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Decompression Modelling of Pipelines Carrying CO2-N2 Mixture and the Influence of Non-equilibrium Phase Transition

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The Carbon Capture and Storage (CCS) is the technology that has been proposed to reduce high concentrations of CO_2 in the atmosphere. This method involves transporting the CO_2 to the storage site, usually in pipelines. In order to ensure safe transport, the required pipe toughness must be accurately estimated. This, in turn, requires an accurate estimate of the decompression wave speed in the fluid. In this paper, a multi-phase Computational Fluid Dynamics (CFD) model is presented to simulate the decompression of a CO_2-N_2 mixture in a pipe. A real gas EOS (GERG-2008) was incorporated into the CFD code. The non-equilibrium liquid/vapour transition was modelled by introducing source terms for mass transfer and latent heat. The model is validated through simulation of a 'shock tube' test. The effects of the non-equilibrium phase transition on the decompression wave speed are discussed.

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Decompression modelling of pipelines carrying CO_2-N_2 mixture and the influence of non-equilibrium phase transition

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Abstract

The Carbon Capture and Storage (CCS) is the technology that has been proposed to reduce high concentrations of CO_2 in the atmosphere. This method involves transporting the CO_2 to the storage site, usually in pipelines. In order to ensure safe transport, the required pipe toughness must be accurately estimated. This, in turn, requires an accurate estimate of the decompression wave speed in the fluid. In this paper, a multi-phase Computational Fluid Dynamics (CFD) model is presented to simulate the decompression of a CO_2-N_2 mixture in a pipe. A real gas EOS (GERG-2008) was incorporated into the CFD code. The non-equilibrium liquid/vapour transition was modelled by introducing source terms for mass transfer and latent heat. The model is validated through simulation of a 'shock tube' test. The effects of the non-equilibrium phase transition on the decompression wave speed are discussed.

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Keywords: Carbon capture and Storage; Equation of State; multiphase flow; CO_2-N_2 mixture

1. Introduction

The Carbon Capture and Storage (CCS) is widely seen as a promising technique to reduce the emission of CO_2 into the atmosphere. CCS requires the transportation of CO_2 from the capture location to the storage site [1]. The commercial-scale transportation prefers to use pipelines. In the design of the pipelines, arresting or preventing the running fracture is a major concern. In terms of operational and economic motivations, the best way to transport CO_2 via pipelines is to transport it in liquid or supercritical state [2]. If an accident occurs leading to fluid release into the ambient, a decompression

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wave is formed inside the pipe. Accurate models for predicting the depressurisation behaviour are required to avoid running-ductile fracture. It has been found that a pipeline transporting CO_2 will be more susceptible to running-ductile fracture than one carrying natural gas. One reason is that severe CO_2 depressurisation in a pipeline tends to generate a two-phase flow. Moreover, captured CO_2 usually contains impurities such as N_2, which can also modify the decompression behaviour quite significantly due to the change of the phase envelope. A number of researchers [3-5] have used transient one-dimensional equations describing mass, momentum and energy conservation expressed in terms of fluid velocity, density and pressure, in conjunction with a 'real gas' Equation of State (EOS) to model such flows. In these models, the fluid is considered to remain at thermal and mechanical equilibrium during depressurisation, and any possible non-equilibrium phase transition is ignored. These models are described as Homogeneous Equilibrium Models (HEMs). Although the overall results predicted by HEM are in reasonable agreement with measurements, there are still relatively great discrepancies between simulation and measurement under some conditions. Specifically, the predicted 'pressure plateau' in the decompression wave speed curve is usually higher than the measured plateau [2, 6]. The discrepancies were probably introduced by the equilibrium assumption. To account for the non-equilibrium liquid/vapour transition, Brown et al. [7] proposed a model by introducing a 'relaxation time', which was empirically determined by Angielczyk et al. [8] based on tests involving the steady flow of CO_2 through a nozzle. In their study, the Peng-Robinson (PR) EOS [9] was employed to model the physical properties of the fluid. Prediction of a CO_2 pipeline full-bore rupture test showed reasonably good agreement with experimental data. However, it was found that the results were strongly dependent on the relaxation time and the improvement compared to HEM results is limited.

In this paper, in order to develop a better understanding of the decompression characteristics of high-pressure CO_2 mixtures, a multiphase CFD model considering non-equilibrium phase transition is proposed. The GERG-2008 EOS was incorporated into the CFD code to obtain precise physical property estimates for the CO_2-N_2 mixture in both liquid and vapour phases. The phase transition was modelled by considering the inter-phase mass transfer and the latent heat due to vaporisation. Validation of the CFD decompression model was carried out against measurements from a 'shock tube' test [8]. The influence of the non-equilibrium phase transition on the decompression characteristics is also discussed.

2. Models and methodology

2.1. Models

In attempting to study the behaviour of pipe flow associated with CO_2 releases, several experiments have been carried out. Among them was a series of 'shock tube' tests performed by Botros et al [10]. In their study, they also proposed a HEM in conjunction with the GERG-2008 EOS to calculate the decompression wave speed. The main section of the shock tube, which was a 'smooth' pipe, was 42 m long with an internal diameter (ID) of 38.1 mm. The tube was fitted with a 'rupture disc' at the discharge end. Controlled rupture initiated release of the contents of the pipe into the atmosphere. The test fluids included pure CO_2 and CO_2 with a range of impurities. In the present study, results of these experiments are used to validate the proposed model.

The physical flow domain in the shock tube test is the fluid initially in liquid form, contained in the horizontal pipe described above. This undergoes a 'full-bore' opening at one end when the rupture disc opens. Fig. 1 shows schematically the physical flow domain and the two-dimensional computational domain, along with a detail of the computational mesh near the outlet.

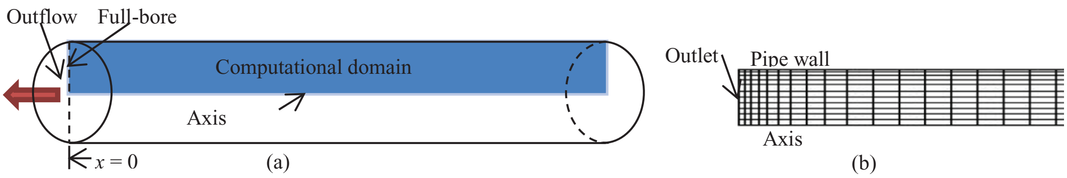


Fig. 1. (a) Schematic of the physical domain (the cylinder) as well as computational domain (blue rectangle), and (b) a two-dimensional computational grid near the exit

2.2. Methodology

A realistic simulation of the depressurisation inside the pipe requires reasonable modelling of the multiphase flow using an accurate EOS. As the GERG-2008 EOS is recommended as the reference EOS for gas pipelines [2], it is employed in this work for modelling the fluid in both liquid and vapour states [11]. As mentioned above, the non-equilibrium phase transition may strongly affect the pipe flow; hence, a non-equilibrium multiphase model was developed in this work. In the multiphase model, during the phase transition, a 'mass transfer coefficient' C is introduced to reflect the phase transfer rate. A simple model for phase transition can be set up as follows:

The mass source terms for each phase can be written as follows:

When $P < P_s$,

$$S_l = -S_v = C_l \alpha_l \rho_l (P - P_s) / P_s \tag{1}$$

When $P \geq P_s$

$$S_l = -S_v = C_v \alpha_v \rho_v (P - P_s) / P_s \tag{2}$$

The energy source term is obtained by taking the latent heat into account:

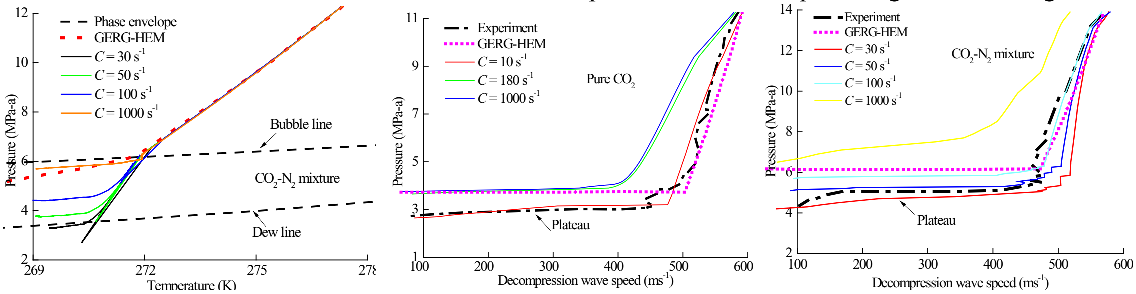
$$S_E = h_{lv} S_l \tag{3}$$

where S, α and ρ represent the mass source term, the volume fraction and the density, respectively; h_{lv} is the latent heat at given temperature. In the above equations, the subscripts l, v, s and E represent the liquid phase, vapour phase, saturation condition and energy. Obviously, C is a time relaxation factor used to regulate the rate of mass transfer, which dominates the phase transition during the depressurisation.

The stagnation condition of CO_2-N_2 mixture were considered as given by P_0 = 14.011 MPa and T_0 = 278.72 K, respectively, which were the same as those in the shock tube test in the Trial 20A [8]. The molar composition of the mixture is: CO_2 94.58% and N_2 5.42%. Trial 32A (P_0 = 11.27 MPa, T_0 = 281.89 K, pure CO_2 test) was also simulated for comparison.

3. Results and Discussion

Fig. 2a shows the P-T curves obtained for CO_2-N_2 mixture test (Trial 20A). The phase envelope consists of two lines – a bubble line (the upper line) and a dew line (the lower line). After crossing the bubble line, the phase change takes place and the fluid will be in a two-phase state. The pressure at bubble line for the mixture at corresponding temperature is much higher than that of saturation pressure of pure CO_2. Therefore, the phase change will occur in a relatively higher pressure. Clearly, compared against that obtained by the multiphase model, after cross bubble line, the P-T curve obtained by HEM will deviate less from bubble line firstly. The P-T curves predicted by the multiphase model deviate more from the bubble line and will end up nearly parallel to the bubble line. A larger value of C creates a smaller deviation from the bubble line. As a result, the pressure in the two-phase region will be higher.

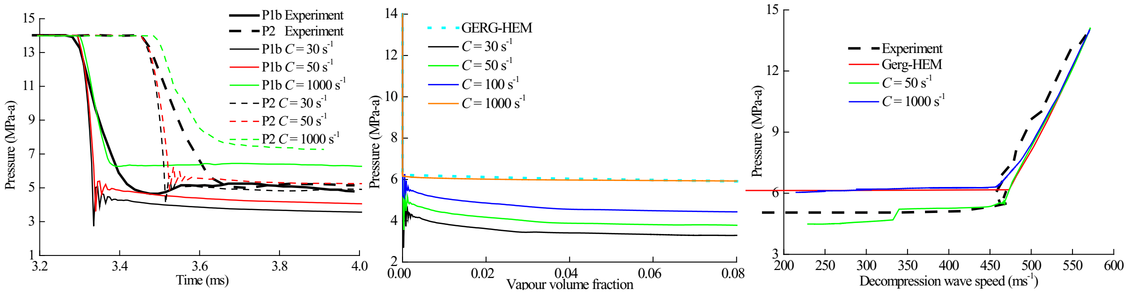


(a) P–T curves (b) Trial 32A, pure CO_2 (c) Trial 20A

Fig. 2 P-T curves and comparison of the measured and simulated decompression wave speeds

The decompression wave speed equals to the speed of sound minus the local 'outflow' velocity. The decompression wave speed curve is important to the fracture control analysis. However, shock tube tests cannot provide the decompression wave speed directly. The decompression wave speed is calculated by determining the times at which a certain pressure level is recorded at several pressure transducers at known locations on the pipe wall. By plotting these locations against time, the decompression wave speed can be obtained by performing a linear regression of each isobar curve. The slope of each regression represents the decompression wave speed for each isobar. In the simulation, the decompression wave speed is calculated using an approach similar to that used in processing the measured data (based on the pressure-time traces). Fig. 2b and Fig. 2c show the predicted decompression wave speeds against measurements for pure CO_2 (Trial 32A) and the mixture (Trial 20), respectively. The predictions obtained by GERG-HEM as proposed by Botros et al. [8] are also presented. It is observed that HEM over-predicts the pressures at plateaus for both pure CO_2 and the CO_2-N_2 mixture. Compared with HEM predictions, the results obtained by multiphase model are closer to the measured at plateau when proper values of C are chosen, both for pure CO_2 and the CO_2-N_2 mixture. Clearly, the value of C will significantly affect the prediction of the decompression wave speed. A smaller value of C can lead to a lower plateau pressure for both pure CO_2 and the mixture. This is because when a smaller value of C is chosen, the pressure drop will be greater due to the stronger non-equilibrium phase transition. The results show that the decompression wave speed predicted using C = 10 s^{-1} agrees well with the experimental data for pure CO_2, while for the mixture, the best value of C is 50 s^{-1}.

Fig. 3a shows the comparison of the measured and simulated pressure histories at two points – P1b and P2, which are located at 102.8 mm and 200 mm from the exit, respectively. The experimental results show that the pressure undergoes an initial sharp drop and then remains at a relatively stable plateau. The overall trend of the pressure drop was successfully predicted by the multiphase model. However, it is clear that the approach of the pressure transients to the plateau is significantly affected by the non-equilibrium phase transition (i.e. the value of C used). In addition, the predicted pressure curve is lower at the plateau when a smaller value of C is chosen. The pressure transient predicted using C = 50 s^{-1} shows the best agreement with measurements near the plateau. Fig. 3b shows the relationship between pressure and vapour volume fraction obtained using different values of C predicted by multiphase model as well as that obtained by HEM. Clearly, a smaller value of C predicts a lower vapour volume fraction at a given pressure. It is also observed that compared with the vapour volume fraction predicted by HEM, there is more deviation when a smaller value of C is chosen. For C = 1000 s^{-1}, the predicted curve is nearly coincident with that predicted by HEM. One can assume that a sufficiently high value of C corresponds to an equilibrium state. The density and speed of sound of the vapour are much smaller than those of the liquid, so that a larger value of *C* will underestimate the density and the speed of sound in 'two-phase' region. This may explain why the decompression wave speed is significantly smaller when a larger value of *C* is chosen. The large discrepancy between decompression wave speeds obtained by HEM and the multiphase model with a larger value of *C* is probably due to the calculation method of the decompression wave speed. In GERG-HEM proposed by Botros et al, the decompression wave speed is calculated as the speed of sound minus the local 'outflow' velocity, rather than performing a linear regression of each isobar curve. The latter technique is used in the experiment and the multiphase model. Fig. 3c shows the decompression wave speed obtained by speed of sound minus the escaping out flow velocity at point PT2. Apparently, the decompression wave speed obtained by $C = 1000\ s^{-1}$ is close to that obtained by GERG-HEM.



(a) Pressure histories (b) Pressure vs vapour volume fraction (c) Decompression wave speed

Fig. 3 Predicted pressure histories, vapour volume fraction and decompression wave speed

4. Conclusions

In this study, a multi-phase CFD model is presented to simulate the decompression behaviour of high-pressure pipelines carrying pure CO_2 and a CO_2-N_2 mixture. The GERG-2008 EOS was incorporated into the CFD code to model the thermodynamic properties of CO_2 in both liquid and vapour states. The inter-phase mass transfer rate was controlled using a 'mass transfer coefficient' in the mass source term. An energy source term was introduced for energy balance to take into account the latent heat due to vaporisation. The proposed model was validated against 'shock tube' tests conducted by Botros et al. It can be concluded that:

1) The non-equilibrium phase transition has a significant influence on the decompression behaviour, both for pure CO_2 and CO_2-N_2 mixture.
2) HEM tends to over-predict the plateau pressure due to the equilibrium assumption. The multiphase model is capable of simulating the non-equilibrium phase transition during the decompression. If the mass transfer coefficient *C* is fine-tuned, the decompression wave speed can be well predicted.

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