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Combustion characteristics and flame bifurcation in repetitive extinction-ignition dynamics for premixed hydrogen-air combustion in a heated micro channel

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A B S T R A C T

The characteristics of repetitive extinction-ignition dynamics of flames are investigated numerically for hydrogen-air mixtures in a heated micro channel. A Low Mach number formulation, detailed chemical kinetics and different molecular diffusivities for each species are utilized in all simulations. In this regard, the effects of inlet velocity, equivalence ratio, and channel width on amplitude and frequency of the repetitive extinction-ignition phenomenon is studied. The results show that the frequency of repetitive extinction-ignition dynamics increases with increasing the inlet velocity, while its amplitude has an ascending-descending behavior. With increasing equivalence ratio from 0.5 to 1 and the channel width from 0.4 to 1, the amplitude of repetitive extinction-ignition dynamics increases and the frequency decreases. Regarding flame bifurcation, the details of the flow field show that the creation of recirculation zones at the wall vicinity causes the flame bifurcation. Investigating the role of chemical kinetics, it is found that the mass fractions of O_2 and H_2O increase inside the zone between the two flame fronts. As a result, the related reactions are activated and produce heavier species such as H_2O, HO_2 and H_2O_2. The heavier species absorb more heat, released from the combustion process, causing temperature reduction and lastly flame bifurcation.

1. Introduction

By recognizing the widespread application of micro scale devices, there is a renewed interest in fundamental investigations of combustion phenomenon in micro scale devices. Coupling between the flame and the walls as a result of reducing the combustion chamber size expands the flammability limits. The effect of wall conductivity, external heat loss and wall thickness on the flammability limits were studied by Norton and Vlachos for stoichiometric CH_4-air [1] and C_3H_8-air [2] combustion. They showed that each variable is bounded by a lower and upper limit with an extreme point located between them. Wan et al. [3] investigated numerically the effect of various pressure levels ($P = 1.0–3.0$ atm) on the blow-off limit of CH_4-air flames. Their results showed that blow-off limit increases first and then decreases by increasing in pressure level. Baigmohammadi et al. [4] studied combustion characteristics of premixed CH_4-H_2/air in a micro reactor equipped with a catalytic bluff body. Their results showed that the use of catalytic bluff body in the center of a micro reactor can significantly increase the flame stability, especially at high velocities.

On the other hand, this coupling between the flame and the walls can dramatically change the characteristics of flame dynamics. Maruta et al. observed experimentally different flame dynamics such as mild combustion, FREI (flame with repetitive extinction-ignition) and steady combustion close to the lower flammability limit (lower velocity), intermediate velocity and close to the upper flammability limit (upper velocity), respectively. They studied flame propagation in the straight [5] and U-shaped [6] heated micro channels for CH_4-air and C_3H_8-air mixtures.

Steady combustion and repetitive extinction-ignition dynamics have been also reported in the experimental work of Richecoeur and Kyritsis for CH_4-air mixture in a curved combustor with various diameters [7].

Pizza et al. studied numerically the premixed lean H_2-air combustion in two- ([8,9]) and three-dimensional [10] heated micro channels with direct numerical simulation. They also distinguished different flame dynamics including mild combustion, FREI,

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Nomenclature

c_p	Heat capacity (J/kg-K)
d	Channel height
D_{im}	Average diffusivity of the ith specie (m^2/s)
hi	Enthalpy (kJ/kg)
I	Identity matrix
L	Channel length
Le	Lewis number
Ng	Species number
p_t	Thermodynamic pressure (Pa)
p_d	Hydrodynamic pressure (Pa)
q_j	rate of each reaction
R	Gas constant(J/kg-K)
R_u	Universal gas constant(J/kmol-K)
S	Stress tensor
T	Temperature (K)
T_w	Wall temperature
T_N	Dimensionless temperature
t	Time
u	Velocity vector (m/s)
U_{in}	Inlet velocity
V_i	Diffusion velocity of the ith specie (m/s)
V_c	Correction diffusion velocity (m/s)
V_i^*	Diffusion velocity of the ith specie (m/s) calculated by kinetic theory
$\overline{W}$	Mean molecular weight of the mixture
x	Coordinate along x axis
Y_i	Mass fraction of the ith specie

Greek Symbols

ρ	Density (kg/m^3)
μ	Dynamic viscosity
λ	Mixture thermal conductivity
$\dot{\omega}_i$	Rate of reaction of the ith specie (kmol/m^3-s)
Φ	Equivalence ratio

Abbreviations

HRR	Heat release rate
FREI	Flame with repetitive ignition-extinction
PLIF	Planar Laser-Induced Fluorescence

Subscripts

w	Wall
in	Inlet
i	ith species
ij	ith species in jth species
im	ith species in mixture

symmetric and asymmetric steady combustion and oscillating flame. However, the physics behind these behaviors is still a topic of discussion and the reasons are not fully understood.

Fan et al. developed a new experimental framework to survey the flame propagation and FREI phenomenon in very thin quartz channels ([11–13]). Their results illustrated that the flame pattern formations are functions of the inlet mixture velocity and equivalence ratio.

Nakamura et al. examined FREI phenomenon for the CH_4-air combustion in a channel with a prescribed temperature gradient on the external wall [14]. In this reference, the detailed behavior of this phenomenon is studied based on a one-dimensional plug flow model for CH_4-air mixture. Their results showed that the flame bifurcation occurs twice for the CH_4-air mixture. The first bifurcation occurs when the flame is propagating toward upstream and downstream. Methane is consumed completely in one of the flame fronts, while CO remains unreacted behind the flame front. By weakening the reactions, the second bifurcation occurs which is due to the presence of the intermediate species such as CH_3, CO, H and OH in the downstream of flow.

Tsuboi studied the CH_4-air combustion in a heated micro-channel of 2 mm inner diameter [15]. Their experimental and numerical results showed the steady combustion and FREI dynamics. They used one-dimensional thermal-diffusive equations in the numerical simulation. Yamamoto et al. [16] investigated the combustion characteristics of n-heptane-air in a heated micro-channel. Weak flame and FREI dynamics were observed in both experiment and numeric.

Stazio et al. [17] developed a new experimental device consist of a micro tabular channel with an external heating source. They reported three distinct flame behaviors (stable flame, FREI and weak flame) over a wide range of equivalence ratios (0.5–1.5) and flow velocities. Miyata et al. [18] conducted a DNS (Direct Numerical Simulation) of micro combustion in a heated narrow circular channel for CH_4-air mixture. They reported unsteady behaviors of the flame such as the oscillating flame and the flame repetitive extinction and ignition (FREI) depending on the inflow temperature and the wall temperature gradient. They also presented that the amplitude and period of FREI have linear relationships with the wall thermal thickness based on the wall temperature gradient. Kamada et al. [19] investigated combustion and ignition characteristics of natural gas components such as methane, ethane, propane and n-butane experimentally and computationally using a micro flow reactor with a controlled temperature profile.

In the recent work of the authors [20], the propagation of H_2-air mixture flame was investigated numerically in a heated micro channel. In this study, FREI, symmetric steady flame and asymmetric steady flame were observed by varying inlet velocity. Upon increasing the inlet velocity, a symmetric flame was formed due to the balance between time scales. Further increase of the inlet velocity made the flame unstable and established an asymmetric steady flame. The detailed behavior of FREI phenomenon was examined using the variations of HRR (heat release rate), temperature and H_2, O_2, OH and H_2O mole fraction. In this study, FREI was classified into five phases namely initiation, ignition, propagation, weak reaction and flowing phase. During the initiation phase, two peaks for HRR are formed. In the ignition phase the HRR peak rises significantly and the flow temperature increases due to the chemical reactions. In the propagation phase, the HRR peak splits into two parts moving toward upstream and downstream. During the weak reaction phase, there are three peaks for the HRR. Finally in the flowing phase, the overall reaction intensity drops and channel is filled again with fuel/air mixture. In the initiation and ignition phases, there is considerable amount of hydrogen/air mixture in downstream, which is consumed in the propagation phase results in flame bifurcation.

Different experimental and numerical works have attempted to investigate FREI phenomenon as a principal dynamics in small-scale combustion. Knowledge of FREI physics is helpful to apply this dynamics in different devices. Since the frequency of temperature variation in this dynamics is high; this temperature variation can be utilized as a source of temperature variation in future applications and in any devices working at high temperature ranges such as thermophotovoltaic devices as well. On the other side, high