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## Modelling ruptures of buried high pressure dense phase CO<sub>2</sub> pipelines in carbon capture and storage applications—Part I. Validation

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#### ABSTRACT

Carbon dioxide  $(CO_2)$  capture and storage presents a short-term option for significantly reducing the amount of  $CO_2$  released into the atmosphere and mitigating the effects of climate change. To this end, National Grid initiated the COOLTRANS research programme to consider the pipeline transportation of high pressure dense phase  $CO_2$ , including the development and application of a mathematical model for predicting the sonic near-field dispersion of pure  $CO_2$  following the venting or failure of such a pipeline. Here, the application of this model to the rupture of a buried pipeline is considered and compared to experimental data obtained through the COOLTRANS programme. The rupture experiment was performed on a 230 m length of 152 mm external diameter pipeline with 300 mm soil cover, equivalent to approximately 1/4 scale when compared to the proposed full-scale 600 mm (24-inch) diameter pipelines with 1.2 m soil cover on average proposed in the UK. The experiment was performed in a pre-formed crater based on experimentally formed craters in other experiments. The comparison demonstrates reasonable quantitative and qualitative agreement. Such validated dispersion flow, to be applied to full-scale rupture modelling in Part II, defines novel, robust, thermodynamically accurate multi-phase source conditions, that enable far-field computational fluid dynamics studies and feed into pragmatic quantified risk assessment models.

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#### 1. Introduction

Carbon dioxide ( $CO_2$ ) capture and storage (CCS) refers to a set of technologies designed to reduce  $CO_2$  emissions from large industrial point sources of emission, such as coal-fired power stations, in order to mitigate greenhouse gas production. The technology involves capturing  $CO_2$  and then storing it in a reservoir, instead of allowing its release to the atmosphere, where it contributes to climate change. Once captured, the  $CO_2$  is transported and stored, typically underground, or used for processes such as enhanced oil recovery.

National Grid initiated the TRANSportation of Liquid  $CO_2$  research programme (COOLTRANS) (Cooper, 2012) in order to address knowledge gaps relating to the safe design and

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http://dx.doi.org/10.1016/j.ijggc.2015.01.020 1750-5836/© 2015 Elsevier Ltd. All rights reserved. operation of onshore pipelines for transporting dense phase CO<sub>2</sub> from industrial emitters in the UK to storage sites offshore. This includes developing the capability for modelling the lowprobability, high-impact worst case scenario - an accidental release from a buried pipeline that contains CO<sub>2</sub> in the dense phase. Learning from these studies can subsequently be combined with a range of other information to inform front-end engineering design (FEED) activities and to develop an appropriate quantified risk assessment (QRA) for a dense phase CO<sub>2</sub> pipeline, currently underway in the UK for two CCS projects (Peterhead, and Don Valley, into which this work specifically contributed). With regard to modelling the worst case scenario, the programme includes theoretical studies by University College London (UCL), the University of Leeds and University of Warwick, carried out in parallel to provide "state of the art" numerical models that connect together in full chain dispersion modelling for the outflow (UCL), near-field dispersion behaviour (Leeds) and far-field dispersion behaviour (Warwick) associated with below ground CO<sub>2</sub> pipelines that are ruptured or punctured. Experimental work and studies using currently available practical models for risk assessment are being carried out by DNV GL

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(Allason et al., 2012; Cosham et al., 2012). The experimental work has provided data against which the modellers can compare their predictions.

In this paper, the Leeds mathematical model (Wareing et al., 2013a), previously validated for free releases into air (Woolley et al., 2013; Wareing et al., 2014a), small-scale laboratory releases and dry ice particle behaviour (Wareing et al., 2013b) and punctures of buried pipelines (Wareing et al., 2014b), is validated against COOLTRANS experimental data from a rupture of a buried pipeline with external diameter of 152 mm and wall thickness of 11 mm, resulting in an internal diameter of approximately 130 mm. This is approximately 1/4-scale when compared to the 600 mm diameter pipelines proposed in the Don Valley CCS project referred to above and henceforth in this article the experiment will be referred to as 1/4-scale. Ruptures occur in pipelines for a number of reasons – from human interference to pipeline defects (Cosham et al., 2012). The validation described in this paper represents a considerable step toward the goal of developing a modelling capability for the transient rupture of a buried pipeline.

In the next section, we review the background literature. In the following Section 3, we present the experimental details of this 1/4 scale rupture experiment. In Section 4, we summarise the model and numerical method. Numerical predictions of this 1/4-scale rupture are presented in Section 5 and compared with experimental data. The comparisons are further discussed in Section 6 and the limits of applicability are discussed in Section 7, Finally, brief conclusions are presented in Section 8. Part II of this two-paper series will apply the model to a full-scale rupture and present numerical simulations of a full-scale transient decompression, as well as sensitivity studies with regard to expected variations of the shape of the crater. As experimental data of the type used here for validation is not currently available for full-scale ruptures, such a sensitivity study is very valuable.

#### 2. Background

In this section, we consider the growing number of recent publications that have examined the release and dispersion of CO<sub>2</sub>, revisiting our review from Wareing et al. (2014a) that summarised the depth provided by Dixon et al. (2012) in the light of new and related additions to the literature.

A study by MMI Engineering (Dixon and Hasson, 2007) presented dispersion simulations employing the ANSYS-CFX computational fluid dynamics (CFD) code. Solid CO<sub>2</sub> particles were simulated by a scalar representing the particle concentration, in order to avoid additional computing associated with Lagrangian particle tracking. Dixon et al. (2012) note that this method assumed a constant particle diameter and temperature (at the sublimation temperature of -78.9 °C) in order to calculate heat and mass exchange between the particles and the gas phase. In a following publication (Dixon et al., 2009), particles were modelled via a Lagrangian particle tracking method, but were still assumed to be at the sublimation temperature. Dixon et al. (2012) note that since the rate of sublimation increases as particle size decreases, an improved distribution of the source of the CO2 gas resulting from particle sublimation could be obtained by allowing for varying particle size and for the fact that temperature is expected to fall below the sublimation temperature in the near-field of a

In 2011, Webber (2011) presented a methodology for extending existing two-phase homogeneous integral models for flashing jets to the three-phase case for CO<sub>2</sub>. Webber noted that as the flow expands from the reservoir conditions to atmospheric pressure, temperature, density and the jet cross-sectional area would vary continuously through the triple point, whilst the mass and

momentum would be conserved. This led to the conclusion that there must be a discontinuity in the enthalpy and  $\mathrm{CO}_2$  condensed phase fraction, in a similar manner to the energy change associated with passing through a hydraulic jump. In the development of our composite equation of state for modelling  $\mathrm{CO}_2$  near-field sonic dispersion (Wareing et al., 2013a), we confirmed this in a conservative shock capturing CFD code and highlighted the importance of fully accounting for the solid phase and latent heat of fusion; the near-field structure of the jet as well as the fraction of solid phase material is different when this is correctly accounted for.

Two recent papers (Witlox et al., 2009, 2011) have discussed the application of the software package PHAST to CO<sub>2</sub> release and dispersion modelling. In the first of these, Witlox et al. (2009) described an extension to the existing model in PHAST (v. 6.53.1) to account for the effects of solid CO<sub>2</sub>, including the latent heat of fusion. The modifications to the model consisted principally of changing the way in which equilibrium conditions were calculated in the expansion of CO<sub>2</sub> to atmospheric pressure. This was done in order to ensure that below the triple point, conditions followed the sublimation curve in the phase diagram, rather than extrapolating the evaporation curve (which diverges considerably from reality, hence the limitations of the Peng and Robinson (1976) and Span and Wagner (1996) equations of state to above the triple point only). In the second paper (Witlox et al., 2011), the results of sensitivity tests were reported for both liquid and supercritical CO<sub>2</sub> releases from vessels and pipes calculated with the revised PHAST model. The public release of the CO2PIPETRANS datasets and associated industrial projects, for example (Ahmad et al., 2013), has validated the development of this approach, which we also adopted in part for our composite equation of state (Wareing et al., 2013a).

E.ON have published a number of studies in support of their proposed CCS programme (Mazzoldi et al., 2008a,b, 2011; Hill et al., 2011). Of these, the most relevant to this work are Mazzoldi et al. (2011) and Hill et al. (2011). These consider atmospheric dispersion from pipeline and vessel releases. The former paper compared simulations from the heavy gas model ALOHA to the CFD model Fluidyn-Panache. Only the gaseous stage of the release was modelled. In the second work (Hill et al., 2011), the authors presented CFD and PHAST simulations of dense-phase CO<sub>2</sub> releases from a 0.5 m diameter hole in a pipeline, located at an elevation of 5 m above level ground. Steady-state flow rates were calculated at the orifice assuming saturated conditions. CFD simulations were performed using the ANSYS-CFX code with a Lagrangian particle tracking model for the the solid CO<sub>2</sub> particles, with three size distributions:  $10-50 \mu m$ ,  $50-100 \mu m$  and  $50-150 \mu m$ . Simulations were also performed without particles. Their results showed that sublimation of the particles led to a cooling of the CO2 plume, affecting dispersion behaviour, although the results were relatively insensitive to particle size. Gas concentrations downwind from the release were reportedly somewhat lower using PHAST (v 6.6) as compared to the CFD results. No comparison to experiment was performed.

Dixon et al. (2012) point out that it appears that in the Lagrangian model of Hill et al. (2011) their particle tracks followed closely the plume centreline, rather than being spread throughout the plume. Dixon et al. (2012) noted that turbulence will have the effect of bringing particles into contact with parts of the jet at a higher temperature and lower CO<sub>2</sub> concentration, thereby tending to increase the rate of sublimation and increase the radius of the region cooled by the subliming particles. In their work, Dixon et al. (2012) included turbulent dispersion effects in the CFX model. Further, they assumed that the solid particles are much smaller with an initial particle diameter of 5 µm. They made that choice based on an analysis of CO<sub>2</sub> experiments. In addition, this particle size distribution is supported by the model recently developed by Hulsbosch-Dam et al. (2012b,a), which suggested that the particle

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