Available online at www.sciencedirect.com

ScienceDirect

journal homepage: www.elsevier.com/locate/he

# Numerical simulation of the effect of hydrogen addition fraction on catalytic micro-combustion characteristics of methane-air

Yunfei Yan [a,b,*], Weimin Tang [b], Li Zhang [a,b], Wenli Pan [b], Zhongqing Yang [a,b], Yanrong Chen [a,b], Jiying Lin [b]

[a] Key Laboratory of Low-grade Energy Utilization Technologies and Systems, Chongqing University, Ministry of Education, Chongqing 400030, PR China

[b] College of Power Engineering, Chongqing University, Chongqing 400030, PR China

ARTICLE INFO

*Article history:*
Received 22 September 2013
Received in revised form
31 October 2013
Accepted 9 November 2013
Available online 15 December 2013

*Keywords:*
Micro-reactor
Combustion
Mathematical modeling
Hydrogen fraction
Stability

ABSTRACT

Understanding of micro-scale combustion mechanism is very essential to the development of micro-power devices, so hydrogen assisted catalytic combustion of methane on platinum was studied in this paper. The combustion of preheated mixtures of methane-hydrogen-air in a micro-combustor was modeled by a two-dimensional model including an elementary-step surface reaction mechanism. It was demonstrated that the model could predict the effects of changes of hydrogen fraction. It was shown that the mole fraction of H, OH and C(s) increase and ignition time decreases with hydrogen addition. It was also shown that the improving effect of hydrogen on the ignition temperature of the fuel and O(s) coverage is particularly evident at relatively low hydrogen fraction. The promotion of the combustion stability is due to the decrease of coefficient of variation with hydrogen addition. The methane combustion will move toward the more stabilized reaction and there is a great potential to reduce the pressure fluctuation.



## 1. Introduction

With concern about energy shortage, investigating the alternative fuels in engines and seeking the way for fuel use are increasingly favored by the scientists. Researches on burning characteristics have been an important study subject now. Methane is regarded as one of the most promising and cleanest fuels in micro-combustion. With the advantages of high power density, longevity, small volume and light weight, the advent of methane-air micro-reactor has had a significant impact on the micro-electronics technology, communication, biology and so on.

Because of small dimension and high rate of heat loss, traditional homogeneous reaction cannot proceed steadily. The research of premixed catalytic combustion of methane in micro-combustor lays the foundation for the technology of

* *Corresponding author*. College of Power Engineering, Chongqing University, Chongqing 400030, PR China. Tel.: +86 23 65103114; fax: +86 023 65111832.
E-mail address: yunfeiyan@cqu.edu.cn (Y. Yan).

0360-3199/$ – see front matter 
http://dx.doi.org/10.1016/j.ijhydene.2013.11.028

hydrocarbon-fueled combustion in micro-engine. Although the catalyst is usually a noble metal, this kind of catalyst for methane catalytic reaction has some disadvantages. Because of a higher sticking probability of $O_2$ in comparison to that of $CH_4$, the surface sites Pt(s) are covered by $O_2$, inhibiting the adsorption of $CH_4$. As a result, oxygen is the dominant species on the catalyst surface and the adsorption rate of methane is considerably lower than that of oxygen. Higher $O_2$ concentration in the gas phase leads to fewer bare surface sites and it is responsible for the increase of ignition temperature [1–3]. Researches show that adding a small amount of hydrogen into natural gas can improve the combustion. When $H_2$ is added, the initial reaction temperature and the ignition temperature of $CH_4$ can decrease. The catalytic oxidation of $CH_4$ occurs on the catalyst (Pt) surface with hydrogen addition, when the reaction of $H_2$ and $O_2$ provides $CH_4$ with necessary uncovered surface sites (Pt(s)) [4–6]. Distribution of species concentrations, mixture fraction, strain rate and temperature were investigated by Amir et al. [7]. The results showed that the hydrogen addition to methane leads to improve mixing, increase in turbulent kinetic energy decay along the flame axis and increase in mixture ignitability. The laminar flame speed increases with hydrogen addition [8]. Hu et al. [9] investigated the activation energy of methane–hydrogen blending and the inner layer temperature with the increase of hydrogen fraction. Both of these contribute to enhance the combustion with hydrogen addition. Moreover, the main effect of hydrogen addition is to extend extinction limits of the flame [10]. The methane oxidation reaction pathways will move to the lower carbon reaction pathways when hydrogen is available and there is the potential in reducing the soot formation [11]. Fairly large experimental and analytic evidences have been reported, that hydrogen can be an effective additive to methane permitting faster combustion rates [12,13]. Christopher et al. [14] also investigated the effect of adding changing amount of hydrogen to methane on the critical ignition temperature in a microtube. Yan et al. [15] studied hydrogen-assisted catalytic combustion of methane for optimization micro combustion. Ilbas et al. [16] have performed an experimental research to study hydrogen-assisted combustion of methane. Their experimental results showed that the combustion efficiency increases and CO emission decreases when the hydrogen content increases in blending fuel. Earlier studies showed that adding a small amount of hydrogen into natural gas could reduce the NO emissions [17–19]. Since hydrogen is very reactive in the presence of catalysts, it may also be used to improve correspondingly the rate of catalytic oxidation of other gaseous fuels [20,21]. Zhang et al. [22] have investigated experimentally the combustion of methane and methane-hydrogen gas in the micro-tube. There is no difference between methane or ethane-added hydrogen and hydrogen alone as fuel when combusting without the platinum, but the result is distinctly different when the platinum is put into the micro-tube.

The objectives of this study are the simulation on the product of combustion, ignition temperature and stability of methane-hydrogen-air mixtures with various hydrogen fraction. The study deepens the understanding of methane-hydrogen-air mixture catalytic micro-combustion.

## 2. Problem description and model

A schematic diagram of the plate type micro-combustor of 12.6 mm channel length, 2.2 mm channel width and 0.5 mm wall thickness is shown in Fig. 1. The combustor has the characteristics of little thermal expansion, high heat resistance and low cost. A total of 45 sticks (0.2 × 0.2 mm) with Pt catalyst arranged in 3 rows are positioned at the center of the burner. The entrance and exit in the reactor have 2 mm space respectively without catalytic sticks. Tiny hybrid screen is placed at the entrance to make the gas mixed well. The premixed and preheated homogeneous fuel-air mixture enters a micro-combustor. This problem is simulated using the computational fluid dynamics software FLUENT which is coupled to external subroutines that model the surface chemistry. The external subroutines calculate the mass fluxes at the wall due to surface reactions and the surface coverage with species adsorbed.

In this model, the reactor operates adiabatically at atmospheric pressure. A two-dimensional description of the flow field is permitted for describing the shape of the channel. The Navier–Stokes equations are solved with the axial and radial spatial coordinates as independent variables. The gas phase reactions in this model are considered to be negligible in comparison to the surface reactions. The fluid volume force, dissipation and gas radiation effect are ignored. The model is described by Navier–Stokes equations, energy conservation equation and additional conservation equations for each chemical species. The governing conservation equations can be written as follows.

$$\text{Continuity}: \quad \frac{\partial \rho}{\partial t} + \frac{\partial (\rho u_i)}{\partial x_i} = 0 \tag{1}$$

where $\rho$ is the density of the gas mixture, $u$ is the velocity and $t$ is time.

$$\text{Species mass balance}: \quad \rho \frac{\partial Y_i}{\partial t} + \rho u_j \frac{\partial Y_i}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D\rho \frac{\partial Y_i}{\partial x_j}\right) + R_i \tag{2}$$

where $Y_i$ is the mass fraction of species $i$, $D$ is diffusion coefficient and $R_i$ is generation/consumption rate. Both gas phase species and surface species can be generated and consumed by surface reactions. The generation/consumption rate $R_i$ is written as below,

$$R_i = \sum_{r=1}^{N_e} \nu'_{ir} k_r \prod_{i=1}^{N_g+N_s} [C_i]^{\nu''_{ir}} \tag{3}$$

where $N_e$ is the total number of elementary surface reactions, $\nu'_{ir}$ is stoichiometric coefficient in forward direction of the reaction $r$, $\nu'_{ir}$ is stoichiometric coefficient in negative direction of the reaction $r$, $k_r$ is forward rate coefficient of the reaction $r$. $N_g$ is the number of gas phase species and $N_s$ is the number of surface species. $C_i$ is the molar concentration of specie $i$. $k_r$ is

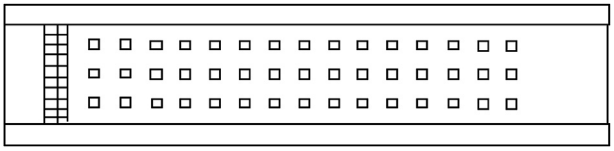

**Fig. 1 – The micro-reactor physical model.**