CO2PipeHaz Newsletter

Winter 2012

Introduction

Welcome to the winter 2012 edition of the EU FP7-funded-project CO2PipeHaz newsletter, highlighting the most recent technical developments. The consortium, led by Prof. Haroun Mahgerefteh at University College London (UCL, UK) comprises 6 other partners: INERIS (France), National Research Centre for Scientific Research (NCSR, Greece), Dalian University of Technology (DUT, PR China), Health and Safety Laboratory (HSL, UK), University of Leeds (UoL, UK) and Gexcon (Norway).

CO2PipeHaz addresses the fundamentally important and urgent issue regarding the accurate predictions of fluid phase, discharge rate, emergency isolation and subsequent atmospheric dispersion during accidental releases from pressurised CO_2 pipelines to be employed as an integral part of large-scale Carbon Capture and Storage (CCS). This information is pivotal to quantifying all the hazard consequences associated with CO_2 pipeline failure, forming the basis for emergency response planning and determining the minimum safe distances to populated areas.

In this newsletter, we report the latest technical developments from NCSR concerning the implementation of advanced equations of state for CO_2, alongside friction theory, for the prediction of the viscosity of CO_2 mixtures. The ability of these approaches to predict a range of viscosities is investigated and sample results presented, which demonstrate good agreement with experimental observations. The need for more detailed experimental data for validation of these models is however highlighted.

The viscosity models developed by NCSR will be subsequently integrated into the respective multi-phase outflow and the near-field dispersion models developed by UCL and UoL.

In this update, UCL reports encouraging results using their CO_2 outflow model and demonstrate its performance using recently acquired data from the large-scale experiments undertaken in China by DUT. UoL discuss the recent developments in relation to their near-field dispersion model, which include multiple particle models, and a higher-order turbulence model. Our GEXCON partners discuss their progress with respect to far-field modelling, and demonstrate the coupling with UoL near-field models and UCL pipe out-flow models. They demonstrate encouraging qualitative preliminary results of calculations considering a realistic pipe-line release and topography.

We hope you find the Newsletter informative and if you would like to find out more please visit our website www.co2pipehaz.eu or e-mail Prof. Haroun Mahgerefteh h.mahgerefteh@ucl.ac.uk.

Project Partners

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Dalian University of Technology, PR China

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SEVENTH FRAMEWORK PROGRAMME

Technical Highlights

CO_2 Mixtures Viscosity Modelling: Assessment of Various Equations of State

N. Diamantonis G. Boulougouris, D.M. Tsangaris, and I. Economou

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One of the objectives of the CO2PipeHaz physical modelling effort is the development of an accurate viscosity model for pure CO_2, and its mixtures with gases of interest to CCS at transportation conditions. Being able to quantify the viscosity change of CO_2 due to the presence of gases such as CH_4, O_2, N_2, H_2S and SO_2 is very important for improving safe design and operation of CO_2 pipelines. To this end, Friction Theory (FT) developed by Quiñones-Cisneros et al. [1] has been employed. FT is a mathematical framework that, when combined with an equation of state (EoS), it can predict the viscosity of both pure components and mixtures. The model has two terms which capture the dilute gas behaviour and also the dense-phase effect. The latter is primarily accounted for by the EoS.

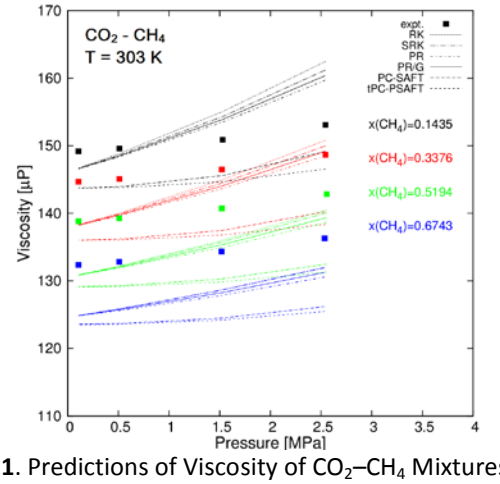

Figure 1. Predictions of Viscosity of CO_2–CH_4 Mixtures Using FT and Several Equations of State at Constant Temperature, Plotted Against Experimental Data.

In a previous newsletter, preliminary results for PC-SAFT and its polar alternative tPC-PSAFT were presented. Here, we present more recent work on validating and comparing different EoS. According to FT, every pure component is modelled by five parameters that are specific to the EoS used. These five parameters are fitted to experimental viscosity data of pure components. In order to tune the model parameters, a multi-variable metaheuristic optimization method, the Particle Swarm Optimization2 (PSO) method, was implemented. The parameter tables that present these values can be found in project's deliverable reports. The values fitted to experimental data were used to model selected CO_2 mixtures and the results were compared to the experimental data available in the literature.

Figure 1 depicts sample viscosity predictions for CO_2-CH_4 systems, plotted against experimental data attributable to Kestin and Yata [2]. One important observation for the CO_2-CH_4 system is that the deviation between experiments and theory seems to be systematic. The theory predicts the trend in viscosity change but it is consistently under-predicting the experimental values. It is hypothesized that this error will not be present at elevated pressures, as at these conditions the dense state term becomes significant and the EoS is expected to compensate for the effect.

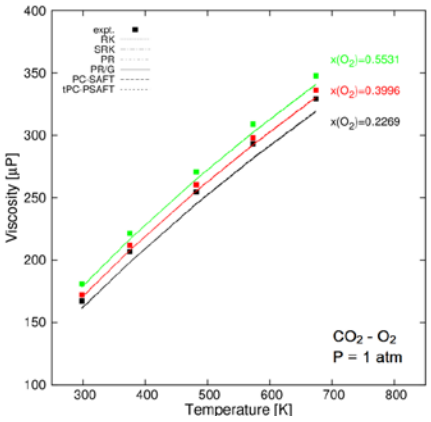

Figure 2. Predictions of Viscosity of CO_2–O_2 Mixtures Using FT and Several Equations of State at Constant Pressure, Plotted Against Experimental Data.

Figure 2 depicts sample viscosity predictions for CO_2-O_2 systems, plotted against experimental data attributable to Kestin et al. [3]. Experimental data were however available only at 1 atm pressure, which is relatively low compared to the expected operating pressure of a CCS pipeline. The error at these conditions is very small and all EoS perform similarly. This behaviour is to be expected as at 1 atm, the

dilute gas term dominates, and all EOS perform equally well.

The different types of EoS compared in this study, display a similar level of accuracy for pure components, especially at low pressures. Such behaviour is expected since the viscosity model depends on five fitted parameters. For mixtures however, PC-SAFT and tPC-PSAFT exhibit superior performance than the other cubic EoS.

In conclusion, FT provides a very reliable framework for viscosity modelling, although there is a requirement for experimental data at elevated pressures for validation. Obtaining experimental data at these conditions is critical for model testing and improvement.

Modelling of an Outflow from a CO_2 Pipeline

S. Martynov, S. Brown and H. Mahgerefteh

University College London, UK

Accurate prediction of CO_2 outflow from an accidently ruptured or punctured transportation pipeline is important for reliable evaluation of the associated hazard profile. A mathematical model of transient compressible flow in such a scenario is being developed by UCL in WP1.3 of the CO2PipeHaz project. The model accounts for the thermal non-equilibrium between the vapour and liquid phases during the rapid process of flash vaporization of liquid CO_2 in a depressurising pipeline, which is described using the relaxation equation for the mass fraction of the vapour phase. To enable accurate calculation of the fluid properties of pure CO_2 in vapour, liquid and also solid states, an extended Peng-Robinson EoS for CO_2 developed by the authors [4] is applied. For calculation of the thermophysical properties of CO_2 and its mixtures with impurities, the computer code for calculation of the flow from a pipeline is linked to the Physical Properties Library developed in WP1.2. Additionally, the flow model developed accounts for the effects of viscous friction and heat transfer, and also has the capability of simulating flow in inclined and segmented pipelines and emergency shutdown isolation [5, 6]. Basic features of the flow model and details of the numerical solution scheme were summarised in the project reports Deliverable 1.3.1, and Deliverable 1.3.3.

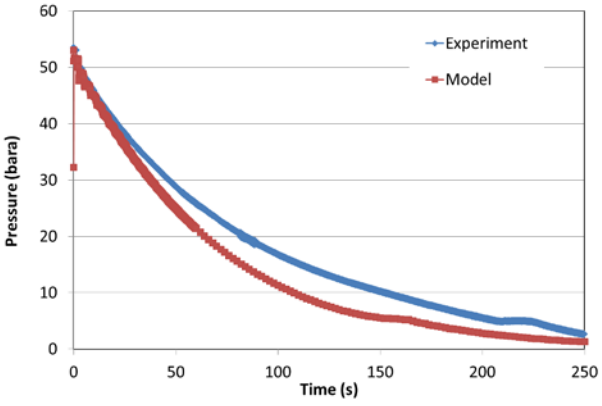

Figure 3. Variation of the Flow Pressure with Time.

In order to assess the validity of the outflow model developed, the predictions were compared against experimental data obtained by the Dalian University of Technology (DUT) in WP2.2 (Deliverable 2.2.3). In the DUT experiments the temperature and pressure of the flow were measured at different locations on the 260 m long, 233 mm internal diameter pipeline during the whole period of its depressurisation.

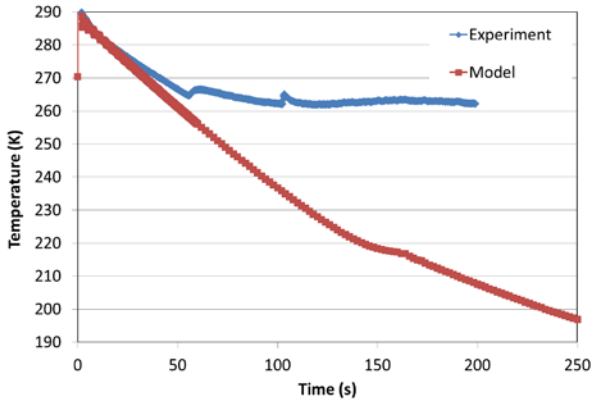

Figure 4. Variation of the Flow Temperature with Time.

Figures 3 and **4** show respectively the time variation of pressure and temperature of the flow at a fixed location in the pipeline as measured in the DUT experiments in comparison with the model predictions. In particular, **Figure 3** shows that the calculated pressures are in reasonable agreement with the measurements. The model captures the experimentally observed stabilisation of pressure around 5 bar corresponding to the triple point pressure of CO_2. This *stagnation* phenomenon is successfully captured by a choked flow model developed

which accounts for CO_2 solids formation in this region.

Figure 4 shows the time variation of temperature of the flow predicted by the model compared with the DUT measurements. It can be seen that in the initial 50 s, the predictions agree well with the measurements. However, after this period, the model predictions significantly deviate from the measurements. This deviation can be attributed to the heat transfer effects which are not currently taken into account in the model. Remarkably, at the late stage of depressurisation, the pressure stabilization around 5 bar predicted by the model (**Figure 3**), is accompanied by corresponding stabilization of temperature about 217 K, which is the triple point temperature of CO_2. The results of the model validation are presently being prepared for publication in a peer-reviewed journal.

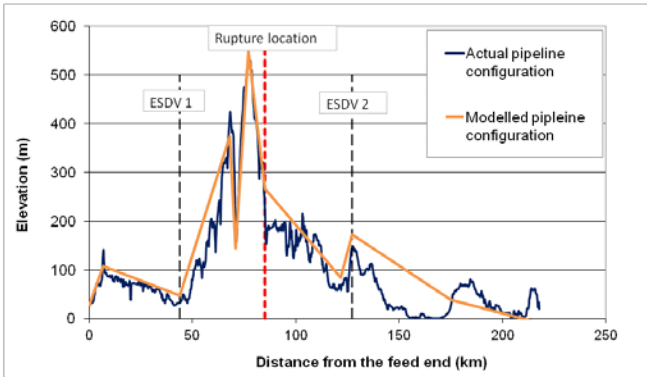

Figure 5. Variation of the Pipeline Elevation Along the Pipeline.

Following testing and validation, the flow model was applied to the prediction of a release form an hypothetical dense-phase CO_2 pipeline passing through different elevations. **Figure 5** shows the elevation profile of the 217 km, 8 inch diameter pipeline containing CO2 at 150 bar and 278 K including the locations of the emergency shutdown valves. The outflow predictions following full bore pipeline rupture are presented in the project progress report, Deliverable 1.3.4. These results serve as input for simulation of the near-field and far-field dispersion of the CO_2 plume and subsequent calculations of the hazard profile of a realistic pipeline using the tools developed in WP3.

Development of Near-field Dispersion Model

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University of Leeds, UK

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. In order to establish the consequences of an accidental CO_2 pipeline puncture or rupture, a near-field dispersion model has been constructed which can predict the concentrations of CO_2 released into the atmosphere and any phase-shift that may accompany such a release. The fundamentals of this fluid dynamic model have been discussed in previous newsletters and more detail can be found in the literature [7].

Predictions were based on the solutions of the ensemble-averaged, density-weighted forms of the transport equations for mass, momentum, and total energy. Closure of this equation set was achieved via the compressibility-corrected $k-\varepsilon$ turbulence model [8] and also a second-moment Reynolds-stress transport model [9]. Within this code, integration of the time-dependent, axisymmetric forms of the descriptive equations employed a second-order accurate, upwind, finite-volume scheme in which the transport equations were discretised following a conservative control-volume approach with values of the dependent variables being stored at the computational cell centres. Approximation of the diffusion and source terms was undertaken using central differencing, and a Harten, Lax, van Leer (HLL) [10] second-order accurate variant of Godunov's method applied with respect to the convective and pressure fluxes. The fully-explicit time-accurate method was a predictor-corrector procedure, where the predictor stage is spatially first-order, and used to provide an intermediate solution at the half-time between time-steps. This is then subsequently used at the corrector stage for the calculation of the second-order fluxes. A further explanation of this algorithm can be found elsewhere [11], and additional descriptions of the applied sub-models can be found in previous CO2PipeHaz newsletters.

The numerical model has now been extended to include the transport of particles within the flow, and two modelling approaches have been adopted. If the particles are large enough for their velocity to be significantly different from that of the fluid, then it is most efficient to integrate the equation of motion for each particle. On the other hand, very small particles are likely to move at their terminal velocity, which depends upon the fluid acceleration. In that case the particles are best described by a distribution. These two descriptions are complementary since, if the particles are large, their number density must be small so that a Lagrangian calculation is not too expensive. Furthermore, their inertia is significant, which means that the equation for the particle motion is not stiff. Small particles are likely to be very numerous if there is a significant mass of particles and the particle equation of motion is stiff due to the small particle mass. One could, of course, cover both cases with a distribution function that depends upon the particle velocity, but this would lead to a seven dimensional problem for three dimensional unsteady flows and would be prohibitively expensive to compute.

Transported Probability Density Function (pdf) Approach –

A transport equation for the number density of particles with masses in the range m_1 to m_2 is constructed. This forms a linear conservation equation in which all terms, except the source, can be established from the fluid state and particle mass. This source is thought to mainly comprise the effects of agglomeration, and as such, within the context of the k-ε turbulence model, Saffman and Turner [12] define a shear agglomeration rate of particles based upon particle sticking efficiency, a collision efficiency factor, and a collision shape factor. This approach can also be applied with a second-moment turbulence closure. This method can then be used with the integration of the particle pdf transport equation to establish the source terms required to describe particle coalescence. Subsequently, a conservative numerical scheme was constructed for the transported pdf, in the same manner as the fluid continuity equation, and hence the efficiency of the numerics was retained.

Figure 6 depicts predictions of particle size pdfs at an initial time, and after a lapse of 1.5 s, in a high-pressure jet release of CO_2. It is evident that the effects of agglomeration cause a lowering of the peak, and a widening of the particle size distribution. Little data are available for the validation of these models, however results do fall in line with recorded observations [13].

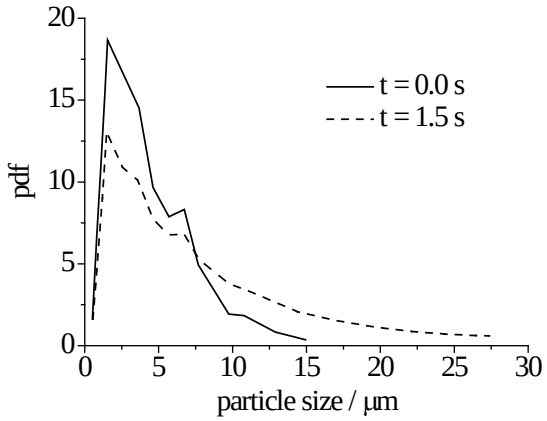

Figure 6. Numerical Predictions of Turbulent Shear Agglomeration in a Typical CO_2 Release Showing Initial (t=0.0 s) and Agglomerated (t=1.5 s) distributions.

Lagrangian Approach –

In the case of individual particles, equations describing the particle motion, the transfer of thermal energy between the particle and fluid, and the evaporation or condensation of the particle require integrating. This must be done for each particle using interpolated values of the fluid variables at the particle position. This is done using a second order Runge-Kutta algorithm. Particle splitting or agglomeration is modelled simply by splitting or merging individual particles, and from a study of the literature, turbulent shear agglomeration is thought to be the dominant driving mechanism as described above.

Unless the particles are very large, it is not expected for them to move significantly faster than the fastest fluid, which means that it is impossible for them to move through more than one cell in one time step. However, for very small particles, it is possible for the acceleration timescale to become very short compared with the fluid time-step, which means that the particles move at their terminal velocity. An explicit integration of the particle equation of motion would then require a very small time-step, which is inefficient. In such cases it is better

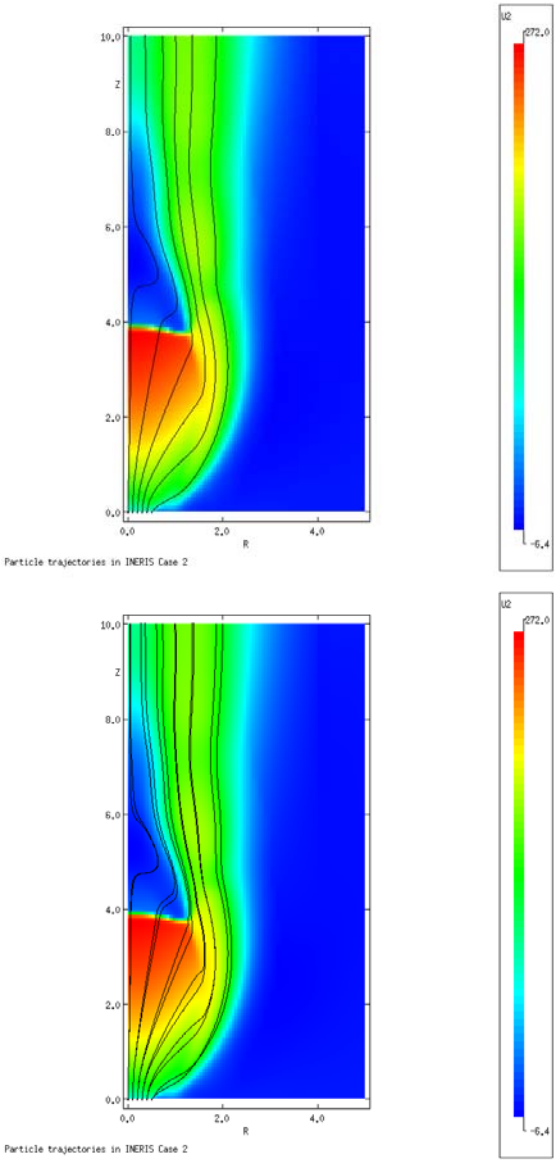

Figure 7. Axial Velocity, Streamlines and Particle Traces for a High Pressure Release of CO_2, with No Relaxation (top), and with Relaxation (bottom).

to assume that the particles move at their terminal velocity, and to neglect their inertia. One can then obtain an equation that relates the particle velocity to the fluid acceleration. This cannot only be used to compute the velocity of individual particles for which the inertia can be neglected, but it also makes it possible to write an evolution equation for the particle distribution function as previously discussed.

Figure 7 shows the axial velocity, streamlines and discrete particle traces for a high pressure release of CO_2. Particles were created at regular intervals across the vent exit at four positions: r = 0.1, 0.2, 0.3, and 0.4. They were initially created at the same origin as the streamlines and also given the fluid velocity. In (a), no relaxation was employed, and the particles clearly follow the velocity streamlines. When an expression for relaxation is introduced to the equation of motion (b), it can be seen that the particles do not follow the streamlines in this case.

A second-moment Reynolds-stress turbulence model has also now been incorporated into the code, and the validation of its performance is on-going.

Dispersion Modelling of a CO_2 Pipeline Release: Influence of Terrain

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A hypothetical scenario involving an accidental pipeline release of pressurized CO_2 and far-field dispersion in a realistic terrain has been studied by means of RANS (Reynolds-averaged Navier-Stokes) simulations using the commercial CFD tool FLACS [14]. Realistic terrain data were obtained from Ordnance Survey and imported into FLACS using complex-polyhedron primitives (CP8) in the FLACS pre-processor CASD (see **Figure 8**). The current setup involves release of pressurised CO_2 (initially at 150 bar and 10 °C) from a pipe of length 217 km and internal diameter of 0.87 m. A full-bore guillotine rupture was considered and the crater dimensions were assumed based on incident data for natural gas in the literature. University College London (UCL) performed the pipeline outflow calculations for the present case and predicted the total released mass as 2690 tonnes. In the present preliminary investigation, a simplified pseudo-source model (developed in-house) was employed to predict the post-expansion jet properties.

The pseudo-source flashing discharge model is based on the Peng-Robinson and Span & Wagner equations of states. For the given fluid conditions and a discharge coefficient of 1.0 (full pipe rupture), post-expansion jet properties as predicted by the pseudo-source model are shown in **Table 1**. Note that the predicted jet velocity 179.17 ms^{-1} and the mass-flux (ρUA) 51590 kg^{-1} are significantly high.

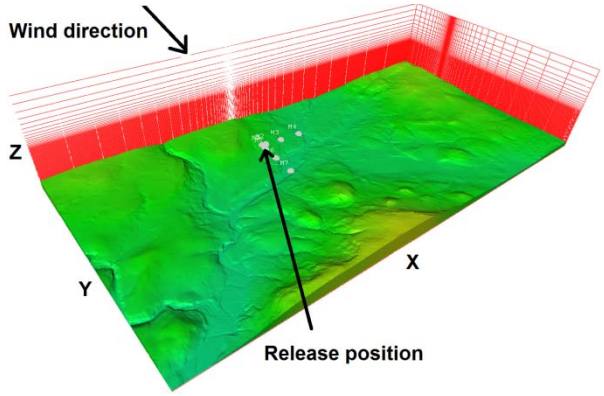

Figure 8. Terrain data loaded in FLACS with a spatial resolution of 12m. Grid, wind direction and crater position are also shown.

Temperature [K]	194.68
Velocity [m/s]	179.17
Dry ice mass fraction [kg/kg]	0.39
Gas density [kg/m^3]	2.81
Dry ice density [kg/m^3]	1500.00
Total density [kg/m^3]	4.61
Jet area [m^2]	102.29

Table 1. Post-expansion jet properties predicted by the FLACS pseudo-source model

The dimensions of the computational domain were 10 km × 5 km × 1.87 km in the streamwise (X), spanwise (Y) and transverse (Z) directions, respectively. This encloses the entire terrain in all the directions. A modest Cartesian mesh of 340000 grid points was used. **Figure 8** show the chosen wind direction, where a velocity of 2 ms^{-1} was prescribed. At all the remaining boundaries, a zero-pressure *Euler* boundary condition was set. For initial conditions, a Pasquill class of type D (neutral) with reference height 10 m and ground roughness 0.1 (rural roughness with low crops and occasional large obstacles) was chosen. Ambient temperature and pressure was set to 10 °C and 1 bar. In FLACS, the release was defined by means of a point-leak function, where the leak duration was set to 52 seconds. Further, relative turbulence intensity and turbulence length scales are assumed as 0.1 and 0.1m, respectively.

Figure 9 and **Figure 10** illustrate some snapshots of the CO_2 volume fraction at corresponding time intervals. After 400 seconds, the CO_2 cloud extends to approximately 2 km from the crater position. Note that the current study adopted a coarser grid resolution and a zero-pressure outflow boundary condition. It is therefore necessary to make further investigations and perform sensitivity studies.

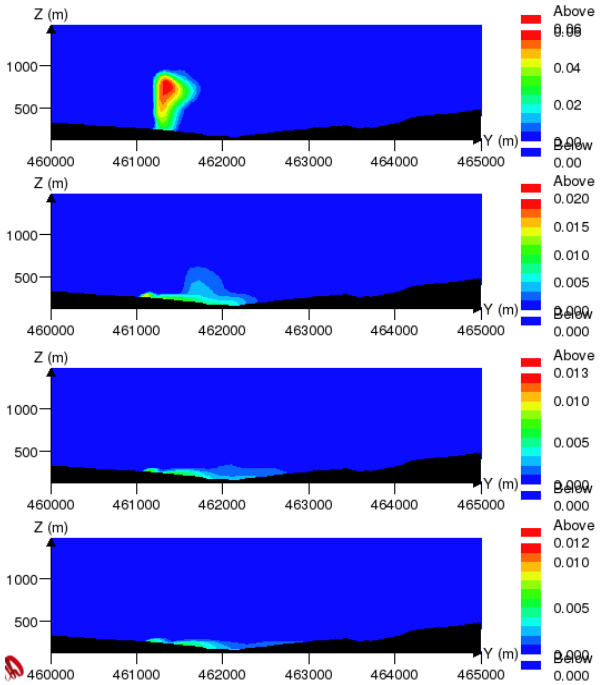

Figure 9. Time-evolution of CO_2 volume fraction (v/v) at a YZ cross-sectional plane corresponding to the crater-position. Snapshots correspond to 100, 200, 300 and 400 seconds after the release starts.

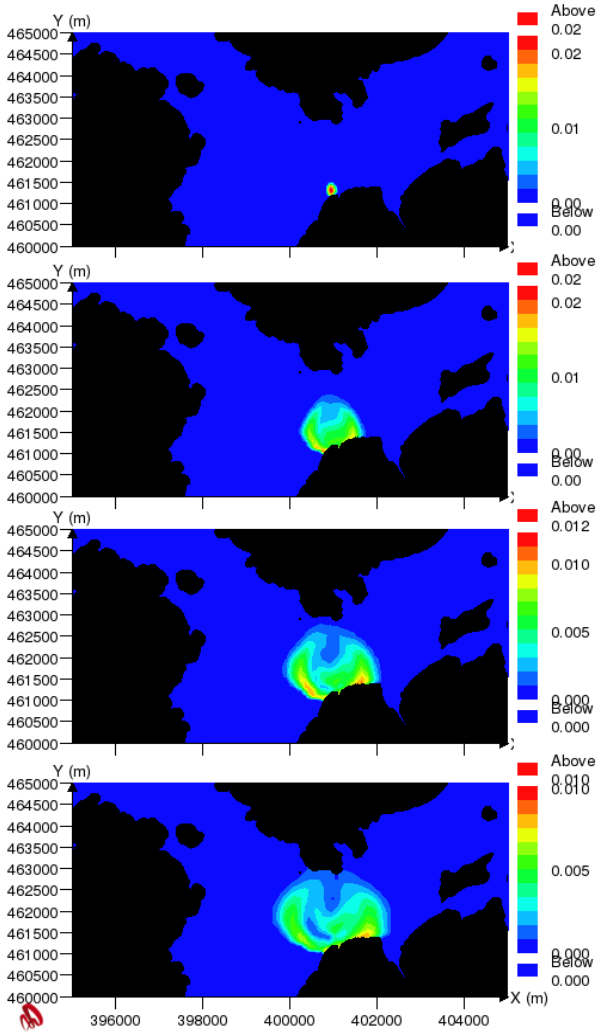

Figure 10. Time-history of CO_2 fraction (v/v) at an XY cross-sectional plane located near crater's altitude.

The results presented here are preliminary in nature. A more robust Nozzle outflow condition and finer grid resolution will be considered in future. In place of FLACS pseudo-source data, the source conditions resulting from the near-field computations of University of Leeds (UoL) will be used. An Euler-Lagrangian two-phase model, which is developed in-house [15], will be employed to track the particulate dispersion. Resulting data will then be compared with the simulations performed using the general-purpose CFD code ANSYS-CFX by the Health and Safety Laboratory (HSL).

Industrial Scale CO_2 Pipeline Rupture Experiments

S. Chen, Y. Zhang

School of Chemical Engineering, Dalian University of Technology, China

Months of painstaking preparation have led to the start of the industrial-scale 260 m long, 233 mm internal diameter pipeline release tests in China. These provide a wealth of valuable experimental data used to validate the outflow and dispersion models developed by the consortium partners. Further discussion regarding the experimental setup including the data acquisition system and the rupture mechanism can be found in previous newsletters available from the project website.

Since the last newsletter, 2 further field-scale tests have been undertaken, which include a 50 mm orifice release, and one full-bore rupture.

Reported in the autumn 2012 newsletter, the first release experiment from the pipeline was conducted on 16th June 2012. In the experiment, pure CO_2 initially compressed in the pipe to a supercritical state (34 ℃, and 80 bar) was released through the 50 mm diameter orifice. The experience and knowledge gained from the first experiment lead to the detailed planning and execution of the whole programme of experimental studies by DUT in the CO2PipeHaz project.

Figure 11 depicts the bursting discs used in the 50 mm releases, and their subsequent condition after the experiments.

Figure 11. Bursting disks after CO_2 release from 50 mm orifice.

Figure 12 displays experimental P-T data obtained from the second 50 mm release at three selected points along the pipeline. The initial pipeline conditions were 21 °C and 52.5 bar which made this test initially a vapour-only release.

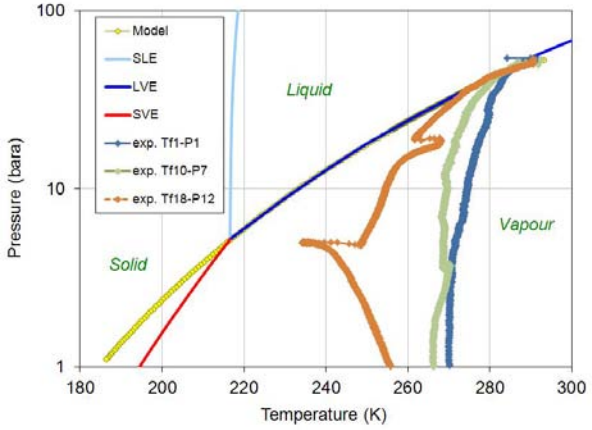

Figure 12. P-T diagram of CO_2 releasing from the pipeline at 21 degree centigrade, 52.5 bar.

The third test undertaken was a full-bore release, and **Figure 13** shows the initial stages of this.

Figure 13. Initial release of the full bore rupture (233 mm i.d., release temperature 3 °C).

The final stages of the experiment are also represented in **Figure 14**, where some solid CO_2 formation can be observed. Having been discharged in the latter part of the release, this can be observed to accumulate underneath the near-field data acquisition assembly.

Figure 14. Near field of the full bore rupture at the end of release

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Publications and Conference Participation

For regular updates on publications please visit:

http://www.co2pipehaz.eu/publications.htm

The most recent CO2PipeHaz event was the multi-disciplinary '**Bridging the gap in CCS infrastructure: Results from European projects**' meeting held in Lisbon, Portugal. All presentations will be available for download from the project website in due course

In addition to CO2PipeHaz, the meeting was co-organised by two major CCS infrastructure projects COMET, and COCATE. A wide range of material was presented and discussed by both academic and industrial contributors, and this material will be subsequently published as a special edition of a leading peer reviewed journal. Again, please monitor the project website for the latest developments.

A number of papers, posters, and presentations are available in the publications section of the project website.

Acknowledgement and Disclaimer

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