Numerical Simulation on Bubble Growth and Micro-explosion Characteristics of Biodiesel/ethanol Fuel Droplets

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Abstract. In this paper, the biodiesel/ethanol gas-containing fuel droplet was numerically simulated at room temperature. The growth characteristics of the bubble growth process were obtained, and the influencing factors affecting the bubble growth and micro-explosion process were explored. Studies have shown that bubble growth and droplet micro-explosion at room temperature are dominated by the pressure difference between the inside and outside of the bubble. Within a certain range, reducing the initial radius ratio of droplets as much as possible can also promote the bubble growth and micro-explosion of droplets. The proportion of fuel in the droplet will also affect the bubble growth and micro-explosion characteristics.

Keywords: Gas-containing Fuel Droplet, Bubble Growth, Micro-explosion

1. Introduction
The key to the development of high-efficiency, low-pollution engine technology is to improve the atomization and evaporation mixing process of fuel jets in the engine cylinder through various technical means [1]. In terms of internal combustion engine engineering, under the micro-explosion effect of gas-containing fuel, oil droplets can turn oil droplets into fine-grained particles, which increases the total surface area of fuel and air contact, and the instantaneous impact of gas-phase jets on droplets. It can increase the turbulent disturbance of tiny droplets, so that the fuel can quickly evaporate and diffuse, greatly improve the mixing quality of fuel and air in the cylinder, and significantly improve the combustion characteristics and emission characteristics of the engine [2].

Existing experimental research shows that the size and proportion of gas-containing droplets and external environmental factors will have a large impact on the micro-explosion process [3-7], but it is difficult to study the growth characteristics of droplets during the micro-explosion process using experimental research methods. In the related numerical simulation research, only various types of emulsified droplet models and schematic diagrams of droplet microburst processes have been proposed, and there are few simulation studies on the growth process of bubbles.

Based on this, this paper uses the phase interface tracking VOF method to build a single biodiesel/ethanol droplet calculation model based on the uniform nucleation theory. On this basis, explore the process of bubble growth and micro-explosion under normal temperature environment,
and study the influence of bubble growth factors and micro-explosion characteristics, and analyze the effect of various factors.

2. Simulation Model of Single Fuel Droplet

In order to reduce the modeling difficulty of single biodiesel/ethanol gas-containing droplet and simplify the complicated bubble growth, droplet evaporation and micro-explosion processes, this paper assumes that the generation of the bubble is based on the theory of uniform nucleation [8], that is, only one inside a single droplet is formed. Inside the droplet is an ethanol bubble, and outside the droplet are a mixed fuel droplet of liquid biodiesel and ethanol. Fig. 1 shows the simplified model of bubble/droplet.

![Figure 1. Simplified model of bubble/droplet](image)

In the fluid flow process, when the gas-liquid two-phase temperature is the same, only the mass conservation, momentum conservation and energy conservation equations need to be satisfied.

According to the mass conservation formula in the system:

\[
\frac{\partial \rho}{\partial t} + \text{div}(\rho \vec{v}) = 0 \tag{1}
\]

Using the VOF model, the stratified flow of liquid-gas two-phase flow in the channel can be solved [9]. After applying the VOF model, the obtained mass conservation equations and the source terms of the liquid and gas phases [10] are shown as:

\[
\frac{\partial a_q}{\partial t} + \vec{v} \cdot \nabla a_q = \frac{S_{aq}}{\rho_q} \tag{2}
\]

\[
a_{q_i} = - m_i \tag{3}
\]

\[
a_{aq} = m_i \tag{4}
\]

Where \(a_q\) is mass fraction of liquid phase; \(S_{q_i}\) is mass source term; \(S_{aq}\) is gas source term; and \(m_i\) is mass flow of component \(i\) at the interface.

The momentum equation obtained after applying the VOF method is:

\[
\frac{\partial}{\partial t}(\rho \vec{v}) + \nabla \cdot (\rho \vec{v} \vec{v}) = - \nabla p + \nabla \cdot [\mu (\nabla \vec{v} + \nabla \vec{v}^T)] + F_{st} + \rho g + S_m \tag{5}
\]

Where \(\vec{v}\) is velocity of fluid; \(F_{st}\) is Surface Tension.

The momentum source term is shown as:

\[
S_m = (1 - 2a) m_i \vec{v} \tag{6}
\]

The energy equation and energy source terms applying the VOF equation are shown as:

\[
\frac{\partial}{\partial t}(\rho E) + \nabla \cdot (\rho (\vec{v} E + p)) = \nabla \cdot (k_{ef} \nabla T - h J) + S_e \tag{7}
\]

\[
S_e = - m_i h_{fg} \tag{8}
\]

Where \(E\) is energy; \(k\) is thermal conductivity; and \(h\) is latent heat of evaporation.
3. Bubble Growth and Droplet Micro-explosion Process

The growth of bubbles inside droplets is one of the key factors that cause droplets to break up, and has an important effect on the atomization mechanism of droplets. Therefore, this section performs a numerical simulation of a single droplet and observes the change process of the droplet from the beginning to the fragmentation.

Fig. 2 shows phase distribution at different times when the initial bubble radius is 15μm.

![Figure 2. Phase distribution at different times when the initial bubble radius is 15μm](image)

As shown in Fig.2, the change of bubble radius of gas-containing droplets is tiny in the time of 0~0.1μs. After 0.1μs, the bubble radius increases rapidly. At 0.4μs, it can be clearly seen that the bubble and droplet increase significantly, and the droplet becomes thinner. At 0.5μs, the droplet is broken by the continuous expansion of the internal bubble and becomes small droplets with a smaller particle size.

Fig. 3 shows phase distribution at different times when the initial bubble radius is 5μm.

![Figure 3. Phase distribution at different times when the initial bubble radius is 5μm](image)

As shown in Fig.3, at first the radius of the bubble gradually increases. When the bubble reaches the maximum radius value, it begins to shrink. After the bubble reaches the minimum radius, the bubble begins to expand again, and goes through the process of secondary shrinkage. Then the droplet continues to expand and retract until it reaches an equilibrium state.

By comparing the two bubble growth processes, it can be found that only when the ratio of the radius of the droplet and the bubble reaches a certain value at the beginning, the micro-explosion may occur.

4. Influencing Factors of Bubble Growth and Droplet Micro-explosion
The growth of the bubble is the first prerequisite for the micro-explosion of the droplet. Therefore, in order to investigate the change of bubble in the droplet in the early stage of micro-explosion, it is necessary to explore the influence of various factors on the growth of bubble.

4.1. Effect of Droplet/Bubble Initial Radius Ratio

In order to compare the effect of the initial droplet/bubble radius ratio \( R/r \) on the bubble growth process, the initial droplet temperature and the ambient temperature are kept at 300K. The initial bubble pressure is set to 1.0 MPa. Set the initial droplet radius to 20\( \mu \)m and change the initial bubble radius to 5\( \mu \)m, 7.5\( \mu \)m, 10\( \mu \)m, 12.5\( \mu \)m, and 15\( \mu \)m, respectively. Fig.4 shows the relationship between the bubble radius and the growth rate of bubble with time at different \( R/r \).

![Figure 4](image_url)

**Figure 4.** Change of bubble radius and growth rate with time at different initial radius ratios

As shown in Fig.4 (a), when the initial bubble radius is too small, the bubble eventually fails to break after growth. When the bubble can be broken, as the initial radius of the bubble increases, the maximum value of the broken radius will also increase accordingly, and the bubble breaking time will be advanced.

As shown in Fig.4 (b), when the initial bubble radius is small, it can inhibit the increase of the growth rate of the bubble. When the initial bubble radius is large, the inertial force that promotes its growth increases, so the growth rate of the bubble increases accordingly.

This article defines the time elapsed from the initial state of the droplet to the moment of fragmentation as the micro-explosion delay time. The maximum micro-explosion intensity value can reflect the maximum degree of deformation during the micro-explosion process with droplets. The formula can be expressed as:

\[
D^2_{\text{max}} = \left( \frac{D}{D_0} \right)^2_{\text{max}}
\]  

(9)

Where \( D^2_{\text{max}} \) is maximum value of normalized squared diameter during droplet micro-explosion.

Fig.5 shows the micro-explosion characteristics of droplets at different initial radius ratios.

![Figure 5](image_url)

**Figure 5.** Change of micro-explosion characteristics at different initial radius ratios
As shown in Fig.5, with the increase of droplet initial radius ratio, the micro-explosion delay time of droplets gradually increases, and the maximum micro-explosion intensity value gradually decreases. This shows that the smaller the initial droplet radius ratio, the greater the promotion effect on the micro-explosion.

4.2. Effect of Pressure Difference Between Inside and Outside of Bubble

In order to find the effect of pressure for the bubble growth processes, the initial pressure inside the bubble is changed to 0.5 MPa, 1.0 MPa, 1.5 MPa, and 2.0 MPa. Fig.6 and Fig.7 shows the variation of bubble growth characteristics with time under different initial pressures inside bubble.

**Figure 6.** Change of bubble growth radius with time under different initial pressures inside bubble.

As shown in Fig.6, the larger the initial pressure difference between the inside and outside of the bubble, the faster the growth rate of the bubble radius, and the breaking time of the bubble will advance. When the initial pressure is too small, the droplet cannot explode, and the bubble grows periodically.

**Figure 7.** Change of bubble growth rate with time under different initial pressures inside bubble.

As shown in Fig.7, with the initial pressure goes up, the growth rate of the bubble increases significantly in turn. This is because as the initial pressure difference between the inside and outside of the bubble increases, the acceleration of bubble growth increases, the growth rate of the bubble also increases. For the case where the bubble is unbroken, the growth rate of bubble shows a periodic change.

Fig.8 shows the micro-explosion characteristics of droplets at different pressures inside bubble.
Figure 8. Change of micro-explosion characteristics at different pressures inside bubble
As shown in Fig.8, with the increase of the pressure difference between the internal and external bubble of droplet, the micro-explosion delay time gradually decreases, and the maximum micro-explosion intensity value increases. This result shows that increasing the pressure difference between the inside and outside of the bubble within a certain range can promote the micro-explosion process.

4.3 Effect of Fuel Volume Ratio
In order to compare the effect of different droplet mix ratios on bubble growth characteristics, the content $c$ of ethanol in the droplets was set to 10%, 30%, 50%, and 70%, respectively, and then the growth process of bubble was numerically simulated. Fig.9 show the relationship between bubble growth characteristics over time under different ethanol contents.

Figure 9. Change of bubble growth characteristics with time at different liquid-ethanol contents
As shown in Fig.9 (a), under the conditions of different ethanol content, the growth trend of the bubbles is basically the same, but the time when the bubbles are broken and the maximum radius reached are different. When the content of biodiesel and ethanol in the droplets are both 50% in the initial state, the growth rate of bubble radius is the fastest. As shown in Fig.9 (b), with the increase of ethanol content, the bubble growth rate will be promoted, but when the ethanol content is too high, the bubble growth rate will be suppressed again.

Fig.10 shows the micro-explosion characteristics of droplets at different liquid-ethanol contents.
Laboratory

Acknowledgments

This paper mainly studies the bubble growth process in gas-containing droplets, explores the micro-explosion process of biodiesel/ethanol gas-containing droplets at room temperature, and the growth characteristics of bubbles during micro-explosion.

1. Through numerical simulation, the microburst history of a single biodiesel / ethanol gas-containing droplet at room temperature was studied, and phase distribution diagrams of gas-containing droplets at different times were obtained.

2. The factors that influence the growth of bubbles in biodiesel/ethanol gas-containing droplets at room temperature were explored, including the pressure difference between the bubbles inside and outside the bubble, the initial radius ratio of the bubbles, and the effect of the ratio of the droplets on the growth of the bubbles. The change of the bubble growth rate and the maximum radius of the bubble under different conditions. It is found that the bubble growth process at room temperature is dominated by the pressure difference between the inside and outside of the bubble. At the same time, the initial radius ratio of the bubble and the different proportions will also affect the bubble growth process.

3. The influencing factors of micro-explosion characteristics of gas-containing droplets of biodiesel/ethanol were studied, and the changes of micro-explosion delay time and maximum micro-explosion intensity of the droplets under different conditions were analyzed. The larger the initial bubble radius ratio, the better the microburst of gas-containing droplets when the fuel is mixed in the same volume.

Acknowledgments

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