



Optimal combustor dimensions for the catalytic combustion of methane-air mixtures in micro-channels



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ARTICLE INFO

Article history:

Received 17 October 2016

Received in revised form 26 November 2016

Accepted 11 December 2016

Keywords:

Micro-combustion
Combustor dimension
Combustion stability
Extinction
Blowout
Catalytic combustion

ABSTRACT

This paper addresses the question of choosing appropriate combustor dimensions for the self-sustained catalytic combustion in parallel plate micro-channels. The combustion characteristics and stability of methane-air mixtures over platinum in catalytic micro-combustors were studied, using a two-dimensional computational fluid dynamics (CFD) model with detailed chemistry and transport. The effects of gap size, wall thickness, and combustor length on the combustion stability and combustor performance were explored to provide guidelines for optimal design of combustor dimensions. Combustion stability diagrams were constructed, and design recommendations were made. The effect of wall thermal conductivity on the mechanisms of extinction and blowout, and its implications on optimal combustor geometry were studied. It was shown that combustor dimensions are vital in determining the combustion stability of the system. The choice of appropriate combustor dimensions is crucial in achieving stable combustion, due to a rather narrow operating space determined by stability, material, and conversion constraints. The optimal gap size depends on whether the flow velocity or flow rate is kept constant. For most practical wall materials in the range of metals to highly conductive ceramics, larger combustors are more stable at a fixed flow velocity, whereas smaller combustors are recommended for a fixed flow rate at the expense of hot spots. The optimal wall thickness increases with flow velocity. Higher flow velocities can be sustained in combustors with low-conductivity materials using thick walls. The optimal combustor length depends on the wall thermal conductivity. Shorter combustors increase the stability against extinction for high conductivity walls, whereas longer combustors increase the stability against blowout for low conductivity walls. Finally, the role of combustor dimensions in conversion and temperature is also presented.

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1. Introduction

Micro-combustion has become an important area of research because of the rapid growth in the field of micro-power systems [1,2]. Currently, quite a few micro-combustors have been successfully fabricated and tested for various applications [3,4]. Micro-combustors can serve as efficient heat sources for endothermic reactions, such as steam reforming [5] and ammonia decomposition [6], in integrated micro-chemical processors for the production of hydrogen for fuel cell applications. Other broad applications include micro-engines [7], micro-thrusters [8], micro-gas turbines [9], and micro-reactors integrated with energy conversion devices, such as thermoelectric [10,11], thermo-

photovoltaic [12,13], and piezoelectric components [14]. In order that these devices be practical, the combustor must not be the limiting component [15,16].

Combustion stability is considered to be the most important issue for any small-scale combustion device [3,4]. Furthermore, understanding and extending the combustion stability limits are essential in designing efficient and robust systems [16], and thus has gained considerable interest. Depending on feed composition, flow rate, and combustor geometry [17,18], hydrocarbon-air flames are typically quenched in sub-millimeter channels due to two primary mechanisms, i.e., thermal and radical quenching [19,20]. High surface-area-to-volume ratios are inherent to gas-phase micro-combustors, resulting in the enhanced heat and mass transfer within the systems [21,22], which makes these systems significantly more prone to both quenching mechanisms [16,23]. In addition to flame quenching, another mechanism for loss of flame stability is blowout due to insufficient residence time derived from small length scales. When blowout occurs, the

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Nomenclature

$c_{p,k}$	specific heat capacity at constant pressure of k -th gaseous species	Y_k	mass fraction of k -th gaseous species
d	gap size	<i>Greek variables</i>	
D_k^T	species thermal diffusion coefficient	γ_k	sticking coefficient of k -th gaseous species
$D_{k,m}$	mixture-average diffusion coefficient of k -th gaseous species	Γ	surface site density
h, h_k^o	total enthalpy, chemical enthalpy of k -th gaseous species	δ	wall thickness
h_o	external heat transfer coefficient	ε	surface emissivity
$k_{ad,k}$	adsorption rate constant of k -th gaseous species	θ_{free}	free surface coverage
K_g	total number of gaseous species	λ_g, λ_s	thermal conductivity of gas and solid
K_s	total number of surface species	μ	dynamic viscosity of gas
l	combustor length	ρ	density of gas
m	total number of gaseous and surface species	σ	Stephan-Boltzmann constant
p	pressure	σ_m	site occupancy of m -th surface species
q	heat flux	φ	fuel-to-air equivalence ratio
Q	volumetric flow rate	$\dot{\omega}_k$	homogeneous molar production rate of k -th gaseous species
R	ideal gas constant	<i>Subscripts</i>	
\dot{s}_m	heterogeneous molar production rate of m -th surface species	<i>amb</i>	ambient
T, T_o	temperature and reference temperature	<i>g</i>	gas
u, u_{in}	streamwise velocity component, inlet streamwise velocity	<i>in</i>	inlet
\underline{v}	transverse velocity component	<i>i, j, k, m</i>	species index
\underline{V}_k	species diffusion velocity vector	<i>o</i>	outer
W_k	molecular weight of k -th gaseous species	<i>rad</i>	radiation
\bar{W}	mixture molecular weight	<i>s</i>	solid
x, y	streamwise and transverse combustor coordinates	<i>w</i>	wall
		<i>x, y</i>	streamwise and transverse components

reaction zone shifts downstream with the increase of flow velocity and eventually exits the combustor [24,25]. Due to the high surface-area-to-volume ratio of these systems, extinction and blowout become significant, limiting the range in which self-sustained combustion can be achieved [20,23–30]. Recent work has highlighted the importance of combustor structure, which is responsible for both heat recirculation through the walls as well as heat losses to the surroundings, in stabilizing combustion in small channels [31]. Additionally, the combustor geometry and combustion mode are also important in determining stability [32].

Combustor dimensions strongly affect combustion stability [3,20,33–36], and it is important to understand their effects for design purposes [37,38]. The first design variable is the gap size. Recent work has shown that the gap size being a critical parameter to be determined in the design of micro-combustors [34]. As the gap size decreases, the surface-area-to-volume ratio increases, resulting in linearly increased transverse heat and mass transfer rates within the system [17]. The effect of this increased transverse heat transfer rates on homogeneous combustion is twofold. In gas-phase micro-combustors, faster transverse heat transfer is desirable in the preheating region, since it tends to preheat the incoming feed faster, but is detrimental in the post-combustion region because of the increased heat loss from the system [39,40]. In catalytic micro-combustors, increasing transverse mass transfer rate results in a substantial improvement in effective heterogeneous reaction rate and thus improve performance when operating in the diffusion-limited regime [23,41]. Since the role of gap size in enhancing transport rates and changing the dominant chemistry in catalytic micro-combustors has been experimentally demonstrated, the tunability of gap size enables one to manipulate transport rates and the contribution of homogeneous and heterogeneous chemistry to achieve desirable operation [42]. Another factor affected by the gap size is the residence time. For

the same flow rate and thus power input, the residence time decreases with gap size. When the flow residence time becomes close to the characteristic reaction timescale, extinction can occur due to incomplete conversion [23].

The wall thickness is another important design variable, since it affects temperature uniformity within the walls and thus the prospect of mechanical failure [16,39,43–46]. Thick walls result in nearly isothermal systems, whereas thin walls cause steep temperature gradients and hot-spots [39]. The wall thickness affects both the rate of heat recirculation and heat loss, and behaves similarly to the wall thermal conductivity [46]. Variation of the wall conductivity can effectively be achieved by making an appropriate change of wall thickness [16]. The wall thickness should not be too thick in order to minimize weight and size, and not be too thin due to material stability [46]. Aside from the gap size and wall thickness, the combustor length is also important since it determines the area for heat loss and can result in the variation of residence time. Substantial recent experimental and theoretical studies have confirmed that self-sustained combustion can be achieved with proper thermal and chemical management, but combustor dimensions, such as the gap size, wall thickness, and combustor length, should be optimized to ensure efficient and robust systems [16,35–42,44–52].

Most of the work on optimizing combustor dimensions was focused on gas-phase micro-combustors. However, the role of combustor dimensions in catalytic combustion is more complex than that in gas-phase combustion. Gas-phase micro-combustors are typically limited by residence time constraints that can be quantified in terms of the Damköhler number [23]. In contrast, the performance of catalytic micro-combustors is typically limited by diffusion of reactant species to the active catalytic surfaces that can be quantified in terms of the Péclet number [23]. Consequently, design principles for catalytic micro-combustors

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