A Turbulent Burning Velocity Model Taking Account of the Preferential Diffusion Effect

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ABSTRACT

In our previous works\textsuperscript{(1)(2)}, we found that the preferential diffusion of highly diffusible molecules played an important role in the turbulent combustion characteristics. The local burning velocity in premixed turbulent combustion was estimated experimentally, taking account of the preferential diffusion effect. In this study, a model, which takes the preferential diffusion effect into consideration, is proposed to predict the turbulent burning velocity and the quenching limit, based on the local burning velocity as a reference instead of the original laminar burning velocity. The model can be simply explained as follows. The turbulence affects the turbulent burning velocity by increasing the flame surface area and stretching the flame. Consequently, the turbulent burning velocity and quenching limit are determined by the balance of both effects. Comparison of the predicted turbulent burning velocities with measured ones showed good quantitative agreement for mixtures where the fuel, equivalence ratio and the laminar burning velocity were varied extensively.

INTRODUCTION

Since the turbulent burning velocity characteristics of premixed mixtures in internal combustion engine is the most important factor which dominates the engine performance, its quantitative prediction studies have been made extensively. Several kinds of prediction models of premixed turbulent burning velocity especially for stoichiometric and near-stoichiometric mixtures have been proposed so far\textsuperscript{(3)-(6)\textsuperscript{a}}. Most of the studies have used the original laminar burning velocity as a basic parameter, in discussing the models.

However, from the viewpoint to solve both environmental and energy problems, attention is focused on lean-burn technique and hydrogen as a fuel of internal combustion engines. Thus, a prediction model of turbulent combustion characteristics for non-stoichiometric mixtures as well as for stoichiometric mixtures of many kinds of fuel is anticipated to be established.

In our previous works\textsuperscript{(1)(2)}, we found that the preferential diffusion effect played an important role in the turbulent combustion characteristics, and estimated the local burning velocity and the value of the change in the local equivalence ratio in premixed turbulent combustion experimentally.

In this study, attempts have been made to examine the turbulent burning velocity characteristics based on the estimated local burning velocity as a basic parameter. It is found in the first place that the Karlovitz numbers at the quenching limit based on the original laminar burning velocity vary with the equivalence ratio and the kind of fuel, whereas those based on the local burning velocity remain nearly constant at about 1.0, irrespectively of the kind of fuel and the equivalence ratio. Then, a model, which takes the preferential diffusion effect into consideration, is proposed to predict the premixed turbulent burning velocity characteristics, using the local burning velocity as a reference instead of the original laminar burning velocity. The predicted velocities by this model are compared with the measured turbulent burning velocities where the fuel, equivalence ratio and the laminar burning velocity are varied extensively. As a result, quantitative accuracy of this simple model is confirmed.

EXPERIMENT

Apparatus and Procedure

The combustion chamber used is a nearly spherical vessel with a mean inner diameter of about 120mm\textsuperscript{(2)}. It is fixed with four perforated plates of 100mm diameter at other four sides. Behind each perforated plate, a fan is equipped to mix gases and generate approximately isotropic and homogeneous turbulence in the central region of the chamber. To conduct combustion experiment, the mixtures with desired composition were prepared at an atmospheric pressure and ignited at the vessel center under controlled turbulent intensity by the fan speed.

The laminar burning velocity, $S_{l0}$, and the turbulent burning velocity, $S_T$, were measured by the pressure history of combustion in the chamber in the early stage of combustion when the pressure rise was 0.01 to 0.02MPa to satisfy the assumption of the flame being nearly spherical\textsuperscript{(7)}. Each experiment was repeated more than 10 times to keep the accuracy of measurements, with the initial pressure and
temperature being 0.101MPa and 298K, respectively. Details of the apparatus and procedure are shown elsewhere(5).

The characteristics of turbulence in the chamber had been obtained by the two-point correlation method using hotwire anemometry(2)(3). From the result, it is found that the longitudinal integral length scale \( L_z \) shows a slight increase and following flattening out and the Taylor's micro scale \( \lambda_z \) shows a negligible increase and following decrease with increasing the turbulence intensity \( u' - 3.67m/s \), being about 3.3±0.3mm and 1.49±0.1mm, respectively.

**Mixture Composition**

Figure 1 shows the contour lines of the laminar burning velocity of hydrogen mixtures with the change in the molar ratio of nitrogen to oxygen and equivalence ratio. Mixtures used in the combustion experiment to estimate the local burning velocity \( S_L \) can be divided into three groups as shown in Fig.1. Here, \( S_L \) used in this paper designates the mean local burning velocity of turbulent flame in the whole combustion field.

The mixtures belonging to group I, denoted by a solid circle in Fig. 1, have nearly the same laminar burning velocity (about 15 cm/s) by adding nitrogen to hydrogen-air mixtures, whose equivalence ratio is varied. These mixtures are used in order to investigate the turbulent combustion mechanism such as the change in local burning velocity and quenching limit. The group II and III mixtures, which are derived from group I mixtures, are used in order to estimate quantitatively the local burning velocity of each specific group I mixture.

Mixtures of the three groups are prepared for methane, ethane, and propane as well. Details of the properties of these mixtures are shown in the references(1)(2).

**RESULTS AND DISCUSSION**

**Local Burning Velocity of Turbulent Flame**

In our previous works(1)(2), the experimental results for the group I mixtures of three hydrocarbons and hydrogen showed large clear difference in the measured turbulent burning velocity \( S_T \) at the same turbulence intensity \( u' \) and also in the quenching limit, even under nearly the same laminar burning velocity \( S_L \). Where, the equivalence ratio was varied. This mechanism was explained by means of Lewis number effect and preferential diffusion effect. Namely, on the basis of Lewis number effect, the convex part of flame toward the unburned mixture have been found out to affect the turbulent burning velocity predominantly. This led to the conclusion that the change of local equivalence ratio at this part could possibly play as if the total equivalence ratio through the flame area had changed.

The preferential diffusion effect can affect the local equivalence ratio of this dominant part, due to the difference in the molecular diffusivity between fuel and oxygen in turbulent flame. At the same time, the probable change of local equivalence ratio inevitably leads to the change of the local burning velocity. Therefore, it naturally follows that the local burning velocity of turbulent flame changes from the original laminar burning velocity.

On the basis of the above discussion, the local burning velocity, \( S_L \), and the value of the local equivalence ratio increase, \( \delta \phi \), were determined quantitatively under the following assumptions, in the weak turbulence condition(\( u' \approx 0.5 \text{ m/s} \)) where the flame surface area increases almost linearly with the turbulence intensity. (1)The surface area of flame solely depends on the turbulence intensity. (2)The increase rate of local equivalence ratio depends only on the property of fuel in the mixture, irrespectively of the original equivalence ratio. (3) The ratio of molar fraction of oxygen to that of nitrogen is constant everywhere in the unburned zone.

Figure 2 shows the relationship between the equivalence ratio and the ratio of the local burning velocity \( S_L \) to the laminar burning velocity \( S_L \). From Fig.2, it is found that the local burning velocity depends on the kind of fuel and the equivalence ratio. In the case of methane and hydrogen mixtures, the lower the equivalence ratio is, the higher the
local burning velocity becomes, while in the ethane and propane mixtures the tendency is reversed. In addition, it is shown that the influence of the preferential diffusion effect can be almost neglected near stoichiometric mixtures regardless of the kind of fuel.

Figure 3 shows the estimated value of the change in the local equivalence ratio \( \delta \phi \) against the ratio of diffusion coefficient of fuel to that of oxygen in the mixture \( D_F/D_O \) for group I mixtures. It is found that the estimated values of the local equivalence ratio increase \( \delta \phi \) of hydrogen mixtures are larger than those of hydrocarbon mixtures due to the higher diffusivity. In addition, there exists an obvious relationship between \( \delta \phi \) and \( D_F/D_O \) regardless of the kind of fuel. This relationship is well approximated as follows:

\[
\delta \phi \approx 0.3 \ln \left( \frac{D_F}{D_O} \right)
\]  

(1)

On the other hand, there exists almost no quantitative relationship between \( \delta \phi \) and Lewis number \( L_e \) which might be thought to affect a flame characteristics. From this experimental result, it is evident that the diffusion of sufficient reactant also plays an important role in the mechanism of turbulent combustion in addition to the Lewis number which considers the diffusivity of the deficient reactant and the thermal diffusivity.

**Discussion Based on Local Burning Velocity.**

A number of turbulent burning velocity models have been proposed so far\(^{10-30}\). Almost all of them uses the laminar burning velocity as one of the basic parameters. Those models seems to be successful in the quantitative explanation of the experimental results for stoichiometric mixtures, however, not enough for non-stoichiometric mixtures. Here, we discuss the quenching limit and the turbulent burning velocity using the estimated local burning velocity as a basis instead of the laminar burning velocity.

**Quenching Limit.** The Karlovitz number \( K_a \), which is used in the discussion on the quenching of flamelets caused by stretch, is known as the following expression\(^{39}\):

\[
K_a = \frac{u'}{\lambda} \frac{a}{S_{L}^{2}}
\]

(2)

where \( u' \) is the turbulence intensity, \( \lambda \) is the Taylor's microscale, \( a \) is the thermal diffusivity, and the \( S_{L} \) is the laminar burning velocity.

On the other hand, taking the estimated changes of the local equivalence ratio and the local burning velocity into consideration, the Karlovitz number can be written as follows:

\[
K_a = \frac{u'}{\lambda} \frac{a}{S_{L}^{2}}
\]

(3)

where \( a \) is the estimated thermal diffusivity based on the local equivalence ratio, and \( S_{L} \) is the estimated (mean) local burning velocity of a turbulent flame.

Figure 4 shows that the Karlovitz numbers at the quenching limit calculated by Eq. (2) and (3) for hydrocarbons and hydrogen mixtures. It is evident that the calculated results by Eq.(2) vary with the equivalence ratio and the kind of fuel, whereas those by Eq.(3) remain nearly constant at about 1.0 under this combustion chamber used. This result is of great interest for the discussion about the quenching mechanism in the turbulent combustion. Because, the extinction of flamelets occurs regardless of the kind of fuel and the equivalence ratio when the Karlovitz number, \( K_a \), which can be determined based on the local burning velocity considering the effect of preferential diffusion, reaches 1.0.

**Turbulent Burning Velocity.** The discussion above suggests that the local burning velocity considering the effect of preferential diffusion can become a decisive parameter in the turbulent combustion mechanism. Then, attempts are made to examine the turbulent burning velocity, taking account of the local burning velocity as the substantial burning velocity of turbulent flame, as follows.
Under the mixture composition, where the ratio of the local burning velocity $S_l$ to the laminar burning velocity $S_{l0}$, $S_l/S_{l0}$, is equal to unity in Fig.2, the local burning velocity in turbulent flame is almost equal to the original laminar burning velocity. Figure 5 shows the change in the product of the increase ratio of turbulent burning velocity to the local burning velocity, $(S_T-S_l)/S_l$, and the preheat zone thickness ($=a_S/S_l$) divided by the Taylor’s microscale, $\eta_L/\lambda_g$, with $K_a$ for the methane, ethane, propane and hydrogen mixtures. From Figure 5, $(S_T-S_l)/S_l(\eta_L/\lambda_g)$ at the same $K_a$ are found to take nearly the same value regardless of the kind of fuel. The data in Fig.5 show the extracted effect of turbulence (intensity and scale) on turbulent burning velocity, since they suffer almost no effect from preferential diffusion. This figure indicates that the local burning velocity and the preheat zone thickness (being proportional to the flame thickness) are the key parameters in determining the turbulent burning velocity.

In addition, the profiles of $(S_T-S_l)/S_l(\eta_L/\lambda_g)$ as shown in Figure 5 may be well divided into two regions. They are the increasing and the following flattening out region of $(S_T-S_l)/S_l(\eta_L/\lambda_g)$ with increasing $K_a$. The tendency of these profiles changes at about $K_a=0.5$. The turbulent burning velocity $S_T$ is well approximated in each region as follows:

$$0 < K_a \leq 0.5$$
$$S_T = (S_L + \frac{\sqrt{2}}{2} \cdot \alpha \cdot u')(1 - K_a^2)$$

$$0.5 < K_a \leq 1.0$$
$$S_T = \frac{3}{8\sqrt{2}} \cdot \alpha \cdot \frac{\lambda_g}{\eta_L} + \frac{3}{4} S_L$$

where

$$\alpha = \left[ \frac{L_f + \eta_L}{L_f} \right]^2$$

$\alpha$ is a flame configuration factor, $L_f$ is the longitudinal integral length scale, $\eta_L$ is the preheat zone thickness based on $a_S/S_L$.

For an example, the dotted dashed line plotted in Fig.5 is calculated by Eq.(4) and (5) for the hydrogen mixture (H113–15). Here, H113–15 shown in Fig.5 denotes a mixture whose fuel, equivalence ratio and laminar burning velocity are hydrogen, 1.13 and about 15cm/s, respectively.

**Modeling of Turbulent Burning Velocity Characteristics**

The expression for the turbulent burning velocity by Eq.(4),(5) can be explained as follows.

The first term of Eq.(4) shows that the increase in turbulent burning velocity from the local burning velocity is in proportion to the geometrical increase of flame surface area by turbulence intensity. Here, the substantial increase of flame surface area is proportional to the square root of 2 over 2 times of turbulence intensity. $\alpha$ is a flame configuration factor taking account of the increase in the flame surface area with increasing the preheat zone thickness (being proportional to the flame thickness) of a turbulent flame of mean scale $L_f$. Thus, the first term expresses the increase of turbulent burning velocity due to the increase in turbulent flame area. Contrarily, the second term shows the decrease in turbulent burning velocity caused by flame stretch, which increases with Karlovitz number squared. Here, the first and second term affect the turbulent burning velocity independently.

In the next place, the Eq.(5) shows that the turbulent burning velocities keep the value of Eq.(4) at $K_a=0.5$ in the region $0.5<K_a\leq 1.0$.

Thus, the model can be simply comprehended as follows. The turbulence affects the turbulent burning velocity by increasing the flame surface area and stretching the flame. Consequently, the turbulent burning velocity and quenching limit are determined by the balance of both effects. The former effect predominates until $K_a=0.5$ is reached, then the two effects conflict over 0.5 of $K_a$ and the flames is finally extinguished when $K_a$ exceeds 1.0.

In Fig.5 the thin broken line represents the Eq.(4) at $L_f$ being infinite when turbulence intensity reaches 0. This line shows the hypothetical case where only the increase in the flame surface area exists under no stretch of flame. From the observation of premixed turbulent flame by using a schlieren-photography and an ion-probe method, and a report on the local configuration of a high-intensity turbulent flame, it was found that the dominant turbulence scale which affects the configuration of flame is about the order of the integral length scale or mean spatial scale of turbulence. On the other hand, the scale which is essential to the flame stretch is about the order of the Taylor’s micro length scale as shown in the Karlovitz number.

Figure 5 shows that the measured turbulent burning velocity at $K_a=0.5$ is about three fourths times as much as the hypothetical turbulent burning velocity where solely the increasing effect of flame surface area by turbulence exists shown by the thin broken line. Thus, the optimum point of both effects exists at $K_a=0.5$ where the decreasing effect of burning velocity by smaller scales of turbulence is about a quarter times as much as the increasing effect of flame surface area by larger scale turbulence. Then, the two effects are conflicting over $K_a=0.5$, of course, the quenching effects
becomes more predominant and at last the chemical reaction cannot be maintained over $K_a=1.0$, where the effect of flame stretch inhibits the existence of any reaction sheets, leading to the extinguishment of whole flame.

Therefore, the turbulence scale depending on the turbulence generating system, as well as the preheat zone thickness and the local burning velocity depending on the composition of mixtures play important roles in the maximum value of turbulent burning velocity.

Equation (4) and (5) have been derived based on the experimental results for mixtures with $S_r/S_{Lo}=1.0$. But, it seems probable that they can be applied not only to the mixtures with $S_r/S_{Lo}=1.0$ but also to the any other mixtures. In order to examine it, the predicted velocities with the model equations, using the local burning velocity given by the relationship in Fig.2, are compared with the measured velocities. Figure 6 shows the measured and calculated ratio of turbulent burning velocity $S_r$ to the laminar burning velocity $S_{Lo}$ against the Karlovitz number $K_a$ for methane, propane and hydrogen mixtures. In Fig.6, the laminar burning velocity is taken as the local burning velocity at $K_a=0$ in Eq.(4), and the predictions by Eq.(5) are drawn to the measured quenching limits. The predictions reproduce quantitatively well the experimental results regardless of the kind of fuel and the equivalence ratio. There are some differences between the predicted and measured velocities over $K_a=0.5$. These differences seem to be caused by the unstable combustion near the quenching limit.

**Generalization of the Model**

The discussion above was only for the mixtures whose laminar burning velocity is about 15cm/s. In order to examine the validity of the above discussion and the generality of the model, comparisons are made between the predicted velocities and the measured velocities for the methane-air and propane-air mixtures whose laminar burning velocities are different from the mixtures shown in Fig.2. Figure 7 shows the result, where the local burning velocity of each mixture $S_r$.

**Fig. 6** Comparison of predictions by a model with measurements of $S_r/S_{Lo}$ (for Mixtures with $S_{Lo}=15cm/s$)
was simply estimated as follows:

\[ S_L = \left( \frac{S_L}{S_{L0}} \right)_{15} \cdot S_{L0} \]  

(6)

where \((S_L/S_{L0})_{15}\) is the value of \(S_L/S_{L0}\) at \(S_{L0} = 15\) cm/s as shown in Fig.2.

Figure 7 shows that there is no measurements until the quenching limit is reached, however, that the predictions well reproduce the measurements for methane-air and propane-air mixtures whose equivalence ratio are varied from 0.7 to 1.0 and 1.0 to 1.5 respectively.

Judging from the results, the quantitative accuracy of the proposed simple model is confirmed for the mixtures where the kind of fuel, equivalence ratio and the laminar burning velocity are varied extensively.

It is desirable to apply the present model to the other existing data of turbulent burning velocities, however, the application of the model is difficult at the present time, due to the lack of information about mixture and turbulence parameters used in those experiments. For this reason, examination of the model is limited only to our data measured.

But, if the turbulence characteristics can be known or well estimated, the turbulent burning velocity of any mixtures may be calculated as follows. In the first place, the local burning velocity for a given mixture can be estimated by using Eq.(1) and a contour lines of laminar burning velocity such as Fig.1, or directly by Fig.2 and Eq.(6). In the second place, the turbulent burning velocity and quenching limit of the mixture can be predicted by Eq.(4) and (5) using the estimated local burning velocity.

Furthermore, it is well known that the turbulent burning velocity characteristic is closely related to the turbulent flame structure. Therefore, the flame structure can be possibly classified based on the Karlovitz number taking the preferential diffusion effect into consideration and may show a dramatical change near \(K_{Lr} = 0.5\), regardless of the kind of mixtures.

**CONCLUSIONS**

In this study, attempts have been made to predict the turbulent burning velocity characteristics based on the local burning velocity estimated experimentally, taking the preferential diffusion effect into consideration for the first time. The following conclusions are obtained.

1. At the quenching limit, the Karlovitz number based on the local burning velocity takes the value of about 1.0 regardless of the kind of fuel and the equivalence ratio.
2. The important factors affecting the turbulent burning velocity are the local burning velocity of turbulent flame, the preheat zone thickness and the turbulence scales.
3. The validity of the simple model proposed is confirmed, as the predicted velocities and quenching limits correspond quantitatively well with a variety of measured ones.

**REFERENCES**