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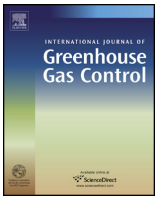

Modelling choked flow for CO_2 from the dense phase to below the triple point

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ABSTRACT

The modelling of the choked flow for CO_2 undergoing expansion from the dense phase state to below its triple point is presented. The choked flow properties, including mass flux, fluid phase composition, pressure, speed of sound and solids mass fraction are determined for the range of stagnation conditions relevant to the pipeline transportation of CO_2 following its accidental failure. The data indicate that the decompression of the dense phase CO_2 results in the stagnation of the flow at its triple point. At pressures below the triple point, the solid/vapour mixture is shown to be released at a mass flux of *ca.* 2000 kg/(m^2s). For a 50 mm diameter puncture in a pipeline transporting CO_2 at its critical point (304.2 K, 73.83 bar), the above translates into a discharge rate of *ca.* 1 kg/s of solid CO_2. Under such circumstances, in the case of buried pipelines, the accumulation of the slow subliming solid CO_2 within the resulting crater may significantly modify the subsequent dispersion behaviour of the migrating CO_2 cloud. As such, the phase transition behaviour of CO_2 around its triple point must be accounted for when performing safety assessment of CO_2 pipelines being considered as part of the carbon capture and sequestration chain.

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1. Introduction

In recent years, the development of carbon capture and sequestration (CCS) as a means of mitigating CO_2 emissions from large industrial sources such as fossil fuel power stations and other industrial plants has attracted considerable attention. An essential element of the CCS chain is the transportation of the large amounts of captured CO_2 to the storage site using pressurised pipelines. Such pipelines may typically be several hundred kilometres long, some passing through or close to populated areas. Given the significant amounts of CO_2 involved (typically several hundreds of tonnes), and considering the fact that CO_2 at high concentrations is an asphyxiant (Kruse and Tekiela, 1996), the safety of CO_2 pipelines is of paramount importance and indeed pivotal to the public acceptability of CCS as a viable means for tackling the impact of global warming (Koornneef et al., 2009; Mahgerefteh et al., 2011).

Central to the safety assessment of pressurised pipelines is the accurate prediction of the flow parameters at the rupture plane including the mass discharge rate, the fluid phase, pressure and temperature. The determination of the chocked flow boundary conditions is the essential first step for simulating such transient data (Mahgerefteh et al., 1999; Oke et al., 2003), the subsequent dispersion behaviour of the escaping CO_2, and hence the minimum safe distances to populated areas.

The rupture of the pipeline results in an almost instantaneous choking of the flow at the rupture plane (Coulson et al., 1999). The prediction of the subsequent outflow requires the determination of the corresponding choked flow condition at the release plane. Elias and Lellouche (1994) reviewed various two-phase liquid–vapour choked flow models ranging in complexity spanning those based on the homogenous equilibrium model (HEM), in which the constituent phases are assumed to be at thermal and mechanical equilibrium, to those accounting for both phase slip and thermal non-equilibrium. For homogeneous equilibrium flows, much the same as single-phase flows, the choked flow velocity equals the local speed of sound. The choked flow condition may then be defined as that corresponding to maximum mass flux with respect to the upstream pressure. For non-homogeneous flows with phase slip, this definition was modified by Moody (1965) who proposed maximising the choked mass flux both with respect to pressure and the ratio of the gas and liquid phase velocities or the slip ratio. More recent developments of the choked flow conditions for real gases and vapour–liquid homogeneous mixtures are reported by Maytal (2006) and Maytal and Elias (2009).

In general, the outflow models based on the HEM flow assumption have been shown to produce reasonably good predictions of the limited experimental data available for the full-bore rupture of two-phase hydrocarbon pipelines (Mahgerefteh et al., 1999,2006,

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Abbreviations: CCS, carbon capture and sequestration; HEM, homogenous equilibrium model; LVE, liquid–vapour equilibrium; SLVE, solid–liquid–vapour equilibrium; SVE, solid–vapour equilibrium.

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2008; Oke et al., 2003). The success of the HEM may be partly justified based on the reasonable proposition that the almost instantaneous significant pressure drop at the rupture plane results in the complete entrainment of any evolving vapour with the high velocity escaping liquid, such that both phases remain in dynamic equilibrium, i.e. no phase slip (Mahgerefteh et al., 1999). However, given the unique thermo-physical properties of CO_2, a two-phase flow model may not be capable of simulating the complete depressurisation of a CO_2 pipeline. Firstly, unlike many common hydrocarbons, CO_2 has a triple point pressure, p_{tr}, of 5.18 bar, i.e. higher than atmospheric pressure. Additionally, CO_2 has a relatively high Joule-Thomson expansion coefficient (Yaws, 2012). As a result, the near-adiabatic decompression process following pipeline rupture may lead to solid CO_2 formation both at the rupture plane and any point within the pipeline where the pressure falls below, p_{tr}. Indeed, as part of our CO_2PipeHaz European Commission Project (CO_2PipeHaz, 2009) involving the controlled rupture of an especially constructed fully instrumented 260 m long, 0.233 m internal diameter pipeline, we have recorded rupture-plane temperatures as low as −75 °C, where solid discharge has been clearly observed.

As such, in the case of CO_2 pipelines, the flow model must be capable of handling solid, liquid and vapour phases, both individually, in pairs, as well as simultaneously at the triple point. In particular, handling the triple point incorrectly will result in the erroneous simulation of the subsequent CO_2 sublimation trajectory. Given the very different hazard profiles of the slowly sublimating solid CO_2 as compared to the vapour, the above will directly impact the reliability of the subsequent CO_2 dispersion behaviour prediction.

The objective of the present study is to formulate the HEM choked flow conditions for CO_2 decompression to atmospheric pressure covering its entire phase transition spectrum. In Section 2, the theory of the choked flow for HEM fluids is presented. This is based on the previous analysis for liquid–vapour equilibrium (LVE) mixtures (Maytal and Elias, 2009), which is extended here to solid–vapour equilibrium (SVE) and solid–liquid–vapour equilibrium (SLVE) mixtures at the triple point. In Section 3, the three-phase model is applied to CO_2 mixtures, where the choked flow properties are determined for the range of stagnation states relevant to the problem of the rapid depressurisation of CO_2 transportation pipelines during accidental failure. Here, the analysis is particularly focused on the choked states around the triple point of CO_2 where the transition from the LVE to SVE mixture occurs. The conclusions of the study are presented in Section 4.

2. Theory

2.1. Properties of HEM fluid

The present study is aimed at modelling the choked flow conditions for equilibrium homogeneous saturated mixtures that can be formed during isentropic expansion of CO_2, including LVE mixtures at pressures above p_{tr}, SVE mixtures at pressures below p_{tr}, and SLVE mixtures at p_{tr}.

For a three-phase SLVE mixture, its specific properties, namely enthalpy, h, entropy, s, and specific volume, v are respectively defined as:

$$h = x_v \cdot h_v + x_l \cdot h_l + x_s \cdot h_s \tag{1}$$

$$s = x_v \cdot s_v + x_l \cdot s_l + x_s \cdot s_s \tag{2}$$

$$v = x_v \cdot v_v + x_l \cdot v_l + x_s \cdot v_s \tag{3}$$

where x is the phase mass fraction. The subscripts v, l, and s refer to the saturated vapour, liquid and solid, respectively. Also,

$$x_v + x_l + x_s = 1 \tag{4}$$

2.2. Expanded states of the flow

An isentropic expansion flow of a fluid from a given stagnation state, defined by pressure, p_o, and entropy, s_o, is accompanied by an increase in the fluid velocity, u, and decrease in the local adiabatic speed of sound, c_s. The expansion states that the fluid passes through before reaching the choked state, where its velocity reaches the local speed of sound ($u = c_s$), is defined by a set of constraining equations. These equations can be obtained based on the one-dimensional mass, momentum and energy conservation equations of homogeneous equilibrium flow (Zucrow and Hoffman, 1975):

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho u}{\partial z} = 0 \tag{5}$$

$$\frac{\partial \rho u}{\partial t} + \frac{\partial(\rho u^2 + p)}{\partial z} = 0 \tag{6}$$

$$\frac{\partial \rho e}{\partial t} + \frac{\partial\left(\rho u\left[h + \frac{u^2}{2}\right]\right)}{\partial z} = 0 \tag{7}$$

where $\rho = 1/v$ and $e = h - p/\rho$ are the density and specific energy of the fluid, t is the time and z is the spatial coordinate. Assuming steady-state and smooth solution of these equations, their integration gives:

$$\Delta(\rho u) = 0 \tag{8}$$

$$\Delta(\rho u^2 + p) = 0 \tag{9}$$

$$\Delta\left(h + \frac{u^2}{2}\right) = 0 \tag{10}$$

Combining Eqs. (8)–(10) with the thermodynamic relation $Tds = dh - vdp$ gives the entropy condition:

$$\Delta s = 0 \tag{11}$$

Eqs. (10) and (11) applied at the release end of the reservoir state respectively conservation of the total enthalpy and entropy of the fluid upon expansion:

$$h + \frac{u^2}{2} = h_o \tag{12}$$

$$s = s_o \tag{13}$$

where h is the thermodynamic enthalpy at the expansion state (p, s) and h_o is the enthalpy at the stagnation state (p_o, s_o).

Eqs. (12) and (13) closed by Eqs. (1), (2) and (4), can be solved simultaneously to determine the velocity of a multi-phase mixture for given stagnation state. In particular, from Eq. (12) the flow velocity can be calculated from:

$$u = \sqrt{2(h_o - h)} \tag{14}$$

For a LVE mixture (i.e. when $x_s = 0$), the vapour mass fraction can be expressed using Eqs. (2) and (4), as:

$$x_v = \frac{s - s_l}{s_v - s_l} \tag{15}$$

Substitution of Eq. (15) and the thermodynamic relation at the triple point $h_v - h_l = T_{tr}(s_v - s_l)$ into Eqs. (1) and (4), and the resulting equation into Eq. (14) produces the following equation for the velocity, u_{lv}, for the LVE mixture:

$$u_{lv} = \sqrt{2\left[h_o - h_l + T_{tr}(s_l - s)\right]} \tag{16}$$

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