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Hetero-/homogeneous combustion of premixed hydrogen–oxygen mixture in a micro-reactor with catalyst segmentation

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ABSTRACT

Numerical simulations with detailed homogeneous (gas phase) and heterogeneous (catalytic) chemistries of premixed hydrogen–oxygen mixture were performed inside a rectangular micro-combustor. The effects of catalytic walls on the homogeneous combustion were investigated via varying catalyst segment layouts and sizes. The interactions between heterogeneous and homogeneous reactions were discussed. It was shown that the heterogeneous reactions become weak when the catalyst disposition is shifted toward the outlet along the streamwise. The homogeneous combustion also becomes obviously weakened downstream behind the catalyst segmentation, except the exit. Moreover, with increasing catalyst segment size, the hydrogen conversion ratio increases and the mean outlet temperature reduces. The competition of the fresh fuel between the heterogeneous and homogeneous reactions result in the inhibition of heterogeneous reactions on homogeneous combustion. In summary, the heterogeneous reactions can obviously improve the combustion efficiency in a micro catalytic combustor. As expected, the effects of catalytic walls were more pronounced for the micro combustor systems.

Introduction

Micro-scale combustors for micro-power generation and micro-propulsion systems have received increasing attention due to their many distinct advantages such as high energy density, low manufacturing cost and environmental friendly, compared with conventional chemical batteries [1,2]. However, it is worth noting that the characteristic scale of micro-combustors ranges from a few millimeters to sub-millimeters, which results in an unstable homogeneous combustion inside the micro-combustor. It is well accepted that there are three primary aspects to generate flame extinction in a micro-combustor, which are high surface-to-volume ratio, thermal quenching and radical quenching on the wall, respectively. The surface-to-volume ratio of micro-combustors is far larger than that of the macro scale combustor, which leads to enhanced heat loss to the surroundings. The heat and radical generated from the reactions also depletes fast on the wall, resulting in the extinction of the homogeneous combustion [1–5]. Conventional flame stability and fuel conversion efficiency can be greatly reduced via controlling these influencing factors in a micro-combustor. In order to solve these problems and extend

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the stable operating range of a micro scale combustor, many useful strategies were proposed, such as use heat-recirculating combustors to reduce heat losses [4,5], utilizing quenching resistant fuel and employing catalytic combustors to enhance reaction and suppress radical depletion on the wall [6–8]. In practice, the catalytic combustion was used for improving combustion stability, which was considered as one of the best available methods. Surface catalytic (heterogeneous) reactions often have lower activation energies than pure gaseous (homogeneous) reactions, and allow sustaining chemical reactions at lower temperature and possess higher heat losses, resulting in lower probability of thermal quenching.

In the catalytic micro-combustor, the catalytic layers are deposited on the combustor walls, and the effect of that can suppress the intrinsic flame instabilities of micro- and meso-scale channels. Many scholars [8–10] have studied the effects of various parameters on the flame stability in the catalytic micro-combustor used by computational fluid dynamics (CFD) simulations or experimental methods, such as equivalence ratio, inlet velocity, wall material, heat loss, blow out behavior and combustor dimension. Maruta et al. [8] numerically studied the extinction limits in a micro-catalytic channel with multi-step reactions. Their research showed that, for adiabatic walls, the equivalence ratio at the extinction limit monotonically decreases with an increasing Reynolds number. However, for non-adiabatic conditions, the extinction curve exhibits a U-shaped dual-limit behavior due to the heat loss and insufficient residence time compared to chemical time. Benedetto et al. [9] reported the effects of cross-sectional geometry on the ignition/extinction behavior of catalytic micro-combustors by three-dimensional CFD simulations, and built the stability maps. Appel et al. [10,11] investigated the numerical and experimental model of catalytic reactions used to stabilize the combustion reactions in micro-channels for H_2-air mixture over platinum (Pt). The understanding of the heterogeneous and homogeneous reaction kinetics is crucial to the development of such systems.

It has been shown that the catalytic wall plays an important role in heterogeneous and homogeneous reactions. Fanaee and Esfahani [12,13] conducted an analysis on effects of the catalytic wall and channel hydraulic diameter on the combustion process in a micro combustor. The results show that the catalytic walls can extend the flammability limits of a lean reactive mixture more than a rich one. Also, they confirmed that using the catalytic wall can decrease the quenching distance in meso and micro scale reactors as compared to the non-catalytic wall case. Chen et al. [14] demonstrated that the catalytic wall has its sustaining and competing effects on homogeneous combustion in a micro tube. In another numerical research conducted by Chen et al. [15], they showed that the existence of catalyst segmentation promotes the performance and conversion ratio of the micro reactor by improving homogeneous combustion. Smyth et al. [16,17] experimentally investigated the surface oxidation on small-scale catalytic coupons of Pt foil for methane/air and propane/air mixtures. The surface reactions can be divided into three phases along the plate. It is suggested that the design of small-scale reactors should proceed by exploiting the intense reaction of phases I (close to the leading edge) and phase II (surface temperature plateaued at a high value) through boundary layer interruption.

It is imperative that the complex heterogeneous–homogeneous interactions should be further studied. There are many interactions between heterogeneous and homogeneous reaction under certain specific factors. It is demonstrated that the heterogeneous reaction can promote the flame combustion due to the catalytically induced exothermicity. It has the inhibition for homogeneous reactions caused by the competition of reactants between the catalytic reaction and homogeneous reaction. Wang et al. [18] investigated the comparison of reaction intensity between catalytic and non-catalytic combustors. The results show that the catalytic combustor displays a high stability and weak reaction intensity. In addition, the experimental data shows that the catalytic combustion can effectively improve the homogenous combustion efficiency in a catalytic micro-reactor [19]. Zade et al. [20] also numerically investigated the importance of gas-phase and surface reactions for H_2/air mixture in planar micro-channels. The results show that lean limitations of the gas-phase reactions become negligible when compared to surface reactions [10]. However, the interactions between homogeneous and heterogeneous reaction are still not clearly understood in the catalytic micro combustor.

In our previous related work [21,22], CFD simulations and related experiments were performed on hetero-/homogeneous combustion of premixed hydrogen–oxygen mixtures inside a sub-millimeter planar combustor with a rectangular channel. The main parameters, such as wall materials, inlet velocity, equivalence ratio and combustor dimensions, have the crucial effects on the combustion characteristics. In this work, we study the effects of catalytic walls described by different sizes and layouts of catalyst on the combustion characteristics. A three-dimensional simulation model was performed to analyze the multi-steps homogeneous and heterogeneous chemistries for premixed hydrogen–oxygen mixture in the special micro combustor coated with a catalyst. Furthermore, an investigation will be carried out to explore the hetero-/homogeneous combustion phenomenon in a micro-combustor by numerical simulations with variable reaction mechanisms.

Numerical model and model validation

Computing models and boundary conditions

A three-dimensional simulation is performed on the micro combustor to simulate the reactive gas flow and reaction characteristics, using the CFD code FLUENT [23]. The rectangular channel has 10 mm in length (- x, L), 10 mm in width (- y, W), and 1 mm in height (- z, H). Thickness of the wall of the combustor is 0.4 mm as shown in Fig. 1. In the CFD modeling, the platinum catalyst at different locations are coated on the inner silicon carbide (SiC) wall. The laminar finite rate model is employed due to the low inlet flow velocity. The mass governing equations are discretized by a first-order upwind scheme in the numerical model, including steady-state Navier–Stokes equations, mass and energy conservation