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Numerical Simulation on BLEVE Mechanism of Supercritical Carbon Dioxide

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Abstract

Greenhouse effect and energy shortage is becoming a more and more serious problem with the fast development of oil refining industry. Oil carbon capture and storage and the enhanced oil recovery (CCS-EOR) is developed to cover the shortage. A simulation was made by CFD method in this paper. The FLUENT software was utilized, and the SIMPLEC method and standard turbulent model are adopted to solve compressible N-S equations. VOF (Volume of Fluid) model are chosen as multiphase model. Numerical simulation is based on physical model and suitable mathematical model. A model was established to illustrate Mechanism and regulation of Supercritical CO_2 BLEVE which can provide technical support to accident prevention and be used as reference for future research.

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Keywords: supercritical CO_2; boiling liquid expanding vapor explosion; blast mechanism; numerical simulation

1. Instruction

Greenhouse gas like CO_2 which is produced in industry and people's daily life makes the climate get warmer and warmer. The application and extension of CCS-EOR (Carbon Capture and Storage-Enhanced Oil Recovery) can not only recycle waste material, but also can save energy. The biggest advantage in the process is the combination of displacing oil and CO_2 burial which can realize social and economic benefits.CO_2 is harmless, odorless and colorless in the natural state. However, CO_2 is in a state of high pressure and high concentrations in CCS-EOR. Many hazards probably happen in this situation, such as CO_2 boiling liquid expanding vapor explosion (BLEVE)[1].It can cause shockwave at high pressure,

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fragments at high speed, asphyxiating gas at high concentration and frostbite caused by rapid phase change. The hazards can not only endanger the operators' personal safety, but also can cause serious damage to the equipment and even have a bad effect on residents and ecosystem nearby.

Most of previous researches focus on the study of thermal response and model of vessel under the thermal effects outside [2-4], the influence of the process of BLEVE pressure relief [5-7], liquid thermal stratification impact on BLEVE[8,9], and the research on the evolution mechanism of microscopic movement[10]. Most of these researches concentrate on macroscopic perspective, and the disadvantage is dramatic because of the experiment measures. Besides, the studies on BLEVE of hydrocarbon like LPG and propane have been in deeply developed. The process of ignition, detonation are also included in these studies. However, the studies on CO_2 which are conducted both theoretically and experimentally are rarely found. So numerical simulation on BLEVE of CO_2 can make the exploration of the mechanism and process of BLEVE better and make it easier to confirm suitable measures to prevent accidents.

2. Simulation settings

In this study, the FLUENT software was utilized, and the SIMPLEC method and standard turbulent model are adopted to solve compressible N-S equations. VOF (Volume of Fluid) model are chosen as multiphase model and the boundary of phases are reconstructed. Body force between molecules should be considered when the calculation starts [11]. UDF (User-Defined Function) should be introduced because the software does not have models to calculate change of phases.

BLEVE is a very complicated physical phenomenon which results from not only the process of thermal transmission, heat exchange between phases and evaporation and condensation, but also the energy release of system and constraint of tank. So the reasonable simplification and assumption are required. Thus, the following assumptions are applied in the model.

- Simplified 2D rectangular model is chosen as the physical model. The real model is symmetrical cylinder. So we can use 2D rectangular model as a simplified model.
- Temperature distribution of medium is uniform and it is equal everywhere when the opening opens.
- The gas in the vessel is ideal gas, the physical property parameters of which change with temperature.
- When heat performance is neglected, and all faces are adiabatic and immovable; when heat performance is necessarily considered, all faces can conduct heat, and the temperature of the faces is constant.

Based on the CO_2-EOR project, we established a physical model as shown in Fig 1.1. 2D rectangle model is used to show the longitudinal section of the cylindrical pressure vessel. The height of the rectangle is 300 mm and the inner diameter of the rectangle is 62 mm. In the middle of the top surface of vessel, there is a circular open. We set monitor line-a and line-b at the trisection of the height and use the method of Facet Average to monitor how the temperature and pressure change with time.

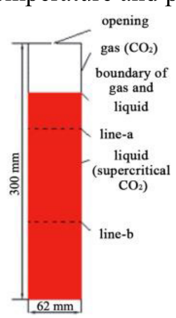


Fig. 1. Physical model

Because Fluent does not have a model to calculate the phase change, UDF should be used to calculate the phase change of BLEVE in the tube. The relationship between gas and liquid is given below[12].

$T > T_{sat}$ (Boiling)

$$R_l = -\lambda \alpha_l \rho_l \frac{|T - T_{sat}|}{T_{sat}}, \quad R_v = \lambda \alpha_l \rho_l \frac{|T - T_{sat}|}{T_{sat}} \tag{1}$$

$T < T_{sat}$ (Condensation state)

$$R_l = \lambda_l \alpha_v \rho_v \frac{|T - T_{sat}|}{T_{sat}}, \quad R_v = -\lambda_v \alpha_v \rho_v \frac{|T - T_{sat}|}{T_{sat}} \tag{2}$$

Where R_l and R_v are mass source item; αl and αv are the volume fraction of liquid and gas; ρ_l and ρ_v are the density of liquid and gas; T is the temperature of system; T_{sat} is saturated temperature; λ_l and λ_v are time relaxation factor of mass transfer, $\lambda_l = \lambda_v = 0.1$[13]

Heat energy at the boundary of phases is given below.

$$q = R_l h_{fg} \tag{3}$$

Where q is the latent heat of vaporization of supercritical CO_2.

The rate of evaporation and condensing is given below[14].

$$\Gamma_{lv} = \frac{h_{lv} A_{lv} (T_{sat} - T_l)}{h_{fg}}, \quad \Gamma_{vl} = \frac{h_{lv} A_{lv} (T_l - T_{sat})}{h_{fg}} \tag{4}$$

Where h_{lv} is heat transfer coefficient; A_{lv} is cross-sectional area of the volumes of cells.

The experimental mediums are supercritical CO_2 and CO_2 steam. The initial time is defined as the moment that the opening opens. The initial conditions and boundary conditions are adopted as follows:

- The liquid in the vessel is supercritical CO_2, the initial amount of which is 90 percent of the vessel volume; Moreover, the gas is CO_2 steam, which permeates the rest of the vessel.
- The initial temperature of the system is 404.15 K, and the distribution of it is uniform.
- The initial pressure of gas is 7.38 MPa which is the saturated vapor pressure at the supercritical point.
- The opening locates in the middle of the upper-wall of vessel, with the diameter is 0.6 mm. The boundary of the opening is *pressure outlet*.
- In this case, heat performance is neglected, and all faces are adiabatic and immovable.

3. Simulation results

3.1 Changing process of flow field

Fig 2 shows the changing process of the phases in the vessel after the opening opens.

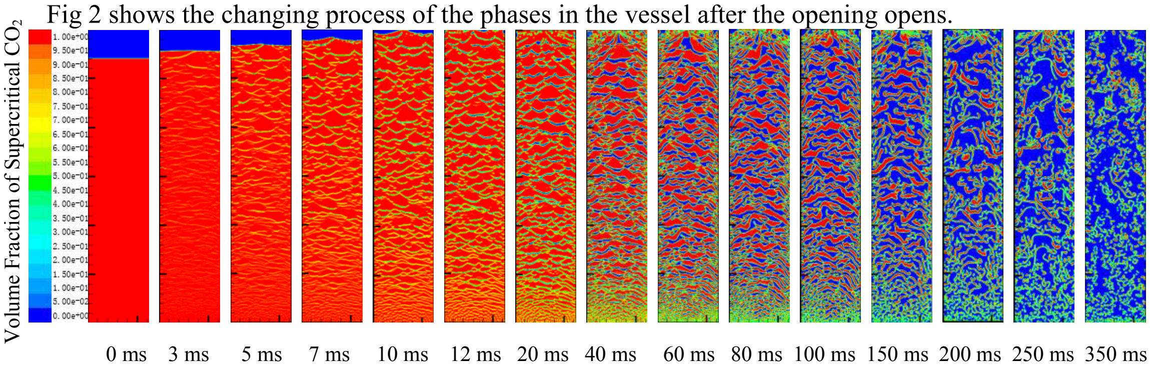


Fig .2. Changing process of gas-liquid flow field

As shown in Fig 2, the medium in the vessel is in thermodynamic equilibrium in the initial state. The gas area is CO_2 steam and the liquid area is supercritical CO_2.

After the opening opens, the pressure inside is much higher than that outside. The pressure of the gas area gets lower because the medium in the area of the vessel release immediately. After the waves are transmitted to the junction of two phases, the pressure of liquid level drops. That makes the supercritical CO_2 overheating in a moment. When the time is 3 ms, bubbles can be seen in the liquid area. Gas-liquid two-phase flow starts to flow upward with the medium faster releasing and the pressure decreasing. At the same time, gas-liquid two-phase flow starts to spread to two opposite sides and squeeze the gas area and liquid area with the rarefaction wave propagating in the liquid area and the degree of superheat increasing continually.

As Fig 2 shows, the whole gas-liquid two-phase flow keeps spreading in a period. When the time is about 10 ms, the gas-liquid two-phase flow spreads to the upper-wall of the vessel. Because of the violent boiling and the impulses on the upper-wall of the vessel caused by two-phase flow, the trend of the pressure increasing is much more obvious than decreasing caused by the medium releasing, with the pressure inside is increasing rapidly. When the time is 12 ms, the pressure is maximum. The gas-liquid two-phase flow erupts rapidly companied with liquid drops. The medium in the vessel is unregulated and superheated boiling. The liquid and gas mingle with each other, and the junction cannot be distinguished. At this moment, the pressure response is maximum during the whole process of supercritical CO_2 BLEVE, so the peak pressure is an important indicator to judge the risk of the process of BLEVE. The peak pressure is also an important parameter in the whole study.

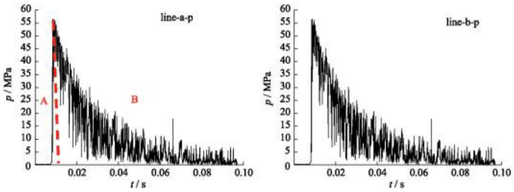
When the time is between 12 ms and 20 ms, the flow field is relatively stable, and the medium is basically unregulated and boiling. The load located on the vessel is the strongest at the moment, and the vessel is thus very easy to distort and even rupture. Later, the temperature of the liquid gets lower and the superheated degree decreases with the energy consumed by the vaporization increases. The trend of the pressure inside increasing is gradually lower than the trend of the pressure inside decreasing with the everlasting releasing of the medium inside. That makes the process of the formation of bubbles restrained, the density of two-phase flow decreased, the spread speed and the push ability reduced, the boiling got weaker and the pressure got lower.

After 80 ms approximately, the energy of the medium decreases, the superheated degree declines, the speed of phase transition gets lower, the density of two-phase flow diminishes with the release of the medium inside. The boiling phrase comes to not so obvious at last and the pressure-dropping process becomes stable and slow. When the time is about 150 ms, the gas area counts larger proportion because CO_2 is gas at ordinary temperatures and pressures. So it can be speculated that the pressure and temperature inside continue to drop and the amount of liquid tapers off as the time goes on. The liquid transforms into gas at last.

3.2 Changing process of the pressure field

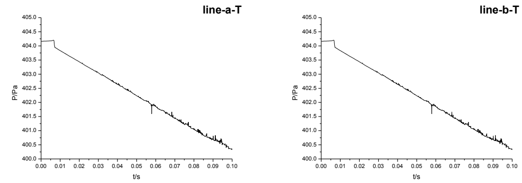
As Fig 3 shows, the changes of pressure which two monitoring lines show are very similar. The beginning of the process of supercritical CO_2 BLEVE is violent and the changes of pressure are even everywhere in the vessel. So the numerical simulation results which Fig 3(a) shows are needed to be discussed only.

There are two stages in the process of the pressure change, which contains increasing pressure stage and decreasing pressure stage. When the time is 0 ms, the medium in the gas area starts to release and the pressure in the vessel declines rapidly at the moment. When the rarefaction wave travels to the liquid area, the liquid is superheated boiling and the two-phase flow puffs up quickly and the liquid impacts on the upper-wall strongly. The shockwave which impacts on the wall called ‘liquid hammer’ is serious destructive and it can even lead to the immediate rupture of the vessel. When the time is about 12 ms, the two-phase flow puffs up to the top of the vessel and the pressure shows the maximum value of supercritical CO_2 BLEVE which is about 56 MPa as Fig 3(a) shows in A area. When the value reaches the peak pressure, the speed of releasing increases and the energy of system reduces. The superheat degree of supercritical CO_2 reduces because of the decrease of temperature. Based upon the interaction of these factors, the boiling phenomenon gets weaker, the density of the two-phase flow reduces, and the upward propulsion of the two-phase flow diminishes. These factors lead to the trend of pressure decreasing surpass the trend of pressure increasing gradually. It is presented as the trend of decrease macroscopically as Fig 3(a) shows in B area.



(a) line-a (b) line-b

Fig. 3. Figure of pressure response



(a) line-a (b) line-b

Fig. 4. Figure of temperature response

3.3 Changing process of the temperature

The temperature responses which two monitoring lines indicate are very similar. As Fig 4 shows, the change of pressure is violent but the change of temperature is relatively stable.

When the time is between 0 and 8 ms, the medium (gas) in gas area releases, the two-phase flow expands rapidly, and the temperature keeps relatively invariable. After 8 ms, phase change process continues with the release of the medium. The temperature of the system falls 4 K in 100 ms, which decreases monotonically without dramatic fluctuations. Supercritical CO_2 BLEVE is an endothermic process. The medium in BLEVE will absorb more energy and can induce more damages if flame outside acting on the system exists.

4. Conclusions

According to the basic assumptions of numerical simulations and the adopted physical and mathematical models, the study explains the process and mechanism of supercritical CO_2 in the change process of the field of flow, pressure and temperature. The study also conducts a research about building of the UDF and describes the method and process of modeling in detail. The study mainly draws these following conclusions.

The pressure declines rapidly at the moment of opening opens, superheated liquid is boiling violently and the rapid expanding and fast-rising two-phase flow is formed. The process of phase change gets weaker gradually and all liquid transforms into gas at last with the releasing of the medium.

There are two stages in the changing process of the pressure, which contains increase pressure stage and decrease pressure stage. The first stage happens at the moment when the opening opens. There is a volume of CO_2 gas produced in the process of phase change. Because the two-phase flow pushes aside the gas area, the pressure increases rapidly. After the value of pressure reaches the peak, the liquid boiling begins to get weaker gradually under the influence of pressure, temperature and the releasing of the medium. It is presented as the trend of decrease macroscopically.

The change of temperature is relatively stable and it diminishes monotonically during the whole process.

Acknowledgements

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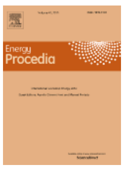

Biography

The first author Yao Zhao is a PhD student in Beijing Institute of Technology studying on the issue of safety assessment of petrochemical system. The corresponding author Zhenyi Liu is an assistant professor in Beijing Institute of Technology working on the topics about safety science and technology.