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Assessment of brittle fractures in CO_2 transportation pipelines: A hybrid fluid-structure interaction model

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Abstract

In order to transport dense-phase CO_2 captured from power and industrial emission sources in the Carbon Capture and Storage (CCS) chain, pressurised steel pipelines are considered the most practical tool. However, concerns have been raised that low temperatures induced by the expansion of dense-phase CO_2, for example following an accidental puncture or during emergency depressurization, may result in a propagating brittle fracture in the pipeline steels.

The present study describes the development of a hybrid fluid-structure model for simulating dynamic brittle fracture in buried pressurised CO_2 pipelines. To simulate the state of the flow in the rupturing pipeline, a compressible one-dimensional Computational Fluid Dynamics (CFD) model is applied, where the pertinent fluid properties are determined using a thermodynamic model. In terms of the fracture model, an eXtended Finite Element Method (XFEM) is used to model the dynamic brittle fracture behaviour of the pipeline steel.

Using the coupled fluid-structure model, a study is performed to evaluate the risk of brittle fracture propagation in a (real-scale) 1.22m diameter API X70 steel pipeline, containing CO_2 at 0°C and 11MPa. The simulated results are found to be in good agreement with the predictions obtained using a semi-empirical model accounting for the pipeline fracture toughness. From the results obtained it is observed that a propagating fracture is limited to a short distance. As such, for the conditions tested, there is no risk of brittle fracture propagation for API X70 pipeline steel transporting dense-phase CO_2.

Keywords: CO₂ pipeline; Brittle fracture; Crack propagation; XFEM, CFD.

1. Introduction

Transport of CO_2 in dense-phase presents a high potential for auto-refrigeration due to depressurization, either during operations or due to pipeline failure. In general, dynamic brittle fractures are not of concern for modern gas transmission pipelines, as discussed by Andrews et al. (2010). It has recently been suggested by Mahgerefteh et al. (2006) for dense-phase CO_2 that the unusually high Joule-Thomson coefficient of CO_2 may induce low temperatures

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in the pipe upon the CO_2 fluid expansion to atmospheric pressure. This may lead to loss of ductility of the pipe wall material, increasing the risk of brittle fracture propagation. As such, to ensure safe operation of CO_2 pipelines, the risk for brittle fracture and its consequences need to be correctly assessed.

Recently several authors have developed methodologies to couple pipeline outflow and crack propagation models, (see for example Mahgerefteh et al. (2012); Nordhagen et al. (2012)). These methodologies are mainly based on the Homogeneous Equilibrium Mixture (HEM) model of pipe flow and utilise various models describing the pipe wall rupture, ranging from the High strength Line Pipe (HLP) model, suggested by Mahgerefteh et al. (2012), to FEM models accounting for ductile fracture of elasto-plastic material, used by Nordhagen et al. (2012). While the above studies have been focused on the simulation of ductile fractures, modelling of the brittle mode of pipeline failure has not received as much attention. Practically this can be attributed to the complex nature of brittle fracture propagation in steel pipes, which accurate description requires accounting for heat transfer and, importantly, the different mechanics of material failure in both ductile and brittle modes. In particular, it has been noted by Andrews et al. (2010) that in contrast to ductile fractures, the pipeline brittle rupture is characterized by a negligible amount of plastic deformation at the crack tip and is governed by the elastic stress in the pipe wall.

The present study develops a hybrid fluid-structure model to simulate scenarios of pressurized pipeline brittle fracture propagation. The model couples the fluid dynamics of the escaping fluid and the fracture mechanics of the deforming pipeline experiencing puncture and back-fill pressures, for example due to surrounding soils. To simulate the state of the fluid in the rupturing pipeline, a one-dimensional compressible CFD model is developed accounting for the propagation of the crack tip along the pipe at a speed predicted by the material failure model. The latter, in turn, is applied to calculate the crack propagation for the instantaneous state of stress (internal pressure) as predicted by the CFD model. In terms of fracture modelling, an eXtended Finite Element Method (XFEM) is used to model the dynamic brittle fracture behaviour of pipeline steel. In this model the Stress Intensity Factor (SIF) and crack propagation velocity are calculated at the crack tip at each crack propagation step.

2. Theoretical Modelling

2.1. Fracture model

Fig. 1 shows the hybrid fluid-structure interaction algorithm for the simulation of pipeline running brittle fracture in the form of variation of crack length with crack propagation velocity. The developed hybrid modelling approach allows the quantitative prediction of the pipeline tendency to long running fractures in the form of the variation of crack length with crack propagation velocity. At the start of the simulation the bulk fluid pressure and the corresponding crack tip pressure are calculated by the CFD model for an arbitrary small initial longitudinal crack opening along the major axis of the pipeline, formed for example, as a result of third party damage. The pipeline internal and back-fill pressures are next implemented in ABAQUS using the DLOAD subroutine. Then, for an arbitrary small time increment, Δt, pipeline rupture is simulated in ABAQUS, by defining a stationary crack, which gives the new position of the crack tip and the corresponding crack propagation velocity. The crack propagation velocity is calculated after obtaining the SIF at the crack tip after each crack propagation step. If the crack tip position reaches the end of the pipe or the crack propagation velocity turns to zero (the crack is arrested) the calculations are terminated. On the other hand, if the crack propagation velocity is positive, it is passed to the CFD code where the position of the pipeline fracture (defined as the point where the pipe opening area expands by an arbitrary small value) is updated based on solution of an advection equation, and the amount of fluid released and the new crack tip pressure are calculated. For a new crack propagation step, the crack length is extended by an arbitrary small Δa. A Python script was written to repeat the above procedure up to the point at which the crack tip position reaches the end of the pipe. In this study the crack propagation velocity is calculated based on the calculated Dynamic Stress Intensity Factor (K_{ID}) at crack tip, as shown in Fig. 1. More information about the relation between the crack propagation speed and K_{ID} can be found in previous work by Talemi (2016); Talemi et al. (2016).

The developed hybrid modelling concept assumes that running pipeline fracture can be modelled as an expansion in the pipe cross-section area from the initial cross-section area of the pipe A_0 to an arbitrary large area A_f. In the one-dimensional flow model pipe rupture is simulated as a continuous expansion in the pipe cross-sectional area, which
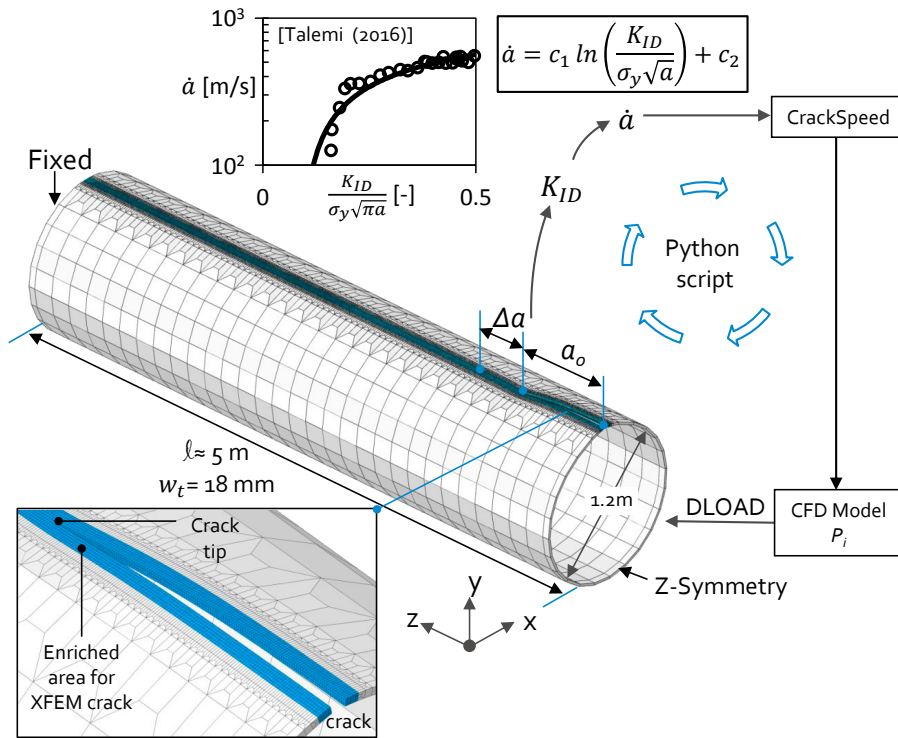
Fig. 1. three dimensional finite element mesh of simulated pipe section along with the schematic representation of the developed coupling algorithm for modelling running brittle fracture and pipeline decompression.

occurs over a short distance interval Δa. Fracture propagation is then modelled as a motion of the expansion front at an instantaneous speed $\dot{a}$.

2.2. Pipeline decompression CFD model

In order to predict the conditions of the fluid in a pipeline during fracture propagation, including its pressure, temperature and the fluid phase, a one-dimensional flow model has been developed by Mahgerefteh et al. (2006); and later modified by Brown et al. (2015) is employed.

A set of equations describing the HEM flow in a pipe includes the mass, momentum and energy conservation equations, proposed by Zucrow et al. (1976), augmented by an advection equation for the pipe cross-sectional area:

$$\frac{\partial \mathbf{U}}{\partial t} + \frac{\partial \mathbf{F}}{\partial x} = \mathbf{S} \tag{1}$$

where $\mathbf{U}$, $\mathbf{F}$ and $\mathbf{S}$ are respectively the vectors of conserved variables, fluxes and source terms, defined as:

$$\mathbf{U} = \begin{pmatrix} \rho A \\ \rho u A \\ \rho E A \\ A \end{pmatrix}, \mathbf{F}(\mathbf{U}) = \begin{pmatrix} \rho u A \\ \rho u^2 A + AP \\ \rho u A \left(E + \frac{P}{\rho} \right) \\ VA \end{pmatrix}, \mathbf{S} = \begin{pmatrix} 0 \\ \rho \frac{\partial A}{\partial x} \\ 0 \\ 0 \end{pmatrix} \tag{2}$$

where u, ρ and P are respectively the fluid velocity, density and pressure, while E is the specific total mixture energy:

$$E = e + \frac{1}{2}u^2 \tag{3}$$

where e is the specific internal energy.

To calculate the properties of the liquid and vapour phases and their equilibrium mixtures formed during CO_2 pipeline decompression, the Perturbed Chain-Statistical Associating Fluid Theory (PC-SAFT) equation of state is applied. This equation of state has proved to provide superior accuracy in predicting the thermodynamic data for multi-component CO_2 mixtures covering the regions of vapour-liquid equilibria (VLE) of relevance for CCS transportation pipelines, as discussed by Diamantonis et al. (2013). In the present study, for the sake of example, the pipeline fracture simulations are performed for a CO_2 stream containing 3.5% of N_2 and 3.4% of H_2S, which are typical impurities found in industrial-grade CO_2 captured using pre-combustion technology, as shown by Porter et al. (2015).

The governing partial differential equations of the flow model can be solved subject to initial and boundary conditions for the flow at either end of the pipeline. At the closed end, the flow velocity set to zero. At the end of the pipe, where the fracture propagation is initiated, the fluid is exposed to the ambient pressure. The numerical solution of the set of above quasi-linear hyperbolic equations, describing flow in a variable cross-section area pipe, is performed using the Finite-Volume Method. Details of the implementation of this method were previously described by Brown et al. (2015).

2.3. Crack propagation model

The XFEM approach is an extension of the conventional finite element method based on the concept of partition of unity, which allows local enrichment functions to be easily incorporated into a finite element approximation. Crack modelling based on XFEM allows simulating both stationary and moving cracks. The method is useful for the approximation of solutions with pronounced non-smooth characteristics in small parts of the computational domain, for example near discontinuities and singularities. In these cases, standard numerical methods such as the conventional finite element method often exhibit poor accuracy.

For the purpose of fracture analysis, the enrichment functions typically consist of the near-tip asymptotic functions that capture the singularity around the crack tip and a discontinuous function that represents the jump in displacement across the crack surfaces. The approximation for a displacement vector function $u^h(\mathbf{x})$ with the partition of unity enrichment is given by

$$u^h(\mathbf{x}) = \sum_{i=1}^{n} N_i(\mathbf{x}) \left[u_i + H(\mathbf{x})a_i + \sum_{\alpha=1}^{4} F_\alpha(\mathbf{x})b_i^\alpha \right] \tag{4}$$

where $N_i(\mathbf{x})$ are the usual nodal shape functions; the first term on the right-hand side of the above equation, u_i, is the usual nodal displacement vector associated with the continuous part of the finite element solution; the second term is the product of the nodal enriched degree of freedom vector, a_i, and the associated discontinuous jump function $H(\mathbf{x})$ across the crack surfaces; and the third term is the product of the nodal enriched degree of freedom vector, b_i^α, and the associated elastic asymptotic crack-tip functions, $F_\alpha(\mathbf{x})$. The first term on the right-hand side is applicable to all the nodes in the model; the second term is valid for nodes whose shape function support is cut by the crack interior. The third term is used only for nodes whose shape function support is cut by the crack tip. The discontinuous jump function across the crack surfaces, $H(\mathbf{x})$, is equal to +1 for $(\mathbf{x} - \mathbf{x}^*)\mathbf{n} \leq 0$ and -1 otherwise, where $\mathbf{x}$ is a sample (Gauss) point, $\mathbf{x}^*$ is the point on the crack closest to $\mathbf{x}$, and $\mathbf{n}$ is the unit outward normal to the crack at $\mathbf{x}^*$. The asymptotic crack tip functions in an isotropic elastic material, $F_\alpha(x)$, are given by

$$\{F_\alpha(r, \theta)\}_{\alpha=1}^{4} = \left\{ \sqrt{r} \sin\left(\frac{\theta}{2}\right), \ \sqrt{r} \cos\left(\frac{\theta}{2}\right), \ \sqrt{r} \sin\left(\frac{\theta}{2}\right)\sin\theta, \ \sqrt{r} \cos\left(\frac{\theta}{2}\right)\sin\theta \right\} \tag{5}$$

where (r, θ) is a polar coordinate system with its origin at the crack tip and $\theta = 0$ is tangent to the crack at the tip. These functions span the asymptotic crack-tip function of elasto-statics, $\sqrt{r}\sin(\theta/2)$ and take into account the discontinuity across the crack face.

2.4. CO_2 Pipe section model

An API X70 grade steel pipe section of 10m long, 1.22m outer diameter and 18mm thickness transporting a CO_2 mixture containing 93.1% of CO_2, 3.5% of N_2 and 3.4% of H_2S, was modelled to test its sensitivity to brittle fracture

propagation. The ambient temperature was assumed to be 0°C. Only half of the pipe section was considered by utilizing the symmetry conditions. The pipe was fixed at one side and a through-wall starter notch with a length equal to the outer diameter is introduced to trigger crack initiation at the other side. The crack propagation distance was limited to 4 times the outer diameter to reduce the computational time.

Isotropic material properties with elasto-plastic behaviour with a yield stress of $\sigma_y = 760$MPa was defined for the pipe section. 3-D structural 8-node linear brick, reduced integration, hourglass control (C3D8R) elements were used for the pipe section model. The minimum mesh size along the crack propagation path was 6mm and increased gradually away from the area of interest. In order to obtain reliable results from numerical simulations, it is essential to apply the correct loading conditions i.e. internal and back-fill pressures during running fracture in the pipe. In the present study a simplified approach was adapted where effect of the back-fill pressure was simulated by applying a constant pressure load of 5MPa on the external surface of the pipe wall, as suggested by Makino et al. (2001).

3. Result and discussion

Fig. 2(a) shows the pipe area which is plastically deformed, also called the process zone, at the crack tip. It should be noted that the crack tip plasticity fulfils the assumption of small scale yielding concept which is necessary for propagating brittle fracture. Fig. 2(b) indicates the variation of the normalised hoop stress versus the normalised pipeline length for different crack lengths. As expected, by advancing the crack, the hoop stress at the crack tip drops due to decompression.

As no experimental data is available for validating the developed hybrid fluid-structure model, a simple semi-empirical crack propagation model previously developed based on the pipeline fracture propagation data was used to verify the obtained numerical results. In particular, in order to calculate the crack propagation speed and verify the developed hybrid numerical model the HLP model was used. The HLP method is a relatively simple algebraic model which is based on the empirical correlation proposed by Makino et al. (2001).

Fig. 3 compares the calculated crack propagation speed of the developed hybrid fluid-structure model (XFEM+CFD) and the above analytical approach for lower shelf energy, which is coupled with the CFD model, (HLP+CFD). Comparing the results of XFEM+CFD model with the HLP+CFD approach at lower shelf energy proves that the estimated numerical results are in good agreement with the calculated analytical solutions.

Fig. 4(a) and (b) depict the variation of the normalised mode I and II (opening and shearing crack propagation modes) SIFs during crack propagation and decompression. As mentioned above the crack front was meshed using three elements through the pipe wall. Therefore, the SIFs can be extracted at four different nodes through the pipe wall's thickness. As shown in Fig. 4(a) these four nodes are named as $n1$ to $n4$, in which $n1$ is the node at the outer
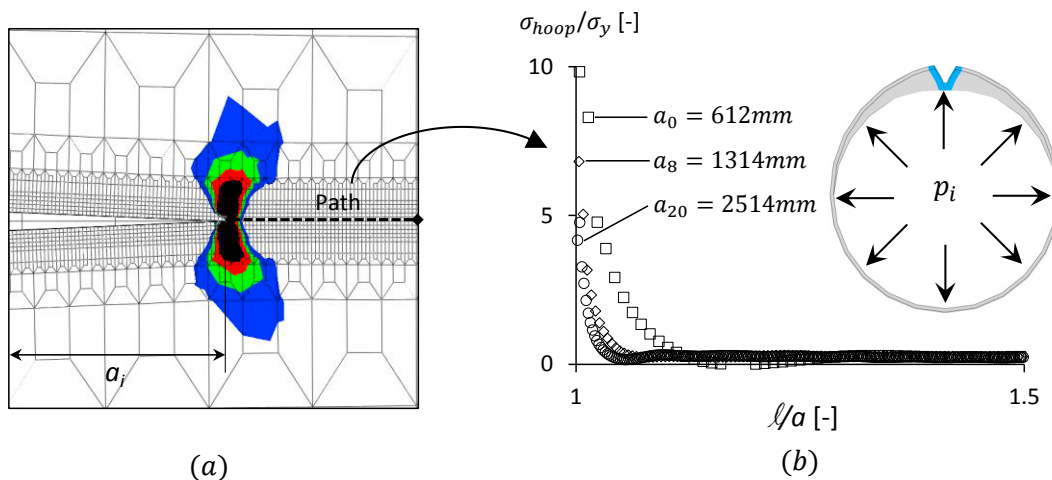

Fig. 2. (a) the plastic stress distribution, which is also call as process zone, at crack tip; (b) the variation of normalised opening stresses versus the normalised pipeline length for different crack lengths

surface and $n4$ is the inner surface. From the figure it can be seen that the mode I SIF (K_I) decreases by advancing the crack, which clearly results from pipe decompression. This drop is severe at the beginning of the pipe's decompression up to a crack length equal to 0.4 times the pipe length and reaches a plateau from 0.4 till 0.8 times the pipe length, following a tendency to drop at the end of the pipe's section. In addition, it can be seen that the obtained mode I SIFs (K_I) follow the same trend at all points through the pipe's thickness as explained above. Nevertheless, the stress intensity is slightly higher inside the pipe, which can be because of the compressive back-fill pressure applied at outer surface of the pipe.

Fig. 4(b) shows the variation of the normalised mode II SIF (K_{II}) versus the normalised crack propagation length. The obtained results reveal that the tendency of mixed mode crack propagation is very low. In addition it can be noted that the variation of K_{II} is not the same for the outside and the inside of the pipe. The mode II SIF inside the pipe has almost the same trend as mode I SIF, as shown in Fig. 4(a), but at the outer surface of the pipe the variation of K_{II} is negligible.

In order to test the propensity of pipeline material to fracture propagation, Battelle Two Curve (BTC) method is commonly applied. This involves comparing the pipeline depressurization rate with the fracture velocity. According to the BTC method the crack is arrested, at any stage during depressurization, once the fracture velocity is lower than or equal to the depressurization velocity. In this study the brittle fracture propagation velocity was calculated using hybrid fluid-structure interaction model described above. Fig. 5 shows the comparison between crack propagation and CO_2 decompression velocities obtained for a pre-combustion CO_2 mixture containing 93.1% CO_2, 3.5% N_2 and 3.4% H_2S. From the figure it can be concluded that around crack tip pressure of 4.5MPa, the crack propagation velocity becomes lower than the gas decompression velocity at which point the crack arrests.

4. Conclusion

In this study, a rigorous hybrid fluid-structure interaction model was presented to simulate brittle fracture propagation in a CO_2 pipeline steel. A one-dimensional compressible CFD model based on the homogeneous equilibrium assumption was employed to simulate the fluid decompression behaviour during pipeline deformation. The XFEM approach was used to model dynamic brittle fracture behaviour of pipeline steel, in which the dynamic SIF and crack velocity were calculated at the crack tip during crack propagation.
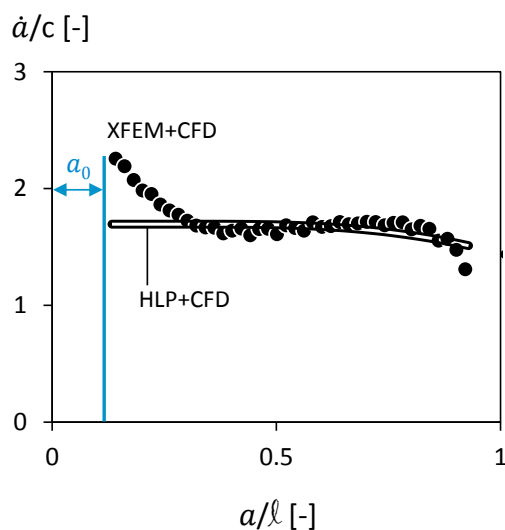

Fig. 3. compares the developed hybrid fluid-structure model (XFEM+CFD) and the analytical approach for both upper and lower shelf energy, which was coupled with FCD model, (HLP+CFD). The crack propagation speed and length are normalised by speed of sound in air (c= 434 [m/s]) and pipe length, respectively.
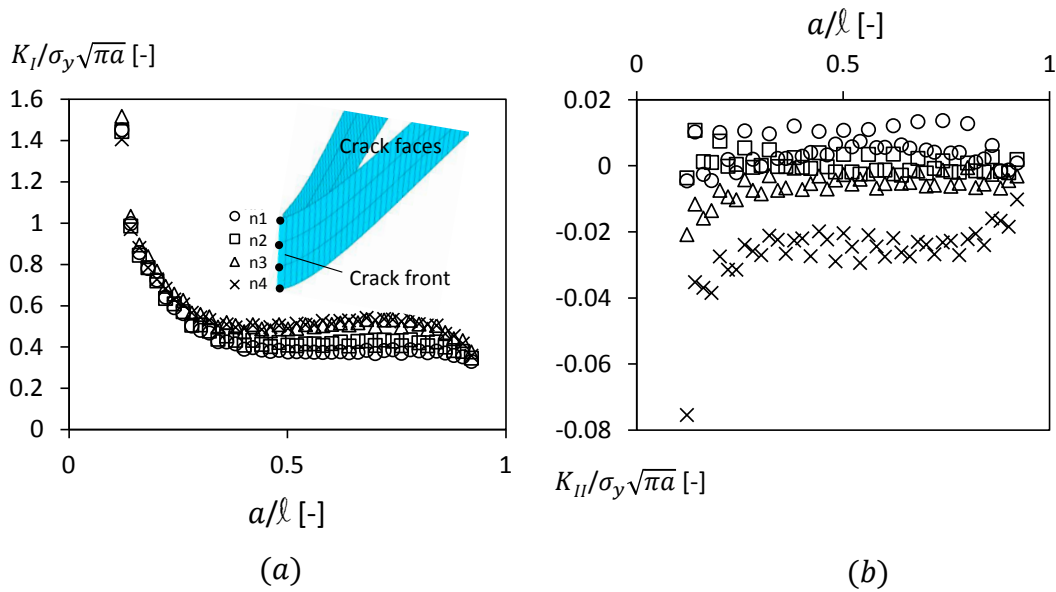
Fig. 4. Variation of normalised (a) mode I (opening crack propagation mode) and (b) mode II (shearing crack propagation mode) during crack propagation and pipeline decompression.

The proposed model was successfully verified by comparing its predictions against those obtained from the available analytical High Strength Line Pipe approach. Based on the application of the rigorous hybrid fluid-structure interaction model to a realistic API X70 steel CO_2 pipeline containing typical operating at conditions expected in CCS, it was shown that in case of a brittle fracture, the propagating crack is arrested at a short distance along the pipe length following its initiation.
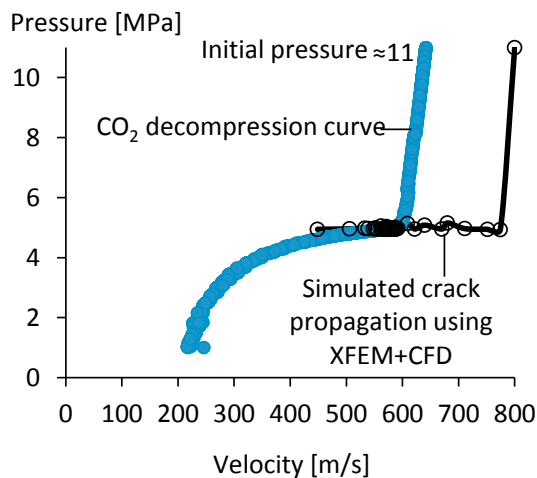

Fig. 5. comparison between the variation of gas pressure versus decompression velocity for CO_2 and the predicted crack velocity during decompression.

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References

Andrews, R., Haswell, J., Cooper, R., 2010. Will fractures propagate in a leaking CO_2 pipeline? Journal of Pipeline Engineering, 9(4).

Brown, S., Martynov, S., Mahgerefteh, H., 2015. Simulation of two-phase flow through ducts with discontinuous cross-section 120, 46–56.

Diamantonis, N.I., Boulougouris, G.C., Mansoor, Erum., Tsangaris, Dimitrios M., Economou, I.G., 2013. Evaluation of cubic, SAFT, and PC-SAFT equations of state for the vapor-liquid equilibrium modeling of CO_2 mixtures with other gases. Industrial & Engineering Chemistry Research 52(10), 3933–3942.

Mahgerefteh, H., Oke, A., Rykov, Y., 2006. Efficient numerical solution for highly transient flows. Chemical engineering science 61(15), 5049–5056.

Mahgerefteh, H., Brown, S., Denton, G., 2012. Modelling the impact of stream impurities on ductile fractures in CO_2 pipelines. Chemical engineering science 7, 200–210.

Makino, H., Kubo, T., Shiwaku, T., Endo, S., Inoue, T., Kawaguchi, Y., Matsumoto, Y., Machida, S., 2001. Prediction for crack propagation and arrest of shear fracture in ultra-high pressure natural gas pipelines. ISIJ international 41(4), 381–388.

Nordhagen, HO., Kragset, S., Berstad, T., Morin, A., Dørum, C., Munkejord, ST., 2012. A new coupled fluid–structure modeling methodology for running ductile fracture. Computers & Structures 94, 13–21.

Porter, R.TJ., Fairweather, M., Pourkashanian, M, and Woolley, Robert M., 2015. The range and level of impurities in CO_2 streams from different carbon capture sources. International Journal of Greenhouse Gas Control 36, 161–174.

Talemi, R.H., and Cooreman, S., Van Hoecke, D., 2016. Finite element simulation of dynamic brittle fracture in pipeline steel: A XFEM-based cohesive zone approach. Journal of Materials Design and Applications DOI: 1464420715627379.

Talemi, R.H., 2016. Numerical simulation of dynamic brittle fracture of pipeline steel subjected to DWTT using XFEM-based cohesive segment technique. Fracture and Structural Integrity 36, 151–159.

Zucrow, M.J., Hoffman, J.D., 1976. Gas dynamics. New York: Wiley.