Effect of the ambient temperature and oxygen concentration in droplet combustion under natural convection conditions

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Abstract. A numerical investigation of combustion of n-heptane droplets in natural convection conditions is presented. The focus is on the effects of ambient temperature and oxygen concentration on the combustion characteristics. Ambient temperatures range from 900K to 1400K, and volume fraction of oxygen range from 17% to 21%, and pressure is 0.1MPa. The results show that ambient temperature and oxygen concentration have a great influence on burning rates and ignition delay times. The ignition delay times decreases with increasing temperature. In addition, the burning rates of with and without natural convection compare to existing theoretical model. The burning rate increase under natural convection.

1. Introduction

Droplet combustion is one of the classical problems in diffusion flame studies. The study of single droplet combustion in static air is the basis of spray combustion research. In recent years, many researchers have studied the droplet combustion by numerical simulations and experiments. Godsave et al. [1] and Spalding et al. [2] studied one-dimensional spherically symmetric droplets combustion in stationary air based on quasi-steady assumption, get the $d^2$ law, i.e., $\frac{d}{dt} = k$, where $k$ is the burning rate constant. In order to simulate the droplet combustion more accurately, it is necessary to consider the change of the physical properties with temperature, the internal flow in droplets and the chemical reactions in gas. Therefore, numerical methods are needed to solve them. Zhang et al. [3] studied an n-decane droplet combustion in high temperature convective air streams, applied VOF method to capture the liquid-gas interface and the physical properties are temperature dependent except surface tension. They captured Stefan flow by numerical simulations clearly. Awasthi et al. [4] studied environment temperature and initial diameter in droplet combustion. With the increase of ambient temperature, the diameter of flammable droplets increased significantly. The ignition delay times decrease near the flammable diameter and increase far from flammable diameter.

In the normal gravity environment, the natural convection has a significant influence on the droplet burning rates and the shape of flames. Sato et al. [5] studied the combustion characteristics of n-octane droplets in a high-pressure environment under natural convection by experiments. They found that burning rates increase with pressure when the ambient pressure is less than the critical pressure. However, burning rates decrease with increasing pressure when ambient pressure greater than the critical pressure. Dzik et al. [6] studied combustion characteristics of n-heptane droplets in high CO$_2$ concentration and normal gravity conditions. They obtained combustible boundary curve about pressure and mass fraction of CO$_2$. They found burning rates of n-heptane increase with increasing of CO$_2$ mass fraction and pressure in the flammable range.
The present work investigates the combustion of n-heptane droplets under natural convection by numerical method. The simulations are based on two-dimensional axisymmetric models. Ambient temperatures and oxygen concentrations can be modified, and pressure is 0.1MPa. Computed ignition delay times and burning rates are compared with the experimental result of Tanabe et al. [7] and Wang et al. [8]. The focus is on the effects of environment temperature and oxygen concentration on the combustion characteristics.

2. Theoretical model

Figure 1 shows the schematic of the computational domain of a droplet under natural convection with the boundary conditions applied. The computational domain employs two dimensional axisymmetric structure. The initial diameter of droplet is 0.75mm and the computational domain is taken as a sphere with a diameter 100 times of the droplet diameter. The outer boundary of computational domain is the pressure outlet. Only two components of oxygen and nitrogen in the initial gas phase, environment temperatures range from 900K to 1400K, and volume fractions of oxygen range from 17% to 21%.

![Figure 1. schematic of the computational domain](image)

The computational domain was discretized into a structured quadrilateral mesh. The mesh is generated along the droplet surface each 1 degrees for improving the calculation accuracy. The number of grids in the whole computational domain is 55168. Numerical simulation are carried out using the finite volume method (FVM) based on the commercial software ANSYS FLUENT V16.0. The time step of this calculation is $1 \times 10^{-5}$s. The convergence criteria are as follows: the residual of the continuous equation and the species transport equation is less than $10^{-3}$, and the residual of the momentum equation and the energy equation is less than $10^{-6}$. The pressure velocity coupling method apply the PISO and the discretization of pressure gradient apply PRESTO! . The energy and momentum equations apply first order and second order upwind schemes respectively and the volume fraction is discretized by the compressive method.

3. Numerical method

3.1. VOF governing equations

The VOF method is used to track gas-liquid interface. The VOF method adds a parameter $\alpha_i$, that represents the volume fraction of someone phase in the control volume. For each control volume, the sum of the volume fractions of each phase is 1. For a gas-liquid two-phase problem as shown in figure 1, there are three conditions for $\alpha_i$:

\[ \alpha_i = 0; \quad \text{in gas phase} \]
\[ \alpha_i = 1; \quad \text{in liquid phase} \]
\[ 0 < \alpha_i < 1; \quad \text{in the interface} \]

3.2. Combustion model

The single step chemical reaction equation for n-heptane is applied in model,
C\textsubscript{7}H\textsubscript{16} + 11O\textsubscript{2} → 8H\textsubscript{2}O + 7CO\textsubscript{2} \quad (1)

The Arrhenius expression of the laminar finite rate model is:

\[ R = -M_{C_{7}H_{16}}k_{f}[C_{7}H_{16}]^{a}[O_{2}]^{b} \quad (2) \]

\[ k_{f} = Ae^{-\frac{E_{a}}{RT}} \quad (3) \]

Where, \([C_{7}H_{16}]\) and \([O_{2}]\) are molar concentration of n-heptane and oxygen, respectively; A is the pre-exponential factor; \(E_{a}\) is activation energy and \(a, b\) are rate exponent of n-heptane and oxygen, respectively. For n-heptane [9], \(a = 0.25, b = 1.5, E = 1.53 \times 10^{8}/\text{kmol}, A = 3.35 \times 10^{10}\).

3.3. Mass diffusion

The diffusion coefficients of each component in gas phase are calculated by Wilke and Lee [10],

\[ D_{AB} = \frac{3.03 - (0.98/M_{AB}^{0.5})(10^{-3})T^{1.5}}{PM_{AB}^{0.5}M_{AB}^{2/3}\sigma_{AB}^{2/3}} \quad (4) \]

Where, \(D_{AB}\) is the two element diffusion coefficient. \(M_{A}, M_{B}\) are molar mass of A and B, respectively.

\[ M_{AB} = 2\left[1/M_{A} + 1/M_{B}\right]^{-1} \quad (5) \]

\[ \sigma_{AB} = \frac{\sigma_{A} + \sigma_{B}}{2} \quad (6) \]

\[ \sigma = 1.18/V_{b}^{1/3} \quad (7) \]

Where, \(V_{b}\) is molar volume of liquid at boiling temperature.

Use the equation to calculate the diffusion coefficients of n-heptane in carbon dioxide, oxygen, water vapor and nitrogen. Then use equation (8) to obtain the diffusion coefficient of n-heptane in the gas mixture.

\[ D_{F-M} = \frac{1-Y_{F}}{D_{F-CO_{2}} + \frac{Y_{CO_{2}}}{D_{F-H_{2}O}} + \frac{Y_{H_{2}O}}{D_{F-O_{2}}} + \frac{Y_{O_{2}}}{D_{F-N_{2}}} + \frac{Y_{N_{2}}}{D_{F-N_{2}}}} \quad (8) \]

3.4. Physical properties

The viscosity, thermal conductivity and specific heat of gas and liquid are referred to in Ref. [11] and calculated by piecewise linear functions.

The surface tension of droplet is a function of temperature. The surface tension due to the non-uniform of surface temperature of droplets is different, and the sheer stress of droplet surface is called the Marangoni effect. Sirignano et al [12] shows that in the droplet combustion, considering the surface tension or not have very small effect on combustion. Therefore the droplet surface tension constant, i.e., not considering the Marangoni effect.

4. Validation

In order to demonstrate the validity of the numerical model, the results of numerical simulations are compared with Tanabe et al.[7] and Wang et al. [8]. Figure 2 are the results of the ignition delay times with the ambient temperature in oxygen volume fraction 21% and absence of gravity. The ignition delay times decrease as the increase of temperature, and the reliability of the model is verified by comparing with the experimental results.

As shown in figure 3, the droplet history of n-heptane droplets with time under the natural convection condition which ambient temperature is 1000K and the oxygen volume fraction is 21%. The results of burning rate are closer to the experimental results. At the beginning of the calculation, the droplet diameters decrease slowly, when the droplets did not start to burn, and then the curve shows an obvious inflection point. At that time the combustion began, the temperature rise rapidly, resulting in the rapid decrease of the droplet diameter.
5. Results and discussion

5.1. Burning rates

The burning rates obtained by numerical simulation can be compared with the semi-empirical correlation of Law and Williams [13]:

$$K = K_0(1 + A_1 Gr^{n_1})$$  \hspace{1cm} (9)

Where, $A_1$ and $n_1$ are constants. Research by Sato et al. [14] shows $A_1 = 0.85$ and $n_1 = 0.52$ for $Gr \approx 1$, Where $Gr$ is the Grashof number:

$$Gr = \left( \frac{\rho g d_0^2}{\mu_2^2} \right) \frac{T_f - T_\infty}{T_2}$$  \hspace{1cm} (10)

The average temperature $T_2$, given by $T_2 = 0.5 \times (T_f + T_\infty)^{-1}$. The $\mu_2$ and $\rho_2$ are viscosity and density at average temperature, respectively. $K_0$ is the burning rate of spherically symmetric flames in a micro-gravity environment, is given by:

$$K_0 = \frac{8\lambda}{\rho_1 C_p f} \ln(1 + B)$$  \hspace{1cm} (11)

Where, $\lambda$ and $C_p f$ are parameters under the temperature of $T_1$, given by $T_1 = 0.5 \times (T_f + T_\infty)^{-1}$. The transfer number calculate by equation (12).

$$B = \frac{\gamma_{0, in} q / i - C_p f (T_b - T_\infty)}{L}$$  \hspace{1cm} (12)

Figure 4 shows the theoretical values of burning rates in gravity and micro-gravity conditions compared with the results of numerical simulations. The presence of gravity increases the burning rate by about 30%, due to the flow of gas caused by natural convection accelerates the diffusion of species. The deviation between the numerical simulation and the semi-empirical correlation is little. The error is acceptable for considering the physical parameters in the semi-empirical correlation are all fixed values at the average temperature.

The decrease in oxygen volume fraction caused two changes: reduction of density and specific heat of gas, as shown in figure 5. With the increase of oxygen mass fraction in the environment, the specific heat of the mixture decrease, caused more heat is absorbed by the fuel resulting in lower ambient temperature. Therefore, the burning rates decrease and the combustion times increase. In the semi-empirical correlation, the reduction of $Gr$ due to decrease of gas density is slightly. The decline of burning rate is mainly due to transfer number.
5.2. Ignition delay times
Figure 6 shows the ignition delay times in the oxygen volume fraction range from 17% to 21% and ambient temperature range from 900K to 1400K.

The figure 6 shows that the ignition delay times are significantly decreased exponentially with the increasing of temperature. The ignition delay times of 900K is 5.6 times as much as that of 1400K. However, the figure also shows that the ignition delay times varies slightly as the oxygen concentration changes. Therefore, volume fraction of oxygen has little influence on ignition delay times.

6. Conclusions
Using a numerical simulation for combustion of n-heptane droplet in the oxygen volume fraction range from 17% to 21% and ambient temperature range from 900K to 1400K. The conclusions of this study are as follows:

1. With the decrease of oxygen mass fraction in the environment, the burning rates of the droplets decrease. The oxygen concentration influences the burning rate by changing the specific heat of the mixture.

2. A droplet combustion semi-empirical correlation under natural convection condition was applied. Gr and transfer number decrease as the mass fraction of oxygen decreases, causing the lower burning rate.

3. The ignition delay times decrease with the increase of temperature significantly, but almost not
change with the oxygen concentration.

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**References**

[1] Godsave G A E. Studies of the combustion of drops in a fuel spray—the burning of single drops of fuel[J]. Symposium on Combustion, 1953, 4(1):818-830.

[2] Spalding D B. The combustion of liquid fuels[J]. Symposium on Combustion, 1953, 4(1):847-864.

[3] ZHANG Xiaobin, XIANG Shijun, CAO Xiaoli, ZHANG Xuejun. Numerical simulation for combustion of droplet with volume of fluid formulation [J]. CIESC Journal, 2011, 62(3):692-698.

[4] Awasthi I, Pope D N, Gogos G. Effects of the ambient temperature and initial diameter in droplet combustion[J]. Combustion & Flame, 2014, 161(7):1883-1899.

[5] Sato J, Tsue M, Niwa M, et al. Effects of natural convection on high-pressure droplet combustion[J]. Combustion & Flame, 1990, 82(2):142-150.

[6] Dzik J, Nayagam V, Williams F A. Ignition and combustion of n-heptane droplets in carbon dioxide enriched environments [J]. International Communications in Heat & Mass Transfer, 2010, 37(3):221-225.

[7] Tanabe M, Bolik T, Eigenbrod C, et al. Spontaneous ignition of liquid droplets from a view of non-homogeneous mixture formation and transient chemical reactions[J]. Symposium on Combustion, 1996, 26(1):1637-1643.

[8] Wang C H, Liu X Q, Law C K. Combustion and microexplosion of freely falling multicomponent droplets [J]. Combustion & Flame, 1994, 56(2):175-197.

[9] Pope D N, Gogos G. Numerical simulation of fuel droplet extinction due to forced convection[J]. Combustion & Flame, 2005, 142(1–2):89-106.

[10] Wilke C R, Lee C Y. Estimation of Diffusion Coefficients for Gases and Vapors[J]. Industrial & Engineering Chemistry, 1955, 47(6):1253-1257.

[11] Monteith J L, Unsworth M H. Properties of Gases and Liquids[M]/ Principles of Environmental Physics. 2013:5-23.

[12] Wu G, Sirignano W A. Transient burning of a convective fuel droplet[J]. Combustion & Flame, 2010, 157(5):970-981.

[13] Law C K, Williams F A. Kinetics and convection in the combustion of alkane droplets[J]. Combustion & Flame, 1972, 19(3):393-405.

[14] Sato J, Tsue M, Niwa M, et al. Effects of natural convection on high-pressure droplet combustion[J]. Combustion & Flame, 1990, 82(2):142-150.