1. Effect of the Joule-Thomson cooling on the leak-before-break approach

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Abstract

Due to the high pressure inside compressed natural gas (CNG) containers, its safety is the first important factor to be considered. Leak-before-break (LBB) is an important methodology of maintaining the integrity of pressure vessels. However, the Joule-Thomson (JT) cooling effect occurred during a leak may impact the validity of the LBB approach. In this paper, a looping model based on MATLAB software is developed starting with the gas at room temperature and 250 bar at the entrance of the crack. From this, the pressure and JT temperature drop is calculated initially, which in turn affects the gas properties, such as viscosity, density, thermal conductivity and heat transfer coefficients. Heat transfer and FEA analysis using a 3D model of the plate with a central through-thickness crack are carried out. Under the internal pressure of 250 bar, the temperature drop and the stress intensity factor in the vicinity of the crack is 59.7 °C and 120 MPa·m^{1/2}, respectively. The stress intensity factor obtained is higher than the fracture toughness of the material at the same low temperature. However, the structure may not experience a catastrophic failure. The reasons for this phenomenon are discussed in the paper.

Keywords: compressed natural gas; leak-before-break; Joule-Thomson cooling effect; fracture toughness

Introduction

Natural gas has become to the forefront of the international energy debate as it is an important environment friendly energy for decreasing pollution and maintaining a clean and healthy environment. Its applications can serve to reduce harmful pollution levels from other fossil fuels. As a result, the transport of natural gas becomes important.^[1] As to the transportation of natural gas, there are only two commercially proven concepts—pipelines and LNG. However, there are many large natural gas reserves that not located near the natural-gas-demand markets. It is considered “stranded” which is defined as gas reservoir fractions that prevent their development or optimal production from an oil or gas field. Neither pipeline nor LNG transportation techniques can economically exploit these stranded gas reserves. The compressed natural gas (CNG) marine transportation concept is one of the most developed and promising natural-gas-transportation concepts that has not yet commercialized.^[2-4]

Due to the high pressure inside CNG containers, the most critical characteristic previously undiscovered in CNG systems with leakage is the Joule-Thomson (JT) effect. At room temperature, all gases except hydrogen, helium and neon cool upon expansion by the Joule-Thomson process.^[5] 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.^[6] As shown in Fig. 1 proposed in a proposal of this research, 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

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is than the critical crack length and leakage flow rate increases to the technology is the development of a small crack continues to grow outward, from length, unstable and rapid growth will ing intervenes to reduce the astic yield strength. The reduction in r than the critical crack length $2C_g$ to leakage and the margin to is safe or not safe with the JT cooling

Fig. 1. Illustration of axial defect growth subjected to mainly cyclic internal pressurization and associated JT cooling.
Summary of experimental work

An experimental study of the JT effect was conducted by Ai et al.^[7] with argon gas. A pressure vessel was designed and fabricated according to ASME Boiler and Pressure Vessel Code Section VIII Division 1 and Section II Part D^[8, 9] as shown in Fig. 2. The test plate containing an artificial, but realistic crack was clamped between the upper and lower flanges of the pressure vessel. The artificial crack was made by first machining a block of steel, then quenching in liquefied nitrogen before cracking in a three point bend rig as shown in Fig. 3. The cracked pieces were mated and welded together into the slot machined in the test plate. The result is tightly fitting realistic crack-like leak path as shown in Fig. 4. In the Joule-Thomson 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. Temperature in the vicinity of the crack and pressure (inside the pressure vessel) were measured by thermocouples and a digital pressure gauge, respectively. 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 mm .

Fig. 2. Set-up of the JT test system.

Fig. 3. Fabrication process of cracked test blocks

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

(b) The test block welded into the test plate.

Fig. 4. The test block welded into the test plate (a) before welding, (b) after welding.

In this experiment, the maximum pressure of argon reaches 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. 5. After investigation and analysis, it is found that the temperature rise on the surface of the test plate at the beginning of the experiment in Fig. 5 is caused by the temperature increase of the gas inside the pressure vessel. The reason for the temperature rise is as follows. At the beginning of the experiment, high pressure gas was trapped into the pressure vessel while the leakage was negligible due to the lower pressure inside the pressure vessel. At this time, the sharp increase of the pressure inside the pressure vessel accounts for the rise of gas temperature which can be explained by the first law of thermodynamics. The gas warming effect disappeared when the pressure inside the pressure vessel tended to be stable. At the same time, the JT cooling effect occurred during gas' leaking through the crack began to dominate to cool the surrounding metal. It is noticed that there is a significant temperature drop during this stage. During the temperature stable stage (between 160 – 400 s), the temperature of the metal increases slightly as the pressure in gas source supply containers reduces continuously. Gas supply was stopped after finishing the test, the metal temperature decreased abruptly with the sharp decreased pressure in the pressure vessel.

Fig. 5. 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).

2. Simulation of the temperature and stress of the test plate under the pressure of 250 bar

The modelling and calculation procedures for the temperature of the test plate are similar to that described in the paper of Ai et al.^[10]. The only difference is that the pressure inside pressure vessel is changed to 250 bar. Therefore, the following only shows the procedure and results which are different from it.

2.1. Evaluation of the properties of leaking argon through a crack under the pipe pressure of 250 bar

Table 1 shows crack geometry parameters and initial state parameters of argon gas inside the pressure vessel. Beck et al.^[11] stated that comparison with experimental results indicates that in the absence of proper measurement, the value of $\pi/6$ for crack surface angle is reasonable. Therefore, the value of $\pi/6$ is selected as the crack surface angle.

Table 1. Crack geometry parameters and initial state parameters of argon gas inside the pressure vessel.

Input parameters	Description	Values
$p(1)$	Initial gas pressure inside the pressure vessel	250 bar
$T(1)$	Initial gas temperature inside the pressure vessel	30 °C
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

Fig. 6 shows the pressure distribution of the leaking argon along the crack depth direction. It is indicated that the pressure decreases greatly along the crack through-wall position from the inside to the outside the pressure vessel. The pressure of the leaking argon drops from 250 bar at the entrance of the crack to 26.05 bar at the exit of the crack. The total pressure drop of the leaking argon through the crack is 224 bar. The fitted pressure formula: $p = (2.5 \times 10^7) e^{-125.6z}$ (z is the crack depth direction) is used as the boundary condition on the crack surface in the structural mechanics module.

The temperature of the leaking argon along the crack depth direction is illustrated in Fig. 7. It is shown that the temperature of leaking argon falls greatly along the crack through-wall position from the inside to the outside the pressure vessel. The temperature of the leaking argon drops from 30 °C at the entrance of the crack to -48 °C at the exit of the crack. The fitted temperature formula $T = (5 \times 10^6) x^3 - 15961x^2 - 5625.1x + 303.74$ (z is the crack depth direction) is used as the boundary condition on the crack surface in the heat transfer module.

The heat transfer coefficient of the leaking argon along the crack depth direction is shown in Fig. 8. It is indicated that the heat transfer coefficient of the leaking argon decreases quickly along the crack through-wall position from the inside to the outside the pressure vessel. The heat transfer coefficient of the leaking argon decreases from $3.15 \times 10^5 \text{ W}/(\text{m}^2 \cdot \text{K})$ at the entrance of the crack to $0.14 \times 10^5 \text{ W}/(\text{m}^2 \cdot \text{K})$ at the exit of the crack. The fitted heat transfer coefficient formula $h = 336869 \times e^{-175.3z}$ (z is the crack depth direction) is used as boundary condition on the crack surface in the heat transfer module.

Fig. 6. The pressure of the leaking argon through the crack.

Fig. 7. The temperature of the leaking argon through the crack.

Fig. 8. The heat transfer coefficient of leaking argon through a crack.

2.2. Simulation of the temperature and stress of the test plate under the pressure of 250 bar

The simulation includes two application modes: heat transfer application mode and structural mechanics application mode. The Thermal-StructureInteraction predefined multiphysics coupling from the Model Navigator in COMSOL program is selected as the application modes. In this case, both application modes are automatically added to the model and the coupling is facilitated by the temperature variable which is automatically defined as the temperature for thermal load in the structural mechanics application mode. At the same time, the pressures inside the pressure vessel and the crack surfaces are defined as the face loads on the internal face of the test plate and the crack surfaces in the structural mechanics application mode.

Due to the structural symmetry, only a 3D quarter model (radius: 0.1778 m) of the test plate is simulated. A three-dimensional quarter model is shown in Fig. 9. The detailed physical conditions about the simulation is illustrated in Fig. 10.

Fig. 9. Quarter model of the test plate.

Fig. 10. Schematic of the simulation model.

2.2.1. Material property

The material used in this model is Steel AISI 4340 which has similar properties to that of the steel used in the experiment. The material properties are listed in Table 3.

Table 3. Properties of the test plate.

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

2.2.2. Boundary conditions

The boundary conditions in the heat transfer module and the structural mechanics module are shown in Table 5.

Table 5. Boundary conditions in the heat transfer module and the structural mechanics module.

Boundaries		Conditions	
		Heat transfer module	Structural mechanics module

1	Arc-shaped boundary	temperature 30 °C	Fixed
2	Crack surface boundary	heat transfer coefficient $h = 336869 \times e^{-175.3z}$, external temperature $T_{inf} = (5 \times 10^6)x^3 - 15961x^2 - 5625.1x + 303.74$	Free, Loads $F_x = (2.5 \times 10^7)e^{-125.6z} \times \sin(9.46)$, $F_y = (2.5 \times 10^7)e^{-125.6z} \times \cos(9.46)$. Where angle 9.46 is the crack slant angle
3	Inner surface boundary (the surface of the test plate towards the pressure vessel)	heat transfer coefficient (forced convection on plates in COMSOL Coefficients library); external temperature 15 °C	Free, Load $F_z = 250$ bar
4	Outer surface boundary (the surface of the test plate towards the outside of the pressure vessel)	heat transfer coefficient (natural convection on plates); external temperature 30 °C	Free
5	Other surfaces boundaries	Symmetry	Symmetry

2.2.3. Calibration of mesh sensitivity

Calibration of mesh sensitivity is shown in Fig. 11. The element employed is a 3D tetrahedral mesh element. In the 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. It shows that the lowest temperature of the test plate and the maximum Von Mises stress in the vicinity of the crack are approaching stable after mesh number C (3420). Element number H (7240) is selected in the present research. The entire mesh and the close-up mesh around the crack surface are shown in Fig. 12&Fig. 13, respectively.

Fig. 11. Calibration of mesh sensitivity.

Fig. 12. Mesh of the test plate.

Fig. 13. Close-up of the mesh around the crack.

2.3. Simulation results and discussion

The temperature distribution in the test plate is shown in Fig. 14. It is shown that the highest and lowest temperatures on the test plate are 30 °C and −29.7 °C, respectively. The maximum temperature drop near the crack is 59.7 °C. Since it is a static simulation, the temperature at the entrance of the crack still keeps at room temperature. Due to the continuous gas leak, in the real dynamic process, this temperature will drop and approach the low temperature at the exit of the crack by the heat transfer from the leaking gas and the metal.

Fig. 14. The temperature distribution in the test plate.

Currently, for the CNG containers, the commonly used steel is X70 or X80 pipeline steel. For the X80 pipeline steel, Reepmeyer et al.^[6] reported that the temperature below −35 °C can result in the embrittlement of the material. Yang et al.^[12] has carried out the studies about the impact of the temperature on the fracture toughness of X70 pipeline steels. The influence of the experimental temperature (−60 to 20 °C) and the specimen thickness (3 – 10 mm) on the fracture toughness is shown in Fig. 15. The crack length has also some influence on the value of fracture toughness and J-integral. From the analysis of the crack morphologies, they concluded that the fracture occurred at the temperature of 20 °C and −20 °C is ductile fracture, and the fracture occurred at the temperature of −60 °C is brittle fracture. Therefore, it could be concluded that the lowest temperature of −29.7 °C in the vicinity of crack simulated in this work could deteriorate its fracture toughness to some extent. In this situation, the material could be in the phase of the ductile-brittle transition which could affect the validity of the traditional leak-before-break philosophy.

Fig. 15. Average of fracture toughness K_{Ic} of X70 steel vs sample thickness B [12].

3. Evaluation of stress intensity factor in the vicinity of the crack tip

A common parameter in fracture mechanics, the so-called stress intensity factor K_I , provides a means to predict if a specific crack will cause the plate to fracture. This critical value of stress intensity determined by Mode I loading in plane strain is referred to as the fracture toughness (K_{Ic}) of the material. When the calculated value of the stress intensity factor K_I becomes equal to the fracture toughness of the material K_{Ic} , then fast, usually catastrophic fracture occurs.^[13-17]

3.1. Mathematical relations

In this model, the stress intensity factor K_I is determined using the so-called J-integral. The J-integral is a two-dimensional line integral along a counterclockwise contour, Γ , surrounding the crack tip. The J-integral is defined as

$$J = \int_{\Gamma} W dy - T_i \frac{\partial u_i}{\partial x} ds = \int (W n_x - T_i \frac{\partial u_i}{\partial x}) ds \quad (1)$$

where W is the strain energy density

$$W = \frac{1}{2} (\sigma_x \cdot \epsilon_x + \sigma_y \cdot \epsilon_y + \sigma_{xy} \cdot 2 \cdot \epsilon_{xy}) \quad (2)$$

and $\mathbf{T}$ is the traction vector defined as

$$\mathbf{T} = [\sigma_x \cdot n_x + \sigma_{xy} \cdot n_y, \sigma_{xy} \cdot n_x + \sigma_y \cdot n_y] \quad (2)$$

σ_{ij} denotes the stress components, ϵ_{ij} the strain components, and n_i the normal vector components.

The J-integral has the following relation to the stress intensity factor for a plane stress case and linear elastic material:

$$J = \frac{K_I^2}{E} \quad K_I = \sqrt{J E} \quad (3)$$

Where E is Young's modulus.

3.2. Stress intensity factor evaluation procedure in COMSOL Multiphysics

The analysis calculates the J-integral for different contours traversing different regions around the crack tip based on the previous results of thermal stress simulation. To calculate the J-integral, the boundary integration variables are defined for the contour. This creates two variables for the contour. The first variable contains the integrated strain energy density, while the second contains the traction vector times the spatial x-derivative of the deformation components. The sum of these two variables then provides the J-integral value as a scalar expression variable. Finally, the stress intensity factor can be computed from the J-integral value by using a scalar expression variable.

3.3. Results and discussion

Von Mises stress distribution along the through-thickness direction in the crack tip is shown in Fig. 16. It is noticed that the highest stress of 7.2 GPa in the crack tip locates at the position of 0.0168 m along the through-wall path of the crack. Therefore, the highest stress intensity factor along the crack tip is calculated at this location (0.0168 m).

Fig. 16. Von Mises stress distribution along the through-thickness direction in the crack tip.

Several J-integral contours around the crack tip at the highest stress location of 0.0168 m are drawn in Fig. 17. The calculated stress intensity factors around the crack tip considering the temperature effect and without considering the temperature effect are shown in Table 6 and Table 8, respectively. The results follow the rule that the stress intensity factor is dependant on the temperature and it is linear with increase in temperature as reported by Rao et al^[18]. However, the extent of the increase is not significant for the metal temperature change of 59.7 °C obtained from this work. In Table 6, the stress intensity factor at the location of 0.0168 m is about $120 \text{ MPa}\cdot\text{m}^{1/2}$.

Fig. 17. J-integral contour path.

Table 6. Stress intensity factors around the crack tip (considering the temperature effect).

J-integral contour location No.	Stress intensity factor ($\text{MPa}\cdot\text{m}^{1/2}$)
No. 1	120.7
No. 2	120.3
No. 3	119.3
No. 4	118.7

Table 8. Stress intensity factors around the crack tip (without considering the temperature effect).

J-integral contour location No.	Stress intensity factor ($\text{MPa}\cdot\text{m}^{1/2}$)
No. 1	125.4
No. 2	124.1
No. 3	121.9
No. 4	119.6

Based on the results obtained for the simulation, it is noticed that the highest value of the stress intensity factor K_I in the crack tip is around $120 \text{ MPa}\cdot\text{m}^{1/2}$. After literature review, it is found that the fracture toughness K_{IC} of the steel at the simulated lowest temperature is about $62.6 \text{ MPa}\cdot\text{m}^{1/2}$ ^[19]. So can we conclude that the leak-before-break concept considering the JT effect is not safe? However, it could be still too early to make this conclusion. The JT cooling is a localized cooling effect in the vicinity of the crack on the test plate. The significant benefit of the heavy wall of the solid steel is that it acts as a large heat buffer. Therefore, it will take a long time to create a significant area in the material at low temperature. This process can be called “crack arrest”. However, the long time continuous leakage will cool the freshly propagated crack and deteriorate the mechanical properties of the material, especially the fracture toughness. Then the crack would extend again. This process can be named as “crack

extension". The cycle of the "crack arrest" and the "crack extension" will greatly slow the speed of the crack growth. Thus, due to the early detection of pressure loss during the period, safety measures will be employed to prevent the unstable propagation of the crack and avoid the catastrophic failure. On the other hand, the traditional failure evaluation criteria could not be applicable to the through-thickness crack. The structure might begin to fracture when the stress intensify factor in the central part in the crack tip line also exceeds the fracture toughness of the material as shown in Fig. 19. Therefore, further study is needed to find appropriate evaluation criteria of the failure for the pressure vessel with a through-thickness crack by considering the JT cooling effect. Once the LBB phenomenon occurs in the steel structure(i.e. the crack grows through the wall of pipe and causes gas leakage, but the pipe structure is still safe), the part of high stresses(with high energy) concentrated in the crack tip will be released quickly. The structure of the pressure vessel could be much safer when the gas leaks out than when the crack has not penetrated the pipe wall because the release of the energy in the crack tip could extend the time of the crack propagation reaching the unstable stage. This is the key point of the leak-before-break philosophy. As the fracture toughness of steels is temperature dependent^[20, 21], the low temperature caused by the JT cooling effect could affect the validity of LBB philosophy. Therefore, the further study about the impact of the Joule-Thomson cooling effect on the leak-before-break approach is necessary to guarantee the integrity of the pressure vessel systems.

Fig. 19. Von Mises stress distribution in the vicinity of the crack.

4. Conclusions

This paper presents the work on the calculation and simulation of the temperature, stress and stress intensity factor in the vicinity of the crack on the test plate under the pressure of 250 bar by considering the Joule-Thomson cooling effect during gas leaks, and the following conclusions can be drawn:

- (1) The temperature of the leaking argon falls quickly along the crack through-wall position from the inside to the outside the pressure vessel. The temperature of the leaking argon drops from 30 °C at the entrance of the crack to -48 °C at the exit of the crack.
- (2) The heat transfer simulation shows that the lowest temperatures in the test plate is -29.7 °C. The total temperature drop of the test plate caused by the JT cooling effect is 59.7 °C. The lowest temperature of -29.7 °C in the vicinity of the crack could deteriorate the material's fracture toughness to some extent. In this situation, the material could be in the phase of ductile-brittle transition.

Stress intensity factor simulation shows that the highest stress intensity factor along the crack tip is about 120 MPa·m^{1/2} which is much higher than the fracture toughness of the steel at the same low temperature. However, the

pressure vessel fails to undergo the catastrophic failure. It is because that the JT cooling is a localized cooling effect in the vicinity of the crack on the test plate. The significant benefit of the heavy wall of the solid steel is to act as a large heat buffer. Therefore, it will take a long time to create a significant area in the material at low temperature. However, the situation will become more severe when huge amounts of high pressure gases are stored in pressure vessels or long-distance pipelines located in cold areas as the long time continuous leak will eventually freeze the surrounding metal and lower its fracture toughness. Consequently, the effect cannot be ignored and a further study of the Joule-Thomson effect occurred during gas leaks is needed to explore the possible impact on the integrity of pressure vessels.

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