

The Numerical Modelling of Laminar H₂ Flame Propagation in Vitiated Coaxial Flow

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1 Introduction

In low NO_x emission furnace, the exhaust gas recirculation is a key technique and has been studied for several decades. Moreover, in order to enhance combustion stability, the hot products can be recalculated and mixed with fresh air for turbulent combustion. It is believed that the flame propagation is an essential issue of considerable fundamental importance to combustor design and is also one of the significant factors controlling flame stability. The triple flames are responsible for flame propagation and stabilization in various nonpremixed or partially premixed stratified mixing layers. According to the previous study [1], during flame propagation, a complex combination of chemical reactions coupled with the fluid dynamics between the stoichiometric line and the preferred equivalence ratio line occurs. They also suggest that the leading point of the propagating flame is still dominated by the redirection effect, while the effect of the intrinsic chemical properties of the fuel mixture on a propagating flame has finite thickness cannot be neglected. To further extend our previous work, and to delineate the effect of temperature and diffusive properties of fuels on the triple flame propagation, the H₂ laminar jet flame propagations in a quartz tube with vitiated coaxial flow are numerically studied to study its burning phenomena, propagation, and flame structures.

With regard to hydrogen combustion, there are still several issues unsolved. Beyond this, however, it is difficult to use hydrogen as fuel with storage due to its low ignition energy, high flammability, and low volumetric energy density. It is well known that hydrogen is the lightest molecular with high diffusivity. It is highly flammable and burnt in air at a range of concentrations between 4 and 75% by volume [2]. It has also been applied to improve emission characteristics, flame stability and performance of combustors by blending hydrogen with hydrocarbon fuels. Several studies have been reported on the hydrogen application to IC engine[3], emissions of hydrogen-hydrocarbon combustion[4], burning velocity of blended fuel [5]and the flame propagation as well as the stabilization phenomena[1][6]. By preliminary paper surveying, several previous papers focused on the propagation of triple flames for the pure fuels and blended fuels. The flame propagation characteristics of pure fuels with high-temperature vitiated coaxial flow that contains combustion products have not been examined as yet. In this paper, a fundamental investigation on the propagation

characteristics of H₂ laminar jet flame in a well confined quartz tube with fresh air and vitiated coaxial flow is numerically studied.

2 Methodology

Similar to the previous study, to numerically model the transient propagation of the fuel-air flame, the time-dependent governing equations of continuity, momentum, energy, and chemical species are solved using the commercial package CFD-ACE+ 2010.0 coupled with chemical kinetic mechanisms from Li's mechanism[7]. The molecular transport and thermal data are obtained from the CHEMKIN package; the code then calculates the thermal conductivity and viscosity of the mixture using Wilke's formula. In addition, the gravitational effect is also included in the present study. The uniform flow of fuel and air at 0.4 m/s are specified at the inflow boundary of the computational domain. Fixed pressure boundary conditions are imposed on the open boundaries of the quartz tube exit. A non-slip, non-catalytic surface reaction and adiabatic conditions are applied to the quartz surface. The transport model also includes thermal diffusion to account for species diffusion due to temperature gradients. An axisymmetric, non-uniform staggered-grid system is used with a control volume formulation in accordance with the SIMPLEC algorithm, which is shown schematically in Fig. 1. To calculate the flame propagation effectively, a compromised grid was used in a grid-independence test. The total number of grids was 61 in the radial direction and 428 in the axial direction for a computational domain of 15 mm×150 mm and a minimum grid spacing of 0.05 mm. The minimum grid size was placed near the axis and the fuel-air mixing layer, and an enlarged grid size was used toward the outer boundaries. Convergence of the solution was declared when the ratio of the change of the dependent variables to the maximum variables in that iteration was less than 1×10^{-4} . The coaxial flow is made of lean premixed hydrogen/air catalytic combustions. The conditions for the present investigations of the fuel-vitiated oxidizer triple flame propagation as well as the calculated flue gas temperature and compositions of flue gas are listed in Table 1.

3 Results and Discussion

Fig. 3 shows the computed temporal propagation traces of flame leading tip for four flames. Note that the plot at $t = 0$ ms corresponds to the instant at which the flame reaches $x = 80$ mm. The results imply that the propagation velocity decreases as the equivalence ratio of mixture which is used to produce vitiated coaxial flow is increased. Despite the temperature of flue gas in the oxidizer stream is apparently increased. The flame structure can be distinguished by the H atom. Hence, the reaction zone in terms of H mass fraction for the cases of flames #1 and #3 are used to identify the propagation and structural transformation of leading flame. As shown in Fig. 3(a), the flame appears to be a bullet-headed structure during the propagation process from $x = 80$ to $x = 25$ mm. As the flame propagates further and approaches $x = 20$ mm, the rich premixed flame branch forms a hollow cone flame structure. For the case of case #3 flame propagation, it shows a similar manner to flame #1. However, the mass fraction of H of flame case #3 is slight weaker than that of flame case #1, and it implies that the pyrolysis rate of fuel need to be further identified.

To illustrate the triple flame structure of the propagating flame, the calculated H and heat release rate contours and the temperature and mixture fraction isopleths are shown in Fig. 4 for flame cases #1 and #3 for when the flame reaches $x = 10$ mm. For both flame case #1 and #3, the triple flame structure can be distinguished by the heat release rate. The distribution of OH and total heat release rate are slightly different.

4 Conclusions

In the present investigation, the propagation characteristics of H₂ laminar jet flame in a well confined quartz tube with coaxial fresh air and vitiated flow is numerically studied. Based on the

distribution of the isopleths of the mixture fractions as well as the chemical reactions, this paper characterizes the formation of the reaction zone, the ignition of fuel, the transformation of the flame base structure, and the propagation phenomena of the jet flame base.

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Table 1: The conditions of the vitiated coaxial oxidizers

case no.	oxidizer (flue gas of H ₂ -air combustion with different ϕ)				
	T(K)	O ₂	N ₂	H ₂ O	
1	300	0.233	0.767	0	
2	631.89	0.209	0.765	0.0262	
3	783.49	0.197	0.764	0.0392	
4	806.88	0.195	0.763	0.0413	

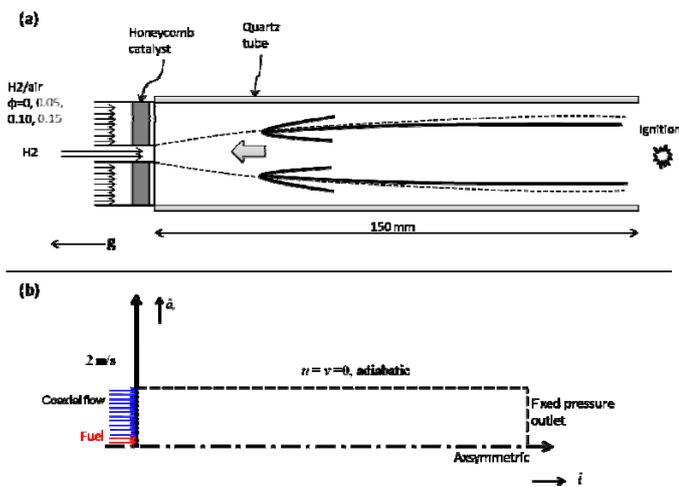


Figure 1. experimental apparatus and numerical simulation domain

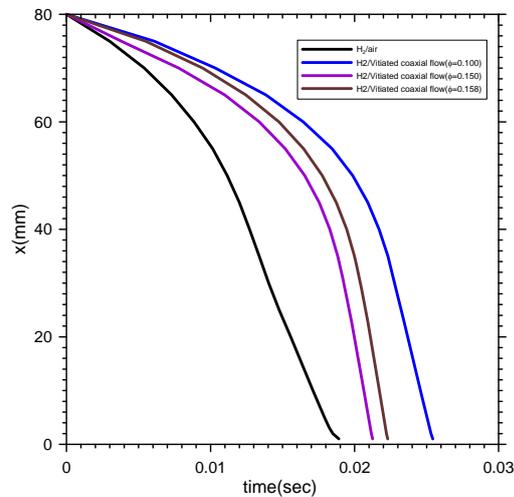


Figure 2. Computed axial flame position

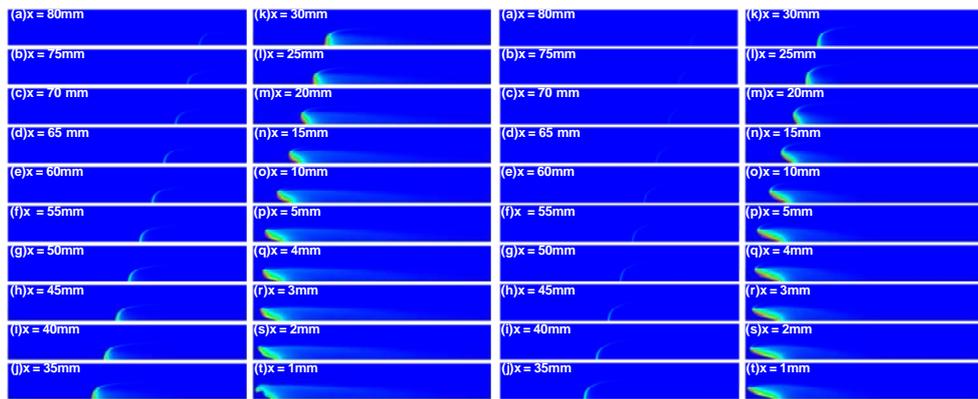


Figure 3. Propagation and structural transformation of H₂-air (flame # 1) flames (left) and H₂-flue gas of $\phi = 0.15$ (case # 3) (right) as the leading point approaches different locations.

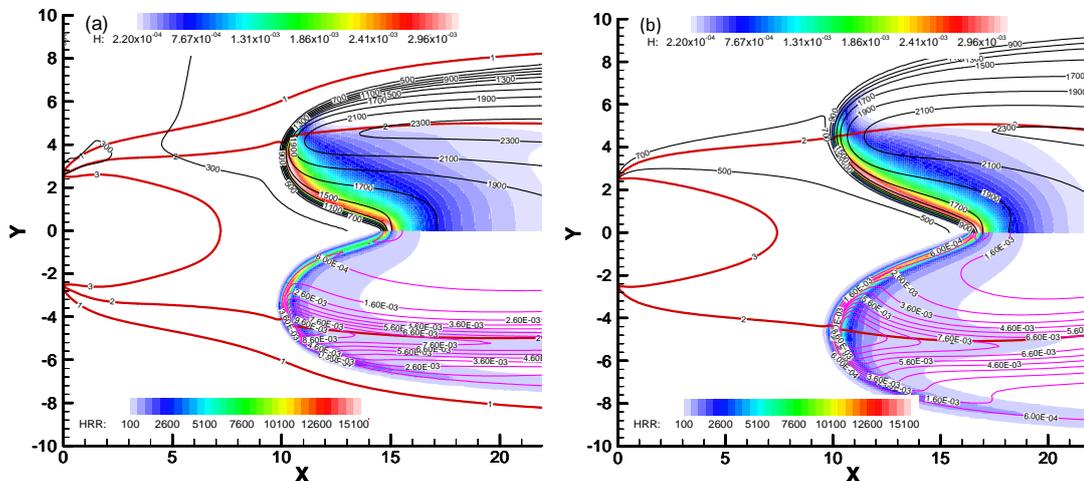


Figure 4. Flame base structure of the propagating flame for flames #1 (a) and 3 (b) in terms of the calculated H and heat release rate contours, the temperature, OH and mixture fraction isopleths.

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