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Research Paper

Hetero-/homogeneous combustion and flame stability of fuel-lean propane–air mixtures over platinum in catalytic micro-combustors

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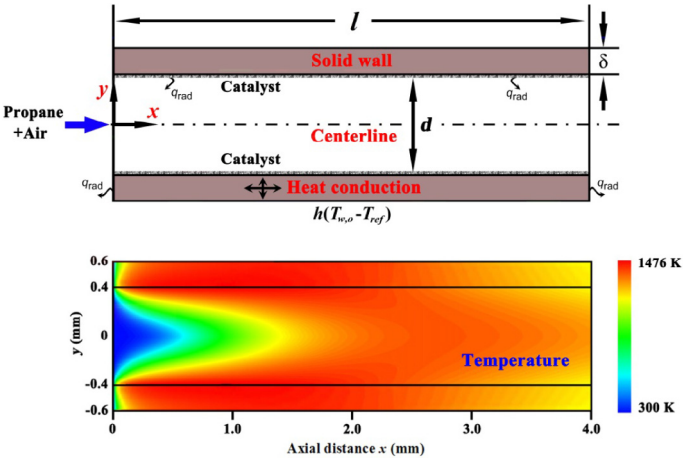
HIGHLIGHTS

- The role of operating conditions was elucidated.
- Combustor dimension and wall material are important design variables.
- An optimum thermal conductivity is found and lower than homogeneous case.
- Operation diagram denoting flame stability was constructed.
- Design recommendations for catalytic micro-combustors were made.

GRAPHICAL ABSTRACT



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ABSTRACT

The hetero-/homogeneous combustion characteristics and flame stability of lean premixed propane–air mixtures over platinum in micro-combustors were numerically studied. For catalytic micro-combustors in particular, numerical studies focused on key thermal management issues, including impact of combustor materials and heat recirculation through the combustor walls. A global heterogeneous reaction step validated over a wide range of parameters has been established, and was further coupled to a detailed homogeneous reaction scheme. Parametric studies were performed with a two-dimensional numerical model to elucidate the role of key operating conditions (wall thermal conductivity, combustor dimension, inlet velocity, flow rate, and equivalence ratio) in determining flame stability and combustion efficiency. Based on these insights, the roles of heat loss and heat recirculation on the mechanisms of flame stability, blowout and extinction were studied. Simulations indicated that the combustor dimension (which includes gap distance and wall thickness) and wall material are important design variables. An optimum thermal conductivity exists for best flame stability, which is lower than that for the homogeneous counterpart. High conductivity materials should be preferred when high-power systems are desired; contrarily, low-power systems would favor more insulating materials to minimize heat losses. Extinction occurs at

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lower values of the external heat transfer coefficient. Operation diagram denoting flame stability (stability maps) was constructed, and design recommendations for catalytic micro-combustors were made. Comparisons to homogeneous micro-combustors were also presented.

1. Introduction

Micro-combustors using hydrocarbon or hydrogen are a promising route for portable production of energy and/or heat [1]. Specifically, the significantly greater energy density of hydrocarbons allows for the realization of micro-scale power generation systems [2,3]. While catalytic combustion is an option for macro-scale power generation [4] and also for household power/heat production [5], it is the preferred route for micro-combustors [6] because of their associated high surface area-to-volume ratios [7,8]. In view of the flame stability issues in micro-combustors, catalytic combustion is promising at micro-scales [9], and becomes an attractive technology with the prototype devices already successfully demonstrated [10]. First, the catalytic surface area per unit volume of combustor along with the transport rates increases linearly with decreasing device size, resulting in process intensification, more stable operation, and faster effective reaction rates [11]. Second, lower ignition temperatures make it possible to self-ignite hydrocarbons on catalysts [12]. Third, compared to their homogeneous counterparts, catalytic micro-combustors can operate with significant heat losses and at lower device temperatures [13]. Experimental investigations of micro-combustion have been carried out using different approaches, such as heat-recirculating or "Swiss-roll" combustors [14], gas-phase burners [15,16] and catalytic combustors; the latter were investigated in terms of fuel conversion efficiency, maximum temperature and combustion stability using a variety of fuels, from methane [17,18] and hydrogen [19] to the more practical propane [20].

Propane is a particular interest fuel for micro-scale systems because it liquefies at moderate pressures and ambient temperatures, and is commercially available in compact containers for a wide range of consumer applications [21]. The study of its complete conversion over catalytic surfaces constitutes the natural first step toward understanding the similar behaviors of higher hydrocarbons [22]. In addition, some of the physical and chemical characteristics of propane are common among higher hydrocarbons, such as the rate of catalytic fuel conversion, the NTC (negative temperature coefficient) of the homogeneous ignition characteristics under certain operating conditions, and the larger-than-unity Lewis number that directly affects the surface temperatures of catalyst [23].

On a fundamental level, the catalytic ignition and combustion behavior in the oxidation of propane on noble-metal catalysts has been investigated along with lower and higher hydrocarbons [24]. An increase in carbon chain length of linear alkanes exhibits higher catalytic reactivity, because of weaker C—C bond strengths of higher hydrocarbons. Furthermore, platinum is found to be the most active noble metal catalyst for the catalytic oxidation of all alkanes (propane, ethane, *n*-butane and isobutane) except methane [25]; the latter is oxidized faster on the nickel catalyst. Detailed heterogeneous scheme for the catalytic oxidation of higher hydrocarbons over platinum has not yet progressed to the same extent as that of methane [26]. Kinetic studies of fuel-lean propane catalytic oxidation over Pt-supported catalysts revealed an overall reaction that is zero order with respect to oxygen, and first order with respect to propane [27]. Accompanying experiments have been carried out to self-ignite propane–air mixtures over platinum in the presence of hydrogen [20].

The lack of heterogeneous scheme for propane over platinum necessitates the use of a global catalytic reaction step, as will be discussed in section 2.3. Furthermore, majority of the numerical studies reported in literatures on propane hetero-/homogeneous combustion in various micro-channels are restricted to simple single-step reaction models, even ignoring the homogeneous (gaseous) chemistry. In other words, homogeneous chemistry is generally ignored, even though experiments provided evidence toward the presence of vigorous homogeneous reactivity under certain operating conditions [10]. In addition, homogeneous chemistry could become very important depending on the gap distance [10] or at some of the higher temperatures [22]. It is emphasized that for catalytic micro-combustors, homogeneous chemistry cannot always be ignored. Finally, in spite of an extensive literature on catalytic combustion of propane on platinum, a kinetic model validated over a wide range of parameters is still not available until recently. Therefore, in the present work, we employed a recently developed global reaction step for the oxidation of propane on platinum, coupled to a detailed homogeneous reaction mechanism.

The fundamentals of heterogeneous (catalytic) combustion at the micro-scale are not as well understood as their homogeneous counterparts [28]. Yet these micro-scale systems are inherently more complex. Heterogeneous combustion at the micro-scale benefits from enhanced mass transfer, but is still subject to heat losses. Loss of flame stability because of high wall temperatures, extinction and blowout are main issues that require careful thermal management. For catalytic micro-combustors in particular, proper thermal management and reducing heat losses are of great importance as is the case for homogeneous counterparts. The catalytic micro-combustor design is a multivariable optimization problem as happens with homogeneous combustion. Elucidating the role of key operation parameters is necessary for the optimization of catalytic micro-combustor design, in terms of flame stability. Moreover, although experimental studies are important criteria toward validations of results, not all aspects of micro-combustion can be measured and studied through detailed experiments because of difficulties associated with smaller dimensions of systems. Furthermore, despite the insight provided by experiments, their inherent limitations at the micro-scale necessitate the use of numerical simulations so as to clarify the underlying physicochemical processes during hetero-/homogeneous combustion. Therefore, appropriate computational tools have been developed, ranging from steady-state to transient models. In addition, numerical studies allow understanding of the hetero-/homogeneous combustion characteristics and flame stability from a different perspective and through a more detailed analysis. CFD (computational fluid dynamics) modeling [29,30] and numerical simulations [31,32] are frequently used to obtain a better understanding of the effect of thermo-fluid processes and geometric parameters on the performance of micro-combustors.

The present work undertakes numerical investigation of the hetero-/homogeneous combustion characteristics and flame stability envelopes of lean premixed propane–air mixtures over platinum in catalytic micro-combustors. The objective of this work is to perform a comprehensive parametric study, by constructing an appropriate global reaction step and then to couple this step with a detailed homogeneous reaction mechanism, so as to understand the role of key operating conditions (wall thermal conductivity, inlet velocity, flow rate, combustor dimension and equivalence ratio) in determining flame stability and combustion efficiency at the micro-scale. A two-dimensional CFD model using a detailed homogeneous reaction scheme and a recently developed global reaction step for the oxidation of propane on platinum, as well as heat and species