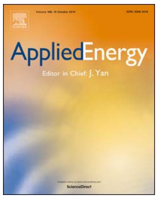
ARTICLE IN PRESS

Applied Energy xxx (xxxx) xxx–xxx

Contents lists available at ScienceDirect

Applied Energy

journal homepage: www.elsevier.com/locate/apenergy



A CFD decompression model for CO_2 mixture and the influence of non-equilibrium phase transition[☆]

Bin Liu, Xiong Liu, Cheng Lu[*], Ajit Godbole, Guillaume Michal, Anh Kiet Tieu

School of Mechanical, Materials and Mechatronic Engineering, University of Wollongong, NSW 2522, Australia

HIGHLIGHTS

- Multi-phase CFD model for decompression simulation of CO_2 mixtures.
- Incorporation of GERG-2008 EOS into CFD code for decompression modelling.
- Predicted decompression wave speed validated by measurements in shock tube experiments.
- Investigation of effects of delayed bubble formation on the decompression wave speed.

ARTICLE INFO

Keywords:
Carbon Capture and Storage
CO_2 pipeline
Decompression
CFD modelling
Multi-phase flow
Delayed bubble formation

ABSTRACT

Carbon Capture and Storage (CCS) is widely seen as an effective technique to reduce what is perceived as excessive CO_2 concentration in the atmosphere. This technique includes transporting CO_2 from source point to the storage site, usually through high-pressure pipelines. In order to ensure safe transport (i.e. to prevent the contents from being released into the atmosphere), it is important to estimate the required pipe toughness in the design stage. This requires an accurate prediction of the speed of the 'decompression wave' in the fluid, which is created when the high-pressure fluid escapes into the ambient. In this paper, a multi-phase Computational Fluid Dynamics (CFD) model is presented to simulate the decompression of high-pressure pipelines carrying CO_2 mixtures. A 'real gas' Equation of State (EOS), the GERG-2008 EOS, is incorporated into the CFD code to model the thermodynamic properties of the fluid in both liquid and vapour states. The non-equilibrium liquid/vapour transition is modelled by introducing 'source terms' for mass transfer and latent heat. The model is validated through simulation of a 'shock tube' test. A 'time relaxation factor' is used to control the inter-phase mass transfer rate. The measured decompression wave speed is compared with that predicted using different values of the time relaxation factor. It is found that the non-equilibrium phase transition has a significant influence on the decompression wave speed. Also, the effects of delayed bubble formation and of various impurities on the decompression wave speed are investigated.

1. Introduction

CO_2 is a major contributor to the 'greenhouse effect' [1]. The worldwide increase in energy demand coupled with a continued reliance on fossil fuel resources has contributed to a significant increase in atmospheric levels of CO_2 in recent years. Currently, power stations running on fossil fuels contribute approximately 40% of the total anthropogenic generation of CO_2. It is estimated that the amount of anthropogenic CO_2 emissions will triple by 2050 if the current trends continue [2]. Although efforts have been put forward to reduce the CO_2 emissions from more energy-efficient power generation processes and the application of renewable energy, many countries are expected to continue using coal and gas as their primary source of fuel [3], leading to continued CO_2 emission into the atmosphere. To combat this trend, the Carbon Capture and Storage (CCS) technique has been widely proposed as an effective technique to reduce CO_2 emissions into the atmosphere in the near future. Large-scale application of the CCS technique involves transporting CO_2 from the points of capture, especially from coal-fired power stations and other industrial facilities, to the storage sites [2,4,5]. This technique is estimated to have the potential to contribute up to 19% reduction of CO_2 emissions into the atmosphere by 2050 [2,6]. In most of the planned CCS projects, CO_2 is transported through high-pressure pipelines [7]. Therefore, issues regarding pipeline safety must be considered [8].

[☆] A shorter version of the paper was presented at the ICAE2016 on Oct 8–11, Beijing, China. This paper is a substantial extension of the short version of the conference paper.

[*] Corresponding author.
E-mail address: chenglu@uow.edu.au (C. Lu).

http://dx.doi.org/10.1016/j.apenergy.2017.09.016
Received 15 January 2017; Received in revised form 6 September 2017; Accepted 8 September 2017

Please cite this article as: Liu, B., Applied Energy (2017), http://dx.doi.org/10.1016/j.apenergy.2017.09.016

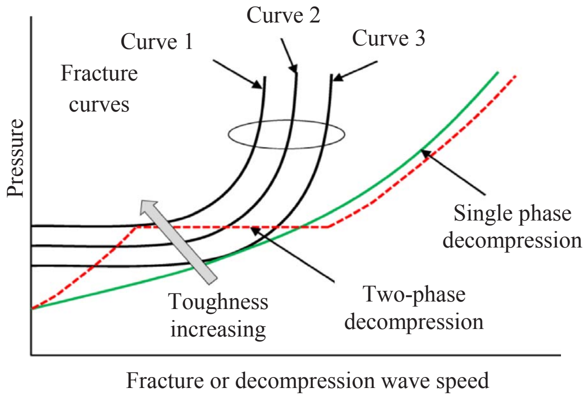


Fig. 1. Schematic diagram of the BTCM.

Under operational conditions, the possibility of running fractures in the pipeline is a major safety concern. Therefore, arresting and/or preventing a running fracture is of paramount importance to the integrity and safety of the pipelines [9,10]. Despite continuing progress over the last several decades, fracture propagation in pipelines is still commonly analysed using the relatively simple semi-empirical Battelle Two-Curve Model (BTCM) [11,12]. The aim is to estimate the resistance of the material to crack propagation. This model involves the superposition of two independently determined curves: the fluid decompression wave speed and the fracture propagation speed (the 'J curve'), each expressed as a function of pressure. Fig. 1 shows a schematic representation of the BTCM. The shape of the fluid decompression wave speed curve depends on the phase of the fluid, as shown by the red (two-phase) and green (single-phase) curves. Curves 1, 2 and 3 represent the fracture speed curves for different toughness values. Intersection of fracture speed curves 2 and 3 with the two-phase decompression curve implies that the fracture and fluid decompression wave move at the same speed. But in this case the fluid pressure at the tip of the fracture no longer decreases as indicated by the 'plateau' in the two-phase curve. This extends the fracture propagation distance. The boundary between arrest and propagation of a running fracture is represented by tangency between the decompression wave speed curve and the fracture speed curve. According to the BTCM, the minimum toughness required to arrest the propagation of a running ductile fracture is the value of toughness corresponding to this condition [13,14].

Clearly, to ensure adequate toughness of the pipe material so that a running fracture can be arrested when an accident occurs, an accurate estimation of the decompression wave speed of the fluid inside the pipeline is essential. To achieve this, a number of 'full-scale burst tests' of natural gas pipelines have been conducted [15–17] to measure the decompression wave velocity as it moves away from the rupture in the pipe. Pipes of increasing toughness are used to identify the toughness required to arrest the fracture. However, a full-scale burst test is very costly. Usually a more economical way is to use 'shock tube' test instead of a full-scale burst test. A shock tube test is designed to determine the decompression wave speed once a 'rupture' is initiated at one end of the tube. In the experiment, the initial fluid pressure and temperature can be adjusted so that different decompression paths can be observed. Cosham et al. [18] experimentally investigated the decompression behaviour of dense-phase pure CO_2 and various CO_2 mixtures, performed using a 144 m long, 168.3 mm Internal Diameter (ID) pipe. Botros et al. [19,20] tested the decompression of pure CO_2 and CO_2 mixtures using a 38.1 mm ID, 42 m long shock tube. As the main concern in these two experiments was to determine the decompression wave speed, the pipeline pressure variation during the depressurisation was only reported for very short duration. Drescher et al. [21] performed three shock tube tests for CO_2-N_2 mixtures. The mass fraction of N_2 in the mixture for three tests was 10%, 20% and 30% respectively. The initial conditions for the experiments were approximately 12.0 MPa and 293.15 K for all tests. The shock tube used was about 140 m long with an ID of 10 mm. These experiments provided valuable data for model validation.

Pipelines transporting CO_2 are more susceptible to a running ductile fracture than those carrying other gases, such as natural gas [22]. Two major reasons for this phenomenon are the tendency of the CO_2 to undergo phase change during depression due to its particular thermodynamic properties, and impurities in the CO_2 pipeline. Firstly, in CCS projects, CO_2 is usually transported in a liquid or supercritical state, as a purely gaseous phase transmission would require significantly larger pipelines to achieve the same mass flow rate. Therefore, if an accident occurs leading to a discharge of the contents of the pipeline, the discharge will involve a two-phase flow. When phase change takes place, the curve of decompression wave speed-vs-pressure will contain a plateau, as shown in Fig. 1. According to the BTCM, in order to avoid a running ductile fracture, the decompression wave speed curve (curve 1) should shift to the left considerably. Therefore, higher toughness is required for CO_2 pipelines. Secondly, the anthropogenic CO_2 that features in CCS projects usually contains impurities. Although the amount of these impurities may be small, their existence can affect the thermophysical properties of the mixture significantly, compared to pure CO_2. In turn, the decompression behaviour will be affected due to a change of the 'phase envelope'. Fig. 2 shows phase envelopes of different CO_2 mixtures and the saturation line of pure CO_2. For a given mixture, the phase envelope is made up of two lines – a 'bubble line' (the upper line) and a 'dew line' (the lower line). Above the bubble line, the fluid is in a liquid state. Between the bubble line and the dew line, the fluid is in a two-phase region. This region does not exist for pure CO_2. Below the dew line, the fluid is in a vapour state. Compared against the phase change condition of the mixture, specifically for the bubble line, the saturation pressure of CO_2 is much lower. This leads to the considerable difference in the decompression behaviour between pure CO_2 and CO_2 mixtures. The impurities also lead to a significant shift in the decompression wave speed curve (curve 1) in Fig. 1 to the left. This is due to a lengthening of pressure plateau, resulting in the higher toughness requirement.

In order to predict the flow of CO_2 in high-pressure pipelines, several numerical models, such as GASDECOM [23], DECOM [18], EPDECOM [24], DECAY [25], Picard and Bishnoi [26,27], PipeTech [22,28] and CFD-DECOM [29], have been proposed. Of these, the most widely used model is GASDECOM, which was originally developed for calculating the decompression curve of hydrocarbons [30]. GASDECOM is capable of modelling mixtures of hydrocarbons including nitrogen, carbon dioxide and methane through to hexane. The model uses the Benedict-Webb-Rubin-Starling (BWRS) EOS, with modified constants known to give accurate estimates of isentropic decompression behaviour. GASDECOM has been shown to predict the decompression curve

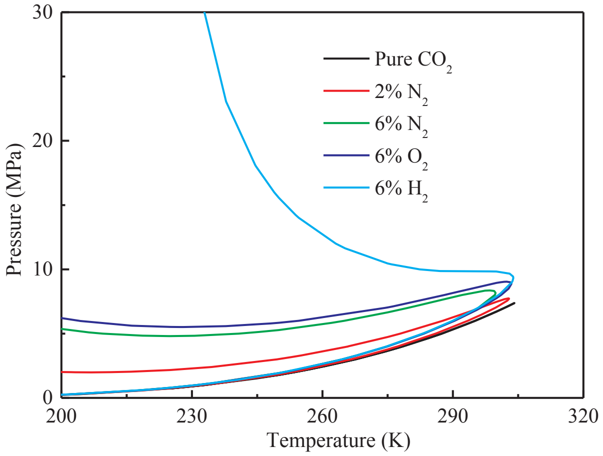


Fig. 2. Phase envelopes of CO_2 mixtures and saturation line of pure CO_2.