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Abstract

Transportation of CO₂ in high-pressure pipelines forms a crucial link in the ever-increasing application of Carbon Capture and Storage (CCS) technologies. An unplanned release of CO₂ from a pipeline presents a risk to human and animal populations and the environment. Therefore it is very important to develop a deeper understanding of the atmospheric dispersion of CO₂ before the deployment of CO₂ pipelines, to allow the appropriate safety precautions to be taken. This paper presents a two-stage Computational Fluid Dynamics (CFD) study developed (1) to estimate the source strength, and (2) to simulate the subsequent dispersion of CO₂ in the atmosphere, using the source strength estimated in stage (1). The Peng-Robinson (PR) EOS was incorporated into the CFD code. This enabled accurate modelling of the CO₂ jet to achieve more precise source strength estimates. The two-stage simulation approach also resulted in a reduction in the overall computing time. The CFD models were validated against experimental results from the British Petroleum (BP) CO₂ dispersion trials, and also against results produced by the risk management package Phast. Compared with the measurements, the CFD simulation results showed good agreement in both source strength and dispersion profile predictions. Furthermore, the effect of release direction on the dispersion was studied. The presented research provides a viable method for the assessment of risks associated with CCS.

Keywords

gas, equation, state, dispersion, co₂, releases, high, pressure, pipelines, cfd, model, source, real, strength

Disciplines

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Source strength and dispersion of CO₂ releases from high-pressure pipelines: CFD model using real gas equation of state

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Abstract

Transportation of CO₂ in high-pressure pipelines forms a crucial link in the ever-increasing application of Carbon Capture and Storage (CCS) technologies. An unplanned release of CO₂ from a pipeline presents a risk to human and animal populations and the environment. Therefore it is very important to develop a deeper understanding of the atmospheric dispersion of CO₂ before the deployment of CO₂ pipelines, to allow the appropriate safety precautions to be taken. This paper presents a two-stage Computational Fluid Dynamics (CFD) study developed (1) to estimate the source strength, and (2) to simulate the subsequent dispersion of CO₂ in the atmosphere, using the source strength estimated in stage (1). The Peng-Robinson (PR) EOS was incorporated into the CFD code. This enabled accurate modelling of the CO₂ jet to achieve more precise source strength estimates. The two-stage simulation approach also resulted in a reduction in the overall computing time. The CFD models were validated against experimental results from the British Petroleum (BP) CO₂ dispersion trials, and also against results produced by the risk management package Phast. Compared with the measurements, the CFD simulation results showed good agreement in both source strength and dispersion profile predictions. Furthermore, the effect of release direction on the dispersion was studied. The presented research provides a viable method for the assessment of risks associated with CCS.

Keywords: Carbon Capture and Storage; CO₂ pipeline; Equation of State; under-expanded jet; CO₂

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the atmosphere by 2050 [7, 8]. CCS is also considered the most economical way to achieve reduction in CO₂ concentration [9]. Transportation of CO₂ in high-pressure (usually ≥ 8 MPa) pipelines from source to storage location constitutes an important link in the CCS chain, especially when transporting large quantities of CO₂ over long distances [10]. It is expected that extensive networks of CO₂ pipelines would be required with the growing application of CCS in the near future [9].

Deployment of CO₂ pipelines is not without risk. Accidental releases may cause damage to human and animal populations. CO₂ is colourless and odourless, and therefore escapes easy detection. It is also an asphyxiant, which can lead to rapid loss of consciousness in humans if the exposure levels exceed 10% [11]. Gaseous CO₂ released from a high-pressure pipeline is colder and denser than air. CO₂ dispersion patterns vary according to local conditions such as wind and terrain. It can be transported some distance from the release point as it can flow downhill, potentially affecting populations that would normally be considered 'safe' from pipeline failure. Therefore it is necessary to gain a better understanding of the atmospheric dispersion of CO₂ released from high-pressure pipelines in different scenarios, to develop controls that may be needed to protect humans, animals and the environment from possible harmful effects of pipeline failures.

The rupture of a high-pressure CO₂ pipeline will be immediately followed by the initiation of a decompression wave inside the pipeline and an under-expanded jet flow exiting from the orifice into the ambient with very high momentum [12]. This is a complicated process that directly affects the strength (e.g. in terms of mass flow rate) of the 'source' of CO₂. The source strength will surely influence the subsequent dispersion of the gas in the atmosphere. Nevertheless, detailed simulations/investigations of the characteristics of the under-expanded jet flow have usually been

ignored in previous CO₂ dispersion studies, due to their complexity. Mazzoldi et al. [13] applied Bernoulli's equation and the choked flow assumption to calculate the jet-release speeds from high-pressure transportation facilities within CCS projects. As those equations over-simplified the physical phenomenon of the discharge process, they cannot be used to obtain a comprehensive expression of the source strength as a function of time. Witlox et al. [14] used the commercial package Phast to study the discharge and the subsequent dispersion behaviour following release of high-pressure CO₂ from pipelines. Phast uses analytical models applying the conservation of mass, momentum, enthalpy and energy, along with the entropy equation, to deduce the source strength and the dispersion profile. The Phast model has been validated against experimental data, but the results have not been reported in detail due to a confidentiality agreement. Wen et al. [15] investigated the far-field CO₂ dispersion of a vertical vent release and a horizontal release from a shock tube, without considering the initial jet. The flow parameters over specific planes downstream from the exit provided by other researchers were directly applied as the inlet conditions. Hsieh et al. [16] studied the dispersion of CO₂ from a CCS-related infrastructure in a complex hypothetical topography. While CO₂ concentration measurements were not available in this scenario, the performance of the Computational Fluid Dynamics (CFD) modelling approach was separately validated using results of the Thorney Island tests, which used a mixture of Freon-12 and nitrogen as the tracer gas. It was found that the presence of an obstacle and/or complex terrain has a significant influence on the dispersion of CO₂. In their studies, the source strength was assumed and the parameters probably did not reflect a real release. Woolley et al. [17] and Wareing et al. [18] proposed CFD models to study the structure of CO₂ jet flows. In their models, only the near-field under-expanded jet region was considered. The source strength at the exit plane was obtained by isentropic decompression calculations and then

applied to the CFD model as inlet conditions. Mazzoldi et al. [9] proposed CFD methods to evaluate safety distances for CO₂ pipelines. In their models, the characteristics of the under-expanded jet flow were not considered. They stated that this treatment will lead to over-prediction of CO₂ dispersion in the near field and consequent under-prediction of CO₂ concentration farther from the source. Koornneef et al. [19] presented a systematic assessment of the impact of knowledge gaps and uncertainties on the results of quantitative risk assessments for CO₂ pipelines. They pointed out that an understanding of the physical phenomena which take place during the accidental release from a pipeline is critical. Factors such as the release rate, release direction, duration of release, exit temperature, vapour mass fraction and diameter of the jet will greatly affect the subsequent dispersion calculation. Therefore, to accurately predict the source strength of a high-pressure CO₂ pipeline leakage, a comprehensive study of the characteristics of under-expanded CO₂ jet flows is required.

Interest in the structure of the under-expanded jet has prevailed for a long time, because of the many areas in which it arises, ranging from design of rocket propulsion systems to consequence and risk assessments associated with high-pressure gas leaks [12, 20]. A number of experiments were carried out in the early days. These aimed to study the flow structure, velocity profile and concentration profile of various gases at different stagnation pressures [20-24]. In recent years, CFD techniques have also been widely used in the studies of high-pressure gas releases due to the availability of enhanced computing resources. Chuech et al. [25] investigated the structure of under-expanded jets using numerical simulations as well as experimental methods. A version of the k - ε turbulence model was proposed, which introduced a compressibility correction factor to the turbulent viscosity. They found that the CFD model yielded encouraging results. CFD studies were also carried out using a modified k - ε model based on the work of Sarkar et al. [26], while a source term for the k equation as well as a

scaling of the turbulent viscosity were introduced [12, 27]. Compared to the standard $k-\varepsilon$ turbulence model, better agreement with the measurements in the prediction of the velocity profile was achieved by the modified $k-\varepsilon$ model. Sand et al. [28] and Novembre et al. [29] studied accidental natural gas releases from high-pressure pipelines. In their work, far-field dispersion was also investigated. In these studies, the tracer gases were all modelled as ideal gases. This treatment considerably simplified the problem but it is not appropriate in the prediction of CO₂ pipeline leakage, where the source strength is of a crucial concern. This is because the ideal gas Equation of State (EOS) is not capable of accurately reflecting the thermodynamic properties of gases at very high pressure or very low temperature, conditions which will surely be experienced by a high-pressure CO₂ jet. Deviations in some properties, for example the density, will significantly affect the prediction of the release rate (source strength). Wareing et al. [18] and Woolley et al. [17] found that a real gas EOS was considerably superior to the ideal gas EOS in predicting the near-field temperature and velocity profiles of CO₂ jet flows. At present, many real gas EOSs [30, 31] which can predict more accurate vapour-liquid behaviour of gases are available. Efforts have also been made to precisely evaluate thermodynamics properties of CO₂ in the solid state [32, 33]. This makes the multi-phase calculation of CO₂ releases possible [34, 35], and provides a perspective of enabling multi-phase simulation of an under-expanded CO₂ jet. In the present study, we would expect that using a real gas EOS to simulate the decompression and under-expansion of CO₂ could achieve more accurate source strength prediction and consequently help the dispersion evaluation.

In this paper, CFD models designed to simulate the CO₂ release from high-pressure pipelines are presented, focusing on (1) estimating the source strength and (2) the subsequent dispersion. To enable more precise modelling of the physical properties of CO₂ over a wide range of temperature and

pressure, a real gas EOS was incorporated into the CFD models. To simplify the problem, CO₂ was treated as a homogeneous fluid and the possible phase change was not considered in the present study. In order to validate the present CFD models, trials of the British Petroleum (BP) DF1 CO₂ dispersion experiments [36] were simulated. Comparative studies were carried out between the results of CFD models using a real gas EOS and the ideal gas EOS. The performance of the CFD models was also validated against DNV Phast [14], a commercial process industry hazard analysis software package.

2. Modelling approach

In this study, simulations were carried out using the commercial CFD software ANSYS Fluent v14.0, which applies the Finite Volume Method (FVM) to discretise the governing differential equations of fluid flow, including the Reynolds-Averaged Navier-Stokes (RANS) equations [37, 38]. Trials of the BP DF1 CO₂ dispersion experiments [36] were employed for validation.

2.1. BP DF1 CO₂ dispersion experiments

The BP DF1 CO₂ dispersion experiments were carried out by Advantica at their Spadeadam test facility located in the North of England in 2006 [36]. The aim of these tests was to investigate and fill the identified knowledge gaps and to generate validation data for dispersion models for liquid and supercritical CO₂ releases. The CO₂ dispersion experiments were conducted on a flat terrain without blockages. The experimental program consisted of a set of twelve CO₂ releases, with stagnation pressures ranging from 8.2 MPa to 15.9 MPa and stagnation temperatures from 5 °C to 147 °C. Fig. 1 is a schematic diagram of the experimental arrangement, showing locations of the measurement instruments.

2.2. Real gas model

The first real gas EOS was developed by van der Waals in 1873 [39], which accounted for the finite intermolecular forces and the finite volume occupied by the molecules by proposing additional terms in the ideal gas EOS. Subsequently, a number of EOSs have been developed in order to accurately predict the thermodynamic properties of fluids [30, 31]. These EOSs can be divided into two categories: (1) cubic equations with simple structures, such as Redlich-Kwong (RK) [40], Soave-Redlich-Kwong (SRK) [41], Patel-Teja (PT) [42], Peng-Robinson (PR) [43] and many others; and (2) equations with more complex structures, including Benedict-Webb-Rubin (BWR) [44], Lee-Kesler (LK) [45], GERG [46], etc. Despite the simple form of cubic EOSs, they are capable of giving reasonable results. EOSs with more complex structures, may give better estimations for some specific properties, but they are usually more difficult to be applied due to their complicated calculation procedure if they are not already included in the original simulation code [30, 31].

Fluent provides built-in implementations for some cubic EOSs and also more complex EOSs from NIST REFPROP. However, these built-in EOSs limit the temperature to above the triple point, making them inappropriate for simulating a high-pressure CO₂ jet flow undergoing significant cooling due to expansion. To overcome this problem, a User-Defined Real Gas Model (UDRGM) was introduced into the simulation, which can be implemented through Fluent User-Defined Functions (UDFs) [47]. In the UDRGM, physical properties of the fluid, such as density, enthalpy, entropy, specific heat, speed of sound, etc. can be solved for given pressure and temperature at runtime using a real gas EOS. In the present work, the PR EOS was employed based on its proven accuracy in modelling the vapour-liquid behaviour of CO₂ [30, 48], and its relative simplicity and computational efficiency. The PR EOS is described by [43]:

$$P = \frac{RT}{V-b} - \frac{a}{V^2 + 2bV - b^2} \quad (1)$$

where P is the pressure, T the absolute temperature, V the molar specific volume, and R the universal gas constant; a and b are empirical parameters accounting for the intermolecular attraction forces and the molecular volume respectively.

The enthalpy H and entropy S of the fluid can be solved using the ‘departure functions’ for the PR EOS [49]:

$$H - H^i = RT(Z - 1) + \frac{T(da/dT) - a}{2\sqrt{2}b} \ln \left[\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right] \quad (2)$$

$$S - S^i = R \ln(Z - B) + \frac{da/dT}{2\sqrt{2}b} \ln \left[\frac{Z + (1 + \sqrt{2})B}{Z + (1 - \sqrt{2})B} \right] \quad (3)$$

where H^i and S^i are the enthalpy and entropy of an ideal gas respectively, $Z = PV/RT$, and $B = Pb/RT$.

The dynamic viscosity is estimated using the following formula [50]:

$$\mu = 6.3 \times 10^{-7} \frac{M^{0.5} (P_C/101325)^{0.6666}}{T_C^{0.1666}} \left[\frac{(T/T_C)^{1.5}}{T/T_C + 0.8} \right] \quad (4)$$

where M is the molar mass of the fluid, T_C the critical temperature, and P_C the critical pressure.

Knowing the viscosity, the thermal conductivity can be estimated by [51]:

$$\lambda = \mu \left(c_p + \frac{5}{4} R \right) \quad (5)$$

where c_p is the isobaric heat capacity of the real gas.

Fig. 2 compares the density, isobaric heat capacity, and speed of sound (denoted by w in Fig. 2) as estimated by both the PR EOS and the ideal gas EOS, against available experimental measurements [52-55]. Overall, compared to the ideal gas EOS, the PR EOS predicts the CO₂ properties with much

better accuracy not only in gaseous state, but also in the liquid and supercritical states. In contrast, the density of CO₂ predicted by the ideal gas EOS shows significant deviations from the experimental data, especially at high pressures. Furthermore, when using the ideal gas EOS, the isobaric heat capacity and speed of sound are assumed constant at a given temperature, contrary to measurements. It can thus be concluded that using the ideal gas EOS to model the fluid dynamics of high-pressure CO₂ pipeline ruptures would introduce considerable inaccuracies in the calculations.

2.3. Turbulence model

In order to accurately predict the source strength at the orifice of the CO₂ pipeline rupture, the under-expanded jet flow following the high-pressure gas release should be studied. As the under-expanded flow involves both turbulent mixing and compressibility effects, it is very important to choose an appropriate turbulence model to reflect these effects [29]. Because the standard k - ε model does not account for the effect of compressibility on turbulence dissipation, Sarkar et al. [26] proposed a modified k - ε model, which has been adopted by many researchers [12, 17, 27, 56] in simulations of under-expanded jet flows, and found to perform much better than the standard k - ε model. The modified k - ε model introduces a source term into the transport equation for the turbulent kinetic energy:

$$S_k = -\rho M_t^2 \varepsilon \quad (6)$$

where M_t is the turbulent Mach number ($= (2k)^{0.5}/w$), w the speed of sound, k the turbulent kinetic energy, and ε the specific eddy dissipation rate. Also, the turbulent viscosity in the standard k - ε model is replaced by

$$\mu_t = C_\mu \rho \frac{k^2}{(1 + M_t^2) \varepsilon} \quad (7)$$

where C_μ is a constant in the standard k - ε model.

The modified k - ε model is already integrated into ANSYS Fluent 14.0. When choosing the ideal gas EOS for the simulation, it is enabled automatically [38]. However, as we used a UDRGM to model the gas properties, in order to test the performance of the modified k - ε model, Eq. (6) and Eq. (7) were introduced explicitly through UDFs. An alternative turbulence model, the Shear Stress Transport (SST) k - ω model, was also tested in this study. In the standard k - ω model, the compressibility effect is considered by incorporating a compressibility function into the equation for calculating the dissipation of ω . The SST k - ω model modifies the standard k - ω model by introducing a damped cross-diffusion derivative term in the equation. Also, the turbulent viscosity is modified to account for the transport of the turbulent shear stress. These features make the SST k - ω model more reliable for modelling transonic shock waves [38].

The free air jet experiment conducted by Eggins and Jackson [21] was used to compare the modified k - ε and SST k - ω models. In this experiment, the air jet was produced by a nozzle having an exit diameter of 2.7 mm, and operating at a pressure of 6.6 atm. The velocity field measurements were made using the Fabry-Perot Laser-Doppler technique. The axisymmetric computational domain for the simulation of this experiment and the mesh around the nozzle are shown in Fig. 3. The overall mesh contains 70,000 cells.

Fig. 4 shows the shadowgraph and also the predicted flow structure of the jet using the two turbulence models. There is generally good agreement. However, the SST k - ω model outperforms the modified k - ε model in resolving the details of the flow structure as seen in the shadowgraph image, in particular

the normal shock (Mach disc), the reflected oblique shocks and the slip line are all better predicted by the SST $k-\omega$ model, while the modified $k-\varepsilon$ model does not capture these details well enough.

Fig. 5 compares the axial velocity predicted by these two turbulence models against measurements. The SST $k-\omega$ model captured the location of the Mach disc and the magnitude of the velocity drop through the Mach disc better than the modified $k-\varepsilon$ model. Downstream of the Mach disc, both models predicted a similar multiple shock structure, but the velocity magnitude estimated by the modified $k-\varepsilon$ model appears to be more reasonable. Further downstream, the SST $k-\omega$ model captured velocity decay better.

Fig. 6 shows the predicted transverse velocity profiles upstream and downstream of the Mach disc against the measurements. Clearly, the SST $k-\omega$ model significantly outperforms the modified $k-\varepsilon$ model.

Generally speaking, both turbulence models produced acceptable estimations but the SST $k-\omega$ model performed better in resolving the detailed flow structure and predicting the overall velocity field. As shown in Fig. 7 (P_0 : stagnation pressure; P_∞ : ambient pressure), downstream of the jet exit, the pressure and temperature tend to reach the ambient pressure and temperature quickly. Prediction of the velocity field is crucial for the accuracy of source strength estimation. Therefore in the subsequent study of the CO₂ jet, the SST $k-\omega$ model was employed.

2.4. Definition of the problem

The above considerations suggest that, following the release of high-pressure fluid, expansion to ambient conditions is marked by the appearance of an under-expanded free jet, with sonic velocity at

the source. In order to capture the details of the jet flow, a very dense mesh is required. Furthermore, the time step required for the transient CFD simulation of the jet appears to be in the range of 10^{-7} s to 10^{-5} s. For an overall CFD model including both the discharge and dispersion domains, the required computing time would be unacceptably long. Therefore the problem was divided into two parts [23, 28, 29], as shown in Fig. 8.

The first part considers only the jet, and determines features of the expanding jet corresponding to the stagnation conditions (P_0 and T_0), and calculates jet conditions in the cross-section (P_s , T_s , and v_s) where the jet flow approaches atmospheric pressure. The obtained values of P_s , T_s , and v_s can be used as inlet boundary conditions for the second part, the dispersion model, within which the fluid can be treated as incompressible.

In the jet model, apart from predicting the mass flow rate at the jet exit and obtaining jet conditions for dispersion modelling, the location of the cross-section (x_s , see Fig. 8) which is to be used as inlet boundary for the dispersion model also needs to be determined. In this work, we assume $x_s = 10x_m$ [29], where x_m is the distance from the jet exit to the Mach disc. In the free jet experiment mentioned above (see the shadowgraph in Fig. 4), the Mach disc was 3.9 mm from the jet exit, while at $10x_m$, the pressure already reached the atmospheric value which was maintained downstream (see Fig. 7). The location of Mach disc was found to be insensitive to the nature of the fluid and can be given as [20]:

$$x_m = 0.6455d_e \sqrt{\frac{P_0}{P_\infty}} \quad (8)$$

where d_e is the diameter of the nozzle exit. Assuming that Eq. (8) is accurate enough for a CO_2 jet, it can be directly applied during model setup.

It should be noted that, in this study, we focused on the CFD model implementation and validation when using real gas EOS to model the decompression, and under-expansion of CO₂ releases from high-pressure pipelines. The possible phase change phenomenon during the discharge process was not considered to simplify the problem. In reality, CO₂ pipelines would usually operate at ambient temperature, while the substance may exit from the orifice in the liquid phase and dry ice may form in the atmosphere due to the substantial temperature drop (see Fig. 7, the jet temperature may fall well below the freezing point of $-78.5\text{ }^{\circ}\text{C}$), which will affect the subsequent dispersion. In order to accurately determine the source strength under such conditions, it is important to know the phase fractions at the source. However, addressing the phase fractions in the source term is beyond the scope of the current study. To avoid touching the vapour-liquid phase boundary, the current jet model is limited to simulations of supercritical releases. In further studies, a multi-phase model may be introduced to consider the vapour, liquid and solid phase separately to account for the phase fractions. To achieve this, more accurate equations for the thermodynamic and transport properties may be needed to model CO₂ in liquid and solid states.

3. CFD model

3.1. Jet model

The jet model was set up based on the dimensions in the experimental setup. As shown in Fig. 9(a), an axisymmetric computational domain was used, which comprises a pipe (*abcd*), a nozzle (*de*) and the ambient atmosphere (*efgh*) initially at rest. Together with the 20 mm long nozzle, the pipe has a length of 5.5 m starting from the end connected to the CO₂ reservoir. The nozzle has an exit diameter of 11.9 mm. The ambient, representing an infinite air reservoir, measures 9 m in depth and 3 m in radius. The computational domain was sub-divided into quadrilateral cells (see Fig. 9(b) for a part of the grid

around the nozzle). Fine resolution was implemented vertically from the pipe wall and also in the near region of the nozzle exit. To ensure grid-independence, simulations of a CO₂ jet with $P_0 = 15$ MPa were carried out with several grid sizes. It was found when the grid size was increased from 0.49 million to 0.96 million cells, the axial velocity component showed only a very small deviation (see Fig. 10). Therefore, in the subsequent simulations, the smaller grid with 0.49 million cells was adopted.

Boundary conditions for the jet model were defined as follows (see Fig. 9):

- a) Inlet (*ab*): pressure inlet, total pressure and temperature equal to those of the CO₂ reservoir (Experimentally measured variations in temperature and pressure described by UDFs were used as inlet conditions for the computational domain);
- b) Wall (*bcd*e): no-slip, adiabatic boundary;
- c) Outlet (*efgh*): pressure outlet with ambient pressure and temperature.

3.2. Dispersion model

Fig. 11(a) shows an ‘exploded’ view of the box-shaped computational domain of the dispersion model with its seven boundary surfaces. The overall dimensions of the computational domain for the dispersion model are 120 m (length) $\times$ 100 m (breadth) $\times$ 40m (height). In accordance with the experimental configuration, the XY plane is the flat ground, with the X axis oriented along the wind and also the jet flow direction. The horizontal Y axis is perpendicular to the wind direction, and the Z axis is vertical. All BP Trials were horizontal releases. The jet exit is located on the Z axis, 1.1 m from the ground. The CO₂ source was represented by a round surface, which is $10x_m$ downstream from the jet exit. The computational domain was discretised in the form of hexahedral cells (see Fig. 11(b)), with refinement around the CO₂ source and also near the ground, which makes a grid with nearly 1

million cells to enable accurate prediction of flow parameters.

In the dispersion model, seven boundary conditions were required to be defined: (1) wind inlet, (2) CO₂ inlet, (3) ground, (4) left side, (5) right side, (6) top, and (7) outlet of the computational domain. The CO₂ inlet was specified by a mass flow rate, using UDFs to describe the time-varying parameters obtained from the jet model, including overall mass flow rate (with air entrainment), average CO₂ fraction, and average temperature over the inlet surface. The ‘top’ and two ‘side’ boundaries were defined as impermeable ‘symmetry’ boundaries with zero normal velocity and zero gradients of all variables, and zero fluxes of all quantities across it. The outlet was set as a pressure boundary with ambient pressure and temperature. The ground boundary was defined as a no-slip, isothermal wall with temperature equal to the ambient temperature. The velocity profile of the wind inlet was specified by a power law correlation [57]:

$$u = u_r \left(\frac{z}{z_r} \right)^\alpha \quad (9)$$

where u_r is a reference wind velocity measured at the reference height z_r , and α is the ‘wind shear exponent’, which depends on the atmospheric stability class and the ground surface roughness.

4. Results and discussion

In order to study the behaviour of high-pressure CO₂ jet, eight separate CFD simulations covering the stagnation pressure range from 1 MPa to 15 MPa were carried out using the present jet model at first. The results for four of these are shown in Fig. 12, in terms of the simulated Mach number contours in the jet flow for four different stagnation pressures. The expansion of the jet outside the nozzle is very clearly seen. The flow structure of the simulated CO₂ jet is similar to the experimental shadowgraph in Fig. 4(a), which consists of an initial curved shock region, where the expanding flow is curved back

towards the axis due to the external pressure, and a reflected shock. Within these simulations, a fully developed Mach disc can be seen. The distance from jet exit to Mach disc (x_m) and the jet diameter increase when the stagnation pressure is raised. In all cases, the location of Mach disc is clear and x_m is easy to measure. The results revealed that the CFD jet model using the real gas EOS is capable of simulating high-pressure CO₂ jets, showing a realistic flow structure.

Table 1 compares the simulated x_m against that calculated by Eq. (8). While generally there was good agreement between theory and simulations, the jet model using a real gas EOS tends to over-predict the distance from jet exit to the Mach disc, compared to Eq. (8). At stagnation pressures greater than the critical pressure, the discrepancy is reduced rapidly with increasing stagnation pressure. In reality, CO₂ pipelines can be assumed to operate at pressures around 15 MPa [58]. Since for this condition, the two methods (theory and simulation) produced very similar estimates of the Mach disc location, Eq. (8) can be considered adequate for determining the value of x_m . Consequently, conditions over the jet cross section $10x_m$ downstream of the nozzle exit can be obtained and applied as the inlet conditions in the dispersion model.

As mentioned above, the current CO₂ jet model is limited to simulations of supercritical releases. To validate its performance, Trial 8 and Trial 8R of BP DF1 CO₂ dispersion experiments [36], both supercritical releases, were simulated. In these two trials, the nozzle diameter was about 12 mm, the stagnation pressures around 15 MPa, with the release lasting 121 s and 141 s respectively. The parameters for the CFD model setup were determined according to the experimental configuration and meteorological measurements (see Table 2). Simulations using the PR EOS and the ideal gas EOS were carried out separately and the results were compared.

Comparative studies were also carried out between the CFD model and a commercial software package, DNV Phast. Phast is a comprehensive hazard analysis software tool, which can examine the progress of a potential incident from the initial release to far-field dispersion, and is widely used in the process industries. In this study, Phast 7.01 was employed, which provides TVDI (Time-Varying Discharge), ATEX (ATmospheric EXpansion) and UDM (Unified Dispersion Model) modules applicable to simulate time-varying release rate, post-expansion conditions and downwind dispersion respectively [14].

4.1. *CO₂ jet simulations*

Reflecting release durations in the experiments, the total transient simulation times were 121 s and 141 s for Trial 8 and Trial 8R respectively in the CO₂ jet simulations. The time step was set as 2×10^{-6} s and the convergence criterion was defined as the residuals becoming equal or less than 10^{-4} . The discharge mass flow rate was evaluated using

$$Q = \bar{\rho}_e \bar{v}_e A_e \quad (10)$$

where ρ_e is the gas density at the nozzle exit, v_e the discharge velocity at the nozzle exit, A_e the area of the nozzle exit, and $(\bar{\quad})$ stands for the average over the exit area.

Fig. 13 compares the predicted release rate against the measurements. The measured release rate was obtained using the measurements from the load cells on the vessel because no direct release rate was reported. The releases initiated at 90.5 s and 20.5 s for Trial 8 and Trial 8R respectively after the start of data logging. It is observed that the measured data fluctuated considerably during the whole period. This is due to the uncertainties in the load cells which measured a nearly 10-tonne vessel, and any tiny error would greatly affect the value of the release rate. However the average value of the release rate

was correctly reflected and the gradually reducing trend was clear. As seen in Fig. 13, the CFD model using the PR EOS reproduced the averaged discharge rate very well: over the whole period, for both Trial 8 and 8R, the predicted value agrees with the averaged measurements and the gradually reducing trend was also well captured. In contrast, when using the ideal gas EOS in the CFD model, the discharge rate was considerably under-predicted. This is mainly because the ideal gas EOS significantly under-predicts the CO₂ density at high pressure. Phast predicted slightly higher release rates than the CFD model using the PR EOS, but the deviation between them tends to reduce gradually.

The total discharged mass is compared with measurements in Table 3. It is seen that for both trials, the ideal gas EOS under-predicted the total discharged mass significantly, but the PR EOS and Phast performed much better. This error would certainly play a part in the subsequent dispersion model and affect the dispersion profile. Phast tends to over-predict the discharge rates and its prediction error is slightly less than the CFD model using the PR EOS. From the risk assessment point of view, Phast is slightly better than the PR EOS coupled CFD model in predicting the discharge rate.

The value of the Mach disc stand-off distance x_m calculated by Eq. (8) during the discharge period ranges from 0.1 m to 0.08 m for both Trial 8 and Trial 8R. In order to set up a uniform dispersion model and allow sufficient space for the reducing of jet pressure and velocity, 0.1 m was selected as the stand-off distance and jet conditions over 1 m downstream cross section were then obtained as inlet conditions for the dispersion model.

Fig. 14 gives the pressure and velocity profiles along the jet axis which were taken 1 s after the start of

release. It is clear that downstream from the jet exit, the jet pressure reduces very quickly and reaches the ambient pressure well before $10x_m$. When approaching $10x_m$, the velocity has also reduced considerably. If the jet cross section at $10x_m$ as the CO₂ inlet surface is used in the dispersion model, the supersonic and oscillating regions can surely be avoided. Fig. 15 shows the jet conditions over the cross section at $10x_m$, also taken 1 s after the start of release. At this location, the highest velocity and lowest temperature occur on the jet axis, while ambient conditions prevail on the lateral jet boundary. The time history of the velocity and temperature (and thus density) over the cross section at $10x_m$ was used to estimate out the CO₂ source strength over the CO₂ inlet surface of the dispersion model.

4.2. CO₂ dispersion simulations

In Trial 8 and Trial 8R, the CO₂ concentration was measured using probe arrays at 5 m, 10 m, 15 m, 20 m and 40 m downstream of the release point. In the first four arrays, the concentration sensors were mounted only at 1 m above ground level, while in the last array, concentration sensors were deployed at 0.3 m, 1.0 m, and 3 m above ground level. Time histories of the measured and predicted centreline CO₂ volume fraction at different downstream locations of Trial 8 and Trial 8R are compared in Fig. 16 and Fig. 17 respectively. Fig. 16(d) and Fig. 17(d) only compare the data 0.3 m above ground level. It is clear that there is very good agreement between the measurements and the results predicted by the CFD dispersion model using the source strength estimated by the PR EOS. During the release, the CO₂ source strength was reducing gradually. This resulted in the gradual reduction in the downstream concentration level. This trend is also captured very well by the model. The CFD model tends to slightly over-predict the downstream concentration, which can be considered good from the risk assessment point of view. One exception is at 40 m downstream in Trial 8R (see Fig. 17(d)), where

only the average concentration was predicted. This may be due to the large wind velocity disturbance during Trial 8R. In this trial, it was observed that 11 m upwind from the release source, the wind velocity was 0.71 m s^{-1} , but 40 m downwind from the release source the wind velocity was 5.34 m s^{-1} . This would certainly affect the downstream dispersion, especially in the far-field region.

CO₂ dispersion simulations using source release rates estimated by the ideal gas EOS were also carried out. As seen in Fig. 16 and Fig. 17, because of diminished source strength estimated by the ideal gas EOS, the CFD dispersion model predicted consistently lower downstream CO₂ concentration. At all monitor points, the concentrations predicted using the source strength estimated by the ideal gas EOS are about 20% less than that predicted using source strength by PR EOS. This agrees with the discrepancy of the released CO₂ mass predicted by the two EOSs mentioned above.

The dispersion during Trial 8 and Trial 8R was also simulated using Phast. As Phast only uses constant source strength for dispersion simulation, two release rates were applied for comparison: the averaged release rate and the initial release rate (maximum instantaneous release rate). Another feature of Phast is that it only predicts time-averaged downstream concentration and the minimum effective averaging time is 18.75 s. Hence 20 s was chosen as the averaging time for Phast simulations and all the measurements and CFD simulation results were 20 s time-averaged for comparison. Table 4 compares the maximum time-averaged CO₂ concentration values between measurements and predictions. The last two columns show the results obtained by Phast using the average release rate and the initial release rate respectively. Despite the greater source strength predicted by Phast, the downstream CO₂ concentration was considerably under-predicted. Even when initial release rate was applied to the dispersion simulation, which was about 25% greater than the average release rate in Trial 8 and Trial

8R, the concentration was still under-predicted by Phast.

Fig. 18 shows the mid-plane concentration of CO₂ 10 s after release in Trial 8R. As a heavier-than-air gas, it is clear that CO₂ tends to sink towards the ground during dispersion. Figure 19 gives the concentration contours of CO₂ over different downwind cross sections. For a horizontal release, the highest concentration is seen at ground level not far from the source point. It is also seen that the hazardous gas disperses quickly downstream. This indicates that, for a specific release, the impact area would be limited. Knowing the meteorological and topography conditions, the safety distance for a given concentration level could be quantitatively determined using the proposed models.

A vertical CO₂ release was also studied, assuming leakage from a DN400 CO₂ pipeline. The orifice was defined as a round hole with a 35 mm diameter, while the estimated maximum release rate was about 100 kg s⁻¹. In the dispersion model, a constant mass flow rate was used, and simulations were carried out using 2 m s⁻¹ and 5 m s⁻¹ wind velocity respectively. Fig. 20 displays the isosurfaces corresponding to 15,000 and 10,000 ppm CO₂ volume fraction, in which the former is the Short Term Exposure Limit (STEL) for human beings, below which no negative impact will be observed on people after a 15-minute exposure [59]. It was found that, in the vertical release scenarios, the high initial momentum will lift the CO₂ cloud to a certain height. Higher wind velocity is able to reduce the cloud height and increase the downwind spread of the cloud. Although gravity still affects the dispersion, the region at ground level in the immediate vicinity of the release will not be the most seriously affected region, as the hazardous gas cloud will be sufficiently diluted before it reaches the ground. This indicates that consideration of release direction is very important in the risk assessment of CO₂ pipelines. In addition, if there are high-rise buildings close to the CO₂ pipeline, the risks

associated with people on the upper floors may also need to be considered.

5. Conclusions

In this study, CFD models for simulating the atmospheric dispersion of CO₂ released from high-pressure pipelines are presented. A UDRGM describing the PR EOS was developed to couple with ANSYS Fluent. Two trials of DNV BP DF1 CO₂ dispersion experiments were simulated for validation of the present models and DNV Phast was employed for comparative studies. It can be concluded that:

(1) For the simulation of the under-expanded free jet, as the SST $k-\omega$ model performs better in resolving the detailed flow structure and predicting the overall velocity field, we recommend using the SST $k-\omega$ model rather than the modified $k-\varepsilon$ model presented by Sarkar et al. [26].

(2) In the determination of the jet cross-section to be used as the inlet surface of the dispersion model, the location of the Mach disc, x_m , should be considered, and $10x_m$ can be used as the location of the inlet surface of the dispersion model. In the model setup stage, the equation proposed by Crist et al. [20] can be employed to determine the value of x_m .

(3) The CFD models using the PR EOS considerably outperform those using the ideal gas EOS. This indicates that CFD models using real gas EOS may be used in the quantitative risk assessment of an accidental CO₂ pipeline release and satisfactory estimations can be obtained.

(4) Phast can predict slightly better discharge rate but may significantly under-predict the dispersion concentration. If using Phast to estimate the dispersion profile, we suggest applying the maximum

instant release rate for its dispersion model and choosing an appropriate safety factor to ensure conservative predictions.

(5) In an accidental CO₂ pipeline release, the fluid exits from the orifice with very high momentum, which may dominate the near-field cloud formation. In the risk assessment, apart from the discharge rate, the release direction is also a very important parameter to be considered.

The present CO₂ jet models are only capable of modelling supercritical CO₂ releases as no phase change was considered. Further studies will be directed to the development of multi-phase model to account for the phase change during discharges, thus enabling the CFD simulation of CO₂ release from liquid state.

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Figure Captions:

- Fig. 1.** Field instrumentation of the BP DF1 CO₂ dispersion experiments [36]
- Fig. 2.** Properties of CO₂, predicted vs measured: PR EOS (—), ideal gas EOS (----), measured (+)
- Fig. 3.** Computational domain and mesh for the air jet
- Fig. 4.** Jet shadowgraph and predicted velocity fields
- Fig. 5.** Velocity profile along the axis of the jet: SST $k-\omega$ (—), modified $k-\varepsilon$ (---), measured (+)
- Fig. 6.** Jet velocity profile: SST $k-\omega$ (—), modified $k-\varepsilon$ (---), measured (+)
- Fig. 7.** Pressure and temperature profile along the axis of the jet: SST $k-\omega$ (—), modified $k-\varepsilon$ (---)
- Fig. 8.** Schematic of the problem partition
- Fig. 9.** Computational domain and mesh for the jet model
- Fig. 10.** Prediction of the along axis velocity profile as a function of the number of grid cells ($P_0 = 15$ MPa, $T_0 = 380$ K)
- Fig. 11.** Computational domain and mesh for the dispersion model
- Fig. 12.** Mach number contours of CO₂ jets initiated with different stagnation pressures (stagnation temperature $T_0 = 380$ K)
- Fig. 13.** CO₂ release rates - predicted vs measured
- Fig. 14.** Axial pressure and velocity profiles of the CO₂ jets (1 s after the start of release): Trial 8 (—), Trial 8R (---)
- Fig. 15.** Velocity and temperature profiles of the CO₂ jets at the $10x_m$ cross section (1 s after the start of

release): Trial 8 (—), Trial 8R (---)

Fig. 16. Downstream CO₂ concentration time history – predicted vs measured (Trial 8)

Fig. 17. Downstream CO₂ concentration time history – predicted vs measured (Trial 8R)

Fig. 18. CO₂ volume fraction over the ZX mid-plane (10 s after release)

Fig. 19. CO₂ volume fraction over downstream cross sections (10 s after release)

Fig. 20. 15,000 and 10,000 ppm concentration isosurfaces for different wind velocities of a vertical CO₂ release

Table Captions:

Table 1 Predicted Mach disc location

Table 2 Parameters used in the CFD models

Table 3 Released CO₂ mass - predicted vs measured

Table 4 Maximum 20 s time-averaged CO₂ volume fraction [%] - predicted vs measured

Fig. 21. Field instrumentation of the BP DF1 CO₂ dispersion experiments [36]

Fig. 22. Properties of CO₂, predicted vs measured: PR EOS (—), ideal gas EOS (----), measured (+)

Fig. 23. Computational domain and mesh for the air jet

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Fig. 25. Velocity profile along the axis of the jet: SST $k-\omega$ (—), modified $k-\varepsilon$ (---), measured (+)

Fig. 26. Jet velocity profile: SST $k-\omega$ (—), modified $k-\varepsilon$ (---), measured (+)

Fig. 27. Pressure and temperature profile along the axis of the jet: SST $k-\omega$ (—), modified $k-\varepsilon$ (---)

Fig. 28. Schematic of the problem partition

Fig. 29. Computational domain and mesh for the jet model

Fig. 30. Prediction of the along axis velocity profile as a function of the number of grid cells ($P_0 = 15$ MPa, $T_0 = 380$ K)

Fig. 31. Computational domain and mesh for the dispersion model

Fig. 32. Mach number contours of CO_2 jets initiated with different stagnation pressures (stagnation temperature $T_0 = 380 \text{ K}$)

Fig. 33. CO_2 release rates - predicted vs measured

Fig. 34. Axial pressure and velocity profiles of the CO₂ jets (1 s after the start of release): Trial 8 (—), Trial 8R (---)

Fig. 35. Velocity and temperature profiles of the CO₂ jets at the $10x_m$ cross section (1 s after the start of release): Trial 8 (—), Trial 8R (---)

Fig. 36. Downstream CO₂ concentration time history – predicted vs measured (Trial 8)

Fig. 37. Downstream CO₂ concentration time history – predicted vs measured (Trial 8R)

Fig. 38. CO₂ volume fraction over the ZX mid-plane (10 s after release)

Fig. 39. CO₂ volume fraction over downstream cross sections (10 s after release)

Fig. 40. 15,000 and 10,000 ppm concentration isosurfaces for different wind velocities of a vertical CO_2 release

Table 5 Predicted Mach disc location

P_0 [MPa]	x_m by CFD [m]	x_m by Eq. (8) [m]	Deviation
1	0.0304	0.0245	23.9%
3	0.0524	0.0424	23.4%
5	0.0684	0.0548	24.8%
7	0.0768	0.0648	18.4%
9	0.0823	0.0735	12.0%
11	0.0852	0.0812	4.8%
13	0.0909	0.0883	2.9%
15	0.0969	0.0949	2.1%

Table 6 Parameters used in the CFD models

Parameter	Trial 8	Trial 8R
Initial stagnation pressure (Pa)	1.574×10^7	1.483×10^7
Initial stagnation temperature (K)	420.3	422.6
Ambient pressure (Pa)	9.6×10^4	9.6×10^4
Ambient temperature (K)	281.0	284.3
Nozzle exit diameter (mm)	11.94	11.94
CO_2 release duration (s)	121	141
Reference wind velocity u_r (m s^{-1})	5.51	0.69
Reference height z_r (m)	8.0	8.0
Wind shear exponent α	0.1168	0.6831

Table 7 Released CO_2 mass - predicted vs measured

	Measured [kg]	PR EOS [kg]	Deviation of PR EOS	Ideal gas EOS [kg]	Deviation of Ideal gas EOS	Phast [kg]	Deviation of Phast
Trial 8	403.9	391.6	-3.0%	306.4	-24.1%	413.0	+2.3%
Trial 8R	424.5	410.2	-3.4%	327.7	-22.8%	434.4	+2.3%

Table 8 Maximum 20 s time-averaged CO₂ volume fraction [%] - predicted vs measured

	Downstream [m]	Measured	PR EOS	Ideal gas EOS	Phast	Phast max
Trial 8	5	8.22	8.93	6.89	5.79	6.31
	10	3.36	3.87	3.00	2.81	3.09
	20	1.85	2.23	1.74	1.49	1.64
	40	1.49	1.62	1.27	0.84	0.92
Trial 8R	5	7.55	8.56	6.82	5.69	6.26
	10	3.23	3.73	2.99	2.94	3.24
	20	1.59	2.21	1.78	1.54	1.70
	40	1.69	1.49	1.20	0.83	0.91