Numerical Simulation of Single Droplet Combustion Characteristics in High Temperature Convection Environment

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Abstract. In order to better study the combustion characteristics of small droplets during spray combustion, a mathematical model of single fuel droplet evaporation and combustion was established based on the numerical simulation method of VOF(Volume of Fluid). Numerical simulation was carried out using FLUENT. The combustion process and flame propagation characteristics of the small droplet in the convection environment under different pressures of 0.1 MPa, 0.2 MPa and 0.3 MPa, were studied respectively, and the influence of different ambient pressures on combustion was analyzed. The results show that due to the influence of air convection, the ignition position was located in the downstream area of the droplet, forming a wake flame. Then the flame gradually overcame the convection effect and developed upstream, and finally transformed into the enveloped flame. With the further development of combustion, the combination of fuel vapor diffusion and combustion promoted the development of the flame front in the direction of airflow. After reaching the balance each other, the position and temperature of the flame front would be relatively stable. The increase of ambient pressure promoted the combustion process, which increased the droplet burning rate and flame temperature. At the initial stage of ignition, the temperature rise rate of the average droplet temperature at 0.3 MPa was 1.18 K/ms, which was 32.6% higher than that 0.89 K/ms at 0.1 MPa.

1. Introduction

Spray combustion is widely used in engineering applications such as liquid rocket engines, jet engines, internal combustion engines and oil-fired boilers. Research on spray combustion is beneficial to improve the combustion efficiency of combustion equipment and reduce pollutant emissions. However, spray combustion is formed by a large number of single small droplets burning together. The single droplet evaporation combustion law is the basis for studying the complex physical and chemical processes of spray evaporation and combustion. Therefore, it is of great significance to study the combustion characteristics of a single droplet for spray combustion.

Theoretical, numerical and experimental studies on fuel droplet evaporation and combustion have been carried out extensively. As early as 1953, Godsave[1] and Spalding[2] established a mathematical model for the combustion process of a single droplet in still air by adopting spherical symmetry and quasi-steady state hypothesis, and obtained the famous "d²-law". Since then, many scholars have conducted more in-depth research on the basis of "d²-law". Sun,F.X. et al. [3-4] considered the thermal expansion effect of droplets in unsteady combustion and the change of gas-liquid phase physical properties, and conducted numerical simulation on the combustion of n-heptane droplets in oxygen.
Ni, P.Y. et al. [5] used the non-equilibrium evaporation model to carry out numerical simulation on the evaporation process of methanol droplets in the static air environment. He, B. et al. [6] simulated the high-pressure unsteady evaporation process of static n-heptane droplet in the nitrogen environment with the transient high-pressure evaporation model under the condition of non-ideal high pressure factors. Li, J.D. et al. [7] established a new droplet evaporation model and simulated the evaporation process of n-dodecane single droplet by considering the effect of Stephen flow on the gas-liquid interface mass transfer. Zhao, P. et al. [8] used gas-liquid two-phase fluid volume method to model the evaporation process of fuel droplets. Ma, Z.H. et al. [9] carried out experimental research on evaporation and combustion characteristics of different hydrocarbon fuel droplets at rest under normal gravity under subcritical and supercritical pressure environment.

The above studies are more inclined to the evaporation and combustion of droplets in the static environment. During the actual spray combustion process, the droplets are affected by convection. The evaporation and combustion processes will be more complicated. The addition of chemical reactions makes the interaction between gas and liquid more complicated. The influencing factors also increases accordingly, which brings great challenges to the realization of numerical simulation. Therefore, this paper uses VOF two-phase numerical simulation method to establish a convection, evaporation and combustion model of n-decane single droplet, simulate the combustion process and flame characteristics of droplet in convection environment, and study the influence of ambient pressure on combustion.

2. Theoretical model

2.1. Description of the model

A single n-decane droplet is placed in the high temperature convection environment for evaporation and combustion. The physical combustion process is shown in Figure 1. To save computing resource, the calculational region is scaled down using an axisymmetric approach. The mass fraction of oxygen and nitrogen in the air is 23% and 77% respectively, and the air flows from the left boundary to the calculational region at the constant velocity. The initial temperature of the droplet is 297 K; the temperature of the inflowing air is 1100 K; and the ambient pressure is varied from 0.1 MPa to 0.3 MPa to investigate the effect of ambient pressure on the combustion of the droplet.

2.2. Assumption

The combustion of liquid fuels is a complex physicochemical phenomenon. In order to enable numerical simulation, it is essential to make appropriate simplifications and assumptions about the model. The assumptions of this model are:

1. The shape of the droplet remains spherical, ignoring the effects of gravity and buoyancy;
2. The flow remains axisymmetric and laminar;
3. Follow the continuity medium assumption, regardless of viscous dissipation;
4. The gas-liquid interface is in thermodynamic equilibrium;
5. The air and combustion products cannot pass through the surface of the droplet;
6. Dufour effect and Soret effect in the gas phase are ignored;
7. The generation of soot is ignored;
8. Do not consider the Marangoni effect.

2.3. Calculation method

Based on the above assumptions, the conservation equation is calculated using the VOF method. The VOF method performs tracking and updating of the phase interface by separately solving the continuity equation of the fluid phase volume fraction. The VOF method shares a set of momentum conservation equations and energy conservation equations in the whole calculational region, which are jointly controlled by the volume fraction of gas-liquid two phases, and the obtained velocity field and energy field are shared by the gas-liquid two phases. In the fuel droplet combustion problem, Stefan flow has an important influence on droplet evaporation and combustion, which can not be ignored. Therefore, the mass transfer model established in this paper considers the mass transfer process of Stefan flow. Since the detailed chemical reaction kinetic mechanism of n-decane combustion involves a series of complicated chemical reactions, if it is used for CFD simulation, it will cause a huge amount of calculation. Therefore, this paper adopts an irreversible, total-package single-step chemical reaction for calculation.

3. Results and discussion

3.1. Model validation

In this paper, the unsteady evaporation and combustion process of a single n-decane fuel droplet in the high temperature convection environment is calculated. In order to verify the validity of the mathematical physical model, the experimental results of Xu et al. \cite{10} under the same conditions are compared. At the same time, in order to make the model verification more rigorous, grid independence validation and time step independence validation are also carried out.

Figure 2 shows the comparison between the experimental results of Xu and the numerical results. The instantaneous diameter of the droplet is normalized to the dimensionless diameter square \((d^2/d_0^2)\) using the initial diameter. It can be seen from Figure 2 that the calculation results in this paper are in good agreement with the experimental results of Xu, and the square of droplet diameter is almost equal each other. In the initial stage of combustion, there is a certain deviation between the two, which is the result of the interaction between droplet thermal expansion and fuel evaporation. Table 1 is a comparison table of grid independence verification and time step independence verification, in which \(l/d_0\) is the ratio of the grid length to the initial diameter of the droplet. It can be seen from Figure 2 with Table 1 that the grid width and time step setting of Case1 can not only ensure the calculation accuracy, but also save computational resource and time. Therefore, this paper uses Case1 grid and time step parameters settings.

![Figure 2. Comparison of experimental and numerical simulation data.](image)
3.2. Analysis of transient combustion process of fuel droplets in convective environment

A single n-decane droplet is placed in the high temperature convection environment for evaporation and combustion. The flow field environmental parameters are set as follows: ambient pressure $P_\infty = 0.1$ MPa, inflow air temperature $T_\infty = 1100$ K, initial droplet diameter $d_0 = 1$ mm, droplet initial temperature $T_0 = 297$ K, inflow air velocity $V_\infty = 0.2$ m/s. The transient evaporation and combustion process of n-decane droplet were analyzed by setting the flow field environment parameters.

Figure 3 shows the flame temperature distribution produced by droplet combustion at different time in this flow field environment parameters setting. After the fuel droplet are placed in the gas phase flow field, since the droplet temperature ($T_0 = 297$ K) is much lower than the flow field temperature ($T_\infty = 1100$ K), it is heated by the action of the external high-temperature gas stream to generate a small amount of fuel vapor. The fuel vapor is blown to the downstream of the droplet due to the interaction of diffusion and convection, and the droplet at the same time is exactly similar to the bluff body from which the air flows, and a low pressure zone is formed on the aft side of the droplet, and the air flow velocity is low. Fuel vapor is accumulated in large quantities here. Since the inflow gas temperature is sufficiently high, when the fuel vapor accumulates to a certain concentration and is sufficiently mixed with oxygen, there is sufficient energy to cause a combustion reaction occurring, and a local high temperature region appears downstream of the droplet, so a fire phenomenon occurs (20 ms). It is called the wake flame and has the characteristics of the premixed flame. After the fire, the temperature of the flow field increases rapidly, the interaction between the gas stream and the droplet is more intense, the droplet generates more fuel vapor, the concentration is continuously increased, and the chemical reaction rate is increasing, and the flame has a tendency to develop upstream (22 ms, 30 ms). In addition, due to the effect of the resistance, the relative velocity of the droplet and the incoming air will gradually decrease, the flame will continue to overcome the convection effect and further develop upstream, and finally the entire droplet will be wrapped in the flame (100 ms), which is called envelope flame, featuring the diffusion flame.

Table 1. Grid and time step independence validation.

| Case number | $d_0/l$ | Time step/s | The number of grids in the calculational region | 8CPU computational time/h |
|-------------|--------|-------------|-----------------------------------------------|--------------------------|
| 1           | 40     | $2 \times 10^{-5}$ | 352000                                      | 144                      |
| 2           | 50     | $2 \times 10^{-5}$ | 550000                                      | 192                      |
| 3           | 40     | $1 \times 10^{-5}$ | 352000                                      | 230                      |

Figure 3. Flame temperature distribution of droplet combustion at different time (Temperature unit: K).

Figure 4 shows the change in mass fraction of fuel vapor downstream of the droplet over time, L being the distance between the downstream region of the droplet and the droplet at the axisymmetric position. At the same position downstream of the droplet, the fuel vapor mass fraction gradually increases with time. With the further development of the flame, the increasing trend in the equal time
interval becomes less and less obvious, reaching a relatively stable state after about 280 ms. This phenomenon is caused by the combination of convection diffusion and combustion reaction. At about 100 ms, the fuel vapor range downstream of the droplet is small, the contact area with air is small, and the fuel vapor consumed by combustion is relatively small. The fuel vapor is accumulated to a certain extent, and the fuel vapor concentration rises rapidly, which is consistent with the fuel vapor accumulation effect mentioned by the scholars Law [11] and Awasthi [12]. At the same time, due to the convection effect of the inflowing air, the fuel vapor is further blown to the downstream region, increasing the contact area with the air. So the amount of fuel vapor consumed by the chemical reaction per unit time increases, and gradually reaching a state of mutual equilibrium with the evaporation amount of the droplet. Furthermore, it can be seen in conjunction with Figure 7 that the temperature of fuel droplet increases rapidly in the initial stage of droplet ignition, which is conducive to droplet evaporation and promotes the accumulation of fuel vapor on the other hand.

Figure 5 shows the distribution of the gas phase temperature on the axisymmetric line downstream of the droplet at different time. As the combustion progresses, the gas phase temperature peak position gradually moves away from the fuel droplet. The position with the highest gas phase temperature is the flame front. The development of the flame front in the direction of the airflow is mainly caused by the two sides. On the one hand, the convection effect of the inflowing air causes the flame front to develop backward. On the other hand, the fuel vapor accumulation and diffusion promote the development of the flame. It is not difficult to find that the temperature of the flame front has increased to some extent, mainly because the combustion is more and more complete with the development of the flame. When the convective diffusion and combustion of the fuel vapor reach a relative balance, the temperature rise amplitude of the flame front gradually decreases and the combustion tends to be relatively stable.

3.3. Influence of environmental pressure on droplet combustion

Figure 6 shows the variation curves of dimensionless diameter square of fuel droplet under different ambient pressures of 0.1 MPa, 0.2 MPa and 0.3 MPa. It can be seen from the Figure 6 that in the initial stage of the fuel droplet entering the high temperature environment, they begin to expand under the heating effect of high-temperature airflow, and the evaporation effect is smaller than the expansion effect. Thus the droplet diameter slightly increases, which does not follow the d^2-law at this stage. After the droplet ignited, the evaporation effect gradually taking the dominant position with the expansion effect gradually reaching the limit. The droplet dimensionless diameter square accordingly appeared inflection point. After the inflection point, the droplet combustion approximated the d^2-law. In addition, it is not difficult to find that the increase of pressure makes the change of fuel droplet diameter more obvious, the combustion rate increases, and the droplet lifetime decreases.
Figure 7 shows the change of the average temperature of the fuel droplet and the central temperature of the fuel droplet with time. The slope of curve represents the rate of temperature rise. The droplet average temperature is the sum of the temperatures at all grid nodes occupied by the droplet divided by the total number of droplet grids. It can be seen from the Figure 7 that the average temperature of the droplet rises rapidly after the droplet ignited, mainly because the gas phase temperature rises rapidly after ignition, and the heating effect on the droplet is enhanced. The difference between the average droplet temperature and the droplet center temperature indicates that the temperature inside the fuel droplet is not uniform during the combustion process, and the temperature near the droplet surface is higher than the droplet center temperature. The ambient pressure has a certain influence on the droplet temperature during the combustion process. The temperature rise rate of the average temperature of the droplet during the heating period is 0.89 K/ms at 0.1 MPa, and the temperature rise rate is 1.18 K/ms when the pressure is increased to 0.3 MPa. The temperature rise rate at 0.3 MPa is about 32.6% higher than that at 0.1 MPa. As a result, the higher the pressure is, the higher the average droplet temperature is at the same time. As the combustion progresses, the droplet temperature gradually increases. But the trend gradually becomes slower and the droplet temperature is lower than the saturation temperature value at the corresponding pressure.

Figure 8 shows the ratio($W_F/d$) of the width of the flame($W_F$) to the transient diameter($d$) of the droplet with time. The so-called flame width refers to the value at the maximum position of the flame perpendicular to the direction of the inflowing air. The ratio shows a tendency to increase with time. At some moments, the curve of the ratio appears to fluctuate. The fluctuation of the ratio is mainly caused by unstable combustion at the beginning of the fire. The ratio is greater in the environment with higher pressure after the same time. Similarly, after the droplet burning for 300 ms, the ratio of the flame width to the transient diameter of the droplet at 0.1 MPa is 7.7, and the ratio at 0.3 MPa is 8.5. It is 10.4% higher than that at 0.1 MPa. This difference is mainly caused by the fact that the higher the pressure is, the higher the flame temperature is, the stronger the heating effect on the droplet is, and the larger the evaporation rate is, so that the droplet diameter decreases at the higher rate, resulting in the relatively higher ratio($W_F/d$) of the width of the flame to the transient diameter of the droplet.

4. Conclusion
(1) Due to the influence of air convection, the ignition position was located in the downstream area of the droplet, forming the wake flame. Then the flame gradually overcame the convection effect and developed upstream, and finally transformed into the envelope flame.

(2) The interaction of fuel vapor convection diffusion and combustion promoted the development of the flame front in the direction of airflow. After reaching the balance each other, the position and temperature of the flame front would be relatively stable.
(3) The increase of ambient pressure promoted the combustion process, which increased the droplet burning rate and flame temperature. At the initial stage of ignition, the temperature rise rate of the droplet average temperature at 0.3 MPa was 1.18 K/ms, which was 32.6% higher than that 0.89 K/ms at 0.1 MPa. The ratio of the flame width to the droplet diameter at the same time after ignition was greater at the higher ambient pressure.

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