

MEASUREMENT AND RANS MODELLING OF LARGE-SCALE UNDEREXPANDED CO₂ 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 CO₂ 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. Comparisons are made with a series of as-yet unreported experimental observations of large-scale, high-pressure CO₂ releases. The effects of corrections to the solenoidal turbulence energy dissipation are tested, and conclusions drawn as to the performance of this approach, with recommendations made for future developments.

INTRODUCTION

Underexpanded flows resulting in velocities greater than the local speed of sound are a feature of a wide number of applications in aviatric, 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 CO₂ 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. CO₂ 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 CO₂, 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 CO₂ 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 CO₂ in the gas and solid states. Model validations have been undertaken using the experimental data described, and suggestions for further developments are presented.

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 CO₂ at a maximum operating pressure and temperature of 200 bar and 200 °C, respectively. It is equipped



Figure 1. Experimental rig, including filling sphere and discharge pipe.

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.

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. These were implemented with the inclusion of a two-equation 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 CO₂,

capable of describing equilibria between the three states observed in a typical release scenario. Solutions of the equation set were obtained for the time-dependent, density-weighted forms of the descriptive equations, and the integration was performed by a shock-capturing, conservative, upwind, second-order accurate, Godunov numerical scheme.

RESULTS AND DISCUSSION

Figure 2 depicts predictions of the normalized centreline axial velocity, plotted against experimental data for a highly under-expanded air jet [3]. As expected, the unmodified $k-\epsilon$ model over-predicts the jet mixing, leading to an over-dissipative solution. Figures 3 to 5 show temperature predictions obtained using the corrected and standard turbulence model, plotted against experimental data in the near-field region of the three investigated releases. Effects of physical phenomena such as CO_2 phase transition are clearly observable in the predicted curves.

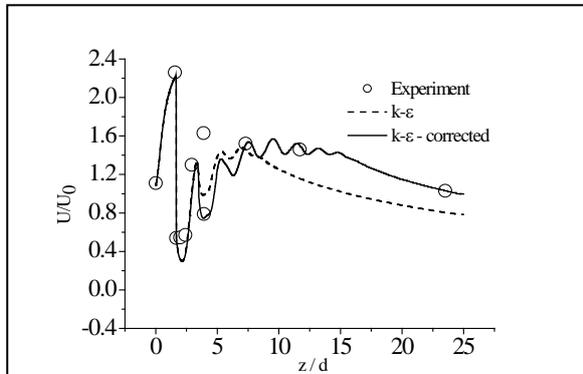


Figure 2. Predictions of normalised centreline velocity obtained using modified and un-modified turbulence model, plotted against data.

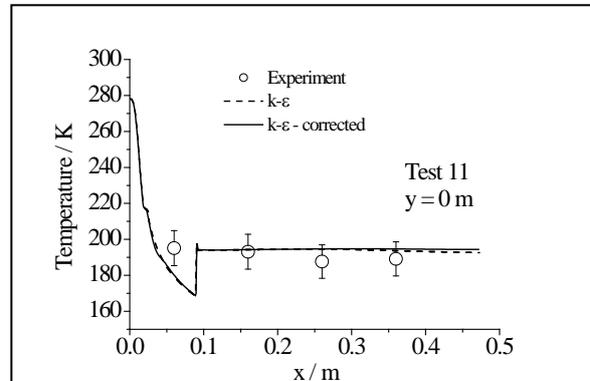


Figure 3. Predictions of centreline temperature obtained using modified and un-modified turbulence model, plotted against data.

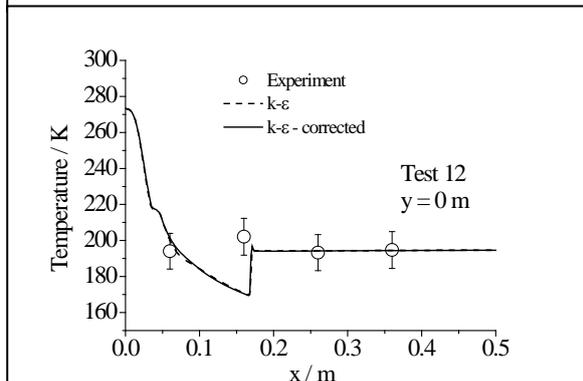


Figure 4. Predictions of centreline temperature obtained using modified and un-modified turbulence model, plotted against data.

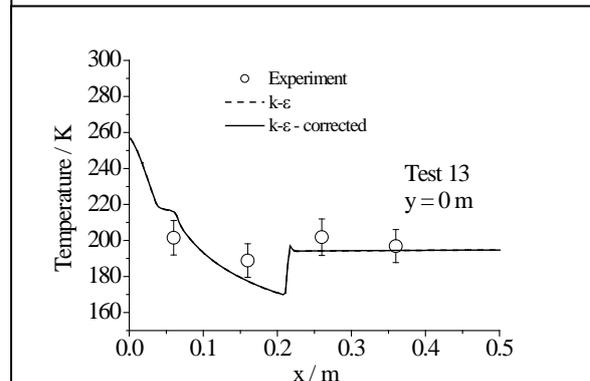


Figure 5. Predictions of centreline temperature obtained using modified and un-modified turbulence model, plotted against data.

CONCLUSIONS

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. The final paper will provide further detailed analyses of the performance of the combined turbulence and state equation closures in the modelling of the experimentally studied releases, including far-field predictions where the effects of compressibility modifications are more significant. Solutions obtained using a second-moment turbulence closure will also be considered. Conclusions will be drawn as to the suitability of these models, considering their accuracy, reliability of the physics employed, and the relative computational expense.

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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