Studies on the flame structure and drag of a combusting droplet group

ARTICLE INFO

Received: 16 December 2022
Revised: 26 January 2023
Accepted: 3 February 2023
Available online: 13 February 2023

Key words: droplet-group combustion; large-eddy-simulation; flame structure; drag force

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1. Introduction

Spray combustion is widely encountered in various engines [1–3]. It was studied by large-eddy simulation [4, 5], where droplets were taken as volume-less point-source particles. Droplet combustion is an important part of spray combustion. The droplet combustion has been studied both experimentally and analytically for many decades since the middle’s years of the last century [6–9]. The experiments were done for suspended droplets, falling droplets and flying droplets of different fuels. The so-called $d^2$-law was examined and the “evaporation constant” $K = \frac{d(d^2)}{dt}$ under different gas relative velocities, gas temperatures and pressures were studied. In analytical studies, most of them are based on simplified 1-D “spherical stagnant-film” models. Even now, the sub-models for spray combustion in modern CFD software are still based on these models. These simplified studies cannot give the detailed structures of droplet flames. In recent years, more detailed theoretical, experimental and numerical studies of droplet combustion were reported. Awasthi et al. [10] simulated the effect of ambient temperature and initial droplet size on the combustion of a heptane droplet. The focus was paid on the heptane-droplet ignition delay and the comparison between the heptane and methanol droplets in flame location and evaporation rates. Kitano et al. [11] simulated single and multiple-droplet combustion, but used a given evaporation model to study the effect of ambient pressure and gas temperature on droplet evaporation. No information on the detailed gas flow, species concentration and gas temperature distributions surrounding the droplets were reported. Zhao et al. [12] simulated the effect of gas temperature on droplet combustion, only the effect of gas temperature on the droplet evaporation rate was reported and the comparison was given with the numerical results of other investigators. Chiu et al. [13, 14] reported an analytical model of droplet-group combustion. Segawa et al. [15] studied experimentally the ignition and early combustion behavior of 49 droplets under microgravity condition. Mikami et al. [16, 17] reported the droplet interactions in flame spreading characteristics of 100 n-decane droplets under micro-gravity conditions. Manish and Sahu [18] used PIV (particle imaging velocimetry) to measure the group combustion of droplet clusters in spray flames.

Regarding to droplet combustion characteristics, the drag force of evaporating/combusting droplets is an important sub-model in spray combustion modeling. Different research results were reported. The measurement results reported by Eisenklam et al. [19] are that evaporation reduces the droplet drag. Yuen et al. [20] did experimental studies, and Renkiszibulat and Yuen [21] did analytical studies of different evaporating droplets; the conclusion is that evaporation does not affect the droplet drag. Makino and Fukuda [22] measured the velocity of a falling combusting sodium droplet. The results show that combustion increases the droplet drag. Sugimoto [23] measured the velocity of a combusting methanol droplet; the results are that combustion reduces the droplet drag.

In general, the flow and flame structures surrounding a combusting droplet-group are unclear and the drag of combusting droplet group has not been reported. In this paper, large-eddy simulation (LES) is used to study a combusting ethanol-droplet group. The obtained flame structures and drag force are reported. The results will help to improve the drag model in numerical simulation of spray combustion in engines.

2. Controlling equations and closure models for LES of a droplet-group combustion

To study the detailed flow and flame structures surrounding ethanol droplet group, the filtered governing equations for 3-D LES are given as

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho \vec{u}}{\partial x_i} = 0$$  \hspace{1cm} (1)

$$\frac{\partial}{\partial t}(\rho \vec{u} \vec{u}) + \frac{\partial}{\partial x_i}(\rho \vec{u} \vec{u} \vec{u} \vec{u}) = \frac{\partial}{\partial x_i} \left( \mu \frac{\partial \vec{u}}{\partial x_j} - \frac{\partial \rho}{\partial x_j} - \frac{\partial \tau_{e s s}}{\partial x_j} \right)$$  \hspace{1cm} (2)

$$\frac{\partial \rho \vec{V}_s}{\partial t} + \frac{\partial}{\partial x_i}(\rho \vec{V}_s \vec{u}) = \frac{\partial}{\partial x_i} \left( \frac{\mu}{5} \frac{\partial \vec{V}_s}{\partial x_j} - \vec{w}_s - \vec{w}_{s s g s} - \frac{\partial \tau_{e s s}}{\partial x_j} \right)$$  \hspace{1cm} (3)
\[ \frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} (\rho \mathbf{u}_j) = \frac{\partial}{\partial x_i} \left( \frac{\mu}{\sigma_v} \frac{\partial \phi}{\partial x_i} \right) - \frac{\partial \sigma_{\text{sys}}}{\partial x_i} \]

(4)

The sub-grid-scale (SGS) stress was closed by the dynamic eddy-viscosity model [24]

\[ \tau_{ij}^{\text{sgs}} = 2 \rho C_s \Delta^2 \left[ \bar{\phi} \phi_i - \phi_i \bar{\phi} \right] \]

(5)

where \( \bar{u}_i \equiv \bar{u}_i \mathbf{u}_j - \bar{u}_j \mathbf{u}_i \), \( \Delta = 2 \tilde{\Delta} \), \( \tilde{\Delta} \) is the filter size/grid size, and

\[ \tilde{\Delta} = \frac{1}{2} \left( \frac{\partial \rho}{\partial x_i} + \frac{\partial \rho}{\partial x_j} \right) | \bar{\phi} | = \frac{\sqrt{2} \rho}{2 \bar{u}_i \bar{u}_j} \]

The SGS mass and heat fluxes are closed by gradient modeling

\[ g_{ij}^{\text{sgs}} = \rho \left( \mathbf{u}_i \mathbf{Y}_j - \bar{u}_i \mathbf{Y}_j \right) = \frac{\mu}{\sigma_v} \frac{\partial \mathbf{u}_i}{\partial x_j} \]

(6)

\[ q_{ij}^{\text{sgs}} = \rho \left( \mathbf{u}_i T - \bar{u}_i \bar{T} \right) = \frac{\mu}{\sigma_T} \frac{\partial T}{\partial x_j} \]

(7)

The sub-grid scale reaction rate is closed by the second-order moment combustion model [25]

\[ w_{\text{sgs}} = \bar{w}_s \left( \frac{Y'_1 Y'_2}{Y_1 Y_2} + \frac{K'_1 Y'_2}{K_1 Y_2} + \frac{K'_2 Y'_1}{K_2 Y_1} \right) \]

(8)

where \( \Phi, \Psi, \phi \) and \( \sigma \) denote the filtered and sub-grid-scale fluctuation values of \( Y_1, Y_2 \) and \( K \) respectively.

\[ \tau_T = 1/|\bar{\phi}| \quad \tau_c = \left[ B \rho \left( \bar{Y}_O + \beta \bar{Y}_C \right) + \exp \left( - \frac{E}{RT} \right) \right]^{-1} \]

For ethanol-oxygen reaction mechanism, a global single-step reaction is used

\[ 2C_3H_6OH + 6O_2 \rightarrow 4CO_2 + 6H_2O \]

(9)

The Arrhenius expression of the single-step global reaction kinetics for the reaction rate is

\[ w_s = 8.345 \times 10^{9} \rho^2 \mathbf{Y}_{I_1} \mathbf{Y}_{O_2} \exp \left( -1.26 \times 10^6 / RT \right) \]

(10)

with boundary conditions at the droplet surface, accounting for the Stefan flux

\[ \lambda_w \left( \frac{dT}{dr} \right) = \rho_w v_w q_e = \]

\[ = \frac{G}{\pi r_w^2} q_e - D_w \frac{d\mathbf{Y}}{dr} - \mathbf{Y}_S q_w v_w = \alpha \rho_w v_w \]

\[ \Delta Y_s = \Delta Y_p + \Delta Y_{ax} + \Delta Y_{pr} + \Delta Y_{in} = 1 \]

where, \( s = F(\text{fuel}), \alpha = 1, s \neq F, \alpha = 0, \alpha \) is a notation for different species. For obtaining the fuel vapor concentration, the fuel vapor partial pressure should be obtained by using the Antoine equation.

3. Computation domain and solution procedure

The computation domain is shown in Fig. 1. The sizes and position of simulated droplets are shown in Fig. 2 and Table 1. The grid sizes in x, y, and z directions are 10–300 \( \mu m \); the time step was taken as 0.000001 s; and the grid number is about 1400000.

![Fig. 1. Computation Domain](image)

![Fig. 2. Droplet sizes and position](image)

The PISO algorithm was used for p–v corrections; the second-order implicit difference scheme was taken for the time-dependent term, the second-order upwind difference scheme was taken for the convection term, and the central difference scheme was taken for the diffusion term. For the gas boundary conditions, a uniform gas inlet velocity was taken. The boundary condition at the exit was based on a fully developed flow assumption, where the gradients for all flow variables in the axial direction were set to be zero.

<table>
<thead>
<tr>
<th>Group No.</th>
<th>Droplet size [( \mu m )]</th>
<th>x [( \mu m )]</th>
<th>y [( \mu m )]</th>
<th>z [( \mu m )]</th>
</tr>
</thead>
<tbody>
<tr>
<td>w1</td>
<td>34.3</td>
<td>301.5</td>
<td>-433.7</td>
<td>515.1</td>
</tr>
<tr>
<td>w2</td>
<td>21.5</td>
<td>-293.9</td>
<td>-420.8</td>
<td>-180.0</td>
</tr>
<tr>
<td>w3</td>
<td>23.3</td>
<td>7.1</td>
<td>-291.0</td>
<td>-364.1</td>
</tr>
<tr>
<td>w4</td>
<td>17.1</td>
<td>238.9</td>
<td>408.9</td>
<td>-289.7</td>
</tr>
<tr>
<td>w5</td>
<td>29.2</td>
<td>409.1</td>
<td>-294.9</td>
<td>-139.3</td>
</tr>
<tr>
<td>w6</td>
<td>36.4</td>
<td>551.1</td>
<td>377.1</td>
<td>343.1</td>
</tr>
<tr>
<td>w7</td>
<td>23</td>
<td>-507.9</td>
<td>451.4</td>
<td>394.6</td>
</tr>
<tr>
<td>w8</td>
<td>27.9</td>
<td>496.1</td>
<td>-17.5</td>
<td>520.8</td>
</tr>
<tr>
<td>w9</td>
<td>20.3</td>
<td>158.8</td>
<td>360.3</td>
<td>214.5</td>
</tr>
<tr>
<td>w10</td>
<td>32.8</td>
<td>-483.0</td>
<td>-429.7</td>
<td>309.3</td>
</tr>
<tr>
<td>w11</td>
<td>19.4</td>
<td>56.3</td>
<td>-498.9</td>
<td>-129.3</td>
</tr>
<tr>
<td>w12</td>
<td>30.6</td>
<td>-257.0</td>
<td>137.0</td>
<td>195.5</td>
</tr>
</tbody>
</table>

4. Simulation results

4.1. Instantaneous flame structures

Figure 3 shows three combustion modes of the droplet group. There are fully-enveloped flame, partially-enveloped flame and wake flame under different gas relative velocity, similar to the numerical results of a single droplet [26], and the PLIF measurement results obtained by Mercier et al.
[27]. However, in case of the droplet group, different combustion modes may exist in the same region, since there are different droplet sizes in a computation domain. Since the Stefan flow surrounding the droplets in the azimuthal direction is non-uniform, which will cause the change of drag with the inlet velocity.

Fig. 3. Three combustion modes of multiple droplets

Fig. 4. Molar fraction of ethanol-vapor concentration

Fig. 5. Molar fraction of H₂O concentration
Figures 4 and 5 show the predicted molar fractions of ethanol-vapor and H₂O surrounding the droplet group respectively. The distribution of ethanol-vapor concentration is axis-symmetrical, but the reaction zones are somewhat declined with an angle of α due the interaction between droplets. Figures 6 and 7 are velocity vectors and streamlines surrounding the combusting droplet group respectively. Obviously, velocities ahead of droplets are larger than those behind droplets due to the Stefan flow, leading to the change of drag. The similar phenomenon was observed in the velocity vectors surrounding a single droplet [26]. The streamlines are distorted due to the interaction between droplets.

![Velocity vectors surrounding combusting droplets](image)

**Fig. 6.** Velocity vectors surrounding combusting droplets

![Streamlines surrounding combusting droplets](image)

**Fig. 7.** Streamlines surrounding combusting droplets

Figure 8 gives the vorticity maps surrounding a droplet group and a single droplet. The vortex shedding in a droplet inside the group is weaker than that in a single droplet owing to droplet-droplet interactions.

![Vorticity maps surrounding a droplet group](image)

**Fig. 8.** Vorticity maps surrounding a droplet group

4.2. Statistics of the combusting droplet drag

The statistics gives the comparison between the widely-used Wallis-Kliachko formula of the drag for non-combusting particles in isothermal flows, modified droplet drag accounting the effect of the Stefan Flow given by the 1-D model [28] and the LES results for a single combusting droplet, as shown in Table 2. The Wallis-Kliachko formula [28] gives

\[
C_D = \begin{cases} 
\frac{24}{Re_p} \left(1 + \frac{Re_p^{2/3}}{6}\right) & Re_p < 1000 \\
0.44 & Re_p \geq 1000 
\end{cases}
\]

\[
Re_p = \frac{\rho d \bar{U} \bar{U}}{\mu_f}
\]

The modified formula in the 1-D stagnant-film theory [28] gives

\[
C_D = C_{D0} \ln(1 + b) / B; \quad B = \frac{c_p(T_g - T_b)}{L}
\]

where B is the transfer number, related to the boiling point and latent heat of the liquid.

![Vorticity maps surrounding a droplet group](image)

**Fig. 8.** Vorticity maps surrounding a droplet group

Obviously, the drag coefficient of combusting droplet is much smaller than that of non-combusting particles in isothermal flows. The physical explanations may be the injection effect of non-uniform Stefan flow surrounding the combusting droplet and the effect of cold droplet-surface temperature on the reduction of friction force due to the reduction of gas viscosity.

<table>
<thead>
<tr>
<th>(\bar{V}_{rel} ) (m/s)</th>
<th>(C_{D0}) (Wallis-Kliachko Formula)</th>
<th>(C_D) (LES)</th>
<th>(C_{D0} \times \ln(1+b)/B)</th>
</tr>
</thead>
<tbody>
<tr>
<td>0.2</td>
<td>3.950</td>
<td>1.100</td>
<td>2.370</td>
</tr>
<tr>
<td>1.0</td>
<td>1.960</td>
<td>0.344</td>
<td>1.176</td>
</tr>
<tr>
<td>4.0</td>
<td>0.963</td>
<td>0.235</td>
<td>0.576</td>
</tr>
</tbody>
</table>

The drag coefficient of a droplet in its group is still smaller than that of a single droplet, as shown in Table 3.

<table>
<thead>
<tr>
<th>(\bar{V}_{rel} ) (m/s)</th>
<th>(C_D) (Wallis-Kliachko)</th>
<th>(C_D) (Single droplet)</th>
<th>(C_D) (Droplet in a group)</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>1.960</td>
<td>0.344</td>
<td>0.297</td>
</tr>
<tr>
<td>4</td>
<td>0.963</td>
<td>0.235</td>
<td>0.144</td>
</tr>
</tbody>
</table>

![Vorticity maps surrounding a droplet group](image)

**Fig. 8.** Vorticity maps surrounding a droplet group

Figure 9 gives the drag coefficient of the single combusting droplet vs droplet Reynolds number, reported in [26]. It is seen that as the droplet Reynolds number increases to be greater than 280, the reduction effect of drag gradually diminishes.

![Vorticity maps surrounding a droplet group](image)

**Fig. 9.** Drag coefficient vs droplet Reynolds number
Figure 10 shows drag coefficients of droplets of different sizes in their group under various gas relative velocities and temperatures, indicating that the effect of gas temperature is more sensitive to drag reduction.

Conclusions

Three modes of flame structures were observed in a droplet group: fully-enveloped, partially-enveloped and wake flames, and Stefan-flow structure was observed for the droplet-group combustion, leading to the change of drag force with the increasing inlet velocity. The drag force of combusting multiple droplets is much smaller than that of non-combusting particles in isothermal flows. Future work should be done for finding a new drag-force model of combusting droplets in numerical simulation of spray-combustion engines.

Acknowledgements

This study was sponsored by the Key Project of National Natural Science Foundation of China under the Grant 51390493.

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