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Hetero-/homogeneous combustion characteristics of premixed hydrogen-air mixture in a planar micro-reactor with catalyst segmentation

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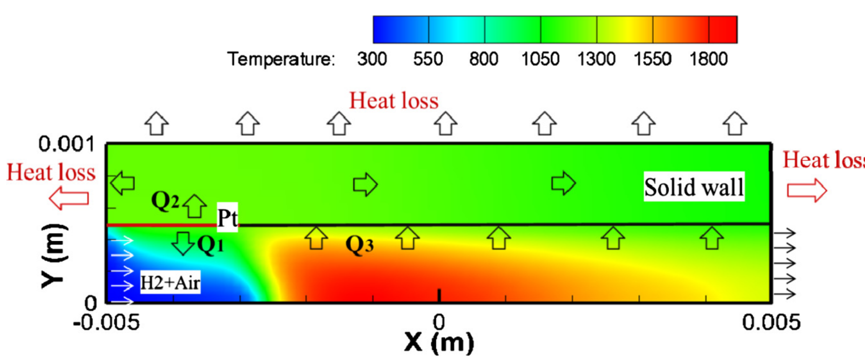
HIGHLIGHTS

- Hetero-/homogeneous combustion characteristics are investigated in a micro reactor.
- The homogeneous ignition distance increases with increasing inlet flow velocity.
- Intense inhibition of heterogeneous reaction on homogeneous reaction at large velocity.
- Flame speed in the catalytic combustor is lower than that in the conventional combustor.

GRAPHICAL ABSTRACT

The heat transfer from the catalytic surface to the gaseous mixture in the catalytic zone exhibited a high intensity under the large flow velocity. The preheated incoming flow improved the heterogeneous reaction to inhibit the homogeneous reaction.



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ABSTRACT

Numerical simulation of stoichiometric hydrogen-air premixed flame in a platinum-coated micro channel was performed to investigate hetero-/homogeneous combustion characteristics. An elliptical two-dimensional (2D) Computational Fluid Dynamics (CFD) model with detailed reaction mechanisms for homogeneous (gas phase) and heterogeneous (catalytic) reactions was adopted. The hetero-/homogeneous reaction characteristics with different inlet flow velocities and flame speeds were used to evaluate the effect of heterogeneous reaction on homogeneous reaction in the combustor with 2 mm length of catalyst segmentation. The effect of heat generation of the heterogeneous reaction was also analyzed. The numerical results indicated that the highest temperature in the catalytic combustor was lower than that in the combustor without catalyst. In the presence of heterogeneous reaction, the species (OH) concentration near the catalytic surface decreased significantly due to the dominated heterogeneous reaction at that region. The homogeneous ignition distance increased with increasing inlet flow velocity. The heat transfer from the catalytic surface to the gaseous mixture in the catalytic zone exhibited a high intensity under the large flow velocity, and the preheated incoming flow improved the heterogeneous reaction to inhibit the homogeneous reaction. The decreased flame speed in the catalytic combustor further demonstrated that the homogeneous reaction was suppressed by the heterogeneous reaction.

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1. Introduction

Catalytic micro combustors have several conspicuous advantages as compared with homogeneous micro combustors and have recently received much attention in the combustion research community. The reactors with catalyst do not only have the advantages with respect to the conventional micro combustors, but also transcends the operated maps of micro scale combustion, due to the exothermicity induced by catalytic reaction and allowing chemical reactions to be initiated under low temperature (Chou et al., 2011; Ju and Maruta, 2011). The well-designed reactors are extensively applied in micro power devices, propellant systems and catalytic reforming systems (Yang et al., 2017; Tang et al., 2015; Deshmukh and Vlachos, 2005; Guan et al., 2008).

It is a fact that, high surface-to-volume ratio is beneficial to the initiation of catalytic reaction in the micro combustor and heterogeneous catalysis is employed to enhance reaction rate and wall temperature (Deutschmann et al., 2000; Li et al., 2010; Kaisare et al., 2008). The physical and chemical processes in the catalytic combustors are intertwined, thus the interplay between heterogeneous and homogeneous reactions is difficult to clearly understand. It has been established in previous works that, the inhibition effect of heterogeneous reaction on the homogeneous reaction is displayed by means of the competitive consumption of reactants and formation or depletion of radicals on the surface (Vlachos, 1996; Lu et al., 2016b). This characteristic is usually conducive to mitigate the intrinsic flame instabilities under the limited conditions. Pizza et al. (2009, 2010) discussed the effect of heterogeneous catalysis on the inhibition of the flame dynamics in a micro scale channel with 1 mm of height. They found that catalytic reaction could inhibit significantly the unsteady and asymmetric flame via coating the channel walls with platinum (Pt). Small perturbations of the gaseous reactivity with the increase of catalytic reactivity resulted in the suppression of the flame dynamics by theoretically predicting sensitivity of the homogeneous ignition distance. The reaction pathway via the transport of the reactant (fuel) mainly affected the homogeneous ignition (Mantzaras and Appel, 2002). In addition, Mantzaras and Benz (1999) proposed a closed-form implicit ignition criterion in terms of non-dimensional groups that were relevant to confined flows and based on the geometrical, flow, chemical, and transport parameters. The increase of the homogeneous ignition distance with increasing inlet velocity was shown analytically in the homogeneous ignition criterion (Mantzaras and Benz, 1999). Nevertheless, the catalytic reaction can effectively enhance the combustion efficiency in the catalytic micro-combustor (Wang et al., 2010).

The purely heterogeneous reaction characteristics have been widely investigated. Smyth et al. (2009, 2012) analyzed the heterogeneous reaction for the heated mixtures (i.e. methane/air and propane/air) over Pt coupons experimentally. The results showed that three phases of the reactive layer along the flat plate were established, and this could be used as a guide for catalytic combustor miniaturization. Subsequently, Badra et al. (2012, 2013a, 2013b) applied series of alkenes to explore the surface-gas chemistry interaction of Pt foils under different initial conditions of the incoming mixture. The corresponding numerical model was developed to simulate catalytic reaction. The results indicated that differential molecular as well as thermal diffusions disrupted the atomic balance resulting in leaner mixtures near the foil. Lu et al. (2016a) reported that the effect of heterogeneous reaction on the homogeneous reaction had an intense inhibition effect when the catalyst segment of 1 mm was placed at the inlet. Lu et al. (2017) investigated the chemical coupling after homogenous ignition under low velocity (1.5 m/s), and the results demonstrated that the heterogeneous reaction mainly occurred at the upstream channel. Chen et al. (2016) investigated numerically the kinetic effects of additional hydrogen on the catalytic self-ignition of lean methane-air mixture. Hydrogen addition could effectively cause catalytic self-ignition of methane-air mixture in micro-channels with 4 mm of length.

Hydrogen is considered as a fine fuel for micro combustors due to its high burning rate and heat value. In our previous works, (Lu et al., 2016a, 2016b, 2017), the oxidization of hydrogen fuel over the Pt catalyst was investigated to illustrate the effect of heterogeneous reaction on the homogeneous reaction. The primary objective of this study is to explore further the interaction between heterogeneous reaction and homogeneous reaction after the homogeneous ignition in the catalytic combustor. An elliptical 2D numerical model was used for the numerical simulation with detailed hetero-/homogeneous reaction mechanisms for H_2/air mixture over Pt catalyst. The combustor with catalyst segmentation of 2 mm length was proposed to demonstrate the characteristics of hetero-/homogeneous reaction under different inlet flow velocities and the effect of heat generation of the heterogeneous reaction on the homogeneous reaction characteristics.

2. Numerical approach

2.1. Physical model

The numerical model used in this work was based on a conventional micro combustor with a rectangular channel used in earlier studies (Lu et al., 2017). Fig. 1 shows the schematic diagram of the micro combustor. The catalyst segment with 2 mm length was placed on the inner surface of the combustor, and the surface site density was 2.7×10^{-9} mol/cm^2. The auxiliary axis located at y = 0.4875 mm was employed to describe clearly the variation of homogeneous reaction characteristics near the inner wall. The high thermostability of 316L stainless steel was used as wall material of the combustor. For the operation process, the premixed gaseous mixture flowed through the channel from left to right.

An elliptical 2D structure (x and y) was considered as computational domain due to the high aspect ratio of the micro combustor (10 in this study). Half of the combustor was employed to reduce the computational load. A structured grid was adopted in the computational domain, and Fluent software was employed for the simulation (Fluent Inc., 1999). Centerline gaseous temperature profiles with different grid sizes in the channel are depicted in Fig. 2. To save computational time and meet the precision requirement, the optimized grid with 12,000 (400 × 30) cells was used in the computational domain. The locally refined mesh was employed to describe the gas-surface reaction near the wall.

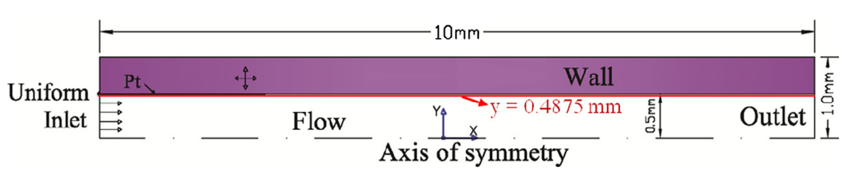

Fig. 1. Schematic of the computational domain.