Study on heat transfer process during leaks of high pressure argon through a realistic crack

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Abstract:

This paper proposes a method for simulating the heat transfer process of high pressure argon gas leaking through a narrow crack which causes the Joule-Thomson cooling effect (JT cooling effect). A once-through (decoupled) model was developed to firstly calculate the gas pressure drop at different crack depth, followed by the temperature drop. A MATLAB code was also developed to iteratively calculate the properties of leaking gas in a crack which was fitted as formula as boundary conditions in heat transfer simulation in COMSOL program. The simulated lowest temperature of the test plate in the vicinity of the crack is 13.8 °C after decreasing from the temperature of 30 °C with initial argon gas pressure of 91 bar. An experiment test rig designed and tested under the same conditions showed a good agreement between the simulation and experiment at the obtained lowest temperature in the test plate. The method is useful for predicting the lowest temperature in the vicinity of the crack caused by the JT cooling effect.

Keywords: cracks, leakage, Joule-Thomson cooling effect, heat transfer simulation

Nomenclature

Latin characters

A	cross-section area, m^2
$a_0, a_1, a_2, \text{ and } a_3$	empirical constants of gas property dependent
C_p	heat capacity at constant pressure, $J/(kg \cdot K)$
D	diameter of microchannels, m
D_e	equivalent diameter, m
dp	pressure drop per depth increment into the crack, Pa or bar
f	friction factor
H	Enthalpy, J
h	heat transfer coefficient, $W/(m^2 \cdot K)$
L	characteristic length, m
M	molar mass, g/mol
N_u	Nusselt number
Nu_{Gn}	Gnielinski modified Nusselt number
P	wetting perimeter, m
p	pressure, Pa or bar
Pr	Prandtl number
Re	Reynolds number
R_{eff}	effective 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_{global}	global roughness, m or μm
R_{local}	local roughness, m or μm
T	temperature, K or $^{\circ}C$
t	crack through-wall thickness (or crack depth), m or mm
t_{eff}	effective crack through-wall thickness, m or mm
v	fluid velocity, m/s
W_c	crack opening displacement (or crack width) perpendicular to the through-wall direction, m or mm

W_{ceff}	effective crack width perpendicular to the average flow direction, m or mm
Greek characters	
α	crack surface angle relative to the crack direction through wall, rad
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
Δp_{recirc}	recirculation term of pressure loss during fluid flowing through a crack, Pa or bar
η	dynamic viscosity, $\mu\text{Pa}\cdot\text{s}$
θ	average flow direction relative to the crack direction through-wall, rad
λ	thermal conductivity, $\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
λ^{c}	thermal conductivity critical enhancement, $\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
λ^0	dilute gas thermal conductivity, $\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
λ^{r}	residual fluid thermal conductivity, $\text{mW}\cdot\text{m}^{-1}\cdot\text{K}^{-1}$
μ_{JT}	Joule-Thomson coefficient, K/Pa or $^{\circ}\text{C}/\text{bar}$
$\hat{v}$	specific volume (which is the reciprocal of density), m^3/kg
ρ	fluid density, kg/m^3

1. Introduction

Natural gas now plays an important strategic role in energy supply as global energy demand rises. The price and environmental advantages render natural gas as one of the most acceptable forms of energy. However, it is more difficult to transport and store gas than oil and therefore it lagged behind oil for a considerable period.^[2-4] In natural gas transportation, large market reserves mainly rely on Pipelined Natural Gas (PNG) and Liquefied Natural Gas (LNG) transportation technologies. However, 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

1 market, lack of transport economy or conversion technology. Neither PNG nor LNG
2 transportation technique can economically exploit these stranded gas reserves.

3 Compressed Natural Gas (CNG) transportation can be considered as a niche that will
4 supplement both PNG and LNG technologies for the monetization of stranded gas. The basic
5 idea of CNG is to compress the natural gas at pressures between 100 and 250 bar, and sometimes
6 chill it to lower temperatures (up to $-40\text{ }^{\circ}\text{C}$). In CNG projects, the gas is stored in high pressure
7 piping or coils inside the CNG ships (up to 250 bar), therefore the reliability of pressure vessel
8 and careful design of CNG transport fleets are very important.

9 The critical technology to maintain the integrity of pressure vessels is the concept of leak-
10 before-break (LBB).^[5-10] The LBB technology **applied** in nuclear industry can be transplanted
11 into CNG systems, although there are significant differences. For CNG system with leakage on
12 the container wall, the temperature of leaking CNG will drop due to Joule-Thomson (JT) cooling
13 effect when CNG passes through the crack. This will chill the vessel wall in the vicinity of the
14 crack and reduce the fracture toughness of the wall. This may push the transition of previously
15 stable crack propagation to become critical. Therefore, it is necessary to assess the impact of the
16 JT cooling effect in cracks on the LBB approach and on the safety and reliability of pressure
17 vessels.

18 There are very few papers on this research topic. The challenges in this study are how to
19 develop a model to represent the JT effect in narrow and tortuous cracks and to evaluate the
20 pressure and temperature drop of leaking gas through cracks. Many factors such as crack
21 opening displacement, crack surface angle, crack turns, surface roughness and temperature
22 dependent properties of the gas critically affect the process. This paper presents an acceptable
23 crack model to calculate the temperature and heat transfer coefficient of leaking gas through a
24 crack and then simulate the metal temperature distribution in the vicinity of the crack.

25 **2. Summary of the experimental work**

26 An experimental study of the JT effect reported in Ai and Ng^[11] was conducted with argon
27 gas. Argon is safer as it is inert compared to flammable methane, the major constituent of natural
28 gas, and it possesses a similar JT coefficient to that of methane.^[12-16] A pressure vessel was

1 designed and fabricated according to ASME Boiler and Pressure Vessel Code Section VIII
 2 Division 1 and Section II Part D^[17, 18] and a JT test system was set up as shown in Fig. 1. The
 3 detailed dimensions of the pressure vessel are shown in Fig. 2. The key part in the experiment is
 4 the data collection of temperature in the vicinity of the crack in the test plate. The test plate is
 5 clamped between the upper and lower flanges of the pressure vessel. The thermocouple
 6 mounting locations on the test plate are shown in Fig. 3.

Fig. 1. Set-up of the JT test system.

Fig. 2. Detailed dimensions of the pressure vessel.

Fig. 3. Thermocouple mounting locations on the test plate.

2.1 Fabrication of the test plate

The test plate contains an artificial, but realistic crack which is made following the procedures shown in Fig. 4. The liquid nitrogen quenching method was adopted in this research. The cracked pieces were mated and welded together into the slot machined in the test plate. The realistic crack-like leak path is shown in Fig. 5. The detailed dimensions of the test plate are shown in Fig. 6.

Fig. 4. Flow chart of the fabrication of test plate with a realistic through-thickness crack.

(a) The cracked test block placed into the test plate before welding

(b) The test blocks welded into the test plate

Fig. 5. The test block welded into the test plate (a) before welding, (b) after welding.

Fig. 6. Detailed dimensions of the test plate.

2.2 Experimental procedure

In the JT experiment, high pressure gas was allowed to leak through the crack in the test plate by tapping the high pressure gas into the pressure vessel. During the test, the valves and regulators on the argon gas cylinders were fully opened to pressurize the pressure vessel. The digital pressure gauge with a relative accuracy of 1% connected to the side nozzle of the pressure

vessel monitored and recorded the pressure inside the pressure vessel. Temperature in the vicinity of the crack was measured by thermocouples connected to a data logger. Once the temperature stabilized for a while, the vessel was depressurized by closing all valves of gas cylinders. The temperature and pressure data were collected until the metal temperature reached room temperature. In addition, prior to the JT experiment, the surface roughness of the surfaces of crack was measured by the surface metrology to be $38.05\ \mu\text{m}$. The crack width (i.e. the crack opening displacement) was measured by feeler gauge to be $0.25\ \text{mm}$.

2.3 Analysis of tested results

In this experiment, the maximum pressure of argon in the pressure vessel is 91 bar. The temperature changes on the outside surface of test plate (in horizontal direction to the crack line) are shown in Fig. 7. With regard to the tested points on the test plate, H1 is the one near the crack and H10 is the one far away from the crack. It is found that the temperature rises on the surface of the test plate at the beginning of the experiment are due to the temperature increase of the gas inside the pressure vessel. At the beginning of the experiment, high pressure gas was tapped into the pressure vessel while the leakage was negligible due to the lower pressure inside the pressure vessel. The gas warming effect disappeared after the pressure inside the pressure vessel increases to maximum value. At the same time, the JT cooling effect occurred during gas leaking through the crack began to dominate to cool the surrounding metal. During the temperature stable stage (between 160 – 400 s), the temperature of the metal increases slightly as the pressure in gas supply containers reduces gradually. When the test finished, the gas supply was stopped, the metal temperature near the crack decreased with the sharply reduced pressure in the pressure vessel.

Fig. 7. Temperature changes in horizontal direction to the crack line on the outside surface of the test plate (the missing H2 and H8 refer to the broken thermocouples).

3. Simulation methodology

Firstly, a crack model with detailed geometry parameters was built to perform the calculation of the pressure loss of leaking gas through a crack and apply JT effect to the gas leakage through the crack. The temperature and heat transfer coefficient of the leaking gas were then calculated by employing MATLAB iterative program to assist the heat transfer simulation between leaking gas and metal in the vicinity of the crack in the COMSOL program.

4. Mathematical modeling

In a real crack, the flow path often deviates from the plane surface and is three dimensional, which is known as tortuosity. Tortuosity increases the distance or path length that the gas will have to travel (shown in Fig. 8). Beck et al.^[19] pointed out that the macroscopic tortuosity, as the crack path wanders (as shown in (a) and (c) of Fig. 8), is much less significant than the

1 microscopic tortuosity arising from the fracture process, provided that the crack faces remain
 2 coincident. Therefore, the planar crack model (b) is considered in this research.

3
 4 Fig. 8. Possible fracture surfaces where sawtooth peaks and valleys represented the roughness
 5 and tortuosity is represented by bends in the crack paths (a) with one bend, (b) planar without
 6 bends and (c) with multiple bends.

7 After comparison among different models, the model proposed by Taggart et al.^[1] is adopted
 8 because it is supported by experimental data.^[1, 19-22] The detailed description of crack geometry is
 9 shown in Fig. 9. α is the crack surface angle relative to the crack direction through-wall, θ is the
 10 average flow direction relative to the crack direction through-wall, W_{ceff} is the effective crack
 11 width perpendicular to the average flow direction, W_c is the crack opening displacement (or crack
 12 width) perpendicular to the through-wall direction, t is the crack through-wall thickness (i.e.
 13 crack depth), t_{eff} is the effective crack through-wall thickness, R_{local} is the local roughness, R_{global}
 14 is the global roughness, and R_{glamp} is the peak-to-trough amplitude of the global roughness
 15 contours for a sawtooth geometry, equal to four times the global roughness R_{global} . W_1 , W_2 and W_3
 16 are geometry parameters which are used for the calculation of W_{ceff} .

Fig. 9. Detailed schematic of flow around several crack turns.

The crack was divided into many equivalent parts along the crack depth direction as shown in Fig. 10. For each increment, the argon gas's pressure, temperature and heat transfer coefficient inside the crack were evaluated by employing the iterative code of MATLAB program as shown in Fig. 11.

Fig. 10. A model of a crack divided into many equivalent parts.

1

(1) Start from the inlet of the crack: define initial gas temperature (T (1)) and pressure (p (1)) (same as experimental condition)

(2) Define crack geometry parameters according to Taggart et al.^[1] model as follows:

Crack surface angle, average flow direction, amplitude of global roughness R_{glamp} , effective roughness R_{eff} , crack through wall thickness t_{eff} , crack width W_c , effective crack width W_{ceff} , effective roughness R_{eff} , and global roughness R_{global} . $R_{eff} = R_{local} + c(R_{global} - R_{local})$, $R_{glamp} = 4R_{global}$

(3) Find the pressure change of gas during leaking through the first small part of the crack, which is the sum of pressure drop by frictional loss, inertial loss and recirculation loss:

$$\Delta p = \Delta p_{fric} + \Delta p_{inert} + \Delta p_{recirc}$$

(4) Calculate the pressure p (2) of gas after leaking through the first small part of the crack

(5) Calculate gas's specific volume $\hat{v}$ (i.e. the reciprocal of density) from the Redlich-Kwong (RK)

$$\text{equation: } p = \frac{R_{con}T}{\hat{v} - b'} - \frac{a'}{\hat{v}(\hat{v} + b')T^{0.5}} \quad \text{where } a' = 0.4278 \frac{R^2 T_c^{2.5}}{p_c} \quad b' = 0.0867 \frac{RT_c}{p_c}$$

(6) Find the change of temperature of gas during leaking through the first small part of the crack. $\Delta T = \int_{p_1}^{p_2} \mu_{JT} dp$, where Joule-Thomson coefficient μ_{JT} is calculated using RK equation:

(7) Calculate the temperature T (2) of gas after leaking through the first small part of the crack

Repeat above procedures (3) to (7) for the calculation of other increments of the crack to obtain the pressure and temperature of leaking gas along the crack, $T(3), T(4), T(5), \dots, p(3), p(4), p(5), \dots$

Calculate gas viscosity by using Lemmon et al. method.
 $\eta = \eta^0(T) + \eta^r(\tau, \delta)$

Calculate thermal conductivity of gas by using Lemmon et al. method.
 $\lambda = \lambda^0(T) + \lambda^r(\tau, \delta) + \lambda^c(\tau, \delta)$

Calculate Prandtl Number, Pr .
 $Pr = \frac{\eta C_p}{\lambda}$

Calculate Reynolds Number, Re .
 $Re = \frac{\rho v l}{\eta}$

Calculate Nusselt Number, Nu .
$$Nu_{Gn} = \frac{\frac{f}{8}(Re - 1000)Pr}{1 + 12.7 \left(\frac{f}{8}\right)^{\frac{1}{2}} (Pr^{\frac{2}{3}} - 1)}$$

$$Nu = Nu_{Gn}(1 + F)$$

Calculate the heat transfer coefficient, h , using the definition of Nusselt number. $h = \frac{Nu \lambda}{L}$

2

3

4

Fig. 11. Calculation flow chart in MATLAB program.

5. Evaluation of the properties of leaking argon through a crack

5.1 Evaluation of the pressure of leaking argon through a crack

Fluid is forced to pass through the crack by the pressure gradient across the pressure vessel wall 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: friction with crack surface Δp_{fric} , inertia pressure Δp_{inert} and the recirculation of the gas Δp_{recirc} ^[1, 19]:

$$\Delta p = \Delta p_{fric} + \Delta p_{inert} + \Delta p_{recirc} \quad (1)$$

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

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

where 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.^[23] gave better agreement with measured results than the use of the relation due to Button et al.^[24]. Therefore, the method of Spence et al. is adopted to calculate the crack friction factor f in the research and is given as

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

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 (4) describes the inertia pressure loss.

$$\Delta p_{inert} = \frac{\rho v^2}{2} \frac{2N\theta W_{ceff}}{W_c} \quad (4)$$

In Equation (4), 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

$$\Delta p_{\text{recirc}} = \frac{\rho v^2}{2} \left(1 - \left(\frac{w_{\text{ceff}}}{w_c} \right)^2 \right) \quad (5)$$

Fig. 12 shows the pressure distribution of leaking argon through a crack. As is evident from Fig. 12, 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. 91 bar is the maximum value of the pressure reached inside pressure vessel during the experiment. The total pressure drop of leaking argon through the crack is 81.5 bar.

Fig. 12. The pressure of leaking argon through a crack

5.2 Flow velocity evaluation of leaking gas through a crack

The mass flow rate can be expressed as

$$Q = C_D (p\rho)^{\frac{1}{2}} W_c L \quad (6)$$

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

$$C_D = \frac{1}{1+\sqrt{F}} \quad (7)$$

where F is the sum of normalized pressure loss terms due to frictional, inertial, and recirculation effects, and is given by Taggart et al.^[1]

$$F = F_{\text{fric}} + F_{\text{inert}} + F_{\text{recirc}} \quad (8)$$

where F_{fric} is the frictional term, F_{inert} is the inertial term, and F_{recirc} is the recirculation term:

$$F_{\text{fric}} = \frac{f t_{\text{eff}}}{2W_{\text{ceff}}} \quad (9)$$

$$F_{\text{inert}} = \frac{2N\theta W_{\text{ceff}}}{W_c} \quad (10)$$

$$F_{\text{recirc}} = 1 - \left(\frac{W_{\text{ceff}}}{W_c} \right)^2 \quad (11)$$

Then flow velocity can be obtained as follows

$$v = \frac{Q}{\rho A} \quad (12)$$

where ρ is the fluid density in kg/m³, and A is the cross-section area of a crack.

5.3 Evaluation of the temperature of leaking argon through a crack

The JT effect is an isenthalpic process, meaning that the enthalpy of the gas remains constant during the procedure.^[25] In thermodynamics, the differential equation of enthalpy is:

$$dH = C_p dT + \left[\hat{v} - T \left(\frac{\partial \hat{v}}{\partial T} \right)_p \right] dp \quad (13)$$

where H is enthalpy, C_p is heat capacity at constant pressure, T is the temperature, $\hat{v}$ is specific volume, dp is the pressure drop per depth increment into the crack.

$dH = 0$, one can obtain:

$$\mu_{JT} = \frac{dT}{dp} = \frac{1}{c_p} \left[T \left(\frac{\partial \hat{v}}{\partial T} \right)_p - \hat{v} \right] \quad (14)$$

then, the expression of the JT coefficient μ_{JT} can be obtained as follows:

$$\mu_{JT} = \frac{1}{c_p} \left[\frac{T \left(\frac{\partial p}{\partial T} \right)_\rho}{\rho^2 \left(\frac{\partial p}{\partial \rho} \right)_T} - \frac{1}{\rho} \right] \quad (15)$$

Partial derivatives $\left(\frac{\partial p}{\partial T} \right)_\rho$ and $\left(\frac{\partial p}{\partial \rho} \right)_T$ in Equation (15) can be derived from the RK (Redlich-Kwong)^[26-28] equation, and then the expression of the JT coefficient μ_{JT} can be obtained and given by

$$\mu_{JT} = \frac{1}{c_p} \left[\frac{RT^2(\hat{v}^2 + \hat{v}b')^2(\hat{v}-b') + 0.5a'T^{0.5}(\hat{v}^2 + \hat{v}b')(\hat{v}-b')^2}{RT^2(\hat{v}^2 + \hat{v}b')^2 - a'T^{0.5}(2\hat{v}+b')(\hat{v}-b')^2} - \hat{v} \right] \quad (16)$$

$$\text{where } c_p = \frac{a_0 + a_1 T + a_2 T^2 + a_3 T^3}{M} \quad (17)$$

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 (16) into the definition formula of μ_{JT} , as follows:

$$\Delta T = \int_{p_1}^{p_2} \mu_{JT} dp \quad (18)$$

The temperature distribution of leaking argon through a crack is illustrated in Fig. 13. 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. The fitted temperature formula $T_{inf} = -2 \times 10^6 z^3 + 144339z^2 - 3533.2z + 303.17$ (z is the crack depth direction) is used as boundary condition on the crack surface in the subsequent heat transfer simulation.

Fig. 13. The temperature of leaking argon through a crack

5.4 Evaluation of heat transfer coefficient of leaking gas through a crack

5.4.1 Petukhov correlation

The heat transfer coefficient is a key input parameter which has to be evaluated and applied in the heat transfer analysis. After a literature survey, it is found that Petukhov correlation^[29] with high accuracy is suitable for the evaluation of the heat transfer in a pipe (not in a crack). It is one of the most accurate correlations for a single-phase forced convection, which has a reported accuracy of ~ 5% and given by

1 Nusselt number
$$N_u = \frac{\left(\frac{f}{8}\right)RePr}{K+12.7\left(\frac{f}{8}\right)^{\frac{1}{2}}\left(Pr^{\frac{2}{3}}-1\right)} \quad (19)$$

2 From the definition formula of Nusselt number (N_u),

3
$$N_u = \frac{hL}{\lambda} \quad (20)$$

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

5
$$h = \frac{N_u \lambda}{L} \quad (21)$$

6 Definitions and meanings of symbols in Equation (19) and Equation (20) are shown in Table 1.

7 Table 1. Definitions and meanings of symbols in Equation (19) and Equation (20).

Symbols	Definitions of symbols	Meanings of symbols in definitions
f	$f = [1.82\lg(R_e) - 1.64]^{-2}$ Refer to Adams' paper ^[30]	R_e is Reynolds number
R_e	$R_e = \frac{\rho v L}{\eta}$	η is dynamic viscosity in Pa·s
Pr is Prandtl number	$Pr = \frac{\eta C_p}{\lambda}$	λ is thermal conductivity in W/(m·K)
K	$K = 1.07 + \frac{900}{R_e} - \frac{0.63}{1 + 10Pr}$	-
L (m) Note: the definition of L in a crack is shown in Section 5.3.2	$L = D_e = \frac{4A}{P}$	D_e is the equivalent diameter in m
		P is the wetting perimeter in m
λ Note: λ of argon is evaluated by employing Lemmon et al. ^[31] method.	$\lambda = \lambda^0(T) + \lambda^r(\tau, \delta) + \lambda^c(\tau, \delta)$	$\lambda^0(T)$ 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

8

9 Reynolds number of the leaking argon through the crack is shown in Fig. 14. It is noticed that

1 the minimum Reynolds number is 1.4×10^4 , and the maximum value of Reynolds number is 1.1
2 $\times 10^5$.

Fig. 14. The Reynolds number of argon leaking through a crack.

5.4.2 Extension of the application of Petukhov correlation to microchannels

Adams et al.^[30] applied Petukhov correlation to microchannels by making some modifications. The microchannels are smaller diameter circular channels with diameters of 0.1 – 1.09 mm. In current research, the heat transfer occurred in a crack, not in a pipe or a circular channel. Therefore, additional modifications were made to apply Adams et al.'s theory to a crack.

(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.^[32] The correlation of the equivalent diameter is,

$$L = D_e = \frac{4A}{P} \quad (22)$$

where L is characteristic length in m, D_e is the equivalent diameter in m, A is the cross-section area of the 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:

$$L = D_e \approx 2W_c \quad (23)$$

(2) Modification of Petukhov correlation to accommodate the small diameters encountered in microchannels

Gnielinski^[33] modified Petukhov correlation to extend the Reynolds number range down to 2300. The Gnielinski correlation is given by

$$Nu_{Gn} = \frac{\frac{f}{8}(Re - 1000)Pr}{1 + 12.7\left(\frac{f}{8}\right)^{\frac{1}{2}}\left(Pr^{\frac{2}{3}} - 1\right)} \quad (24)$$

where

$$f = (1.82 \log(Re) - 1.64)^{-2} \quad (25)$$

Adams et al.^[30] modified the Gnielinski correlation to accommodate the small diameters encountered in microchannels by using the following form:

$$Nu = Nu_{Gn}(1 + F) \quad (26)$$

where

$$F = CR_e \left(1 - \left(\frac{D}{D_0}\right)^2\right) \quad (27)$$

where: $C = 7.6 \times 10^{-5}$, $D_0 = 1.164 \text{ mm}$, Re is Reynolds number, D is the diameter of microchannels. In this paper, D denotes the crack width (W_c).

5.4.3 Evaluation results of heat transfer coefficient of leaking argon through a crack

The heat transfer coefficient of leaking argon through a crack is shown in Fig. 15. It is shown 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 $6.7 \times 10^4 \text{ W/(m}^2\cdot\text{K)}$ at the entrance of the crack to $0.26 \times 10^4 \text{ W/(m}^2\cdot\text{K)}$ at the exit of the crack. The fitted heat transfer coefficient formula $h = 65291e^{-183z}$ (z is the crack depth direction) is used as boundary condition on the crack surface in the subsequent heat transfer simulation.

Fig. 15. The heat transfer coefficient of leaking argon through a crack.

6. Simulation of the temperature changes in the test plate

6.1 Establishment of mathematical model

A heat transfer application model was developed to simulate the temperature change in the test plate by employing the COMSOL Multiphysics program. The side view of 2D geometry of the test plate with the through-thickness crack is shown in Fig. 16. The material used in this model is Steel AISI 4340 which is a built-in material in COMSOL Materials library, which has

1 similar properties to that used in the experiment. Due to symmetry conditions, only a 3D quarter
2 model of the test plate is simulated as shown in Fig. 17.

3
4 Fig. 16. Diagram of the model of a gas leaking through a crack on the wall of a pressure vessel.

5
6 Fig. 17. Quarter model of test plate.

6.2 Problem description

As a matter of fact, the heat transfer process between the leaking gas and the surrounding metal under study is a two-way coupling problem (consider both heat transfers from gas to metal and from metal to gas), that is, the leaking gas cool the surrounding metal due to the JT cooling effect, and at the same time, the surrounding metal and atmosphere warm 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 JT 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. For these reasons, the problem treated as a one-way coupling problem (only consider heat transfer from gas to metal) is a reasonable approximation.

6.3 Governing equations in heat transfer application model

The fundamental law governing all heat transfer is the first law of thermodynamics, commonly referred to as the principle of conservation of energy. However, internal energy, U , is a rather inconvenient quantity to measure and use in simulation.^[34, 35] Therefore, the base law is usually rewritten in terms of temperature, T . For a fluid, the resulting heat equation is:

$$\rho C_p \left(\frac{\partial T}{\partial t} + (\mathbf{u} \cdot \nabla) T \right) = -(\nabla \cdot \mathbf{q}) + \tau : \mathbf{S} - \frac{T}{\rho} \frac{\partial \rho}{\partial T} \bigg|_p \left(\frac{\partial p}{\partial t} + (\mathbf{u} \cdot \nabla) p \right) + Q \quad (28)$$

where

- $\mathbf{u}$ is the velocity vector (m/s)
- $\mathbf{q}$ is the heat flux by conduction (W/m²)
- p is pressure (Pa)
- τ is the viscous stress tensor (Pa)

- $\mathbf{S}$ is the strain rate tensor (1/s):

$$\mathbf{S} = \frac{1}{2}(\nabla \mathbf{u} + (\nabla \mathbf{u})^T) \quad (29)$$

- Q contains heat sources other than viscous heating (W/m^3)

The above heat Equation (28) assumes that mass is always conserved, which means that density and velocity must be related through:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \quad (30)$$

The heat transfer application mode employed in current study uses Fourier's law of conduction which states that the conductive heat flux, $\mathbf{q}$, is proportional to the temperature gradient:

$$q_i = -k \frac{\partial T}{\partial x_i} \quad (31)$$

where k is the thermal conductivity ($\text{W}/(\text{m}\cdot\text{K})$).

Inserting Equation (31) into Equation (28), reordering the terms and ignoring viscous heating and pressure work puts the heat equation on a perhaps more familiar form:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q - \rho C_p \mathbf{u} \cdot \nabla T \quad (32)$$

The heat transfer application mode solves this equation for the temperature, T . If the velocity is set to zero, the equation governing pure conductive heat transfer in a solid can be obtained:

$$\rho C_p \frac{\partial T}{\partial t} + \nabla \cdot (-k \nabla T) = Q \quad (33)$$

6.4 Initial conditions

Table 2 shows crack geometry parameters and initial state parameters of argon gas inside the pressure vessel same as that in the experiment. The comparison with experimental results performed by Beck et al.^[19] indicates that in the absence of proper measurement, the value of $\pi/6$ for crack surface angle is reasonable. And the calculation results in MATLAB are not sensitive to

1 the value of crack surface angle (α). Therefore, the value of $\pi/6$ is selected as the crack surface
2 angle.

3 Table 2. Experimental crack geometry parameters and initial state parameters of argon gas inside
4 the pressure vessel.

Input parameters	Description	Values (Refer to experiment data)
$p(1)$	Initial gas pressure inside the pressure vessel	91 bar
$T(1)$	Initial gas temperature inside the pressure vessel	30 °C
$\rho(1)$	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

5 6.5 Boundary conditions

Boundaries			Conditions

1	Arc-shaped boundary		temperature 30 °C (same as room temperature on the day of the experiment)
2	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)

<div style="text-align: center;"> Boundaries </div>			<div style="text-align: center;"> Conditions </div>
3	Inner surface boundary (the surface of the test plate towards inside of 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 the pressure vessel during test)
4	Outer surface boundary (the surface of the test plate towards the outside of 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)
5	Other surfaces boundaries		Symmetry

1

2 6.6 Mesh calibration

3 The results of mesh sensitivity study are shown in Fig. 18. The finite element (FE) meshes of
4 the whole test plate and the close-up on the crack surface are shown in Fig. 19. The element used
5 is a 3D tetrahedral mesh element with total number of elements of 8122. The element type is
6 linear Lagrange element with integration order 2. Most of the mesh concentrates on the crack
7 surface to accurately model the temperature changes of the metal in the vicinity of the crack.

Fig. 18. Calibration of mesh sensitivity.

Fig. 19. FE meshes of the test plate.

7. Simulation results and discussion

Fig. 20 shows the simulated temperature distribution on the test plate. It is noticed that the lowest temperatures in the vicinity of the crack is 13.8 °C. The maximum temperature drop of the test plate from the ambient temperature is 16.2 °C.

Fig. 20. Simulated temperature distribution on the test plate.

7.1 Selection of appropriate experimental data for comparison with simulation results

The lowest metal temperature on the outside surface of the test plate in the diagonal direction to the crack line is lower than that of horizontal direction to the crack as shown in Fig. 21.^[11] However, there is a depression along the diagonal direction which is caused by the machining process as illustrated in Fig. 22. The temperature results may be affected by the depression in the diagonal direction to the crack line as the leaking gas impacts the depression directly. 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 the test plate in the horizontal direction to the crack line are selected to compare with the simulation results. As shown in Fig. 21 (a), the measured lowest temperature on the outside surface of the test plate (in the horizontal direction to the crack line) during the JT cooling period is 12.5 °C, and the lowest temperature obtained from simulation is 13.8 °C. It can be concluded that the simulation results agree well with the experimental results on the evaluation of the low temperature in the vicinity of the crack. It should be noticed that the location of the calculated lowest temperature in simulation is not same as that of the tested lowest temperature in this experiment which will be explained in the following section.

(a) In horizontal direction to the crack line.

(b) In diagonal direction to the crack line.

Fig. 22. A recess near the crack on the surface of the test plate.

7.2 Analysis of results

In Fig. 21 (a), it is noticed that the JT cooling effect decays with the decreasing of the gas pressure inside the containers due to the limited supply of gas which ran out. If there is enough gas source (such as in a long gas pipeline or large vessel) i.e. under the infinite source condition, the JT cooling effect can continue indefinitely. Furthermore if the pressure difference between inside and outside of pressure vessel is kept constant, the pressure induced stresses is maintained to drive the propagation of the crack. In this regard, the JT cooling effect is much more dangerous for larger pressure vessels or pipeline with a large volume of gas.

Reepmeyer et al.^[36] have carried out several hydraulic full scale fatigue tests to test the JT effect during leakage in accordance with the requirements in Det Norske Veritas (DNV) rules for CNG carriers (carrying pressure vessels of 250 bar). The lowest temperature close to the exit of the crack during leakage was around $-70\text{ }^{\circ}\text{C}$ at the steel surface. They stated that temperatures below $-35\text{ }^{\circ}\text{C}$ can result in the embrittlement of the X80 pipeline steel. From the inspection of the fracture, however, no evidence was found for a brittle crack growth during the cooling down test. Therefore, it is not appropriate to evaluate the severity of the impact of the JT cooling effect on the reliability of pressure vessels based on the lowest temperature on the crack surface as the area of extreme low temperature is very small due to the localized cooling effect. In addition, it

1 takes enough time to create a significant volume of material at low temperature as the heavy
2 cylinder wall acts as a large heat buffer. In comparison, the lowest temperature simulated in this
3 paper is more useful as it predicts the temperature located at a certain distance from the crack
4 (the yellow circle as shown in Fig. 23).

5 The heat transfer among leaking gas, test plate and surrounding environment would
6 eventually result in a significant temperature gradient on the test plate. According to previous
7 report^[11], the temperature distribution on the test plate is radial direction dependent, the
8 temperature change in horizontal and diagonal direction to the crack line has a similar trend. The
9 sharp temperature gradient will cause tensile thermal stresses with a tendency to open the crack
10 further at the crack tip which coincides with the highest temperature gradient. If the lowest
11 temperature obtained at the circle location in Fig. 23 is below materials' embrittlement
12 temperature, then the temperature of materials inside the rectangular area will drop to much
13 lower temperature than that at the location of the lowest temperature test point. Then, the whole
14 low-temperature region in the vicinity of the crack may trigger the transition of previously stable
15 crack propagation to rapid unstable growth and affect the validity of LBB principle. Therefore, it
16 is necessary to carry out further studies about the JT cooling effect during leakage to increase the
17 safety and reliability of pressure vessels, especially the pressure vessels storing or transporting
18 gas under higher pressure located in cold regions.

Fig. 23. Location of the lowest temperature test point

8. Conclusions

In this paper, a two-stage simulation method is proposed to simulate the heat transfer of high pressure argon leaking through a narrow crack to identify the impact of the JT cooling effect occurred during leakage. The first stage is the properties evaluation of the leaking argon through a crack by using MATLAB program followed by the second stage which is the temperature simulation of the test plate by employing the heat transfer model in the COMSOL Multiphysics program.

The calculated 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 lowest temperature of the test plate in the vicinity of the crack obtained from the simulation is 13.8 °C. There is a good agreement between the simulation and experiment at the obtained lowest temperature in the test plate. The lowest temperature obtained from the proposed method predicts the temperature located at a certain distance (regional cooling) from the crack in the experiment. Compared with the localized cooling, the regional cooling is likely to affect the validation of LBB approach. Therefore, the proposed two-stage simulation method is a useful tool for predicting the regional lowest temperature and paving the way for the further study of the JT cooling effect during leakage.

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