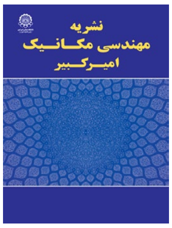

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Maps of Flame Dynamics for Premixed Lean Hydrogen-Air Combustion in a Heated Microchannel

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ABSTRACT: In the present work, flame dynamics are extracted for combustion of premixed lean hydrogen-air in a heated microchannel using numerical simulation. In order to simulate the combustion phenomenon at this scale, Navier-Stokes equations along with energy and species conservation equations are considered by formulation of low Mach number and with consideration of detail chemical kinetics. Regarding different conditions, three dynamics is observed in the micro channel including periodic repetitive ignition-extinction, steady symmetric flame and steady asymmetric flame. Effects of different parameters such as inlet velocity, equivalence ratio, and channel width are investigated on the flame dynamics. .

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1- Introduction

In recent years, many efforts have been done to develop energy supply systems based on the small-scale combustion. Maruta et al. [1] experimentally investigated the combustion characteristics in a mesoscale combustor. They observed that variation of inlet flow velocity will be affected by the type and location of the flame. Ju et al. investigated the propagation and extinction of propane-air [2] and methane-air [3] in mesoscale by analytical and experimental methods. Pizza et al. reported periodic repetitive ignition-extinction flame, steady symmetric flame, static asymmetric flame, and oscillating and pulsating flames in a Two-Dimensional (2D) channel [4] and the Three-Dimensional (3D) tube [5] by direct numerical simulation approach.

In the present work, the effects of geometrical and flow parameters on microscale combustion dynamics are investigated by numerical simulations with further details. The effects of flow velocity, equivalence ratio, and channel diameter are investigated on the dynamics of periodic repetitive ignition-extinction flame, steady symmetric flame, and steady asymmetric flame.

2- Numerical Method and Governing Equations

In the present work, in order to simulate the combustion in the small-scale, Navier-Stokes equations along with the energy conservation and species conservation equations are solved using low Mach number formulation [5].

Mass conservation:

$$\frac{\partial \rho}{\partial t} + \nabla.(\rho u) = 0 \qquad (1)$$

Momentum conservation:

$$\rho\left(\frac{\partial u}{\partial t} + u.\nabla u\right) = -\nabla p_d + \nabla.(\mu S) \qquad (2)$$

where ρ, u and μ are density, velocity vector, and dynamic viscosity, respectively. Stress tensor *(S)* is expressed as $\nabla u + (\nabla u)^{T} - \frac{2}{3}(\nabla u) I$ in which I is the unit matrix.

Energy equation in fluid:

$$\rho c_p\left(\frac{\partial T}{\partial t} + u.\nabla T\right) = \nabla.(\lambda \nabla T) - \sum_{i=1}^{N_g} h_i \omega_i - \rho\left(\sum_{i=1}^{N_g} c_{p,i} Y_i V_i\right).\nabla T \qquad (3)$$

where λ is the thermal conductivity of the mixture, and c_p and h_i are the thermal capacity and enthalpy of the i^{th} species.

According to the above explanation, it can be said that in flow with a Mach number lower than $\hat{p}_d \ll \hat{p}_t$, the equation of state of the perfect gas is written as follows:

$$p_t = \rho \frac{R}{\overline{W}} T \qquad (4)$$

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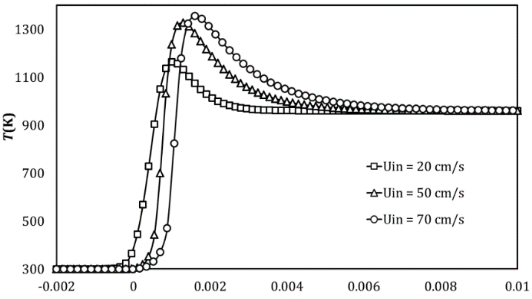

Fig. 1. Flow temperature variations along the channel symmetry line for different inlet velocities

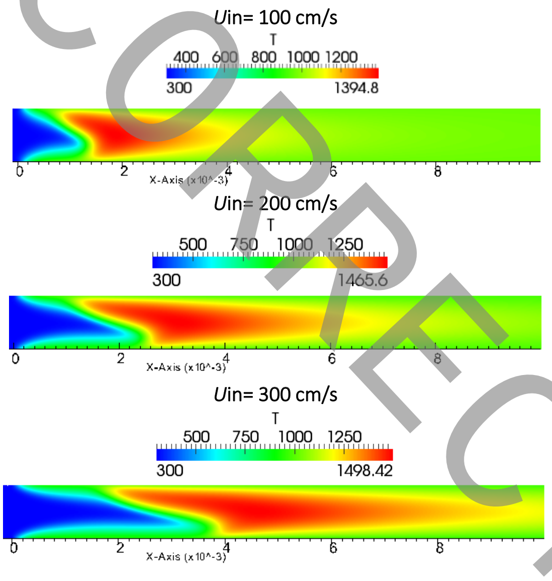

Fig. 2. Temperature contours for different inlet velocities

where $\overline{W}$ and R are the average molecular weight of the mixture and the ideal gas constant, respectively.

Mass conservation equation of ith species:

$$\rho\left(\frac{\partial Y_i}{\partial t}+u.\nabla Y_i\right)=-\nabla.\left(\rho Y_i V_i\right)+\dot{\omega}_i \tag{5}$$

where $\dot{\omega}_1$ is the rate of reaction of i^{th} chemical species, and Y_i and V_i are the mass fraction and the diffusion velocity vector. D_{mi} is the diffusivity of i^{th} species in the mixture.

One of the common geometries for analysis of small-scale combustion is heated microchannel which has been used in many studies [5-7]. A specific part of the channel is considered as the test section and the temperature of its walls is increased with the use of an external source. The mixture of hydrogen and air enters from one channel side with an equivalence ratio of 0.5 and temperature of 300 K.

The mechanism of 9 species and 27 reactions from Yetter et al. [8] are used for the kinetics of the gas phase, which is shown in Fig.1. Also, to calculate the molecular diffusion coefficients, the data of Chemkin [9] has been used.

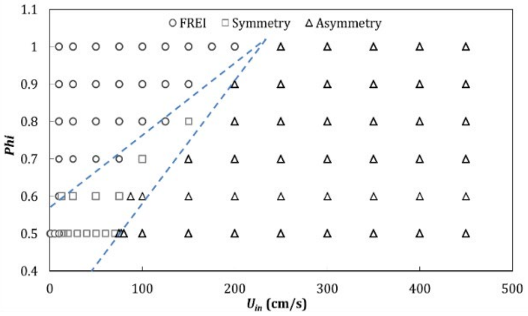

Fig. 3. Flame dynamics diagram-Effect of velocity and equivalence ratio for a channel width of 1 mm

3- Results and Discussion

In the heated microchannel, the temperature of the outer side is risen by external high-temperature source. Regarding different conditions, there exist three specific dynamics for flame: periodic repetitive ignition-extinction dynamics, steady symmetric flame, and steady asymmetric flame. In each dynamics, the effects of inlet flow velocity, equivalence ratio and channel width on the flame dynamics are investigated. The range of 10 to 400 cm/s is considered for inlet flow velocity as well as the range of 0.4 to 1 mm for the channel width and the range of 0.5 to 1 for the equivalence ratio.

The maximum value of the Reynolds number for the predetermined ranges is 212 by considering the value of 0.1887 cm2/s for the kinematic viscosity. Given the calculated value of the Reynolds number, it can be ensured that the flow is laminar and finally the maps of flame dynamics could be presented.

3- 1- Periodic repetitive ignition-extinction dynamics

Near the lower flammability limit, the periodic repetitive ignition/extinction dynamics is observed. Due to the high temperature of the wall (960 K), the flow temperature increases gradually by entering into the channel from 300 K and the reactions will begin. By increasing the intensity of chemical reactions and increasing the flow temperature due to the increase in the reaction rate, the maximum mass fraction of OH radical will shift toward the symmetry line. This distribution propagates toward the downstream and upstream and a wide region of reaction rate is observed throughout the channel. A portion of the flame which moves to the downstream consumes the unburned gases of that region, and another part of the flame which flows to upstream consume its unburned fresh. By moving the flame fronts toward the downstream and upstream, a bifurcation is created between the reaction zones. The downstream part is quickly weakened due to the lack of fuel, but in the upstream part a more resistant is observed due to the existence of fresh fuel-air mixture. However, it has been also influenced by the low-temperature region of the wall, consequently, the reaction rate weakens with time. As long as the inlet flow velocity overcomes the propagation velocity of the flame, the inlet flow will be dominated to the flame and moves it's toward end of the channel. After heating again by walls, the flow begins again by the next cycle wall.

3- 2- Steady symmetric flame dynamics

By increasing the inlet flow velocity in a channel with a specific width, the periodic repetitive ignition-extinction dynamics disappear and the steady symmetric dynamics are observed.

As the inlet flow velocity increases, the flame front moves the downstream and since the wall temperature value at the downstream is higher than the temperature of the beginning of the channel, the flow has a more chance of preheating, which results in an increase in the flame front temperature.

According to the obtained results, it is observed that the flame front is thicker at lower velocities. By increasing the inlet flow velocity, the thermal thickness of the flame front decreases, and then this amount increases by more increment in the inlet flow velocity. Hence, the descending-ascending behavior for the thermal thickness of the flame front is observed by increasing more in the inlet flow velocity.

3- 3- Steady asymmetric flame

By increasing the inlet flow velocity of flow through a channel with a specific width, the steady symmetric flame becomes unstable due to the flow perturbation and then it will restore in the steady state by forming an asymmetric shape. These flames are arranged at angles greater than or equal to 90° relative to the direction of flow, called upper asymmetric flames or lower asymmetric flames [10]. The effect of the inlet flow velocity on the steady asymmetric flame in channel width of 1 mm and fuel-air mixture with an equivalence ratio of 0.5 is shown in Fig. 2 using temperature contours and mass fraction contours of OH radical. With an increase in the inlet flow velocity from 100 to 300 cm/s, the flame front becomes larger in a way that the point of flame closer to the bottom wall is moved toward the downstream.

By moving the flame front toward the downstream, the surface of the flame front increases, leading to an increase in the rate of heat release and thus rise the temperature. As the flow temperature increases, reactions of the light radicals become more active and the number of light species such as OH increases in the channel. Therefore, the maximum temperature and the mass fraction of OH radical increase by increasing the inlet flow velocity. The temperature distribution on the symmetry line for the different inlet velocities at an equivalence ratio of 0.5 for a channel width of 1 mm is shown in Fig. 2. As the inlet flow velocity increases, the flame front extended, so the location of the flame front (the region between the minimum and maximum value of temperature) is shifted to the downstream symmetry line.

3- 4- Maps of flame dynamics for microscale combustion

The flame dynamics diagrams for variations in the inlet flow velocity, the equivalence ratio for a channel width of 1 mm is shown in Fig. 3. According to the results, it is observed that the amplitude of the flame dynamics is extended with increasing channel width.

4- Conclusions

In the present work, the combustion of hydrogen-air premixed in a heated microchannel has been simulated to observe the flame dynamics. To simulate the combustion phenomenon at this scale, the Navier-Stokes equations with energy and species conservation equations were considered with the formulation of a low Mach number. The periodic repetitive ignition-extinction dynamics are observed at low velocities near the lower flammability limit. By increasing the inlet flow velocity and balancing between the reaction time scale and fluid residence in channel time scale, a steady symmetric flow is observed in the channel. In this case, the maximum value of temperature and the mass fraction of species are located on the symmetry line of channel. By increasing the inlet flow velocity in a specific channel, the flame moves toward the channel downstream in the symmetry line of the channel and it stretches near the wall. In this case, the surface of the flame front is susceptible to instability and is converted to unstable flame due to the turbulences in the channel. The maps of flame dynamics in small-scale for a hydrogen-air mixture were presented based on three parameters of inlet flow velocity, equivalence ratio, and channel width in a microchannel. According to the obtained results, it is observed that the steady symmetric dynamics are eliminated by increasing the equivalence ratio, channel width, and inlet flow velocity and replaced by steady asymmetric dynamics.

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