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Evaluation of multi-phase atmospheric dispersion models for application to Carbon Capture and Storage

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A dispersion model validation study is presented for atmospheric releases of dense-phase carbon dioxide (CO_2). Predictions from an integral model and two different Computational Fluid Dynamics (CFD) models are compared to data from field-scale experiments conducted by INERIS, as part of the EU-funded CO_2PipeHaz project.

The experiments studied consist of a 2 m^3 vessel fitted with a short pipe, from which CO_2 was discharged into the atmosphere through either a 6 mm or 25 mm diameter orifice. Comparisons are made to measured temperatures and concentrations in the multi-phase CO_2 jets.

The integral dispersion model tested is DNV Phast and the two CFD models are ANSYS-CFX and a research and development version of FLACS, both of which adopt a Lagrangian particle-tracking approach to simulate the sublimating solid CO_2 particles in the jet. Source conditions for the CFD models are taken from a sophisticated near-field CFD model developed by the University of Leeds that simulates the multi-phase, compressible flow in the expansion region of the CO_2 jet, close to the orifice.

Overall, the predicted concentrations from the various models are found to be in reasonable agreement with the measurements, but generally in poorer agreement than has been reported previously for similar dispersion models in other dense-phase CO_2 release experiments. The ANSYS-CFX model is shown to be sensitive to the way in which the source conditions are prescribed, while FLACS shows some sensitivity to the solid CO_2 particle size. Difficulties in interpreting the results from one of the tests, which featured some time-varying phenomena, are also discussed.

The study provides useful insight into the coupling of near- and far-field dispersion models, and the strengths and weaknesses of different modelling approaches. These findings contribute to the assessment of potential hazards presented by Carbon Capture and Storage (CCS) infrastructure.

1. Introduction

The introduction of CCS will result in CO_2 being produced and transported in much greater quantities than it is today. It has been estimated that in order to generate 1 GW of electrical power from a coal-fired power station fitted with CCS will require around 30,000 tonnes/day of CO_2 to be captured and sequestered into long-term storage facilities (Harper, 2011).

To transport CO_2 from emitters, such as power stations, to sequestration sites, it is likely that pipelines will be used that will operate with the CO_2 in a dense-phase state, as either a supercritical fluid or liquid, i.e. at a pressure higher than 74 barg, and a temperature above or below its critical temperature of 31 °C. As part of the design and risk assessment process for CCS infrastructure, an understanding is required of the consequences of an intentional or accidental release of dense-phase CO_2.

When dense-phase CO_2 is discharged into the atmosphere, it is transformed into a mixture of gaseous and solid CO_2 (dry ice) at ambient temperature and pressure. The drop in pressure from the

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operating conditions to atmospheric pressure is also accompanied by significant cooling, since CO_2 has a high Joule–Thomson effect. For CO_2 at saturation conditions of 300 K and 67 bar, the Joule–-Thomson coefficient is approximately 0.9 K/bar (Perry, 2007). In comparison, for nitrogen at a similar temperature and pressure, the Joule–Thomson coefficient is slightly negative at around −0.01 K/bar. The positive coefficient value for CO_2 indicates a reduction in temperature with pressure, whereas the small negative value for nitrogen indicates a slight increase in temperature with falling pressure.

This unusual release behaviour of CO_2 presents a number of challenges for dispersion models that are used to predict the extent of the toxic cloud. This paper provides a review of the recent research in this area, followed by a description of the experiments, modelling and results of the validation exercise that was conducted as part of the EU-funded CO_2 PipeHaz project.[1]

2. Review of related research

Over the last decade, there have been a number of major research projects directed towards understanding the new safety issues presented by industrial-scale CCS. Perhaps the earliest study looking specifically at validation of dense-phase CO_2 dispersion models was undertaken in support of BP's Decarbonised Fuels 1 (DF1) project, in which it was planned to capture CO_2 emitted from the Peterhead power station in the UK and sequester it in the Miller oilfield under the North Sea. As part of this project, experiments were conducted at the GL Noble Denton Spadeadam test site and a number of consultancies performed dispersion model predictions. Some results from the MMI Engineering contribution to that project were published by Dixon and Hasson 2007 and Dixon et al. 2009. In the first of their two papers, results were presented using the CFD code ANSYS-CFX, in which the solid CO_2 particles in the jet were modelled using a transported scalar to represent the particle concentration. This approach was taken to avoid the additional computing time associated with the alternative particle-tracking approach. However, one of its limitations was that in calculating the heat and mass exchange between the particles and the gas phase it was necessary to assume a constant particle diameter. The CO_2 gas distribution within the jet may have therefore been poorly predicted, since the sublimation rate increases as the particle size decreases in the jet. In addition, the particle temperature was assumed to remain constant at the sublimation temperature of −78 °C, i.e. a "boiling" assumption was made. In their second paper (Dixon et al., 2009), solid CO_2 particles were modelled using a Lagrangian particle-tracking approach. However, the particles were still assumed to remain at a constant temperature of −78 °C, whereas in reality the particle temperature is expected to fall in the jet, to perhaps as low as −100 °C. In both of their papers (Dixon and Hasson, 2007; Dixon et al., 2009), scales were omitted on the axes of graphs showing the comparison of model predictions against experiments, due to confidentiality of the experimental data.

E.ON have published a number of studies in support of their proposed CCS programme (Mazzoldi et al., 2008a, 2008b, 2011; Hill et al., 2011). The most relevant of these, for the present work, are by Mazzoldi et al. (2011) and Hill et al. (2011), which considered atmospheric dispersion from pipelines and vessels. The former paper compared simulations from the heavy gas model ALOHA to the CFD model Fluidyn-Panache. Although the work focused on discharges of dense-phase CO_2 from a 100 bar release, only the gaseous stage of the discharges were modelled. The bulk of the analysis consisted of comparisons between the two models, rather than validation against experimental data.

Hill et al. (2011) presented CFD and Phast simulations of dense-phase CO_2 releases from a 0.5 m diameter hole in a pipeline, located at an elevation of 5 m above flat ground. CFD simulations were performed using the ANSYS-CFX code with a Lagrangian particle-tracking model for the solid CO_2 particles. To examine the effect of the particle size, Hill et al. (2011) performed simulations using three different particle size distributions: from 10 to 50 μm, 50 to 100 μm and 50 to 150 μm. Simulations were also performed using no solid CO_2 particles. The results showed that sublimation of the particles led to cooling of the CO_2 plume, which affected its dispersion behaviour, but the results were relatively insensitive to the particle size. Predicted gas concentrations were lower using Phast version 6.6 than with ANSYS-CFX, but there was no comparison of model predictions to experiments.

One of the differences between the ANSYS-CFX model used by Hill et al. (2011) and that used in the present study is that Hill et al. (2011) used a Lagrangian model that did not account for the effect of turbulence on the dispersion of the solid CO_2 particles. The particle tracks were not spread throughout the plume but instead followed closely the plume centreline. Ignoring turbulent dispersion effects can have a significant influence on the model predictions, particularly the temperature. Turbulence has the effect of bringing particles into contact with parts of the jet at a higher temperature and lower CO_2 concentration. This tends to increase the rate of sublimation and increase the radius of the region cooled by the sublimating particles.

DNV Software has produced several key papers on CO_2 release and dispersion modelling (Witlox et al., 2009, 2011, 2012). In the first of these, Witlox et al. (2009) described an extension to the existing model in Phast version 6.53.1 to account for the effects of solid CO_2. The modifications consisted principally of changing the way in which equilibrium conditions were calculated in the expansion of CO_2 to atmospheric pressure, to ensure that below the triple point, conditions followed the sublimation curve in the phase diagram. Furthermore, two-phase vapour/solid effects instead of vapour/liquid effects were included downstream of the orifice, after the CO_2 jet had depressurised to ambient pressure. Although the revised model was validated against experimental data, the measurements were confidential and were not reported. In the second paper (Witlox, 2010), the results of a sensitivity analysis were reported for both liquid and supercritical CO_2 releases from vessels and pipes, using the revised Phast version 6.6 model. Again, no experimental validation was presented due to data confidentiality. In more recent work (Witlox et al., 2012), results were finally compared to experimental data that was made publicly available as part of the CO_2PipeTrans joint industry project.[2] These experiments, which were originally funded by BP and Shell, consisted of above-ground, horizontal releases of supercritical and liquid CO_2, using orifice diameters from ¼″ to 1″ diameter (6.5 mm to 25.4 mm). The measured flow rates were predicted by Phast with an error of less than 10% and the dispersion model predictions were in good agreement with data (well within the factor-of-two criteria often used to assess the performance of atmospheric dispersion models).

The same Shell experiments were also modelled independently by Shell and HSL using the Shell FRED integral dispersion model, and two different CFD codes, OpenFOAM and ANSYS-CFX (Dixon et al., 2012). Both FRED (Betteridge and Roy, 2010) and the OpenFOAM models assumed Homogeneous Equilibrium (HE) between

[1] http://www.co2pipehaz.eu, accessed 28 January 2014.

[2] http://www.dnv.com/ccs, accessed 28 January 2014.