Numerical study of the effect of ambient air oxygen concentration on the combustion behaviour of fuel films

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Abstract

This study presents three-dimensional unsteady numerical simulations to clarify the effect of oxygen concentration conditions in a constant volume chamber on the combustion behaviour of the fuel film. The numerical simulation results show that the behaviour of the flame varies significantly with the oxygen concentration. Specifically, at high oxygen concentrations of 30%, the flame exhibited laminar characteristics and flickering was observed, where the flame fluctuates vertically and periodically due to vortex rings generated by the shear layer at the outer edge of the flame. Additionally, under these conditions, the temperature of the flame is higher, and the buoyancy effect increases. Conversely, at low oxygen concentrations of 16%, the flame transitioned to a turbulent one. Under these conditions, the temperature of the flame was also lower, and the buoyancy effect decreased. These variations in flame behaviour with oxygen concentration were found to be related to variations in the relationship between buoyancy and viscosity as the flame temperature changes, and can be explained by the Grashoff number.

Keyword: *Fuel film combustion, Ambient oxygen concentration, flame, Buoyancy, Large Eddy Simulation*

1. Introduction

Gasoline direct injection engines (GDI-E) are an effective technology for reducing greenhouse gas emissions from internal combustion engines, with the advantage of significantly higher thermal efficiency and fuel consumption than conventional port fuel injection engines. However, it has also been pointed out the problems regarding carbon dioxide emissions and the formation of soot due to the combustion of residual fuel film on the piston surface [1]. The effects of ambient conditions such as pressure and oxygen concentration on the combustion process of the fuel film and the formation of soot have not been clarified. Understanding the combustion process of the fuel film and the formation process of soot could lead to the development of new technologies to reduce emissions from GDI engines, and therefore researches focusing on the combustion of the fuel film have been carried out.

The authors constructed a experimental system to reproduce the flame behaviour of fuel films exclusively in a constant-volume chamber and conducted combustion experiments of fuel films with the pressure and oxygen concentration in the chamber as parameters [2]. The visualization of the formation process of soot by applying an optical method revealed that the flame behaviour of the fuel film varies significantly depending on the environmental conditions, which leads to a variation in the formation process of soot. Additionally, the authors carried out three-dimensional unsteady numerical simulations to investigate the effect of pressure in the chamber on the flame behaviour of the fuel film, and found that the variation of flame behaviour due to pressure is related to the increase in buoyancy effect with increasing pressure and the resulting increase in flow velocity at the outer flame edge, and that this effect can be summarized by the Grashoff number.

The aim of this study is to investigate the effect of oxygen concentration conditions in a constant volume chamber on the combustion behaviour of the fuel film using three-dimensional unsteady numerical simulations. The present paper presents firstly the validity of the numerical simulation method and results, and then the results of the evaluation of the influence of the oxygen concentration conditions on the flame

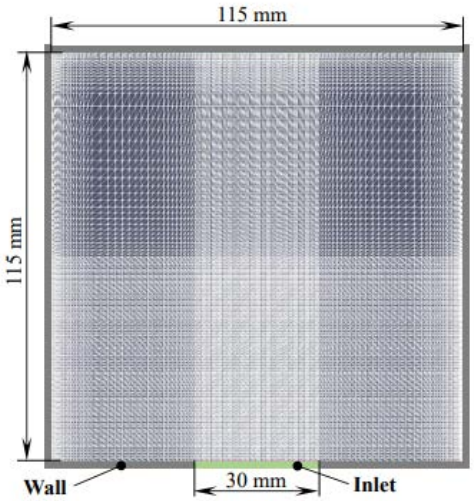


Fig. 1 Computational grids

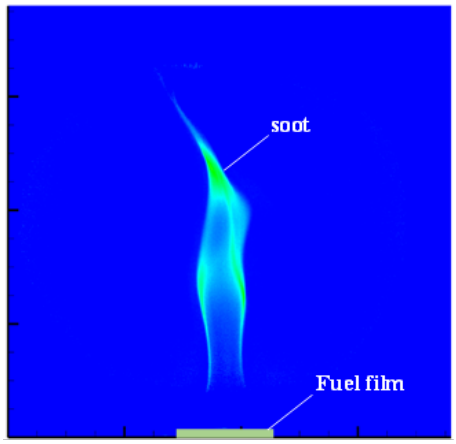


Fig. 2 Experimental results at 3 bar

behaviour of the fuel film.

2. Numerical method

The present study has been carried out based on the experimental conditions of the previous study [2] to set up the conditions for the numerical simulation and the numerical method was the same as in the previous study [3]. The fuel used was iso-octane. As the present study focuses on the relationship between the ambient oxygen concentration conditions and variations in flame behaviour, the combustion reaction was assumed to be a one-step overall reaction, expressed by the following chemical equation.

$$2C_8H_{18} + 25O_2 \rightarrow 16CO_2 + 18H_2O \quad (1)$$

Large Eddy Simulation (LES) was performed to simulate the unsteady turbulent flow field with the combustion reaction. The governing equations were considered the effect of density changes and a gravity term to estimate the effect of buoyancy caused by the density distribution. Sub Grid Scale model for the LES was chosen to be the Wall-Adapting Local-Eddy viscosity model. The Infinitely Fast Chemistry model was used as the combustion model. This model is a one-equation model in which the reaction rate is determined in proportion to the mass fractions of the fuel and oxidiser, and is characterised by the fact that the reaction rate increases as the mixture of the two increases. In this simulation, the effect of radiation is also considered, and the fvDOM model was used as the radiation model.

The flow field is implicitly solved by the finite volume method and discretised with respect to space using a second-order accurate finite difference method. For the discretisation with respect to time, an implicit second-order precision backward differencing was used. The PIMPLE method was used as the computational scheme and the number of pressure correction loops was set to two. The simulations described above were carried out using the simulation code OpenFOAM Ver. 9. The thermodynamic properties and transport coefficients required in the simulations were obtained from the CHEMKIN database.

The computational grid used in this simulation is shown in Fig. 1. The computational domain simulates the inside of a constant volume chamber used in a previous study [2], see Fig. 2, and the size of the domain is a cube with 115 mm on a side. An inlet boundary with a diameter of 30 mm was set up at the centre of the bottom of the computational domain, from which the evaporation process of the fuel film was simulated by giving iso-octane an inflow velocity estimated from experimental results (U_{in} = 3×10^{-5} m/s) under the condition of stoichiometric ratio. Surfaces except the inlet boundary were assumed to be wall surfaces and adiabatic conditions with no slip were given. Hexahedral cells were used as the computational grid, with non-uniform grid spacing. In order to simulate in detail the flame evolution and vortex structures generated by the combustion of the fuel film, the cells about three times larger than the Kolmogorov scale were arranged in the region downstream of the inlet boundary to increase the spatial resolution. The total number of computational cells is 2.88 million, with the number of grid divisions set to 120, 200 and 120 in the x-, y- and z-directions, respectively.

A preliminary study of the effect of the grid resolution on the numerical simulation has confirmed that the

grid convergence is achieved under the present grid conditions and that the behaviour of the flame is in qualitative agreement with the experimental results [3]. The time step was set at a value for which the Courant number is less than 1 (2.5×10^{-4} s). The ambient pressure in the computational domain was set to 3 bar, in accordance with the experimental conditions of the previous study [2]. The oxygen concentration of the ambient air in the computational domain was also simulated under four different conditions, 16%, 21%, 25% and 30%, as in the previous study [3].

3. Results and Discussion

3.1 Comparison of numerical simulation results with experimental results

To validate the results from the present numerical simulation, comparisons with the experimental results [2] were performed. Note that, in the experiment, only a specific amount of fuel (30 μL) is supplied just before ignition, so that the remaining amount of fuel decreases as combustion proceeds, causing the evaporation rate of the fuel to vary over time. This differs from the conditions of the present numerical simulation, where the inlet velocity was set to be constant regardless of time. Therefore, the evaluation of the numerical results was carried out using the results up to 1.5 s after the start of combustion, when the difference in the inlet velocity between the simulation and the experiment is relatively small.

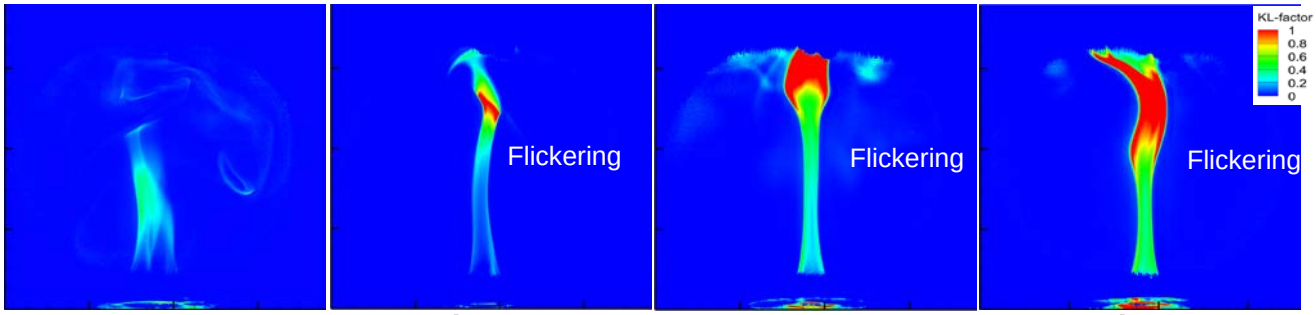
The experimental and numerical results for varying the oxygen concentration of the ambient air in the constant volume chamber from 16% to 30% are shown in Fig. 3 and Fig. 4, respectively. Here, the experimental results show the KL values, which indicate the presence of soot, and the higher the amount of soot, the higher the KL value. The distribution of the KL values can be used to determine the shape and behaviour of the flame. Meanwhile, the simulation results show the mass fraction of iso-octane, and the shape and behaviour of the flame can be confirmed from the distribution. Experiments have confirmed that, in the case of an oxygen concentration of 30%, a phenomenon called Flickering is observed, in which, after ignition, the flame extends vertically upwards and reaches the top of the constant volume chamber, after which the upper part of the flame breaks off, splitting in two and the lower flame extends vertically upwards again, repeating this behaviour in cycles. The frequency of flickering was approximately 10 Hz. The flame behaviour was close to laminar flame characteristics. Flickering has been known to occur due to the formation of vortex rings at the flame edge. Namely, shear layers are generated by an increased upward velocity at the flame edge due to the buoyancy effect caused by the temperature distribution due to the combustion reaction, and these shear layers periodically roll up to form vortex rings. The behaviour of the flame changes gradually as the oxygen concentration is reduced, and it can be observed that, under conditions of 16% oxygen concentration, the behaviour of the flame is significantly different from that of 30% oxygen concentration. Under these conditions, the periodic vertical flame behaviour due to flickering, observed in the case of 30% oxygen, disappears and the flame becomes dominated by horizontal, irregular flame behaviour, resulting in a turbulent flame. The height of the flame is also reduced.

The experimental results described above are also shown in the numerical simulation results shown in Fig. 4. In the case of an oxygen concentration of 30%, the flame forms a laminar flame, and the flame behaviour fluctuates periodically in the vertical direction due to flickering. The frequency of this flickering is approximately 15 Hz, which is close to the experimental value, and thus qualitatively represents the experimental results. The behaviour of the flame gradually changes as the oxygen concentration decreases, and the flame at 16% oxygen concentration becomes a turbulent flame with no flickering and an irregular horizontal fluctuation, and the flame height is lower than that of the 30% oxygen concentration, thus confirming that the behaviour changes are the same as the experimental results.

The results of the present numerical simulation are in qualitative agreement with the experimental results and can simulate the effect of the oxygen concentration of the ambient air on the variation in the behaviour of the flame, as confirmed by the experiment.

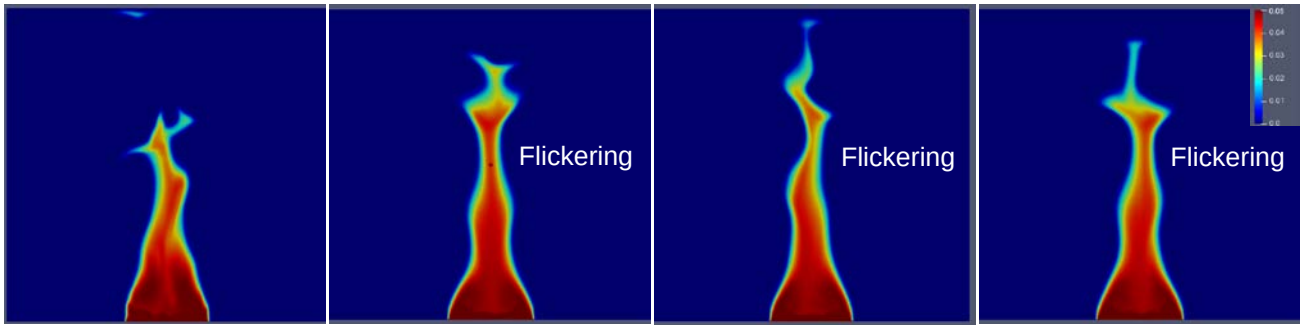
3.2 Effect of oxygen concentration on combustion behaviour

To investigate the mechanism of the variation of flame behaviour with the oxygen concentration of the ambient air as described in the previous section, a comparison of the simulation results for oxygen concentrations of 16% and 30% was conducted. The temperature distributions at each oxygen concentration are shown in Fig. 5 for t = 0.10 s, 0.30 s and 0.50 s. At t = 0.10 s, the flame begins to extend upwards at both oxygen concentrations, and the rapid temperature rise associated with the flame formation results in the rapid generation of an upward air flow. Vortex rings are formed at the flame tip due to the upward airflow generated by the rapid temperature rise associated with the flame formation. The flame temperature shows



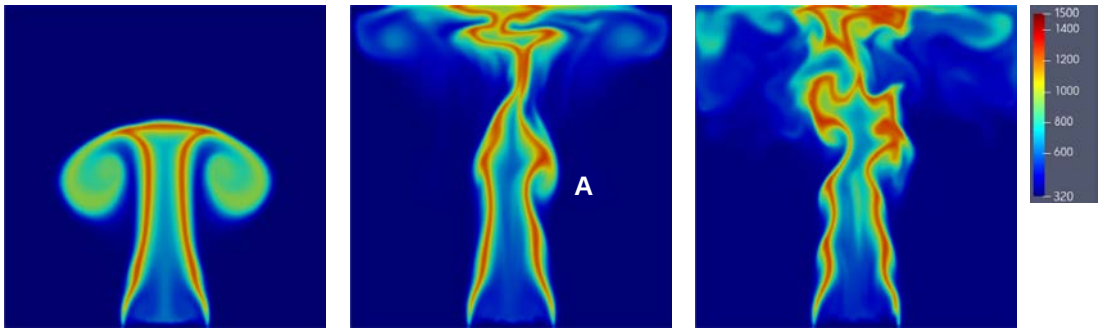
(a) 16 % (b) 21 % (c) 25 % (d) 30 %

Fig. 3 Distribution of KL factors obtained by DBI-EI (experiments)



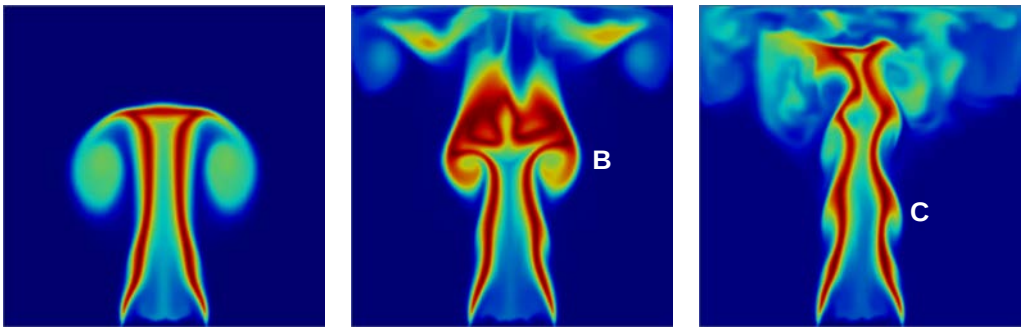
(a) 16 % (b) 21 % (c) 25 % (d) 30 %

Fig. 4 Distribution of mass fractions obtained by LES



t = 0.10 s t = 0.30 s t = 0.50 s

(a) 16 % oxygen concentration



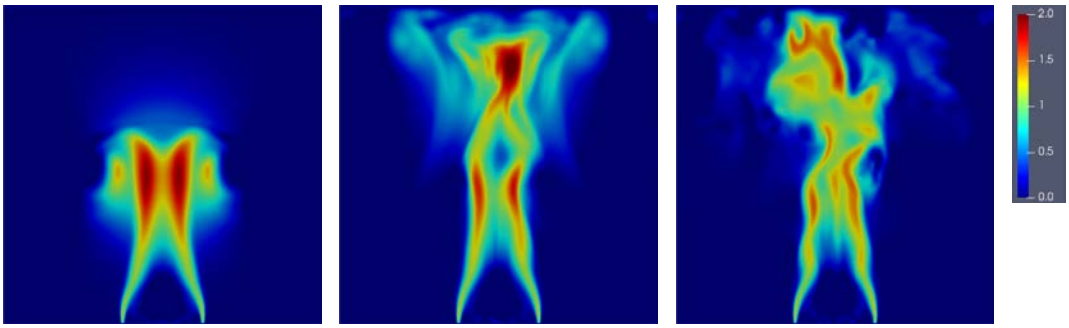
t = 0.10 s t = 0.30 s t = 0.50 s

(b) 30 % oxygen concentration

Fig. 5 Comparison of flame temperature distributions at 16 % and 30 % oxygen concentration

higher values at 30% oxygen concentration, with a difference of 250-300 K between the two maximum flame temperatures. This may indicate that the combustion reaction progresses with increasing oxygen concentration.

At t = 0.30 s, the two oxygen concentrations show differences not only in the temperature distribution of the flame but also in the flame shape. Focusing on the outer edge of the flame, a small distortion of the temperature layer indicating the formation of a vortex structure, shown “A” in the diagram, is observed at



t = 0.10 s t = 0.30 s t = 0.50 s

(a) 16 % oxygen concentration

t = 0.10 s t = 0.30 s t = 0.50 s

(b) 30 % oxygen concentration

Fig. 6 Comparison of upward velocity distributions at 16 % and 30 % oxygen concentration

16% oxygen concentration, but this distortion shows a non-axisymmetric shape, which indicates that it is not a vortex ring. The formation of this non-axisymmetrical vortex structure is considered to be the cause of the turbulent characteristics of the flame. On the other hand, at an oxygen concentration of 30%, the distortion of the temperature layer, shown “B” in the diagram, shows an axisymmetric shape, which confirms that vortex rings continue to be generated, and that these vortex rings are the cause of flame flickering. The vortex rings do not have enough effect to significantly promote mixing and diffusion at the outer edge of the flame, and as a result the flame is considered to exhibit a laminar shape.

At t = 0.50 s, the vortex formation behaviour at the outer edge of the flame is almost the same as that at t = 0.30 s. The flame at 16% oxygen concentration is a turbulent flame due to the formation of non-axisymmetric vortices, whereas at 30% oxygen concentration the flame is more like a laminar flame due to the formation of axisymmetric vortices, shown “C” in the diagram. The flame shows a shape similar to a laminar flame due to the formation of axisymmetric vortices, shown “C” in the diagram. Thus, the variation of flame behaviour with different oxygen concentrations occurs at an early stage immediately after the start of combustion and is considered to be related to the variation of the temperature distribution in the flame area and the consequent variation of the vortex ring structure.

The reason for the variation of the vortex structure due to changes in the temperature distribution seems to be related to the variation of the relationship between buoyancy and viscosity caused by the temperature difference. The variation of the buoyancy force appears in the vertical, or y-direction, velocity of the combustion field. Fig. 6 shows the y-directional velocity distribution at each of the times shown in Fig. 5. The figure shows that the velocity at the outer edge of the flame at each time is 30% higher in the case of 30% oxygen concentration than in the case of 16% oxygen concentration, confirming that the upward velocity at the outer edge of the flame increases with the increase in oxygen concentration. This means that the temperature of the flame increases with increasing oxygen concentration, thereby increasing the buoyancy effect. However, for the flame to become laminar with increasing oxygen concentration, the effect of viscosity must be enhanced with increasing temperature. The relationship between buoyancy and viscosity in this combustion field is considered here on the basis of the Grashoff number given below.

$$Gr = \frac{g\beta\rho^2 l^3}{\mu^2}\Delta T \tag{2}$$

where g is the acceleration of gravity, β is the coefficient of volume expansion, ρ is the density, l is the

representative dimension, ΔT is the temperature difference between the flame temperature and the ambient temperature and μ is the viscosity coefficient. Since β, ρ and μ in the equation vary with temperature T, introducing the equation of state and Sutherland's equation for μ into equation (2) to determine the effect of the variation of these values with temperature on the Gr number, the Gr number can be expressed by the following equation using temperature.

$$Gr = C_1 l^3 \frac{\Delta T}{T^4}\left(1+\frac{S}{T}\right)^2 P^2 \tag{3}$$

where S is Sutherland's constant, P is the ambient pressure and C_1 is a constant expressed by the following equation

$$C_1 = \frac{T_0^3 g}{\mu_0^2 R^2 \left(T_0 + S\right)^2} \tag{4}$$

where T_0 is the reference temperature, μ_0 is the viscosity coefficient at the reference temperature and R is the gas constant. Equation (3) shows that as the flame temperature increases, the Glashoff number decreases and the buoyancy effect decreases. This means that when the oxygen concentration is high, the flame temperature is high and the viscous effect dominates, resulting in a laminar flame, whereas when the oxygen concentration is low, the flame temperature is low and the buoyancy effect dominates, resulting in a turbulent flame.

In summary, it was confirmed that the variation of flame behaviour with oxygen concentration is related to the variation of the relationship between buoyancy and viscosity with flame temperature, and that this variation can be summarized by the Grashoff number.

4. Conclusion

The present study aimed to clarify the influence of oxygen concentration conditions in a constant volume chamber on the combustion behaviour of fuel films by using three-dimensional unsteady numerical simulations of fuel film combustion. The results are summarized below.

The results of the numerical simulation of fuel film combustion performed under the numerical simulation conditions presented in this paper are in qualitative agreement with the experimental results and successfully simulate the effect of oxygen concentration on the variation of flame behaviour.

The numerical simulation results showed that the behaviour of the flame changed significantly depending on the oxygen concentration, with a high oxygen concentration of 30%, the flame became laminar and Flickering was observed, where the flame fluctuated vertically and periodically due to vortex rings generated by the shear layer periodically rolling up at the outer edge of the flame. The temperature of the flame under these conditions is high, which increases the buoyancy effect. However, when the oxygen concentration was reduced to as low as 16%, the flame was found to be turbulent. The temperature of the flame under these conditions was also lower, which reduced the buoyancy effect.

Flame behaviour changes with oxygen concentration as described above are related to changes in the relationship between buoyancy and viscosity as the flame temperature changes, which can be explained by the Grasshoff number. In other words, in the case of high oxygen concentration, viscous effects dominate due to the high flame temperature and the flame becomes a laminar flame, whereas in the case of low oxygen concentration, buoyancy effects dominate due to the low flame temperature and the flame becomes a turbulent flame.

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