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A novel catalytic-homogenous micro-combustor

Almerinda Di Benedetto [a,*], Valeria Di Sarli [a], Gennaro Russo [b]

[a] Istituto di Ricerche sulla Combustione, Consiglio Nazionale delle Ricerche (CNR), Via Diocleziano 328, 80124, Naples, Italy
[b] Dipartimento di Ingegneria Chimica, Università degli Studi di Napoli Federico II, Piazzale Tecchio 80, 80125, Naples, Italy

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ABSTRACT

Miniaturizing combustors from macro- down to micro-scales leads to an increase of the surface area to volume ratio and, thus, thermal and radical quenching may prevail. The ranges of operating conditions at which micro-combustors exhibit stable behaviors are very narrow unless a catalyst is employed. However, catalytic combustors face the problems of thermal control related to the formation of hot spots and the subsequent catalyst deactivation.

In this paper, two-dimensional computational fluid dynamics (CFD) simulations are run to investigate into the opportunity of setting up a novel scheme of micro-combustor divided into two parts. In the first part, the walls of the micro-combustor are catalyst-coated, while in the second part, the catalyst is absent and only homogenous combustion can take place.

Numerical results show that this hybrid micro-combustor (HμC) allows operating at high inlet gas velocities and thus high input powers, without encountering blow-out and maintaining almost complete fuel conversions. This enlargement effect of the operating map on the high inlet velocity side increases on increasing the solid thermal conductivity. Furthermore, the catalytic wall temperature of such HμC is controlled and taken below 1200 K, thus preserving the catalyst.

1. Introduction

Owing to their high specific energy (45 kJ/g), micro-combustors may substitute traditional lithium batteries (specific energy = 1.2 kJ/g) in micro-electromechanical systems (MEMS) [1].

When scaling down from macro- to micro-reactors, phenomena negligible at the macro-scales become relevant at the micro-scales. Miniaturizing macro-combustors leads to an increase of the surface area to volume ratio and, thus, thermal and radical quenching may prevail [1–6]. It has been shown that the ranges of operating conditions at which micro-combustors exhibit stable behaviors are very narrow [3–6]. Conversely, catalytic micro-combustors exhibit wider stability maps than homogenous micro-combustors [7,8]. The catalytic layer deposited on the reactor walls may allow sustaining chemical reactions at lower temperatures and in the presence of higher heat losses, thus reducing the impact of thermal quenching.

However, catalytic micro-combustors face the problems of thermal control related to hot spots, traveling heat waves and wrong way behaviors, which all lead to the catalyst deactivation. Furthermore, the use of micro-combustors for MEMS requires high power density, which can be obtained by increasing the inlet mass flow rate and thus gas velocity. On the other hand, to reach high conversions, the residence time should be relatively high which means that low inlet gas velocities are needed to prevent blow-out conditions. As a result, a trade-off in the choice of the inlet gas velocity has to be reached.

In this framework, it would be beneficial to define a novel reactor configuration in which combustion is stabilized also at high inlet gas velocities with complete conversions.

By means of numerical simulations, we have shown that it is possible to operate a catalytic micro-combustor, fed with lean propane–air mixtures, at high inlet gas velocities (i.e., up to the velocity value limiting the laminar regime for the incoming flow, ~100 m/s for the geometry investigated) with wall temperatures higher than gas temperatures (1600 K *versus* 800 K) and fuel conversions of around 30% [9].

Based on these results, in this paper, we present a novel scheme of micro-combustor divided into two parts. In the first part, the walls of the micro-combustor are catalyst-coated, while in the second part, the catalyst is absent and only homogenous combustion can take place.

In such hybrid micro-combustor (HμC), the catalytic part is used to provide light-off. The heat generated at the catalytic walls is transferred downstream by conduction. This allows both the cooling of the catalytic walls and the preheating of the walls of the

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[*] Corresponding author.
E-mail addresses: almerinda.dibenedetto@irc.cnr.it (A. Di Benedetto), valeria.disarli@irc.cnr.it (V. Di Sarli), genrusso@unina.it (G. Russo).

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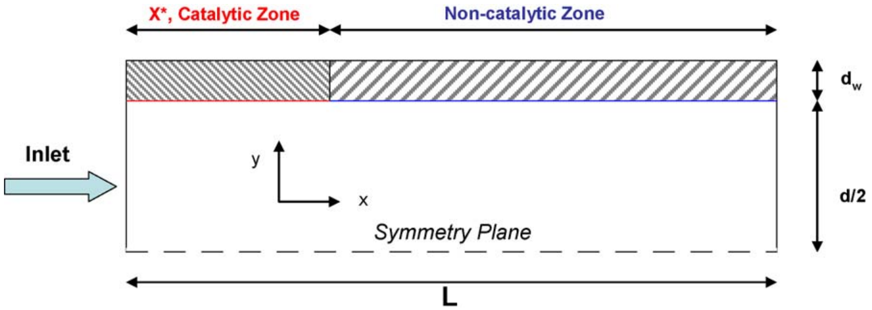

Fig. 1. Scheme of the hybrid micro-combustor (parallel plate reactor). The dashed line is the axis of symmetry.

homogenous section, where volumetric combustion is stabilized, thus completing fuel (propane) conversions.

The opportunity of setting up the HμC scheme is investigated by means of computational fluid dynamics (CFD) simulations.

2. The model

A two-dimensional CFD model is developed to simulate the coupling of the fluid flow and the chemical processes at the gas–solid interface and in the gas phase.

In Fig. 1, the scheme of the hybrid micro-combustor (HμC) is shown which consists of two parallel (infinitely wide) plates (gap distance, $d = 600\ \mu m$; wall thickness, $d_w = 200\ \mu m$; length of the catalytic zone, $X^* = 0.01$ m; total length, $L = 0.06$ m).

The model solves the mass, momentum, species and energy conservation equations in the fluid along with the energy equation in the solid wall. Steady-state simulations are carried out.

The conservation equations in the fluid are listed below (conventional notation is adopted):

Continuity

$$v_x \frac{\partial \rho}{\partial x} + v_y \frac{\partial \rho}{\partial y} + \rho\left(\frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y}\right) = 0 \tag{1}$$

Momentum

$$\frac{\partial \rho v_x v_x}{\partial x} + \frac{\partial \rho v_x v_y}{\partial y} = -\frac{\partial p}{\partial x} + \frac{\partial \tau_{xx}}{\partial x} + \frac{\partial \tau_{yx}}{\partial y} \tag{2}$$

$$\frac{\partial \rho v_x v_y}{\partial x} + \frac{\partial \rho v_y v_y}{\partial y} = -\frac{\partial p}{\partial y} + \frac{\partial \tau_{xy}}{\partial x} + \frac{\partial \tau_{yy}}{\partial y} \tag{3}$$

Species ($i = 1, \ldots, N_s - 1$, with N_s species number)

$$\frac{\partial\, \rho v_x Y_i}{\partial x} + \frac{\partial\, \rho v_y Y_i}{\partial y} = \frac{\partial}{\partial x}\left(\rho D_{i,m}\frac{\partial Y_i}{\partial x}\right) + \frac{\partial}{\partial y}\left(\rho D_{i,m}\frac{\partial Y_i}{\partial y}\right) + R_i \tag{4}$$

Energy

$$\frac{\partial\, \rho v_x h}{\partial x} + \frac{\partial\, \rho v_y h}{\partial y} = \frac{\partial}{\partial x}\left(\lambda\frac{\partial T}{\partial x}\right) + \frac{\partial}{\partial y}\left(\lambda\frac{\partial T}{\partial y}\right) + \sum_{i=1}^{N_S}\left(\frac{\partial(h_i \rho D_{i,m}\partial Y_i/\partial x)}{\partial x} + \frac{\partial(h_i \rho D_{i,m}\partial Y_i/\partial y)}{\partial y}\right) - \sum_{i=1}^{N_S} h_i R_i \tag{5}$$

The above equations are coupled to the ideal-gas equation:

$$\rho = \frac{p W_{\mathrm{mix}}}{\Re T} \tag{6}$$

The energy equation in the solid wall reads:

$$0 = \lambda_w\left(\frac{\partial^2 T_w}{\partial x^2} + \frac{\partial^2 T_w}{\partial y^2}\right) \tag{7}$$

where λ_w is the solid thermal conductivity.

At the inlet of the micro-combustor, a fixed flat velocity profile is assumed. For species and energy, Danckwerts boundary conditions are used. At the exit, the static pressure is imposed as equal to the atmospheric pressure, and far-field conditions are specified for the remaining variables. At the fluid-wall interface, a no-slip boundary condition is assigned (the fluid has zero velocity relative to the boundary) which, in the catalytic zone, is coupled to the species balances (the mass flux of each species, ρJ_i, is equal to its rate of production/consumption, $\omega_{y,i}$):

$$\rho J_i = \omega_{y,i} \tag{8}$$

and the energy balance:

$$\lambda \frac{\partial T}{\partial y} = \lambda_w \frac{\partial T_w}{\partial y} + \omega_{\mathrm{h}} \tag{9}$$

where ω_{h} is the heat surface production rate.

Heat losses from the ends of the micro-combustor are not considered (insulated ends), while Newton's law of convection is used at the outer surface of the wall:

$$q = h(T_{w,\mathrm{ext}} - T_{a,\mathrm{ext}}) \tag{10}$$

where h is the exterior convective heat transfer coefficient, $T_{w,\mathrm{ext}}$ is the temperature at the exterior wall surface, and $T_{a,\mathrm{ext}}$ is the external temperature (=300 K).

The reaction rate for homogenous propane combustion is calculated according to the single-step reaction rate by Westbrook and Dryer [10]:

$$R_H = 4.836E + 9 \cdot \exp\left(\frac{-1.256E + 8}{\Re T}\right) \cdot (C_{C_3H_8})^{0.1} (C_{O_2})^{1.65} \left[\frac{\mathrm{kmol}}{\mathrm{m^3\,s}}\right] \tag{11}$$

where the activation energy is in J/kmol and the concentrations in kmol/m^3.

The catalytic reaction is assumed to be irreversible, first order in fuel concentration and zeroth order in oxygen concentration [11]. The reaction rate, referred to platinum as the catalyst, is calculated according to:

$$R_C = 2.4E + 5 \cdot \exp\left(\frac{-9.06E + 7}{\Re T}\right) \cdot C_{C_3H_8} \left[\frac{\mathrm{kmol}}{\mathrm{m^2\,s}}\right] \tag{12}$$

where the activation energy is in J/kmol and the concentration in kmol/m^2.

The molecular viscosity is approximated through Sutherland's law for air viscosity. The fluid specific heat and thermal conductivity are calculated by a mass fraction weighted average of species properties. The species specific heat is evaluated as a piecewise fifth-power polynomial function of temperature.

The model equations are discretised using a finite volume formulation on a structured mesh built by means of the Gambit pre-processor of the Fluent package (version 6.3.26) [12]. Grid