Proceedings Paper:

Woolley, RM, Proust, C, Fairweather, M et al. (4 more authors) (2013) Measurement and RANS modelling of large-scale under-expanded CO2 releases for CCS applications. In: AIP Conference Proceedings. AIP Conference, 21–27 September 2013, Rhodes, Greece. AIP Publishing LLC , 107 - 111. ISBN 9780735411845

https://doi.org/10.1063/1.4825432

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Citation: AIP Conference Proceedings **1558**, 107 (2013); doi: 10.1063/1.4825432
View online: http://dx.doi.org/10.1063/1.4825432
View Table of Contents: http://scitation.aip.org/content/aip/proceeding/aipcp/1558?ver=pdfcov
Published by the AIP Publishing

Measurement and RANS Modelling of Large-scale Under-expanded CO_2 Releases for CCS Applications

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Abstract. The deployment of a complete carbon-capture and storage chain requires a focus upon the hazards posed by the operation of CO_2 pipelines, and the consequences of accidental release must be considered as an integral part of the design process. Presented are results from the application of a shock-capturing numerical scheme to the solution of the Favre-averaged Navier-Stokes fluid-flow equations, coupled with a compressibility-corrected turbulence model, and a novel equation of state for CO_2. Comparisons are made with a series of as-yet unreported experimental observations of field-scale, high-pressure CO_2 releases. The effects of corrections to the solenoidal turbulence energy dissipation are tested, with conclusions drawn, and recommendations made for future developments.

Keywords: CCS, CO2, multi-phase flow, experimental measurement, mathematical modelling, pipeline depressurization
PACS: 02.60.-x, 07.05.Tp, 47.11.-j, 47.11.Df, 47.40.Ki, 47.40.-x, 47.55.-t, 93.85.Tf

INTRODUCTION

Under-expanded flows resulting in velocities greater than the local speed of sound are a feature of a wide number of applications in aviatic, astronautical, and process engineering scenarios including those relating to the accidental release of high-pressure fluids from pipelines. Such pipelines are considered to be the most likely method for transportation of captured CO_2 from power plants and other industries prior to subsequent storage, and their safe operation is of paramount importance as their contents are likely to be in the region of several thousand tonnes. CO_2 poses a number of dangers upon release due to its physical properties. It is a colourless and odourless asphyxiant which has a tendency to sublimation and solid formation, and is directly toxic if inhaled in air at concentrations around 5%, and likely to be fatal at concentrations around 10%. The developments presented in this paper concern the measurement of large-scale jet releases of CO_2, and the formulation of a multi-phase homogeneous discharge and dispersion model capable of predicting the near-field fluid dynamic and phase behaviour of such CO_2 releases. Predicting the correct fluid phase during the discharge process in the near-field is of particular importance given the very different hazard profiles of CO_2 in the gas and solid states. Model validations have been undertaken using the experimental data described, and suggestions for further developments are presented.

MATHEMATICAL MODELLING

The calculations employed an adaptive finite-volume grid algorithm, the major advantage of which being a great reduction in execution times. The model to describe the fluid flow field was cast in an axisymmetric geometry and transport equations representing continuity, momentum, mixture fraction, and the total energy per unit volume (internal energy plus kinetic energy) were solved. In Cartesian tensor notation, these equations take the form:

$$\frac{\partial \bar{\rho}}{\partial t} + \frac{\partial}{\partial x_i}\left(\bar{\rho}\tilde{u}_i\right) = 0 \tag{1}$$

$$\frac{\partial}{\partial t}\left(\bar{\rho}\tilde{u}_i\right) + \frac{\partial}{\partial x_j}\left(\bar{\rho}\tilde{u}_i\tilde{u}_j + \bar{p} - \bar{\rho}u_i''u_j''\right) - s_u = 0 \tag{2}$$

11th International Conference of Numerical Analysis and Applied Mathematics 2013
AIP Conf. Proc. 1558, 107-111 (2013); doi: 10.1063/1.4825432

$$\frac{\partial \tilde{E}}{\partial t}+\frac{\partial}{\partial x_i}\left[(\tilde{E}+\overline{p})\tilde{u}_i-\tilde{u}_i\overline{\tau}_{ij}\right]-\frac{\partial}{\partial x_i}\left(\mu_t T\frac{\partial S}{\partial x_j}\right)-s_E=0 \tag{3}$$

where t, ρ, u, p, E, τ, μ, T, and S, s respectively represent time, density, velocity, pressure, total energy, turbulence stress tensor, viscosity, temperature, entropy, and source term. An overbar represents conventional averaging, a tilde Favre averaging, a double prime a fluctuating component, and summation convention is used.

These equations were implemented with the inclusion of a two-equation k-ε model [1] to represent the turbulent Reynolds stresses. A number of modifications to these models have been proposed by authors, and previous work has indicated that for flows typical of those being studied here, the model proposed by Sarkar et al. [2] provides the more reliable predictions. The equation set was also supplemented with an equation of state for CO_2, capable of describing equilibria between the three states observed in a typical release scenario. The Peng-Robinson equation of state is satisfactory for predicting the gas phase properties of CO_2, but when compared to that of Span and Wagner, it is not so for the condensed phases. Furthermore, it is not accurate for gas pressures below the triple point and, in common with any single equation, it does not account for the discontinuity in properties at the triple point. In particular, there is no latent heat of fusion. Span and Wagner give a formula for the Helmholtz free energy that is valid for both the gas and liquid phases above the triple point, but it does not take account of experimental data below the triple point, nor does it give the properties of the solid. In addition, the formula is too complicated to be used efficiently in a computational fluid dynamics code. A composite equation of state has therefore been constructed to determine the phase equilibrium and transport properties for CO_2. The inviscid version of this model is presented in detail elsewhere[3] and the method reviewed here is now extended for the turbulent closure of the fluid equations detailed in the previous section. In this, the gas phase is computed from the Peng-Robinson equation of state, and the liquid phase and saturation pressure are calculated from tabulated data generated with the Span and Wagner equation of state and the best available source of thermodynamic data for CO_2, the Design Institute for Physical Properties (DIPPRR) 801 database.

Since any computational model of CO_2 releases must be able to represent mixtures of air and CO_2 in liquid, solid, and gas phase, an appropriate methodology is required. An initial step was the implementation of a homogenous equilibrium model (HEM), in which all phases are considered to be in dynamic and thermal equilibrium. This can be considered true in the case of a well mixed system in which any dense-phase particles are sufficiently small. There are some indications in test calculations that this will however not be true in rupture sizes of the order of centimeters. Hence, a full model will require the inclusion of transport of dense-phase particles, which is currently under investigation and beyond the scope of this paper. In the present work however, the HEM has been extended to account for the relaxation to dynamic equilibrium by the introduction of a source term to the transport equation for the condensed phase fraction.

Solutions of the equation set were obtained for the time-dependent, density-weighted forms of the descriptive equations, and these were discretised following a conservative control-volume approach. Approximation of the diffusion and source terms was undertaken using central differencing, and a Harten, Lax, van Leer [4]second-order accurate variant of Godunov's method applied with respect to the convective and pressure fluxes. This upwind scheme, although one of a number of variants, is selected for its robustness and ability to highly resolve stationary discontinuities.

EXPERIMENTAL MEASUREMENT

Figure 1 depicts the 2 cubic metre spherical experimental pressure vessel, with the filling sphere in-situ in the foreground, and the discharge pipe exiting the building wall to the right. This is thermally insulated, and can contain up to 1000 kg of CO_2 at a maximum operating pressure and temperature of 200 bar and 200 ºC, respectively. It is equipped internally with 6 thermocouples and 2 high precision pressure gauges as well as sapphire observation windows. Various orifices can and are used at the exit plane of the discharge pipe, and are all drilled into a large screwed flange. The thickness of this flange is typically 15 mm and the diameter of the orifice is constant over a length of 10 mm and then expanded with an angle of 45° towards the exterior. Three experiments representative of pipeline punctures were undertaken in this study, incorporating an 83, 77, and 69 bar release from a 12mm, 25mm and 50mm orifice respectively. The 50 mm release is undertaken without the use of an orifice flange, and represents a full-bore release. The parameters of these releases are given in Table 1.

TABLE 1. Parameters of the experimental releases.

Test Number	Observed Mean Mass Flow Rates / kg s^{-1}	Ambient Temperature / K	Air Humidity / %	Reservoir Pressure / bar	Nozzle Diameter / mm
11	7.7	276.15	>95	83	12
12	24.0	276.15	>95	77	25
13	40.0	276.65	>95	69	50

RESULTS AND DISCUSSION

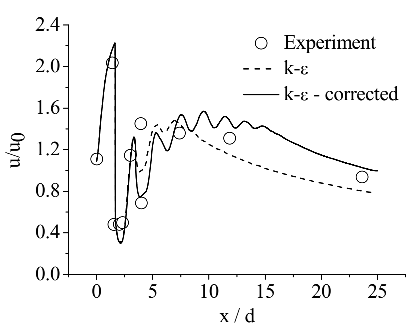

FIGURE 2. Predictions of normalised centreline velocity obtained using modified and un-modified turbulence model, plotted against data.

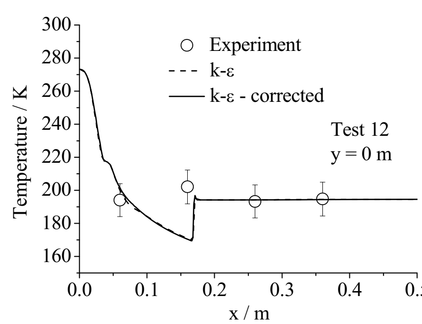

FIGURE 3. Predictions of centreline temperature obtained using modified and un-modified turbulence model, plotted against data.

Figure 2 depicts predictions of the normalized centreline axial velocity, plotted against experimental data for a highly under-expanded air jet [5]. As expected, the unmodified k-ε model over-predicts the jet mixing, leading to an over-dissipative solution. Figure 3 shows temperature predictions obtained using the corrected and standard turbulence model, plotted against experimental data in the near-field region of one of the investigated releases. Effects of physical phenomena such as CO_2 phase transition are clearly observable in the predicted curves. The step-change in gradient of the curve located at the triple-point temperature in Figure 3 is due to the equilibrium transition from liquid-vapour to that of liquid-solid, and the effects of the heat of fusion which is implemented at this point. Although the data set represents the most detailed currently available, it is difficult to ascertain how well the fine structure of the near-field jet is predicted due to the number of sample points in this narrow region. It is however clear that predictions and data are in excellent qualitative and quantitative agreement. As to be expected in what is a near-inviscid region, the effect of the solenoidal dissipation correction can be seen to be negligible.

Figure 4 shows predictions of radial temperature profiles plotted against experimental data measured along a vertical plane through the release for tests 11, 12, and 13, at an axial location of 5 m. The model qualitatively and quantitatively captures the thermodynamic structure of the sonic releases well, and although there is a small discrepancy between the observed and predicted spreading rates leading to a general under-prediction of temperature, calculations lie within the accepted error range of the experimental data. It is possible that dense phase CO_2 is removed from the system due to such phenomena as agglomeration, which would affect the higher temperatures observed. Hence, recent developments of the model include the incorporation of sub-models for the distribution of solid and liquid particles within the flow, and it is expected that the effects of phenomena such as particle coagulation will have an impact upon the predicted temperatures. Also, the system may not be in equilibrium due to this, or generated turbulence, which may cause the discrepancies.It is notable that discrepancy between prediction and experiment is most evident in the near-field of the flow. Hence, the under-prediction of the spreading rate is accentuated in the plot of Test 13 which relates to a downstream distance of 125 nozzle diameters. This is consistent with previous comparisons of calculations and data sets of other experimental releases [6].

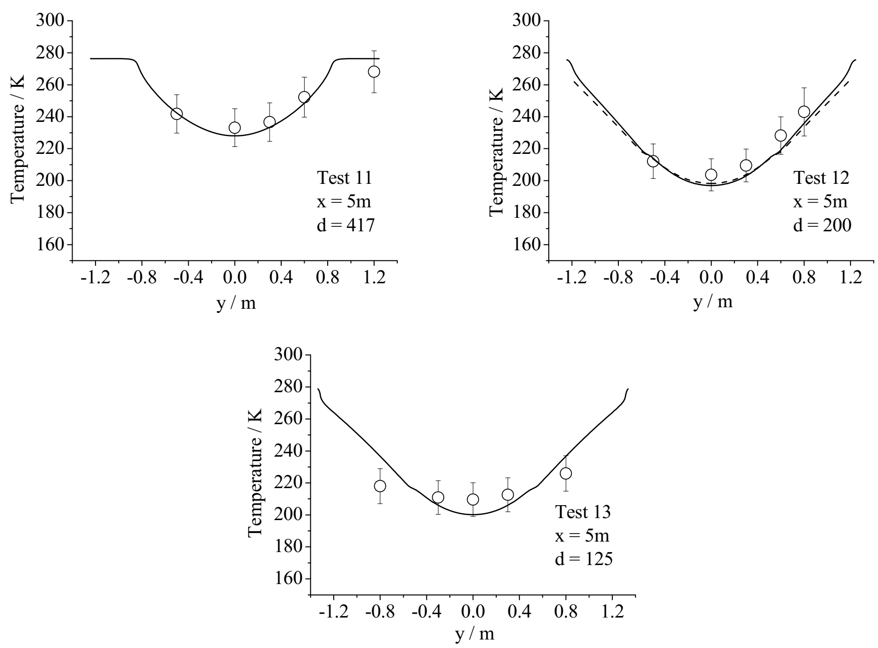

FIGURE 4. Predictions of radial temperature profiles (solid line – Sarkar corrected, dash line – no correction) in all three tests, plotted against data at an axial location of 5 m.

Predictions of Test 12 made without the compressibility correction can be seen to be in line with expectation in that enhanced mixing raises the temperature at the centre of the jet, and effects a widening of the jet structure. Although greater than observations within the inviscid region of the jet, the effect of this correction is seen to be relatively small in these jet releases.

CONCLUSIONS

A turbulent computational fluid dynamic model capable of predicting the near-field structure of high pressure releases of multi-phase carbon dioxide representative of those arising from an accidental pipeline puncture or rupture has been presented. Alongside this, previously unreported experimental observations are used in the validation of the model.

It is evident that the modelling approach quantitatively and qualitatively reproduces the experimental data and physical phenomena very well, and the methodology employed is suited to aiding in the design of CCS technologies. It has been identified that the inclusion of discrete particlesmay be required for more accurate representation of the thermophysical interactions between the phases, and this is currently under development by the authors.

ACKNOWLEDGEMENTS

The research leading to the results described received funding from the European Union 7th Framework Programme FP7-ENERGY-2009-1 under grant agreement number 241346. The paper reflects only the authors' views and the European Union is not liable for any use that may be made of the information contained therein.

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