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The Effect of Differentiating the Thermal Conductivity between Inner and Outer Walls on the Stability of a U-Bend Catalytic Heat-Recirculating Micro-Combustor: A CFD Study

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Abstract: The effect of differentiating the thermal conductivity between inner and outer walls on the stability of a U-bend catalytic heat-recirculating micro-combustor was investigated. To this end, a two-dimensional computational fluid dynamics (CFD) model was developed using the commercial code ANSYS Fluent (release 2020 R1) and, for different combinations of values for the inner and outer thermal conductivities, simulations of lean pre-mixed propane/air combustion were performed by varying the inlet gas velocity. Numerical results have shown that extinction is mainly ruled by the inner wall, whereas the outer wall controls blowout. Differentiating the thermal conductivity has been found to be an effective strategy to jointly exploit the better extinction resistance of low-conductive (i.e., insulating) materials, required by the inner wall, and better blowout resistance of highly conductive materials, required by the outer wall, thus enlarging the stable operating window of the catalytic micro-combustor compared to the use of the same material for both walls.

Keywords: catalytic micro-combustors; heat recirculation; excess enthalpy; U-bend; wall thermal conductivity; extinction; blowout; computational fluid dynamics

1. Introduction

Over the past decades, a trend has been set in the miniaturization of mechanical devices [1]. In line with this trend, combustion of high-energy density fuels, such as hydrocarbons and hydrogen, in micro-reactors has attracted growing interest for applications in portable power generation and in process intensification for improving energy efficiency [2,3]. The heat evolved from combustion can be converted into electricity by coupling with thermoelectrics [4], thermophotovoltaics [5], or thermoionics [6] for use in portable devices. Furthermore, it can be utilized to conduct endothermic reactions, such as in the case of the steam reforming of methane, by close thermal coupling with combustion [7].

Despite its benefits, miniaturization leads to several issues [8]. For micro-combustors, one of the most challenging issues is stability [2,3]. Micro-combustors lose stability via two primary mechanisms, extinction and blowout [9]. As the scale of the device decreases, the surface-to-volume ratio increases, whereas the residence time decreases and, thus, heat losses increase, adversely impacting stability. In the case of extinction, most of the heat is lost through the walls to the surroundings. In the case of blowout, most of the heat is lost in the form of hot exhaust gases. Extinction occurs when heat losses lower the temperature of the system to values at which combustion does not self-sustain, i.e., when the input power is insufficient compared to the power lost from the system. Blowout, on the other hand, occurs when there is insufficient pre-heating of
the reactants to ensure ignition and stabilization of combustion, i.e., when there is insufficient residence time compared to the chemical reaction time.

Under the conditions of the sub-millimeter confinement of micro-reactors, homogeneous combustion is especially susceptible to quenching [10]. Hence, catalytic combustion, with its lower operating and light-off temperatures, is the focus area for research in the field of micro-power generation systems [11]. Indeed, the catalytic coating of the walls of the micro-combustors, even if only partial [12–14], favors their ignited state.

Although to a lesser extent than homogeneous micro-combustors, catalytic micro-combustors still suffer from stability issues and, thus, even for them, the non-trivial task of minimizing heat losses is crucial to the development of more robust configurations [15–18].

A key approach to minimize the detrimental effects of heat losses in combustion systems is based on recovering heat from the reaction zone, i.e., on recirculating part of the sensible heat of the hot exhaust gases to pre-heat the cold incoming reactants. This concept was first proposed by Lloyd and Weinberg [19] for conventional-sized combustors as a means to burn fuels with very low heat content in a double-spiral counter-current heat-recirculating geometry called “Swiss roll”. Due to the large ratios of internal heat exchange area to external heat loss area, the Swiss-roll configuration causes “excess-enthalpy” combustion, i.e., large super-adiabaticity, in both macro-scale [20] and micro-scale [21] systems.

Excess-enthalpy reactors other than the Swiss-roll configuration have been proposed and also investigated in the context of homogeneous micro-combustion. They are the porous-media [22], reverse-flow [23], and heat-recirculating [24,25] reactors, the latter often being simplified Swiss-roll configurations. In contrast to excess-enthalpy combustors, standard straight-channel combustors exhibit worse stability, the only mechanism of heat recirculation on which they can rely being the mechanism of axial heat conduction in the upstream direction along the solid walls [24].

The concept of excess-enthalpy combustion has also been transferred to catalytic micro-reactors through studies carried out by different research groups and mainly focused on heat-recirculating configurations [26–29]. However, the knowledge acquired in the field of homogeneous micro-combustors cannot be directly applied to their catalytic counterparts due to a substantial difference: in the former, heat is first generated in the gas phase and then transferred to the walls, whereas, in the latter, heat is released on the walls, possibly determining better heat-recirculation performance due to accelerated heat transfer within the walls [27].

Achieving a complete understanding of the mechanism of thermal stabilization in catalytic heat-recirculating micro-combustors is essential to fully exploit the potential of such systems through a proper choice of design parameters. To this end, experimental [26,30] and, above all, numerical [26–29,31–34] investigations have been performed. Indeed, the fact that to obtain space-resolved measurements in micro-scale devices is difficult renders the contribution from computational fluid dynamics (CFD) particularly important.

The stability of micro-combustors is strongly dependent on the solid thermal conductivity, given that heat is transferred upstream via axial conduction through the walls and also lost to the surroundings through the walls (see, for example, [10,11,35]). Besides that, in heat-recirculating configurations, the solid thermal conductivity also comes into play via the transverse heat exchange between the hot combustion products and the cold incoming reactants that takes place through the inner walls separating the inlet and outlet channels (see, for example, [26,29,31,32]). While exhibiting high resistance to extinction, micro-systems with insulating walls typically lose stability via blowout, i.e., insufficient pre-heating. In heat-recirculating micro-combustors, thanks to the additional pathway of transverse heat transfer, the effective thermal conductivity of the inner walls increases [28], thus making the issue of blowout less critical than in single-channel configurations [26,32]. Furthermore, there is a feature of heat-recirculating micro-combustors
that makes them unique: in order to minimize the heat losses to the surroundings and, at the same time, facilitate pre-heating, thus improving stability, different materials can be used for the inner and outer walls [25].

The effect of differentiating the thermal conductivity between inner and outer walls on the stability of a catalytic heat-recirculating micro-combustor has been preliminarily studied by Chen’s group [32]. Their configuration is that of a symmetric system having an inlet/reaction channel and two outlet/recirculation channels, one on each side of the inlet channel. These outer channels also protect the inner one from the heat losses to the surroundings (see, for example, [29,36]). Stability was quantified in terms of the critical external heat transfer coefficient (i.e., the external heat loss coefficient beyond which combustion does not self-sustain). Numerical results have shown that stability is strongly dependent on the thermal conductivity of the inner walls and, thus, can be significantly improved when using highly insulating materials, especially for such walls. However, it is not clear whether these findings also apply to configurations in which the inlet channel is not surrounded on both sides by outer recirculation channels, i.e., configurations in which the reaction zone is more exposed to external heat losses.

In order to effectively improve the stability of catalytic heat-recirculating micro-combustors assigning them a double functionality (reduced external heat losses and enhanced pre-heating), it is essential to identify conditions under which there is a clear distinction of the roles played by the inner and outer walls in determining extinction and blowout. On the other hand, improving the stability of such systems is also crucial to enlarge their operability limits in terms of a key parameter, the inlet gas velocity, i.e., the input power. At low inlet gas velocity (i.e., at low input power), extinction is likely to occur and, thus, low-power systems require insulating materials, and conversely, at high inlet gas velocity (i.e., at low residence time), blowout is likely to occur and, thus, high-power systems require conductive materials [10,35]. Once a clear distinction of roles is identified, differentiating the thermal conductivity between inner and outer walls could lead to systems capable of working at both low inlet gas velocity, thanks to the resistance to extinction imparted by the material with low thermal conductivity, and high inlet gas velocity, thanks to the resistance to blowout imparted by the material with high thermal conductivity.

The present paper fits in this framework focusing on the effect of differentiating the thermal conductivity between inner and outer walls on the stability, assessed in terms of critical inlet gas velocities (i.e., the velocity below which extinction occurs and the velocity beyond which blowout occurs), of a non-symmetric U-shaped catalytic heat-recirculating micro-combustor. In this configuration, the inlet channel is protected by the outlet channel on the one side and directly exposed to external heat losses on the other side. The aim was to understand the role played by the inner and outer walls in determining extinction and blowout, and whether differentiating the thermal conductivity could be an effective strategy to improve stability, thus enlarging the operating window of the catalytic micro-combustor compared to the use of the same material for both walls. To this end, a two-dimensional CFD model was developed and, for different combinations of materials (i.e., different combinations of values for the inner and outer thermal conductivities), simulations of lean pre-mixed propane/air combustion were performed by varying the inlet gas velocity.

2. Mathematical Model

Two-dimensional steady-state CFD simulations were carried out to investigate the stability of the U-bend catalytic heat-recirculating micro-combustor schematized in Figure 1.
After entering the micro-combustor, the gas stream flows through the inlet channel, turns around the inner wall, flows through the outlet channel and then exits.

Table 1 lists the values of the geometrical parameters for the configuration of Figure 1.

| Parameter                          | Value  |
|-----------------------------------|--------|
| Channel gap size, $d$ [mm]        | 0.6    |
| Wall thickness, $\delta$ [mm]     | 0.2    |
| Length of the micro-combustor, $L$ [mm] | 12.5   |

The model was developed using the commercial CFD software package ANSYS Fluent (release 2020 R1). The processes simulated include conduction and convection in the gas phase, solid-phase conduction within the walls, external convective heat losses, and chemical reactions both in the gas phase and at the gas-solid interface (green lines in Figure 1). The model equations are the conservation equations for mass, momentum, energy, and chemical species in the fluid as well as the conservation equation for energy in the solid walls. Laminar flow was assumed. In the momentum equation, the stress tensor took the standard form for a Newtonian fluid.

Simulations were run for lean pre-mixed propane/air. Among alkanes, propane is particularly suitable for catalytic micro-combustion [11,37].

The reaction rate of homogeneous (i.e., gas-phase) propane combustion was calculated according to the single-step reaction rate by Westbrook and Dryer [38]:

$$ r_{\text{hom}} = -4.836 \times 10^9 \exp\left(-\frac{1.256 \times 10^7}{RT}\right) C_{\text{C}_3\text{H}_8}^{0.1} C_{\text{O}_2}^{1.65} \left[ \text{kmol} / (\text{m}^3 \text{s}) \right] $$

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

A single-step reaction rate was also assumed for heterogeneous (i.e., catalytic) propane combustion (occurring at the gas-solid interface) [39]:

$$ r_{\text{cat}} = -2.4 \times 10^9 \exp\left(-\frac{9.06 \times 10^7}{RT}\right) C_{\text{C}_3\text{H}_8} \left[ \text{kmol} / (\text{m}^3 \text{s}) \right] $$

where the activation energy is expressed in J/kmol and the concentration of propane in kmol/m$^3$.

At the inlet boundary, uniform profiles were specified for (axial) velocity, temperature and species mole fractions. The inlet conditions are detailed in Table 2. Stability was
assessed in terms of critical inlet gas velocities, i.e., the velocity below which extinction occurs, \( V_{in} \) for extinction, and the velocity beyond which blowout occurs, \( V_{in} \) for blowout.

**Table 2. Inlet conditions.**

| Parameter                        | Value       |
|----------------------------------|-------------|
| Inlet gas velocity, \( V_{in} \) [m/s] | 0.12–24.5   |
| Inlet gas temperature [K]        | 300         |
| Inlet fuel equivalence ratio [-]  | 0.5         |
| (Inlet) Reynolds number, Re [-]  | 4.6–937.5   |

The (inlet) Reynolds number, \( Re \), defined based on the inlet gas velocity, gas kinematic viscosity at ambient conditions, and channel gap size, is also reported in Table 2. At the highest value of \( V_{in} \) explored (24.5 m/s), \( Re \) is equal to around 940, thus confirming the assumption of laminar flow.

At the outlet boundary, a condition of fixed static pressure was assigned. At the gas-solid interface, no-slip boundary conditions were used for both velocity components (the fluid had zero velocity relative to the boundary). All the external surfaces exposed to the surroundings were assumed to lose heat through convection. The convective heat transfer coefficient was set equal to 10 W/m²K (value within the range of natural convection), and the ambient temperature to 300 K.

The ideal gas law was used to compute the fluid density. The fluid viscosity and thermal conductivity were assumed to vary with temperature according to the laws reported—for nitrogen—in Canu [40]. The specific heat capacity for each species was calculated as a piecewise fifth-power polynomial function of temperature. The mixture-averaged specific heat capacity was computed as a mass-fraction average of the pure species heat capacities.

The wall thermal conductivity was assumed to be constant. Cordierite, stainless steel, silicon carbide (SiC), and cast iron were considered as materials. Table 3 details the values of thermal conductivity for the outer and inner walls adopted in the computations run by varying the inlet gas velocity.

**Table 3. Values of thermal conductivity for the outer and inner walls adopted in the computations.**

| Thermal Conductivity of the Outer Wall [W/m K] | Thermal Conductivity of the Inner Wall [W/m K] | Nomenclature          |
|-----------------------------------------------|-----------------------------------------------|-----------------------|
| 2                                             | 2                                             | All Cordierite        |
| 32.8                                          | 32.8                                          | All SiC               |
| 2                                             | 32.8                                          | Cordierite + SiC      |
| 32.8                                          | 2                                             | SiC + Cordierite      |
| 23.3                                          | 23.3                                          | As SiC + Cordierite   |
| 10                                            | 10                                            | All Stainless Steel   |
| 10                                            | 2                                             | Stainless Steel + Cordierite |
| 50                                            | 50                                            | All Cast Iron         |
| 50                                            | 2                                             | Cast Iron + Cordierite|

\(^1\text{In this case, the thermal conductivity of both outer and inner walls was set equal to the same value of volume-averaged solid thermal conductivity as the case SiC + Cordierite.}\)

The value of thermal conductivity for SiC was taken from [41]. The values 10 W/m K and 50 W/m K are typical of thermal conductivity for stainless steel and cast iron, respectively [29].

Simulations were performed using a uniform grid with square cells. In order to check the grid independence, three cell sizes were tested: 0.08 mm–coarse grid; 0.04 mm–intermediate grid; 0.02 mm–fine grid. The maximum wall temperature was as-
sumed as a criterion for convergence. For the case All Cordierite (see Table 3) at $V_{in} = 0.5$ m/s, Figure 2 shows the axial profiles of temperature along the center line of the inner wall, where the maximum temperature was attained, as computed by varying the grid resolution.

![Axial profiles of temperature along the center line of the inner wall at different grid resolutions: $V_{in} = 0.5$ m/s; All Cordierite.](image)

Reducing the cell size from 0.04 mm to 0.02 mm resulted in variations of the wall temperature lower than 5%, without affecting its maximum value. Thus, the intermediate grid, with cell size equal to 0.04 mm, was employed in this work.

The conservation equations were solved semi-implicitly with a segregated solver. The SIMPLE (Semi-Implicit Method for Pressure-Linked Equations) algorithm was adopted to treat the pressure-velocity coupling. The spatial discretization used second-order schemes for all terms. Convergence was confirmed by: (1) the residual of each equation going below $1 \times 10^{-12}$; (2) the global mass and energy balances being satisfied at the end of each simulation; (3) the constancy of temperature and propane mole fraction monitored at various locations for at least $1 \times 10^5$ iterations.

3. Results and Discussion

3.1. All Cordierite versus All SiC

In this sub-section, results obtained for the U-bend catalytic micro-combustor with both inner and outer walls made of the same material, cordierite and SiC, are presented and discussed. With reference to the nomenclature of Table 3, these are the cases All Cordierite and All SiC.

3.1.1. Base Cases

Figure 3 shows the maps of temperature, $T$, and propane mole fraction, $X_{Propane}$, as computed when setting the inlet gas velocity, $V_{in}$, equal to 0.5 m/s.
As expected, in the case of low thermal conductivity (cordierite), the thermal profile was much less uniform, and higher values of local temperature were attained. In addition, when looking at the inlet channel, it can be noticed that, in the case of SiC, there was a substantial symmetry with respect to the center line for temperature and, above all, for propane mole fraction. Conversely, in the case of cordierite, there was no symmetry.

For both cases of Figure 3, Figure 4 shows the axial profiles of (catalytic) reaction rate along the inner and outer walls of the inlet channel.

![Figure 3](image1)

**Figure 3.** Maps of temperature, T, and propane mole fraction, X<sub>Propane</sub>, at V<sub>in</sub> = 0.5 m/s: All Cordierite; All SiC. A scaling factor equal to 2 was used to scale the computational domain along the transverse direction.

![Figure 4](image2)

**Figure 4.** Axial profiles of (catalytic) reaction rate along the inner and outer walls of the inlet channel at V<sub>in</sub> = 0.5 m/s: All Cordierite and All SiC.
In the case of SiC, the reaction zone was located close to the inlet on both inner and outer sides. In the case of cordierite, symmetry was lost, the reaction zone being located close to the inlet on the inner side and further downstream on the outer side.

On the inner side of the inlet channel, two mechanisms of heat recirculation allow for pre-heating of the cold feed. The first mechanism is that of transverse heat transfer, i.e., heat recirculation from the reaction zone: following reaction, the product mixture that flows down the channel first gets cooled due to the heat losses from the outer wall, but later, close to the outlet, it picks up the heat released in the reaction zone of the inlet channel and pre-heats the cold feed. The second mechanism of heat recirculation is the classical mechanism of axial conduction in the upstream direction along the solid wall. In the case of cordierite, despite its low thermal conductivity, this latter mechanism was facilitated by the presence of the outlet channel that also acted as a protection for the reaction zone. On the outer side of the inlet channel, which is directly exposed to the heat losses toward the external environment, the only pre-heating mechanism is that of axial heat conduction. However, in the case of cordierite, the thermal conductivity was too low and, thus, the reaction zone was pushed downstream.

3.1.2. Effect of the Inlet Gas Velocity

Figure 5 shows the plots of maximum wall temperature, $T_{\text{wall max}}$ (outlet) bulk gas temperature, $T_{\text{inlet}}$, and (outlet) propane conversion versus $V_{\text{in}}$.

In the case of the low-conductive cordierite, temperatures were higher and extinction, which is regulated by competition between the heat losses toward the external environment and the heat produced by combustion, occurred at a lower value of $V_{\text{in}}$ than with SiC (0.13 m/s versus 0.32 m/s). In contrast, in the case of SiC, blowout occurred at a higher value of $V_{\text{in}}$ than with cordierite (19.75 m/s versus 8 m/s).

From a practical point of view, the trend depicted in Figure 5, with better extinction stability at low thermal conductivity and better blowout stability at high thermal conductivity, implies that, for low-power systems, insulating materials are needed and, conversely, for high-power systems, conductive materials are needed.

Figure 5 also shows some features that have already been found by Kaisare’s group, although for a different configuration of catalytic heat-recirculating micro-combustor [29]: at extinction, both the maximum temperature and the fuel conversion are substantially independent of the thermal conductivity, whereas at blowout, the fuel conversion decreases with increasing thermal conductivity.

In Figure 6, the maps of temperature and propane mole fraction are shown at different values of $V_{\text{in}}$.

As the inlet gas velocity was increased, the reaction front was progressively shifted downstream. However, this effect was particularly marked on the outer side of the inlet channel of the micro-combustor made of cordierite. In this case, the outer wall remained cold along much of its length, and unconverted propane left the inlet channel, turning around the inner wall, already at $V_{\text{in}} = 4$ m/s. Conversely, in the case of SiC, temperature was sufficiently high also for the outer wall, and the inlet channel could be fully exploited as a reactor to obtain (almost) complete propane conversion up to $V_{\text{in}} = 7$ m/s.

The reason behind the fact that cordierite exhibited higher susceptibility to blowout than SiC is directly linked to its low thermal conductivity. The geometrical asymmetry of the U-bend configuration—with the inlet channel directly exposed to the heat losses toward the external environment on one side and protected by the presence of the outlet channel on the other side—seems to have made the low thermal conductivity of the outer wall especially responsible for the poor resistance to blowout of the micro-reactor made of cordierite. In this case, if we consider the inlet channel, the outer wall remained cold due to insufficient pre-heating of the fresh incoming reactants, i.e., insufficient axial heat conduction in the upstream direction. Conversely, the inner wall attained high temperatures as heat recirculation (transversely across and axially along the solid wall) was effective in pre-heating the cold feed.
On the basis of the above-presented results, differentiating the thermal conductivity between inner and outer walls can be expected to have an impact on the stability of the U-bend catalytic micro-combustor.

**Figure 5.** Maximum wall temperature, $T_{\text{wall,max}}$, (outlet) bulk gas temperature, $T_{\text{bulk}}$, and (outlet) propane conversion versus $V_{\text{in}}$: All Cordierite and All SiC. Arrows indicate extinction (at low values of $V_{\text{in}}$) and blowout (at high values of $V_{\text{in}}$).
Figure 6. Maps of temperature, $T$, and propane mole fraction, $X_{\text{Propane}}$, at different values of $V_{\text{in}}$: All Cordierite; All SiC. A scaling factor equal to 2 was used to scale the computational domain along the transverse direction.

3.2. Differentiating the Thermal Conductivity between Inner and Outer Walls

This sub-section is focused on results obtained for the U-bend catalytic micro-combustor with inner and outer walls made of different materials. From these results, the role played by the two walls in determining stability was first quantified, and the optimal combination of materials was then identified.
3.2.1. Roles of the Inner and Outer Walls

Figure 7 shows the plots of $T_{\text{wall,max}}$, $T_{\text{bulk}}$, and propane conversion versus $V_{\text{in}}$ for the cases of Table 3 Cordierite + SiC (outer wall made of cordierite and inner wall made of SiC) and SiC + Cordierite (outer wall made of SiC and inner wall made of cordierite). For the sake of comparison, the plots obtained in the cases All Cordierite and All SiC are also shown.

![Figure 7: Maximum wall temperature, $T_{\text{wall,max}}$ (outlet) bulk gas temperature, $T_{\text{bulk}}$, and (outlet) propane conversion versus $V_{\text{in}}$: Cordierite + SiC and SiC + Cordierite. For the sake of comparison, the plots obtained in the cases All Cordierite and All SiC are also shown. Arrows indicate extinction (at low values of $V_{\text{in}}$) and blowout (at high values of $V_{\text{in}}$).]
Let us focus on extinction. The outer wall surely plays a role in determining extinction, given that the case All Cordierite resulted in the best extinction resistance. However, in spite of its higher volume-averaged solid thermal conductivity (23.3 W/m K versus 11.5 W/m K), the case SiC + Cordierite exhibited a better extinction stability ($V_{in@extinction} = 0.23$ m/s) than the case Cordierite + SiC ($V_{in@extinction} = 0.25$ m/s). This means that extinction was mainly ruled by the inner wall. On the other hand, Chen et al. [32] have highlighted the key role of the inner walls in determining stability on the basis of CFD simulations of a catalytic heat-recirculating micro-combustor with symmetric configuration performed by varying the external heat transfer coefficient.

Figure 8 shows the temperature maps at extinction for the three cases All Cordierite, Cordierite + SiC, and SiC + Cordierite.

![Temperature Maps at Extinction](image)

**Figure 8.** Maps of temperature at extinction: All Cordierite; Cordierite + SiC; SiC + Cordierite. A scaling factor equal to 2 was used to scale the computational domain along the transverse direction.

In all cases, the hottest zone was located downstream. However, the thermal pattern established in the case SiC + Cordierite was rather similar to that predicted in the case All Cordierite, with the inner wall attaining the maximum temperature. In the case Cordierite + SiC, the thermal pattern was completely different: the wall that attained the maximum temperature was the outer one and, thus, the stabilizing action of the inner wall was lost.

As far as blowout is concerned, Figure 7 shows that the cases Cordierite + SiC and SiC + Cordierite exhibited the same behavior as the cases All Cordierite and All SiC, respectively. This confirms what conjectured in the previous sub-section: the outer wall controls blowout.

In Figure 9, the maps of temperature and propane mole fraction are shown as computed at $V_{in} = 7.5$ m/s for All Cordierite and Cordierite + SiC, and at $V_{in} = 13$ m/s for All SiC and SiC + Cordierite. According to Figure 7, these were the highest values of $V_{in}$ that still allowed for 100% propane conversion.
Let us look at the inlet channel. Thanks to heat recirculation, the inner wall attains high temperatures regardless of the material it is made of and, therefore, does not play a substantial role in determining blowout. The differences in the high-velocity behavior are in fact to be attributed to the outer wall. As in the case All Cordierite, even in the case Cordierite + SiC, due to its low thermal conductivity, the outer wall remained cold along much of its length and, thus, the inlet channel could be only partially exploited as a reactor. Conversely, as in the case All SiC, even in the case SiC + Cordierite, due to its high thermal conductivity, the outer wall attained high temperatures and, thus, the inlet channel could be fully exploited as a reactor.

3.2.2. Optimal Combination of Materials

The above-presented results have shown that heat recirculation creates a distinction of the roles played by the inner and outer walls in determining stability. The outer wall controls blowout. It also plays a role in affecting extinction. However, this is mainly ruled by the inner wall.

Figure 10 shows the inlet gas velocity at blowout ($V_{in}$ @ blowout) as a function of the inlet gas velocity at extinction ($V_{in}$ @ extinction) for the four cases All Cordierite, Cordierite + SiC, SiC + Cordierite, and All SiC, and the additional case As SiC + Cordierite. In this latter case, the thermal conductivity of both outer and inner walls was set equal to the same value of volume-averaged solid thermal conductivity as the case SiC + Cordierite (23.3 W/m K—see Table 3).
These results clearly contradict the intuitive idea that the best combination of materials is that of a low-conductive outer wall, which minimizes the heat losses toward the external environment, and a highly conductive inner wall, which facilitates pre-heating of the cold feed to get easier ignition. Indeed, the case Cordierite + SiC was the worst case, as it exhibited lower resistance to extinction than the case All Cordierite and, at the same time, lower resistance to blowout than the case All SiC. Conversely, the case SiC + Cordierite exhibited much better resistance to extinction than the case All SiC and, at the same time, much better resistance to blowout than the case All Cordierite. This can be attributed only to a lesser extent to the fact that the volume-averaged solid thermal conductivity for the case SiC + Cordierite was lower than the thermal conductivity of SiC and higher than the thermal conductivity of cordierite. Indeed, better resistance to extinction was mainly imparted by the low thermal conductivity of the inner wall, whereas better resistance to blowout was mainly imparted by the high thermal conductivity of the outer wall.

Global assessment of Figure 10, thus, demonstrates that the distinction of the roles played by the inner and outer walls offers the opportunity of differentiating the thermal conductivities to enlarge the stable operating window of the U-bend catalytic micro-combustor compared to the use of the same material for both walls. From this perspective, the configuration SiC + Cordierite, with a low thermal conductivity for the inner wall and a high thermal conductivity for the outer wall, represents the optimal combination of materials. This combination is suitable for both low- and high-power systems.

For the optimal configuration with an insulating inner wall and conductive outer wall, simulations were also run by varying the thermal conductivity of the outer wall, while keeping the thermal conductivity of the inner wall constant and equal to that of cordierite. The results of these simulations are shown in Figure 11, where $V_{in} @ extinction$ and $V_{in} @ blowout$ are plotted as a function of the volume-averaged solid thermal conductivity. In the same figure, the results obtained for the configuration with both walls made of the same material are also shown.
At a fixed solid thermal conductivity, as a result of higher resistance to both extinction and blowout, the optimal configuration exhibited a wider stable operating window than the configuration with both walls made of the same material. Moreover, the benefit in terms of widening of the stable operating window increased with increasing solid thermal conductivity.

4. Conclusions

The effect of differentiating the thermal conductivity between inner and outer walls on the stability of a U-bend catalytic heat-recirculating micro-combustor was investigated. To this end, a two-dimensional CFD model was developed and, for different combinations of values for the inner and outer thermal conductivities, simulations of lean pre-mixed propane/air combustion were performed by varying the inlet gas velocity.

Numerical results have shown that heat recirculation creates a distinction of the roles played by the inner and outer walls in determining stability. The outer wall controls blowout. It also plays a role in affecting extinction. However, this is mainly ruled by the inner wall. This distinction of roles offers the opportunity of differentiating the thermal conductivities to enlarge the stable operating window of the catalytic micro-combustor compared to the use of the same material for both walls. It has been found that the optimal combination of materials is that of a low-conductive (i.e., insulating) inner wall, which imparts better resistance to extinction, and a highly conductive outer wall, which imparts improved resistance to blowout.

Although obtained on a prototypical configuration, these results highlight the great potential and flexibility of catalytic heat-recirculating micro-combustors, and also provide directions on how to improve their operability limits through a careful design in terms of wall thermal conductivity.
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