

$$p = 3625.9436 \text{ psi (250 bar)}$$

$$R = 3.5005 \text{ in (I.D. = 7.001 in)}$$

$$S = 1.2 \times 10^4 \text{ psi}$$

$$E = 0.60$$

So the minimum required thickness of cylindrical shell after forming is

$$t_s = \frac{PR}{2SE + 0.4P} = \frac{3625.9436 \times \frac{7.001}{2}}{2 \times 12 \times 1000 \times 0.6 + 0.4 \times 3625.9436} = 0.8008 \text{ in.}$$

Note: For easy fabrication, the thickness of hemispherical head has been rounded up to same thickness of 0.875 in^[126].

The nozzle on pressure vessel shell

The input values for the calculation of the thickness of the nozzle on pressure vessel shell are as follows:

$$p = 3625.9436 \text{ psi (250 bar)}$$

$$R = 0.125 \text{ in (I.D. = 1/4 in)}$$

$$S = 1.2 \times 10^4 \text{ psi}$$

$$E = 0.65$$

So the minimum required thickness of the nozzle on pressure vessel wall after forming is

$$t_n = \frac{PR}{2SE + 0.4P} = \frac{3625.9436 \times \frac{0.25}{2}}{2 \times 12 \times 1000 \times 0.65 + 0.4 \times 3625.9436} = 0.027 \text{ in}$$

For the thick part of this nozzle, nominal thickness used is $\frac{3}{4}$ in. For the thin part of this nozzle, nominal thickness used is 0.2 in.^[1, 126]

The nozzle on hemispherical head of pressure vessel

The input values for the calculation of the wall thickness of the nozzle on hemispherical head of pressure vessel are as follows:

$$p = 3625.9436 \text{ psi (250 bar)}$$

$$R = 0.25 \text{ in (I.D. = } 1/2 \text{ in)}$$

$$S = 1.2 \times 10^4 \text{ psi}$$

$$E = 0.65$$

So the minimum required thickness of the nozzle on hemispherical head of pressure vessel after forming is

$$t_n = \frac{PR}{2SE + 0.4P} = \frac{3625.9436 \times \frac{0.5}{2}}{2 \times 12 \times 1000 \times 0.65 + 0.4 \times 3625.9436} = 0.054 \text{ in}$$

Note: For easy fabrication, the wall thickness of the nozzle on hemispherical head takes same nominal thickness as the nozzle on cylindrical shell. For the thick part of this nozzle, nominal thickness used is $\frac{3}{4}$ in. For the thin part of this nozzle, nominal thickness used is 0.2 in.^[1, 126]

- **Flange of pressure vessel**

The minimum required thickness of flange in present research is calculated by the formula:

$$t_f = d \sqrt{\frac{CP}{SE} + \frac{1.9Wh_G}{SEd^3}}$$

where t_f = minimum required thickness of circular flat plate or blind flange, in

d = diameter, or short span, in

C = a factor depending upon the method of attachment of head, shell dimensions, and other items, dimensionless

h_G = gasket moment arm, equal to the radial distance from the center line of the bolts to the line of the gasket reaction, as shown in Table 2-5.2 in reference^[1], in. $h_G = \frac{C-G}{2}$, where G is diameter, at location of gasket load reaction, in

W = flange design bolt load, for the operating conditions or gasket seating, as may apply, lb

(1) For operating conditions,

$$W = W_{m1}$$

where W_{m1} = minimum required bolt load for the operating conditions, lb.

$$W_{m1} = H + H_p = 0.785G^2P + (2b \times 3.14GmP)$$

Symbols	Description	Definition
H	total hydrostatic end force, lb	$\frac{\pi}{4} G^2 P$
H_p	total joint-contact surface compression load, lb	$2b\pi GmP$
G	diameter, at location of gasket load reaction, in	<p>(1) when $b_0 \leq \frac{1}{4}$ in., G = mean diameter of gasket contact face, in.</p> <p>(2) when $b_0 > \frac{1}{4}$ in., G = outside diameter of gasket contact face less $2b$, in.</p> <p>(3) where b_0 = basic gasket seating width, in.</p>
b	effective gasket seating width, in	<p>(1) when $b_0 \leq \frac{1}{4}$ in., $b = b_0$, in.</p> <p>(2) when $b_0 > \frac{1}{4}$ in., $b = 0.5\sqrt{b_0}$, in.</p>
m	gasket factor	

(2) For gasket seating,

$$W = \frac{(A_m + A_b)S_a}{2} \quad (6-2)$$

Symbols	Description	Definition
A_m	Total required cross-sectional area of bolts, taken as the greater of A_{m1} and A_{m2} , sq in.	<p>A_{m1} is total cross-sectional area of bolts at root of thread or section of last diameter under stress, required for the operating conditions, sq in.</p> $A_{m1} = W_{m1}/S_b$ <p>where W_{m1} is minimum required bolt load for the operating conditions, lb; S_b is allowable bolt stress at design temperature, psi</p>
		<p>A_{m2} is total cross-sectional area of bolts at root of thread or section of last diameter under stress, required for gasket seating, sq in.</p> $A_{m2} = W_{m2}/S_a$ <p>where S_a is allowable bolt stress at atmosphere temperature, psi; W_{m2} is minimum required bolt load for gasket seating, lb</p> $W_{m2} = \pi b G y$
A_b	Total actual bolt area, sq in.	-
S_a	Allowable bolt stress at atmosphere temperature, psi	-

- **Calculation procedure of the minimum required thickness of the flange of pressure vessel**

Calculation condition: cylindrical shell I.D.=7.001 in., design pressure = 250 bar (3625.94 psi).

Figure App IIIa-2: Location of gasket load reaction ($b_o > 1/4$ in.)

The calculation steps of minimum flange thickness are as follows:

- (1) The allowable tensile stress of the bolts from ASME Boiler and Pressure Vessel Code Section II Part D^[118] at gasket seating and operating conditions (design temperature) is $S_a = S_b = 20.2$ ksi

- (2) The allowable tensile stress of the flange from ASME Boiler and Pressure Vessel Code Section II Part D^[118] at gasket seating and operating conditions (design temperature) is $S_{fa} = S_{fo} = 12.0$ ksi
- (3) Gasket is spiral-wound metal, asbestos filled (type 2 of gasket material), 7.001 in. I.D. $\times$ 1.0 in. wide. (the reason of the selection of gasket material is explained by the following Step (5))

The diameter of the gasket's line-of-action, G , is determined as follows:

$$N = 1.0 \text{ in.}, b_0 = N/2 = 0.5 \text{ in.},$$

$$\text{As } b_0 > 1/4 \text{ in.}, b = 0.5\sqrt{b_0} \approx 0.3535 \text{ in}$$

$$G = 7 + (2 \times 1.0) - (2 \times 0.3535) = 8.293 \text{ in}$$

- (4) With $N = 1$, $b = 0.3535$, $m = 3.0$, and $y = 10,000$, the bolt loadings and the number and diameter of bolts are

$$H = \frac{\pi}{4} G^2 p = \left(\frac{\pi}{4}\right) \times 8.293^2 \times (3625.9436) \approx 195854.8 \text{ lb}$$

$$H_p = 2b\pi Gmp = 2 \times 0.3535 \times \pi \times 8.293 \times 3.0 \times 3625.9436 \approx 200365.6 \text{ lb}$$

$$W_{m1} = H + H_p = 195854.8 + 200365.6 \approx 396220.4 \text{ lb}$$

$$W_{m2} = \pi b G y = \pi \times 0.3535 \times 8.293 \times 10,000 \approx 92098.16 \text{ lb}$$

$$A_m = \text{the larger of } A_{m1} (=W_{m1}/S_b) \text{ or } A_{m2} (=W_{m2}/S_a)$$

$$A_{m1} = W_{m1}/S_b$$

$$= 396220.4 / (20.2 \times 1000)$$

$$\approx 19.6 \text{ in}^2$$

$$A_{m2} = W_{m2}/S_a$$

$$= 92098.16 / 20,200$$

$$\approx 4.559 \text{ in}^2$$

So $A_m = 19.6 \text{ in}^2$

Outside diameter of flange (r)	19	
Bolt size	1.625	
8-thread Series	No. of Threads	8
	Root Area	1.68
Bolt Spacing	Minimum B_s	3.5
Bolt circle diameter (C_b)	15.5	
Minimum Radial Distance (R_m)	2.125	
Edge Distance (E)	1.625	
Nut Dimension (across flats)	2.5625	
Maximum Fillet Radius at base of hub	0.625	

A_b = actual bolt area

$$= 12 \times 1.68$$

$$\approx 20.16 \text{ in}^2$$

For gasket seating condition

$$W = 0.5(A_m + A_b)S_a$$

$$= 0.5 \times (19.6 + 20.16) \times 20,200$$

$$= 401576 \text{ lb}$$

For operating condition

$$W = W_{m1} = 396220.44 \text{ lb}$$

(5) Gasket crushout width

If the gasket material is elastomer without fabric or high percent of asbestos fiber (type 1 of gasket material),

$$N_{min} = \frac{A_b S_a}{2y\pi G} = \frac{20.16 \times 20.2 \times 1000}{2 \times 200 \times \pi \times 8.293} = 39.077 \text{ in} > 1.0 \text{ in actual}$$

If gasket is Spiral-wound metal, asbestos filled (type 2 of gasket material),

$$N_{min} = \frac{A_b S_a}{2y\pi G} = \frac{20.16 \times 20.2 \times 1000}{2 \times 10,000 \times \pi \times 8.293} = 0.78 \text{ in} < 1.0 \text{ in actual}$$

Therefore, type 2 of gasket material is selected in present research.

(6) The total flange moment for gasket seating condition is:

Flange load

$$H_G = W_a = 401576 \text{ lb}$$

Lever Arm

$$h_G = \frac{C_b - G}{2} = \frac{15.5 - 8.293}{2} = 3.6 \text{ in}$$

Flange Moment

$$\begin{aligned} M_G &= H_G \times h_G \\ &= 401576 \times 3.6 \\ &= 1445673.6 \text{ in. lb} \end{aligned}$$

(7) The total flange moment for operating condition is:

Flange loads

$$\begin{aligned} H_D &= (\pi/4)B^2p \\ &= (\pi/4)7^2(3625.9436) \\ &= 139542.66 \text{ lb} \\ H_G &= H_p = 200365.6 \text{ lb} \end{aligned}$$

$$\begin{aligned}
 H_T &= H - H_D \\
 &= 195854.8 - 139542.66 \\
 &= 56312.14 \text{ lb}
 \end{aligned}$$

Lever Arms

$$\begin{aligned}
 h_D &= 0.5(C_b - B) = 0.5 \times (15.5 - 7.001) = 4.25 \text{ in} \\
 h_G &= 0.5(C_b - G) = 0.5 \times (15.5 - 8.293) = 3.6 \text{ in} \\
 h_T &= 0.5(h_D + h_G) = 0.5 \times (4.25 + 3.6) = 3.925 \text{ in}
 \end{aligned}$$

Flange moments

$$\begin{aligned}
 M_D &= H_D \times h_D = 139542.66 \times 4.25 = 593056.305 \text{ in. lb} \\
 M_G &= H_G \times h_G = 200365.6 \times 3.6 = 721316.16 \text{ in. lb} \\
 M_T &= H_T \times h_T = 56312.14 \times 3.925 = 221025.15 \text{ in. lb} \\
 M_0 &= M_D + M_G + M_T = 1535397.615 \text{ in. lb}
 \end{aligned}$$

- (8) Shape factor from Appendix 2 of ASME Boiler and Pressure Vessel Code Section VIII, Division 1^[1] is $K = A/B = 19/7 = 2.714$

Using the equation of Y factor from Fig. 2-7.1 of ASME Boiler and Pressure Vessel Code Section VIII, Division 1^[1],

$$Y = \frac{1}{K-1} \left[0.66845 + 5.71690 \frac{K^2 \log_{10} K}{K^2 - 1} \right] = 2.06$$

- (9) The minimum required thickness of the flange is the larger $t_{\min}$ of gasket seating condition and operating condition:

For gasket seating condition:

$$t_{\min} = \sqrt{\frac{M_G Y}{S_{fa} B}} = \sqrt{\frac{721316.16 \times 2.06}{12,000 \times 7}} = 4.206 \text{ in}$$

For operating condition:

$$t_{min} = \sqrt{\frac{M_o Y}{S_{fo} B}} = \sqrt{\frac{1535397.615 \times 2.06}{12,000 \times 7}} = 6.136 \text{ in}$$

Therefore, $t_{min} = 6.136 \text{ in}$.

• **Calculation results for thicknesses of pressure retaining components of pressure vessel**

According to ASME Boiler and Pressure Vessel Code Section II: Part D^[118] and Section VIII, Division 1^[1], the calculation results of minimum required thicknesses of pressure retaining components of pressure vessel at the design pressure of 250 bar are shown in Table Table IIIa-4. The engineering drawings for the fabrication of Joule-Thomson test rig is presented in Appendix III.

Table IIIa-4: Dimensions of pressure retaining components of pressure vessel at the design pressure of 250 bar

Inside diameter of cylindrical shell (in.)	Minimum required thicknesses of different parts (in.)				
	t_s (cylindrical shell) (E = 0.6)	t_h (hemispherical head) (E = 0.65)	t_n (nozzle) (E = 0.65)		t_f (flange)
I.D.: 7.001	0.8008	0.8533	on shell	on head	6.136
			0.027 (I.D. = 0.25)	0.054 (I.D. = 0.5)	
	Nominal thickness used is 0.875 ^[126] O.D.: 8.751 I.D.: 7.001	Nominal thickness used is 0.875 ^[126] O.D.: 8.751 I.D.: 7.001	Nominal thickness Thick part= ¾ O.D.: 1.75 I.D.: 0.25 Thin part = 0.2 O.D.: 0.65 I.D.: 0.25	Nominal thickness Thick part= ¾ O.D.: 2.00 I.D.: 0.50 Thin part = 0.2 O.D.: 0.90 I.D.: 0.50

Nanyang Technological University		
TITLE: Pressure vessel	SCALE: 1:5	DRAWN:
DWG NO:	DATE:	
MATERIAL:	PROJ:	ALL DIMENSIONS IN INCH

Figure App IIIa-3: Overall view of pressure vessel with manifold casing

APPENDIX IIIb ENGINEERING DRAWINGS FOR THE FABRICATION OF PRESSURE VESSEL

Figure App IIIb-1: Cross-section view of test equipment

Figure App IIIb-2: Components of pressure vessel

Figure App IIIb-3: Engineering drawing of upper flange

Figure App IIIb-4: Engineering drawing of test plate

Figure App IIIb-5: Engineering drawing of gasket

Figure App IIIb-6: Engineering drawing of lower flange

Figure App IIIb-7: Engineering drawing of bolts

Figure App IIIb-8: Engineering drawing of manifold casing

Figure App IIIb-9: Engineering drawing of the door of manifold casing

Figure App IIIb-10: Engineering drawing of pressure vessel

Figure App IIIb-11: Welding requirement between hemispherical head and cylindrical shell

Figure App IIIb-12: Welding requirement between flange and cylindrical shell

Figure App IIIb-13: Welding requirement between nozzle and hemispherical head

Figure App IIIb-14: Welding requirement between nozzle and cylindrical shell

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