Numerical simulation of liquid CO₂ accidental release at atmospheric environment

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Abstract. Investigation of the transient behaviour of high-pressure CO₂ sudden release is important for the pipeline transportation safety of carbon capture and storage technology. A CFD model based on the volume of fluid method and non-equilibrium phase transition is established to simulate the high-pressure liquid CO₂ release at atmospheric environment, which considers the flow domain out of the opening. The pressure drop and decompression wave speed predicted by CFD are in good agreement with the “shock tube” test results, which verifies the established CFD model. On this basis, we further investigate the transient behaviour of liquid CO₂ release. The results show that the liquid-gas two-phase flow continues expanding outward from the rupture opening and sucking up the surrounding air, forming a complex three-phase under-expanded jet. It is found that the distance from rupture opening to Mach disk increases with the increase of initial pressure. It is also found that the liquid-gas CO₂ mixture spurted from the rupture opening is mainly composed of liquid CO₂ and a small amount of gaseous CO₂ by analyzing the mass flow composition. Moreover, The static pressure and the total mass flow at the rupture opening both increase with the increase of the initial pressure, while the mass flow of the gas CO₂ decreases with the increase of the initial pressure.

1. Introduction
As the most direct and effective carbon reduction option, carbon capture and storage (CCS) technology has good development prospects in the next few decades [1]. It is believed that by 2050, the deployment of CCS plants will reduce CO₂ emission to a minimum of 19% [2]. In CCS technology, the pressurized CO₂ is usually transported through long-distance pipelines in a liquid or supercritical state. The operating temperature and pressure are recommended be in a range of 13-44°C and 8.5-15 MPa respectively in order to reach a stable flow of single-phase CO₂ within the pipelines [3]. As a result of equipment failure, corrosion, maintenance errors, external impacts and operator errors, accidental release from CCS plants are most likely due to a rupture or puncture of pipelines [4]. During the release process, the pressure and temperature of pressurized CO₂ within the pipe will drop
sharply and cause a phase transition, which will lead to a long pressure plateau and aggravate the extension of pipeline cracks. Moreover, understanding the release behaviour is essential for the early detection and prevention of any significant hazards related to the transportation of high-pressure CO₂.

In recent years, a large number of experiments have been conducted to study the release behaviour of high-pressure CO₂ [5,6]. Botros et al used a “shock tube” with a total length of 42 m and an inner diameter (ID) of 38.1 mm to study the transition behaviour of high-pressure CO₂ decompression within pipe [7]. Furthermore, Xie et al investigated the pressure drop within pipe and the structure of the under-expanded jet flow at the rupture opening during the CO₂ release based on a minor-caliber test pipeline with a ID of 30 mm [8]. To reveal the flow characteristics and dispersion in the process of high-pressure CO₂ discharge from a large caliber pipe, Guo et al conducted a series of CO₂ release tests based on an industrial scale pipeline with a total length of 258 m and an ID of 233 mm [9].

CO₂ release often involves complex phenomena, including liquid-gas phase transition and multiphase flow, which bring great challenges to numerical simulation. However, with the development of multiphase flow technology in recent years, numerical simulation has been applied to study the transient behaviour of high-pressure CO₂ release. In order to calculate the mass transfer and heat transfer of liquid-gas phase transition, the homogeneous equilibrium model (HEM) and homogeneous relaxation model (HRM) have been proposed. The HEM easily leads to a higher predicted “pressure plateau” value, while the HRM takes into account the delayed phase transition, which has more accurate prediction results [10,11]. Although many release models have been proposed, most of them are based on one-dimensional flow assumptions, ignoring some flow details [12,13]. In the recently proposed numerical model based on non-equilibrium phase transition and multiphase flow, Liu et al set up a computational fluid dynamics (CFD) model for CO₂ mixture based on mixture multiphase model and GERG-2008 equation of state (EoS) [14]. And Xiao et al established a CFD model for high-pressure liquid CO₂ with mixture multiphase model and Span-Wagner EoS [15]. However, none of them have considered the complex phase transition and multiphase flow of the flow domain out of the rupture opening.

In this paper, a CFD model based on the volume of fluid (VOF) method and non-equilibrium phase transition was developed to simulate the high-pressure liquid CO₂ release at atmospheric environment, which considers the flow field out of the opening. And the effects of initial pressure on the transition behaviour within the pipe and the development of under-expanded jet structure near the opening were further investigated. The results will provide a reference for the numerical investigation of CO₂ pipeline release.

2. Computational model

2.1. Multiphase VOF model
In the VOF model, the volume fraction equation of k phase is defined as:

\[ \frac{1}{\rho_k} \left[ \frac{\partial}{\partial t} \left( \alpha_k \rho_k \right) \right] + \nabla \cdot \left( \alpha_k \rho_k \vec{V}_k \right) = S_m, \] (1)

where \( \rho \) is the density, \( \alpha \) is the volume fraction, the sum of the volume fractions of all phases is equal to 1. \( \vec{V} \) represents the velocity, and \( t \) is the flow time. \( S_m \) is the source term of mass transfer between liquid phase and gas phase.

The momentum equation for the mixture can be expressed as

\[ \frac{\partial}{\partial t} \left( \rho \vec{V} \right) + \nabla \cdot \left( \rho \vec{V} \vec{V} \right) = -\nabla p + \nabla \cdot \left[ \mu \left( \nabla \vec{V} + \nabla \vec{V}^T \right) \right] + \rho \vec{g} + \vec{F}, \] (2)

where \( p \) is the fluid pressure, \( \mu \) is the viscosity, and \( \vec{g} \) represents the gravitational acceleration.

The energy equation for the multiphase model takes the following form:

\[ \frac{\partial}{\partial t} \left( \rho E \right) + \nabla \cdot \left( \vec{V} \left( \rho E + p \right) \right) = \nabla \cdot \left( k \nabla T \right) + S_e, \] (3)
where \( k_e \) is the effective conductivity, and \( T \) is the temperature. \( S_E \) represents the volumetric source, which is defined as the latent heat of phase transition in this study.

In the VOF model, the energy \( E \), temperature \( T \) and velocity \( V \) of mixture are mass-averaged variables, and are defined as follows:

\[
E = \frac{\sum_{k=1}^{n} \alpha_k \rho_k E_k}{\sum_{k=1}^{n} \alpha_k \rho_k},
\]

(4)

Other mixture properties, such as density and viscosity, are treated as volume-fraction-averaged variables, which take on the following form:

\[
\rho = \sum_{k=1}^{n} \alpha_k \rho_k,
\]

(5)

\[\text{Figure 1. CFD computational model.}\]

2.2. Thermodynamic property model

The Lee model was commonly used to study the liquid to gas phase transition process [15]. The pressure-driven mass transfer between liquid phase and gas phase can be expressed as follows:

If \( P_l < P_{sat} \) (evaporation), then

\[
m_{lg} = \tau \alpha_l \rho_l \frac{P_{sat} - P_l}{P_{sat}},
\]

(6)

If \( P_g > P_{sat} \) (condensation), then

\[
m_{gl} = \tau \alpha_g \rho_g \frac{P_{sat} - P_g}{P_{sat}},
\]

(7)

where \( m_{lg} \) and \( m_{gl} \) are the mass transfer of liquid phase to gas phase and gas phase to liquid phase respectively, and the sum is defined as the source term \( S_E \). \( \tau \) can be regarded as the relaxation time coefficient, and the value is 15 s\(^{-1}\) [15]. The subscripts \( l, g, \) and \( sat \) are the corresponding parameters of liquid CO\(_2\) phase, gas CO\(_2\) phase and saturation phase, respectively.

Here, the Span-Wagner EoS was embedded into the CFD model by programming to predict the thermodynamic properties of CO\(_2\). More details were discussed in our previous work [15].

\[\text{Table 1. Initial computational parameters of cases.}\]

| Cases | \( P_0 \) (MPa) | \( T_0 \) (K) | \( \rho_0 \) (kg/m\(^3\)) |
|-------|----------------|--------------|----------------------|
| 1     | 5.067          | 281.89       | 880.0                |
| 2     | 11.270         | 281.89       | 936.9                |
| 3     | 23.388         | 281.89       | 1000.0               |

2.3. Computational domain and numerical method

The computational domain includes the CO\(_2\) domain inside the pipe and the air domain out of the rupture opening, as shown in Figure 1. The length of the CO\(_2\) domain inside the pipe is 10 m, and the radius \( R \) is 19.05 mm. The height and length of the air domain are 20\( R \) and 100\( R \), respectively. A two-dimensional (2D) axial symmetric model, which was suitable for current calculations, was used to speed up the calculations [14,15]. The pressure outlet boundaries were adopted at the upper and side
edges of the air domain. Rest of the boundaries were set as adiabatic walls. To ensure the computational accuracy, the grid sizes along radial and axial in the CO₂ domain were set as 2 mm and 5 mm respectively [14,15]. The meshes near the rupture opening and the pipe walls were refined, and the minimum size is 1 mm. The total number of grids in the computational domain was 32930.

Figure 2. Comparison of pressure drop at PT1A. The experiment was implemented by Botros [7]. $P_0$ and $T_0$ are 11.27 MPa and 281.89 K respectively.

Figure 3. Decompression wave speed by CFD and experiment. $P_0$ and $T_0$ of the simulation are 11.27 MPa and 281.89 K respectively.

The pressure-based solver was selected to match the VOF model, which are applicable to a broad range of flows—that is from incompressible to highly compressible [16]. The realizable $k$-$\varepsilon$ turbulent model was adopted to simulated the under-expanded jet flow. The “Least squares cell based” and “PRESTO” schemes were used for gradient and pressure discretization, respectively, while “QUICK” scheme was used for all others. The time step was set to be $1 \times 10^{-8}$–$1 \times 10^{-6}$s. In order to study the effect of initial pressure $P_0$, three different cases were set up, as shown in Table 1. The initial temperature $T_0$ of the CO₂ domain inside the pipe, however, were always 281.89 K. The air domain out of the rupture opening was assumed to be ideal gas, and the initial pressure and temperature are 101325 Pa and 281.89 K, respectively.

Figure 4. Velocity and volume fraction with a flow time of 10 ms: (a) velocity, (b) volume fraction of vapor CO₂, (c) volume fraction of liquid CO₂ and (d) volume fraction of air. $P_0$ and $T_0$ are 11.27 MPa and 281.89 K, respectively.
3. Results and discussion
A same “shock tube” experiment as case 2 in Table 1 was conducted by botros [7]. Figure 2 shows the pressure drop of monitoring point “PT1A”, which is located at 92.4 mm away from the rupture opening. The instantaneous pressure drop is fully captured by numerical simulation. The decompression wave speed curves by numerical calculation and experiment are shown in Figure 3, which are in good agreement. Therefore, it can be concluded that the established CFD model can effectively predict the release behaviour of high-pressure CO2 pipelines at atmospheric environment.

Table 2. Comparison of $x_m$ by CFD and Equation 8.

| Cases | $P_s$ (MPa) | $x_m$ (mm)     | Errors (%) |
|-------|-------------|----------------|------------|
| 1     | 2.22        | 132.13         | 115.12     | 14.78      |
| 2     | 2.43        | 140.05         | 120.44     | 16.23      |
| 3     | 2.79        | 156.01         | 129.05     | 20.89      |

Figure 4 shows the velocity and volume fraction flow fields. One can see that high-pressure liquid CO2 spurts from the rupture opening rapidly, and part of them is transformed into gaseous CO2 to form a high-pressure liquid-gas two-phase mixture, which continues expanding outward and sucking up the surrounding air, forming a complex three-phase under-expanded jet by entrainment. At the same time, the high-pressurizes liquid CO2 in the pipe is continuously transferring into gaseous CO2 to form a two-phase flow. It is found that a Mach disk is formed at about 7.35R away from the rupture opening. This is due to the continuous vaporization and expansion of the formed two-phase flow, which is compressed when the pressure is lower than the ambient pressure, as shown in Figure 5 (a).

Figure 5. Variation of pressure and mass flow: (a) pressure distribution along the axis, (b) static pressure, (c) total mass flow, and (d) mass flow of gas CO2 at the rupture opening.
The distance $x_m$ from the rupture opening to the Mach disk can be approximately given as [17]:

$$x_m = 1.291 \frac{P_s}{P_a}$$

(8)

where $P_s$ is the stagnation pressure at the rupture opening. The CFD predicted values of $P_s$ are shown in Table 2. $P_a$ is the ambient pressure. The distances of $x_m$ by CFD and Equation 8 are also shown in the table, which indicate that the CFD results are slightly larger than the calculation results of Equation 8, and the maximum error reaches 20.89 %. This is mainly due to the fact that Equation 8 is applicable to a single phase gas, while not to a liquid-gas mixture. In spite of this, the value of $x_m$ increases with the increase of initial pressure. The errors in the table, however, were calculated by

$$\frac{(X_{m(CFD)} - X_{m(Eq8)})}{X_{m(Eq8)}}$$

The volume fraction of the liquid CO$_2$ on the left side of the Mach disk is lower than that on the right side, as shown in Figure 4 (c). It can be inferred that the gas-liquid phase transition occurs on the right side of the Mach disk, which is mainly due to the excessive expansion of the two-phase flow. The air mainly exits in the jet outer edge area, which shows little effect on the main structure of the jet. The maximum flow velocity, however, is only about 180 m/s when the flow time is 10 ms. This may be due to the fact that the jet is a liquid-gas two-phase flow.

Figure 5 (a) shows the pressure distribution along the axis by difference initial pressure at a flow time of 8 ms. Affected by the decompression wave, the fluid pressure in the pipe ($x < 0$) suddenly drops to a plateau pressure value. In the air domain near the rupture opening ($x > 0$), the pressure near the Mach disk has a sudden change. The pressure on the left is lower than the ambient pressure, while on the right is higher than the ambient pressure.

Figure 5 (b) shows the static pressure at the rupture opening. Reference [15] did not consider the air domain, while in this paper, the air domain out of the opening was considered. As a result, the opening pressure are the same as the atmospheric pressure at the initial moment, and continue to increase slowly. Figure 5 (c) shows the total mass flow at the rupture opening, which have a maximum value at a flow time of about 1 ms, and then slowly decreases. The mass flow of gas CO$_2$, which is very small compare to the total mass flow, continues to increase with the flow time, as shown in Figure 5 (d). It can be inferred that the fluid spurted from the rupture opening is mainly composed of liquid CO$_2$ and a small amount of gaseous CO$_2$. In addition, the pressure and the total mass flow at the rupture opening both increase with the increase of the initial pressure, while the mass flow of the gas phase decreases with the increase of the initial pressure. This is because the state point with a smaller initial pressure is closer to the saturated state when temperature is constant, and the vaporization is more fast.

4. Conclusion

A CFD model based on the VOF method and non-equilibrium phase transition was established to simulate the high-pressure liquid CO$_2$ release at atmospheric environment. The CFD model is verified by comparing the numerical results with the “shock tube” test results. The transient behaviour of liquid CO$_2$ accidental release at atmospheric environment was further investigated. It was found that the liquid-gas two-phase flow continuously expanded outward from the rupture opening and sucked up the surrounding air, forming a complex three-phase under-expanded jet by entrainment. A Mach disk was clearly observed near the rupture opening, and the value of $x_m$ increases with the increase of initial pressure. The static pressure at the opening, however, was the same as the atmospheric pressure at the initial moment, and continued to increase. The total mass flow at the rupture opening reached a maximum value at a flow time of about 1 ms, and then slowly decreased. The mass flow of gas CO$_2$ was very small compare to the total mass flow, and continued to increase with the flow time. Further analysis indicated that the mass flow composition of the liquid-gas CO$_2$ mixture spurted from the rupture opening consisted of a large amount of liquid CO$_2$ and a small amount of gaseous CO$_2$. In addition, the pressure and the total mass flow at the rupture opening both increased with the increase of the initial pressure, while the mass flow of the gas phase decreased with the increase of the initial pressure.
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