A CFD computational model for high-pressure liquid CO₂ decompression

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Abstract. A CFD decompression model with considering external flow field is established based on the non-equilibrium phase transition. The results of pressure and decompression wave speed calculated by CFD are compared with the results of “shock tube” test, showing good agreement. On this basis, the effects of external flow field on the transient behaviour of liquid CO₂ decompression in the pipe is further investigated. It is found that the external flow field basically has no effect on the variation of pressure and decompression wave speed in the pipe. Moreover, a Mach disk is formed at about 7.35R (R is the radius of rupture opening, 19.05 mm) away from the rupture opening in the process of jet expansion. Although the external flow field has a significant influence on the static pressure at the rupture opening, the mass flow in the case without considering external flow field is larger than that with considering external flow field, and the overall difference between the two cases is within 6%.

1. Introduction

A large amount of CO₂ generated by fossil fuel combustion aggravates the trend of global warming. According to the monitoring data of National Oceanic and Atmospheric Administration (NOAA), the concentration of atmospheric CO₂ has been increasing continuously since 1960, as shown in Figure 1. Up to the latest data (September 2020), the atmospheric CO₂ concentration has been recorded at 412.55 ppm [1]. To control the concentration of atmospheric CO₂ effectively, the Carbon Capture and Storage (CCS) technology has been proposed and implemented. According to a report by the Intergovernmental Panel on Climate Change (IPCC) [2], CCS will be of great significance in reducing carbon emissions.

In the CCS system, the pressurized CO₂ is mainly transported through the onshore/offshore pipelines [3]. To reach a stable flow of single-phase CO₂ within the pipelines, the operating temperature and pressure are recommended be in a range of 13-44°C and 8.5-15 MPa respectively [4]. Under such operating conditions, CO₂ is usually transported through long-distance pipelines in liquid or supercritical state, which will lead to leakage accidents inevitably. During the leakage process, the
sudden pressure drop and temperature drop of the liquid CO$_2$ within the pipe will cause a liquid-gas phase transition, which will then lead to a long pressure plateau and intensify the pipeline crack extension. According to the recorded accidents related to CO$_2$ pipelines in the USA from 1990 to 2009, about 32.9% of these accidents are from pipeline ruptures, 41.9% from pinhole and puncture, and 25.2% from system failures [5].

At present, researchers have conducted a large number of experimental researches on CO$_2$ leakage, especially on high-pressure CO$_2$ pipeline leakage/decompression [6,7]. Cosham et al investigated the liquid CO$_2$ discharge through a “shock tube” test, which is commonly used to simulate a pipeline rupture. It was found that the pressure of CO$_2$ fluid within the pipe dropped sharply and a long pressure plateau appeared during the decompression process [8]. Botros et al established a small-bore “shock tube” test device with an inner diameter of 38.1 mm, and conducted a series of high-pressure liquid CO$_2$ decompression tests. The results show that the fluid pressure and decompression wave speed drop sharply during decompression [9].

![Figure 1. Monitoring concentration of atmospheric CO$_2$ from 1960 to 2020 by NOAA.](image)

In recent years, numerical simualtions of CO$_2$ decompression based on the CFD multiphase flow technology have been developed, which can be used to obtain more flow field details. In order to describe the phase transition during the high-pressure liquid CO$_2$ decompression, the Homogeneous Equilibrium Model (HEM) and Homogeneous Relaxation Model (HRM) have been proposed. The HEM predicted results are likely to be excessive, while the HRM shows a higher prediction accuracy by introducing a relaxation time coefficient to simulate the “delayed phase transition” [10,11]. Elsahomi et al established a CFD model for rich-CO$_2$ mixture decompression based on the GERG-2008 Equation of State (EoS) and a assumption of homogeneous equilibrium [12]. On this basis, Liu et al further introduced a relaxation time coefficient into the CFD model, taking into account the effects of “delayed phase transitions” [13]. Xiao et al established a non-equilibrium phase transition decompression model for high-pressure liquid CO$_2$ with Span-Wagner EoS [14]. Although these CFD models have achieved good prediction results, the effect of external flow field was ignored due to its complex transition behaviour, and a pressure outlet boundary where the specified static pressure was equal to the ambient pressure, was commonly adopted at the location of pipe rupture.

In this paper, a CFD model based on the non-equilibrium phase transition was used to simulate the decompression of liquid CO$_2$ with and without external flow field. The results will provide a reference for the numerical investigation of CO$_2$ decompression.

2. CFD computational model

2.1. Computational domain and numerical method

Two cases named case A and case B were carried out to investigate the effects of external flow field on the transient behaviour of liquid CO$_2$ decompression in the pipe. The external flow field was considered in case A, while ignored in case B, as shown in Figure 2. The length of the calculation
domain of pipe is 10 m, and the radius R is 19.05 mm. The height and length of external flow field in case A are 20R and 100R, respectively. A two-dimensional (2D) axial symmetric computational model was used to speed up the calculation. The static pressure of the outlet was set to be the same as the atmospheric pressure. Other boundaries that not specified were set as adiabatic walls. The initial pressure and temperature of the pipe domain were 11.27 MPa and 281.89 K, respectively. In order to simplify the calculation, the external flow field was assumed to be gaseous CO₂, and the initial pressure and temperature are 101325 Pa and 281.89 K, respectively.

The grid sizes along radial and axial in the pipe domain were 2 mm and 5 mm, respectively. To capture the larger pressure gradient around the rupture opening, the meshes near the opening were refined, and the minimum size was 1 mm. Five boundary layers were set near the pipe wall; the thickness of the first layer was defined as 1 mm, and the growth factor was set to be 1.2. The total number of grids in case A was 32930, and 23055 in case B.

The pressure-based solver was selected to calculate the CFD decompression model. The spatial discretization schemes of gradient and pressure were “Least squares cell based” and “PRESTO!” method, respectively, while all others were “Third-order QUICK” method.

Figure 2. Computational meshes of case A and case B.

2.2. Mixture multiphase model
As the calculation model involves the interactions in different phases, the mixture multiphase model was used. Here the continuity equation of the mixture phase takes the following form:

$$\frac{\partial}{\partial t} (\rho_m) + \nabla \cdot (\rho_m \bar{v}_m) = 0,$$

where $\rho_m$ and $\bar{v}_m$ are the mixture density and mass-averaged velocity, respectively. $t$ is the flow time. In the mixture model, the density of mixture phase can be expressed as

$$\rho_m = \alpha_\ell \rho_\ell + \alpha_v \rho_v,$$

The mass-averaged velocity takes the following form:

$$\bar{v}_m = \frac{\alpha_\ell \rho_\ell \bar{v}_\ell + \alpha_v \rho_v \bar{v}_v}{\rho_m},$$

where $\alpha$ represents the volume fraction, $\bar{v}$ is the mass-averaged velocity, and the subscripts “$\ell$” and “$v$” indicate the liquid phase and the gas phase parameters, respectively. The sum of the volume fraction of the phases is equal to 1.

The momentum equation for the mixture phase in the mixture multiphase model is defined as follows:

$$\frac{\partial}{\partial t} (\rho_m \bar{v}_m) + \nabla \cdot (\rho_m \bar{v}_m \bar{v}_m) = -\nabla P + \nabla \cdot \left[ \mu_m \left( \nabla \bar{v}_m + \nabla \bar{v}_m^T \right) \right] + \rho_m \bar{g}$$

$$+ \bar{F} + \nabla \cdot \left[ \sum_{k=1}^{s} \alpha_k \rho_k \bar{v}_{\ell,k} \bar{v}_{\ell,k} \right],$$

where $P$ and $g$ are the pressure and gravitational acceleration, respectively.

The energy equation of the mixture phase can be defined as:
\[ \frac{\partial}{\partial t} \sum_{i} \left( \alpha_i \rho_i E_i \right) + \nabla \cdot \sum_{i} \left( \alpha_i \mathbf{v}_i \left( \rho_i E_i + p \right) \right) = \nabla \cdot \left( k_e \nabla T \right) + S_E, \]

where \( S_E \) and \( k_e \) are the volumetric source and effective conductivity, respectively.

Similar to the continuous equation, the volume fraction equation takes the following form:

\[ \frac{\partial}{\partial t} \left( \alpha_k \rho_k \right) + \nabla \cdot \left( \alpha_k \rho_k \mathbf{v}_k \right) = -\nabla \cdot \left( \alpha_k \rho_k \mathbf{v}_{k_{dr}} \right) + S_m, \]

where \( S_m \) represents the mass transfer source between the liquid phase and gas phase.

2.3. Thermodynamic property model

In this paper, the Lee model was used to calculate the mass transfer between the liquid phase and gas phase [15]. The mass transfer can be expressed as follows:

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

\[ \dot{m}_{lv} = \tau \alpha_l \rho_l \frac{P_{sat} - P_l}{P_{sat}}, \]

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

\[ \dot{m}_{lv} = \tau \alpha_l \rho_l \frac{P_{sat} - P_l}{P_{sat}}, \]

where \( \dot{m}_{lv} \) and \( \dot{m}_{vl} \) are the mass transfers from the liquid phase to gas phase and from the gas phase to liquid phase, respectively. The sum of \( \dot{m}_{lv} \) and \( \dot{m}_{vl} \) is defined as the mass transfer source \( S_E \). \( \tau \) represents the relaxation time coefficient, the value is 15 s\(^{-1} \) [14]. Here, The subscripts “\( \text{sat} \)” is defined as the corresponding saturation state parameters.

To predict the thermodynamic property accurately, the Span-Wagner EoS was used to calculate the thermodynamic parameters of liquid phase and gas phase. Specifically, the EoS of the liquid phase was imported into the model through User Defined Real Gas Model (UDRGM), while the EoS of the gas phase was by Use Defined Function (UDF). More details were discussed in literature [14].

3. Results and discussion

A same “shock tube” experiment was conducted by Botros [9]. The pressure drop of the experimental monitoring point “PT1A”, which was located at 92.4 mm away from the rupture, was compared with the CFD results, as shown in Figure 3. The results show that the pressure drop curves of case A and case B by CFD simulation are slightly different, but they are in good agreement with the experimental results. Figure 4 shows the variations of decompression wave speed by CFD and experiment. The results of case A and case B are consistent with the experiment results. This indicates that the simulation results have high calculation accuracy, and the external flow field basically has no effect on the variation of pressure and decompression wave speed within the pipe.

**Figure 3.** Comparison of pressure drop at “PT1A”. The experiment was implemented by Botros [9].

**Figure 4.** Variations of decompression wave speed by CFD and experiment.
The velocity flow fields of case A and case B are shown in Figure 5. It can be seen from case A in the figure that high-pressure liquid CO$_2$ is rapidly spurted from the rupture opening, and part of the liquid CO$_2$ is transformed into gaseous CO$_2$ to form a high-pressure liquid-gas two-phase mixture, which continues to expand outward, forming an under-expanded jet in the external flow field. The structure of under-expanded jet, however, is clearly visible in the figure. A Mach disk is formed at about 7.35R away from the rupture opening in the process of jet expansion. Since it is a two-phase mixture, the maximum speed is only 150 m/s when the flow time is 6 ms. The flow field structure in case B is relatively simple, and the flow velocity at the rupture location is the largest, which is about 67.3 m/s when the flow time is 0.5 ms.

Figure 5. Velocity flow fields of case A and case B.

Figure 6 shows the average static pressure of the rupture opening surface. The pressure value in case A continues to increase with the increase of flow time, but the growth rate (the slope of the pressure curve) continues to decrease. The value in case B is always the same as the specific pressure value. The mass flow of the rupture opening predicted by case A and case B is shown in Figure 7. Case B has a larger prediction result, which is about 5.36% higher than case A. In addition, from the mass flow curves of case A and case B, it can be seen that the mass flow reaches the maximum at a flow time of about 1 ms, which is 34.87 kg/s and 36.74 kg/s respectively, and then slowly decreases. Although the static pressure values on the rupture opening in case A and case B are quite different, the difference between the two predicted mass flow values is small, and the overall error is within 6%.

Figure 6. Comparison of average static pressure of the rupture opening.  
Figure 7. Comparison of mass flow of the rupture opening.

4. Conclusions
The effects of external flow field on the transient behaviour of liquid CO$_2$ decompression in the pipe were investigated based on a non-equilibrium phase transition decompression model, which was
verified by a “shock tube” experiment. The external flow field was considered in case A, while ignored in case B. By analyzing the two case, some conclusions are as follow:

1. The external flow field basically has no effect on the pressure drop and the decompression wave speed in the pipe;
2. In case A, a Mach disk is formed at about 7.35R away from the rupture opening in the process of jet expansion, while in case B, the flow field structure is relatively simple;
3. Although the static pressure values of the rupture opening in case A and case B are quite different, the mass flow of the rupture opening in case B is larger than that in case A, and the overall difference between the two case is within 6%.

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