Application of FGM Method Considering Preferential Diffusion and Flame Stretch to a Cylindrical Propagating Hydrogen Flame

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1 Introduction

To reduce greenhouse gas emissions, hydrogen (H_2), which emits no carbon dioxide when combusted, has been gathering attention as an alternative energy source to fossil fuels. Accordingly, the development of H_2 engines has been more and more advanced.

Numerical simulation is a powerful tool for the development of engines because it costs lower than the experiment and can calculate physical properties that are difficult to be measured in experiments. In numerical simulations of combustion, to rigorously predict the physical quantities, it is necessary to consider many chemical species and reactions by solving the chemical species' conservation equations and Arrhenius formulas. However, the computational cost of this approach is so high that the use of a turbulent combustion model is inevitable to perform three-dimensional numerical simulations of a full-scale combustor. A flamelet method [1] is a widely used combustion model that solves turbulent flames at a low computational cost using the laminar flamelet database. In particular, a flamelet-generated manifold (FGM) method [2], which is a type of flamelet method, is widely used for premixed flames.

The conventional FGM method assumes that Lewis numbers of all chemical species are unity. However, preferential diffusion induced from differential diffusivities of chemical species greatly influences H_2 flame properties because H_2 has a very high diffusivity. Therefore, the FGM method considering preferential diffusion (FGM-PD method) [3,4] is necessary. Previous studies (e.g., [4]) have shown that the FGM-PD method can accurately reproduce unstretched flame behaviors. In addition, it is known that the flame stretch strongly interacts with the preferential diffusion [5]. Therefore, the FGM method considering flame stretch (FGM-S method) [6] is also necessary to accurately predict H_2 flame properties. De Swart et al. [7] proposed the FGM method considering preferential diffusion and flame stretch (FGM-PD-S method) and applied it to a H_2/methane/air premixed flame. They performed the simulations at an equivalence ratio of 0.7, which is a condition where the effect of flame stretch on flame speed is small [8], and therefore more investigation at another equivalence ratio is required. Moreover, little research has been conducted on the applicability of the FGM-PD-S method to pure H_2 flames.

In this research, two-dimensional numerical simulations of outwardly propagating cylindrical H_2/air premixed flames are performed to investigate the applicability of the FGM-PD-S method to H_2/air premixed flames. The simulations are performed under various equivalence ratio conditions using a direct

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method, which directly solves the Arrhenius equation without any combustion model, the FGM-PD-S method, the FGM-PD method, and the FGM-S method. Those results are compared with respect to the prediction accuracy of flame speed and flame stretch rate.

2 Numerical method

In this study, two-dimensional numerical simulations are performed in four methods: the direct, FGM-PD-S, FGM-PD, and FGM-S methods. In the direct method, the governing equations are the conservation equations of mass, momentum, enthalpy, and mass fraction of chemical species. The details of the formula are given in [9]. A detailed reaction mechanism with 33 chemical species and 214 reactions, which is obtained by excluding reactions involving C atoms from AramcoMech3.0 [10] and considering N sub-mechanism by Glarborg et al. [11], is used to describe the reacrions of H_2/air combustion. The FGM-PD, FGM-S, and FGM-PD-S methods are all a type of combustion model called the flamelet method. The flamelet method assumes that a turbulent flame can be regarded as a set of laminar flamelets. In the flamelet method, instead of directly solving Arrhenius formulas in physical space, flame properties such as the temperature and the reaction rate are obtained from a pre-tabulated database comprised of laminar flamelet data.

In the FGM-PD method, a conservation equation of progress variable C written as follows is solved in addition to the conservation equations of mass and momentum.

$$\frac{\partial \rho C}{\partial t} + \nabla \cdot (\rho C \boldsymbol{u}) = \nabla \cdot \left\{ \rho \frac{D_C}{W} \nabla (WC) \right\} + \rho \dot{\omega}_C,$$

where ρ is the density, $\boldsymbol{u}$ is the velocity, D_C is the diffusion coefficient of C, W is the molar mass, and $\dot{\omega}_C$ is the reaction rate of C. In this study, C is defined as the mass fraction of H_2O (Y_{H_2O}). D_C is defined as $D_C = \lambda / (\rho c_p Le_{H_2O})$, where λ is the heat conductivity, c_p is the specific heat capacity at constant pressure, and Le_{H_2O} is the Lewis number of H_2O. D_C and $\dot{\omega}_C$ are obtained from the flamelet database using C as a reference parameter. The database is a compilation of characteristics of a one-dimensional unstreched freely propagating premixed flame as a function of C.

In the FGM-S and FGM-PD-S methods, the flamelet database contains not only unstretched flame data, but also data of stretched counter premixed flames with various flame stretch rates. Another reference parameter corresponding to the flame stretch rate is needed to characterize the stretched flames. This study adopts a mixture fraction Z based on Bilger's definition [12] as the additional reference parameter. Therefore, in the FGM-S and FGM-PD-S methods, a conservation equation of Z written as follows is solved in addition to the conservation equations of mass, momentum, and C.

$$\frac{\partial \rho Z}{\partial t} + \nabla \cdot (\rho Z \boldsymbol{u}) = \nabla \cdot (\rho D_{ZZ} \nabla Z) + \nabla \cdot (\rho D_{ZC} \nabla C)$$

The FGM-PD-S method, as well as the FGM-PD method, considers non-unity Lewis number that varies with chemical species and also varies locally, while the FGM-S method uses the unity Lewis number. D_C, $\dot{\omega}_C$, D_{ZZ} and D_{ZC} are obtained from the flamelet database, which compiles the flame characteristics as a function of C and Z. D_{ZZ} and D_{ZC} are written as,

$$D_{ZZ} = \frac{\lambda}{W \rho c_p} \sum_k \frac{z_k}{Le_k} \frac{\partial W Y_k}{\partial Z}, \qquad D_{ZC} = \frac{\lambda}{W \rho c_p} \sum_k \frac{z_k}{Le_k} \frac{\partial W Y_k}{\partial C},$$

where z_k is the coefficients, and Le_k is the Lewis number of chemical species k.

Here it is noted that although the computational cost of the one-dimensional numerical simulation of a spherical flame in spherical coordinate is low, one-dimentional calculation in a spherical coordinate

does not completely reproduce flame behaviors, such as the wrinkled flames often seen in lean hydrogen flames. Moreover, three-dimentional simulations are difficult to perform because of the computational cost. For these reasons, the simulations in this research are performed in a two-dimentional Cartesian coordinate system. It is also noted that stretch and curvature effects are different between spherical flames and cylindrical flames. The main focus of this research is to investigate the applicability of the proposed model to hydrogen flames with strain and curvature rather than to investigate the phenomenon of spherical flames. Therefore, the objective of this research can be achieved even by considering cylindrical flames in a two-dimentional Cartesian coordinate.

The computational domain is a square area ($20.48\,\mathrm{mm} \times 20.48\,\mathrm{mm}$), and outflow boundary conditions are given in all the boundaries. The computational grid is a uniform staggered grid with a grid spacing of 40 μm in a Cartesian coordinate system. As initial conditions, an unburnt H_2/air premixed gas with pressure $P = 0.1$ MPa, temperature $T = 300$ K, and equivalence ratios $\phi = 0.3$, 0.45, 0.7, 1.2 are given to the whole region except an ignition area. The ignition is achieved by giving the temperature and composition of burnt premixed gas to the center of the domain, and then the flame propagates outward. The computations are performed using an in-house code, FK^3 [13].

3 Results and discussion

Figure 1 shows the time series of temperature distributions at $\phi = 0.45$ obtained employing the direct, FGM-PD-S, FGM-PD, and FGM-S methods. As shown in this figure, the FGM-PD-S method predicts the temperature distribution well. Figure 2 shows the flame speed plotted against the flame stretch rate obtained employing the direct, FGM-PD-S, FGM-PD, and FGM-S methods. The flame stretch rate ε is defined according to a cylindrical geometry as follows.

$$\varepsilon = \frac{1}{A}\frac{dA}{dt} = \frac{1}{r}\frac{dr}{dt},$$

where A is the surface area of the flame front, r is the radius of the flame front, and the flame front is defined as the isoline of mass fraction of H_2O at 0.02. The FGM-PD-S method reproduces the tendencies of the direct method: an increase in flame speed under lean conditions and a decrease under rich conditions as the flame stretch rate decreases. These tendencies have also been observed in the experiments [8]. The FGM-S method does not agree well with the direct method, especially for $\phi = 1.2$. This is because the relation between flame speed and flame stretch rate is influenced by the Lewis number effect, while the FGM-S methods assumes unity Lewis number. On the other hand, the result of the FGM-PD method does not agree with that of the direct method under lean conditions. Only the FGM-PD method shows a negative flame speed for the case of $\phi = 0.3$, which can be explained as follows. $\phi = 0.3$ is an extremely lean condition and is close to the flammability limit for unstretched flames. In contrast, the lean flammability limit for highly stretched flames is much leaner. Therefore, the reaction rate of progress variable C ($= Y_{H_2O}$) in the FGM-PD method at $\phi = 0.3$ is much lower than the production rate of H_2O calculated with the direct method. In addition, the profile of C obtained with the direct method, which has a large gradient of C near the flame front, is used as an initial distribution for the calculation with the FGM-PD method. Hence, the underpredicted reaction rate of C in the FGM-PD method is not large enough to overcome the diffusion of C, and the flame shrank inwardly, which means the negative flame propagating speed, immediately after the start of the simulation. The minima in flame speed seen only in the FGM simulations can also be explained by the effect of initial conditions. For the direct simulation, $t = 0$ is set to the time when the effect of the initial condition has sufficiently disappeared, while for the FGM simulations, the profile of the direct simulation at $t = 0$ is used as the initial condition at $t = 0$. Therefore, the effect of the initial condition appears for the FGM simulations but does not appear for the detailed simulation in Figure 2.

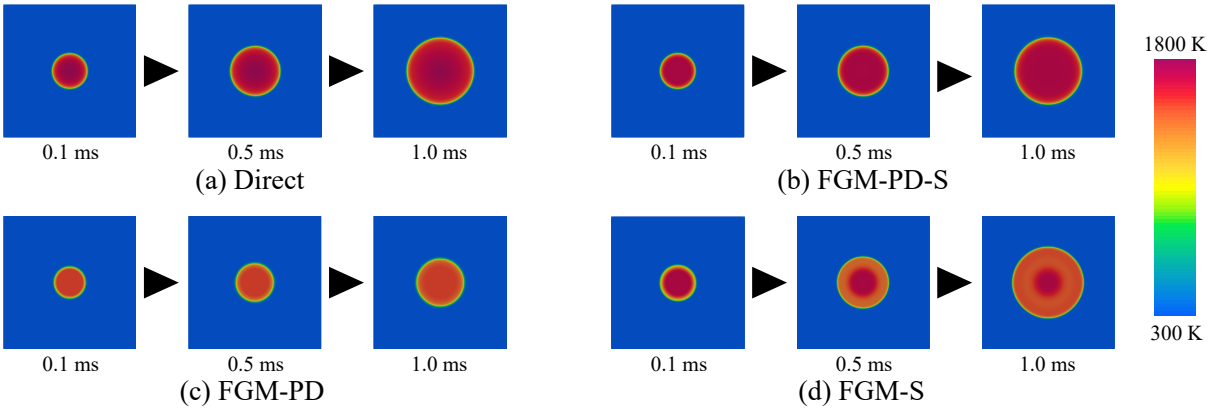

Figure 1: Comparison of time series of temperature distributions among (a) direct method, (b) FGM-PD-S method, (c) FGM-PD method, and (d) FGM-S method at an equivalence ratio of 0.45.

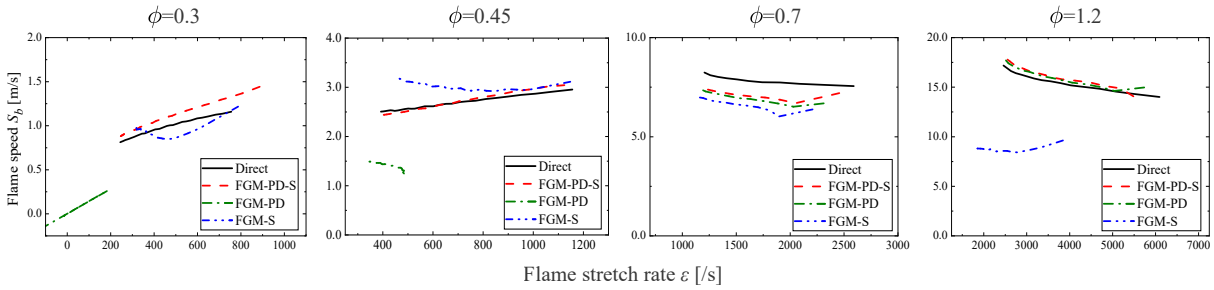

Figure 2: Comparison among the results obtained by the direct, FGM-PD-S, FGM-PD, and FGM-S methods about flame speed against flame stretch rate at equivalence ratios of $\phi = 0.3$, 0.45, 0.7, and 1.2.

4 Conclusions

In this study, two-dimentional numerical simulations of outwardly propagating cylindrical H_2/air premixed flames at equivalence ratios of $\phi = 0.3$, 0.45, 0.7, 1.2 was performed using the FGM-PD-S method considering preferential diffusion and flame stretch. It was found that the FGM-PD-S method could predict the H_2 flame properties more accurately than the FGM-PD and FGM-S methods under all equivalence ratio conditions.

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