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Numerical study on catalytic combustion and extinction characteristics of pre-mixed methane–air in micro flatbed channel under different parameters of operation and wall

Yunfei Yan [a,*], Weipeng Huang [a], Weimin Tang [a], Li Zhang [a], Lixian Li [b,*], Jing Ran [b], Zhongqing Yang [a]

[a] Key Laboratory of Low-grade Energy Utilization Technologies and Systems, Chongqing University, Ministry of Education, Chongqing 400030, PR China
[b] Chongqing Key Laboratory of Translational Research for Cancer Metastasis and Individualized Treatment, Chongqing Cancer Hospital & Institute & Cancer Center, Chongqing 400030, PR China

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ABSTRACT

The pre-mixed methane–air catalytic combustion on platinum is numerically modeled in steady condition. The aim of work goes to better understand how the operation and wall parameters affect the combustion of methane, especially the extinction, Pt(s) coverage and hot spot. For this purpose, a micro flatbed channel for pre-mixed methane–air catalytic combustion is investigated. It is clearly shown through a numerical study that lower inlet velocity increases methane conversion, however, it is easier to generate hot spot near the entrance. In addition, the optimum surface site density is 2.72×10^{-9} mol/cm^2 according to methane conversion and surface coverage of Pt(s). When surface site density is greater than 2.72×10^{-9} mol/cm^2, the effect of surface site density on methane conversion rate is not observable. At the case of heat insulation for external wall, wall material with higher thermal conductivity is chosen to preheat mixed gas and avoid generating thermal stress and hot spot. The mixed methane–air can combust steadily at the conditions of thermal isolation external wall, equivalence ratio of 0.8 and inlet velocity of 0.35 m/s, only when the thermal conduction property $b \times \lambda > 3.9 \times 10^{-3}$ W/K.

1. Introduction

With the rapid development of all kinds of micro devices, the demands for miniaturized and sustainable power sources are growing rapidly [1–3]. However, the dominant power sources for portable electronics are currently batteries whose limited energy density and adverse effects on the environment upon disposal are driving the emergence of a new class of micro power sources [3,4]. With the advantages of high power density, longevity, small volume and light weight, the advent of pre-mixed methane–air micro-combustor has a significant impact on the micro power sources [5].

Because of an obvious decrease of residence time and a strong heat loss of wall, micro combustor is difficult to maintain combustion efficiency and stability compared to the conventional combustors. In the past several years, researchers have increasingly studied on methane catalytic combustion in micro scale to widen the range of stable operating parameters and lower the ignition and combustion temperature [2]. Federici et al. [6] experimentally and numerically observed that different thermal conductivity and surface site distance impact on combustion stability significantly. Yan et al. [5,7,8] investigated the effect of hydrogen addition on micro-combustion of methane, which indicates that O(s) coverage decreases with hydrogen addition, especially under the condition of catalytic. Suzanne et al. [9] experimentally investigated the surface oxidation on small-scale catalytic coupons of Pt foil for methane–air mixture. Lee et al. [10] studied the methane–air combustion characteristics in a micro heat-regenerative combustor space with and without catalytic platinum wires. Mohammadreza et al. [11] numerically investigated the combustion characteristics of pre-mixed CH_4-H_2/air in a micro reactor equipped with a catalytic bluff body. They found that the catalytic bluff body in a micro-combustor significantly increases the flame stability. Seung et al. [12,13] explored the minimization of hot spot in a microchannel reactor for the steam reforming of methane with response surface methodology to select the optimum stripe catalyst layer. Ran et al. [14,15] used CFD simulation to investigate the catalytic surface reaction and heat loss characteristics of premixed CH_4/air in micro-channels with platinum catalyst.

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* Corresponding authors.
E-mail addresses: yunfeiyan@cqu.edu.cn (Y. Yan), lilixian2010@yahoo.com (L. Li).

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Nomenclature

A	pre-exponential factor
b	temperature exponent
C_i	molar concentration of specie i, mol m^{-3}
C_p	specific heat at constant pressure, kJ K^{-1} mol^{-1}
D	diffusion coefficient, m^2 s^{-1}
E_a	activation energy of the reaction, kJ mol^{-1}
h	enthalpy, J kg^{-1}
k_r	forward rate coefficient of the reaction r, kg mol^{-1} s^{-1}
M	molar mass of specie i, kg mol^{-1}
N_e	number of elementary surface reactions
N_g	number of gas phase species
N_s	number of surface species
p	pressure, Pa
q	heat of reaction, J kg^{-1}
R	universal gas constant, J K^{-1} mol^{-1}
R_i	generation/consumption rate, kg m^{-3} s^{-1}
S_{0i}	adsorption coefficient of specie i
u	axial velocity, m s^{-1}
X	co-ordinate distance in x direction, m
Y_i	mass fraction of species i

Greek symbols

λ	thermal conductivity, w m^{-1} K^{-1}
ϕ	equivalent ratio
ρ	density, kg m^{-3}
τ	number of active sites occupied
ε_{ir}	surface coverage parameter
μ	viscosity, kg m^{-1} s^{-1}
μ_{ir}	surface coverage parameter
Θ_i	surface coverage rate of species i
Γ	surface site density of the catalyst, mol m^{-2}
v'_{ir}	stoichiometric coefficient in forward direction of the reaction r
v''_{ir}	stoichiometric coefficient in negative direction negative direction of the reaction r

Veeraragavan et al. [16,17] have concluded that heat recirculation from the post-flame to the pre-flame can promote flame stabilization and burning rate deeply, in addition, the flame speed primarily depends on total heat recirculation. Meanwhile, a procedure using manufacture solutions for compressible conjugate heat transfer solvers which are required for micro combustor simulations is verified [18]. Kang et al. [19] have experimentally studied the flame stability limits with thermally orthotropic walls, which found the flame stability can be widen by enhancing the heat conduction of walls at large mixture flow rates.

The catalytic combustion and heat recirculation have been shown effectively from above-mentioned studies to help stabilize fuel combustion in micro-combustors [5–19]. However, there are a few studies on the extinction characteristic and hot spot of methane–air catalytic combustion under different operation and wall parameters. Especially, there is no clear answer to the specific effect of operation and wall parameters on extinction of methane catalytic micro-combustion. The research of operation and wall parameters contributes to realize efficient combustion and the optimized configuration of micro-combustor, respectively.

Table 1
Elementary reaction mechanism of methane catalytic combustion.

	Reactions	A (mol, cm, s)	E_a (kJ/mol)	S_0
1	$H_2 + 2Pt(s) \Rightarrow 2H(s)$			4.6×10^{-2}
2	$2H(s) \Rightarrow H_2 + 2Pt(s)$	3.7×10^{21}	67.4	
3	$H + Pt(s) \Rightarrow H(s)$			1.0
4	$O_2 + 2Pt(s) \Rightarrow 2O(s)$			7.0×10^{-2}
5	$2O(s) \Rightarrow O_2 + 2Pt(s)$	3.7×10^{21}	213.2	
6	$O + Pt(s) \Rightarrow O(s)$			1.0
7	$H_2O + Pt(s) \Rightarrow H_2O(s)$			7.5×10^{-1}
8	$H_2O(s) \Rightarrow H_2O + Pt(s)$	1.0×10^{13}	40.3	
9	$OH + Pt(s) \Rightarrow OH(s)$			1.0
10	$OH(s) \Rightarrow OH + Pt(s)$	1.0×10^{13}	192.8	
11	$O(s) + H(s) \Rightarrow OH(s) + 2Pt(s)$	3.7×10^{21}	11.5	
12	$H(s) + OH(s) \Rightarrow H_2O(s) + Pt(s)$	3.7×10^{21}	17.4	
13	$2OH(s) \Rightarrow H_2O(s) + O(s)$	3.7×10^{21}	48.2	
14	$CO + Pt(s) \Rightarrow CO(s)$			8.4×10^{-1}
15	$CO(s) \Rightarrow CO + Pt(s)$	1.0×10^{13}	125.5	
16	$CO_2(s) \Rightarrow CO_2 + Pt(s)$	1.0×10^{13}	20.5	
17	$CO(s) + O(s) \Rightarrow CO_2(s) + Pt(s)$	3.7×10^{21}	105.0	
18	$CH_4 + 2Pt(s) \Rightarrow CH_3(s) + H(s)$			1.0×10^{-2}
19	$CH_3(s) + Pt(s) \Rightarrow CH_2(s) + H(s)$	3.7×10^{21}	20.0	
20	$CH_2(s) + Pt(s) \Rightarrow CH(s) + H(s)$	3.7×10^{21}	20.0	
21	$CH(s) + Pt(s) \Rightarrow C(s) + H(s)$	3.7×10^{21}	20.0	
22	$C(s) + O(s) \Rightarrow CO(s) + Pt(s)$	3.7×10^{21}	62.8	
23	$CO(s) + Pt(s) \Rightarrow C(s) + O(s)$	1.0×10^{18}	184.0	

Our objectives are to develop a plate-type micro-combustor for methane–air catalytic combustion and investigate the effects of operation and wall parameters on the Pt(s) coverage, methane conversion rate, threshold convective heat transfer coefficient, hot spot, extinction characteristic and so on. This study deepens the understanding of catalytic combustion and extinction characteristics with different operation and wall parameters.

2. Physical model and control equation

As shown in Fig. 1, the physical model consists of a parallel-plate channel which is 20 mm and 1 mm in length and height respectively. Aluminum is used to be wall material whose thickness is 0.2 mm. The pre-mixed methane and air flow with a constant velocity into the micro-combustor and the inlet temperature is 300 K. The axial diffusion velocity is ignored in the calculation, because it is much less than the axial velocity. In this work, the upper part of the micro combustor is chosen as calculation model to reduce the computation load, because the structure of combustor is plane-symmetry.

At the case of heat insulation for external wall, which means there is no heat loss exist between the external wall and environment, the Reynolds number is approximately 25 based on the constant inlet velocity of 0.35 m/s and inlet temperature of 300 K. The wall materials have a specific thickness which allows heat transfer from downstream to upstream to preheat premixed gas. Laminar model is selected in this paper, since Kuo et al. [20] had recommended that laminar model is more appropriate to investigate the characteristics of micro reactor as the Reynolds number below 500, which means that volume force and dissipative effect for the mixture can be neglected. In addition, gas radiation and gravity are ignored. In this paper, the continuous hypothesis is suited to our work for the Knudsen number is less than 0.01.

Based on the above assumptions, the mathematical equations can be written as follows.

$$\text{Continuity equation}: \quad \frac{\partial(\rho u_j)}{\partial x_j} = 0 \tag{1}$$

where ρ is the density of the gas mixture, u_j is the velocity of direction j, x_j is the displacement of direction j.

$$\text{Composition equation}: \quad \rho u_j \frac{\partial Y_s}{\partial x_j} = \frac{\partial}{\partial x_j}\left(D\rho \frac{\partial Y_s}{\partial x_j}\right) + R_s \tag{2}$$