

Article

Combustion Characteristics of Premixed Hydrogen/Air in an Undulate Microchannel

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Abstract: This work reports a numerical investigation of microcombustion in an undulate microchannel, using premixed hydrogen and air to understand the effect of the burner design on the flame in order to obtain stability of the flame. The simulations were performed for a fixed equivalence ratio and a hyperbolic temperature profile imposed at the microchannel walls in order to mimic the heat external losses occurred in experimental setups. Due to the complexity of the flow dynamics combined with the combustion behavior, the present study focuses on understanding the effect of the fuel inlet rate on the flame characteristics, keeping other parameters constant. The results presented stable flame structure regardless of the inlet velocity for this type of design, meaning that a significant reduction in the heat flux losses through the walls occurred, allowing the design of new simpler systems. The increase in inlet velocity increased the flame extension, with the flame being stretched along the microchannel. For higher velocities, flame separation was observed, with two detected different combustion zones, and the temperature profiles along the burner centerline presented a non-monotonic decrease due to the dynamics of the vortices observed in the convex regions of the undulated geometry walls. The geometry effects on the flame structure, flow field, thermal evolution and species distribution for different inlet velocities are reported and discussed.

Keywords: numerical study; microcombustion; hydrogen; complex geometry



Citation: Resende, P.R.; Morais, L.C.; Pinho, C.; Afonso, A.M. Combustion Characteristics of Premixed Hydrogen/Air in an Undulate Microchannel. *Energies* **2022**, *15*, 626. <https://doi.org/10.3390/en15020626>

Academic Editors: Alexandre M. Afonso, Pedro Resende, Mohsen Ayoobi and Dimitrios Katsaprakakis

Received: 14 October 2021

Accepted: 1 January 2022

Published: 17 January 2022

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1. Introduction

The technology advances in the last years allowed the development of integrated system devices at microscale, including both electro and mechanical components designated by MEMS (Micro Electro-Mechanical Systems) [1]. This type of system needs external power supply and, given the typical battery limitations, efforts have been made to develop alternatives based on microcombustion in order to take advantage of the high-density energy of the hydrocarbon and hydrogen fuels. Nevertheless, early experimental studies involving microcombustion presented some difficulties to obtain a stable flame caused mainly by two phenomena: the low residence time inside of the microcombustor to complete combustion and the higher heat losses from the combustion chamber walls [2,3].

In order to better understand the microcombustion dynamics and overcome some of the referred limitations, several numeric studies were carried out to obtain more detailed information. Raimondeau et al. [4] presented a numerical study on flammability limitations that relied on simple models to analyze the radical and thermal effects in the flame quenching using a methane/air mixture. They established that both effects were caused by the wall, the thermal quenching resulted from the high heat losses through the combustor walls, leading to a situation where the auto-sustainable combustion is no longer possible, and the radical quenching was due to a deficit homogeneous chemistry caused by the radicals absorption at the wall and their subsequent recombination. This establishes the importance of a good choice of the wall properties to achieve a stable flame. For this

reason, Norton and Vlachos [5] performed a numerical study to analyze the impact of different combinations of the wall thermal conductivity and thickness in the external heat losses, also changing the dimensions of the combustion chamber and operation conditions. Their study allowed to define the optimal values of terms of wall thermal conductivity, dimensions and flow velocity to obtain an auto-sustainable methane/air mixture flame.

In sequence, Norton and Vlachos [6] performed a similar study using a propane and air mixture, obtaining similar conclusions for the scale reduction to micro. However, the range of thermal conductivity to be used for a stable combustion is higher due to lower ignition temperature of the propane. In an attempt to improve the thermal efficiency, Federici and Vlachos [7] simulated a propane and air mixture combustion inside of a simple channel reactor with and without recirculation to analyze the flame stability. They reported that the flame is more susceptible to extinction at the limits of highly conductive inner walls or lower fuel inlet velocities, obtaining the same stability effect in both situations. In addition, in the case of low-conductivity walls or high inlet velocities, the system became more stable with the presence of the recirculation due to the heat transferred to the cool reactants provided by the recirculation gases through the outer wall, causing ignition and flame stabilization. Federici et al. [8] continued their work by experimentally and numerically studying the flame stabilization on catalytic microburners with and without recirculation using the same fuel. At the limits of highly conductive walls, they achieved the same stabilization effect in both geometries, but for low conductivity walls, the microburner with recirculation became more effective when compared with the single channel due to the lower capacity to preheat the cool reactants.

To further understand the external heat losses impact in the combustion due to material properties of the combustor chamber walls, Li et al. [9,10] numerically studied the effect of different physical and boundary conditions on the flame temperature for H_2 and CH_4 microscale mixture combustion using stainless steel walls. They simulated both gas and solid phases and highlighted the importance of the reactants preheating through the axial heat conduction of the chamber walls to obtain a stable flame, suggesting the use of geometries with recirculation. These types of studies consisted essentially of 2D geometries, so to analyze the 3D effect, Pizza et al. [11] simulated a premixed hydrogen/air flame in a 3D microtube with different diameters and velocities, and they were able to observe three axisymmetric combustion modes by varying the inlet velocity: steady mild combustion, oscillatory ignition/extinction, typically known as FREI (flame with repetitive extinction-ignition), and steady flames. The FREI phenomenon was also reported in their previous work [12]. For higher diameter, the combustion dynamics became more complex, presenting a steady non-axisymmetric flame and a spinning flame which rotated azimuthally. They reported the existence of a critical tube diameter for the transition combustion modes. Later, Aikun et al. [13] simulated the combustion in a 3D rectangular microchannel using a hydrogen/air mixture and analyzed the impact on the flame in terms of flame temperature and length for different wall material, channel height and the inlet velocity. The temperature field showed three distinct regions, the preheating, the combustion and the cooling region, with the flame anchoring near the entrance in a cone-shaped structure. For the tested velocity range, the flame remained stable even in the limited cases, without extinction. In addition, in relation to wall materials, they reported that, in case of lower heat conductivity, the wall temperature becomes more intense, which could lead to thermal stress fracture. However, on the opposite side, with higher heat conductivity, the external heat losses increase, leading to a decrease in the reaction and probably to the extinction of the flame.

In order to improve the combustion efficiency, Pan et al. [14] studied a hydrogen/oxygen premixed combustion in microporous media combustor to achieve higher conversion efficiency of a micro thermophotovoltaic system and concluded that it is possible to obtain a more intense combustion with porous media materials with low specific heat and high thermal conductivity. By using a different fuel, Yan et al. [15] analyzed the geometrical parameters on CH_4 /air premixed combustion in a 3D heat recirculation micro-combustor with baffles. Recently, Peng et al. [16] investigated the combustion and thermal performance enhancement of a nozzle inlet microtube using hydrogen/air. Moreover,

Resende et al. [17,18] studied the impacts of N_2 dilution on a premixed H_2 /air combustion in terms of flame structure and pollutant emissions, NO_x , for a large range of equivalence ratios and dilution amounts. More recently, other numerical studies were performed to understand the geometrical effects on the microcombustion phenomenon. Li et al. [19] numerically investigated the behavior of a H_2 /air blend in a microcombustion chamber with cavities and found that these cavities can also expand the working range of the inlet velocity. Abbaspour and Alipoor [20] investigated the combustion characteristics of hydrogen/air premixed mixture in 1 mm converging–diverging microtubes with heated walls. Chabane et al. [21] performed a numerical study of catalytic combustion in a meso-scale channel with non-planar walls by exploring four different wall configurations and combining either obstacles or cavities and a continuous or segmented Pt-coating. Zuo et al. [22] developed a ribbed micro-cylindrical combustor, and performed a study with micro-cylindrical reduced wall thickness [23,24] and an elliptical cross-section microcombustor [25].

The present work numerically investigates the combustion characteristics in a complex geometry of one undulate microchannel using a H_2 and air mixture. The objective is to verify if the flammability at microscales can be improved by designing non-straight microchannels as an alternative to the burner with recirculation of reaction products. The effect of the geometry on the combustion characteristics is analyzed by varying the inlet velocity but keeping the same boundary conditions, equivalence ratio and external heat flux losses. In the methodology section, the fundamental governing equations that describe the physics of this work are presented, followed by the computational domain section, which provides detailed information regarding the specific problem addressed in this study. In the results section, the main findings of this study are presented and discussed in detail and, finally, the paper is concluded by summarizing the main achievements of this work.

2. Methodology

The governing equations used in the simulations to describe the microcombustion phenomenon are the conservation equations of total mass, momentum, species mass fractions and energy, for a compressible, continuous, multi-component and thermally perfect gas mixture, considered as Newtonian fluid, in a laminar flow, and can be expressed as :

$$\frac{\partial \rho}{\partial t} + \nabla(\rho \mathbf{u}) = 0 \quad (1)$$

$$\rho \left[\frac{\partial \mathbf{u}}{\partial t} + \nabla \cdot \mathbf{u} \mathbf{u} \right] = -\nabla p + \nabla \tau + \rho \mathbf{g} \quad (2)$$

$$\frac{\partial}{\partial t}(\rho Y_k) + \nabla(\rho Y_k \mathbf{u}) = -\nabla(\rho Y_k \mathbf{V}_k) + \dot{R}_k \quad k = 1, \dots, N_C \quad (3)$$

$$\rho C_p \frac{\partial T}{\partial t} + \rho C_p \mathbf{u} \nabla T = -\nabla \mathbf{q} - \rho \sum_{k=1}^{N_C} C_{p,k} Y_k \mathbf{V}_k - \sum_{k=1}^{N_C} h_k \dot{\Omega}_k \quad (4)$$

Here, $\mathbf{u}$, ρ , t , p , $\mathbf{g}$ and $\boldsymbol{\sigma}$ represent the mixture velocity vector, the mixture density, time, the pressure, the acceleration vector due to gravity and the fluid stress tensor, respectively. N_C is the total number of species, T is the temperature, and $\dot{\Omega}_k$, $\dot{R}_k$, h_k , Y_k and $\mathbf{V}_k$ are the net production rate of the k^{th} species, the formation rate, the enthalpy, the mass fraction and the diffusion velocity, respectively. $\mathbf{q}$ the heat flux vector and C_p represents the specific heat coefficients. The gas mixture is assumed to be an ideal gas and its density is calculated through the equation of state.

The diffusion velocities of species k are calculated from Fick's law and the thermal diffusion effect:

$$\mathbf{V}_k = -\frac{D_k}{Y_k} \nabla Y_k - \frac{D_k \Theta_k}{X_k} \frac{1}{T} \nabla T \quad (5)$$

where X_k , D_k and Θ_k are the mole fraction, the mixture-averaged diffusion coefficient of species k and the thermal diffusion.

The heat flux vector, $\mathbf{q}$, is defined as:

$$\mathbf{q} = -\lambda \nabla T + \mathbf{q}_{rad} \quad (6)$$

where $\mathbf{q}_{rad}$ is the radiative heat transfer and λ is the mixture thermal conductivity. However, some studies demonstrated that the radiative heat transfer could be neglected due to the smaller impact at microscale.

The radiative heat transfer can be modeled by assuming the optically thin radiation hypothesis in which self-absorption of radiation is neglected. The radiative heat transfer contribution in the energy equation is described as:

$$\nabla \mathbf{q}_{rad} = -4\sigma a_p (T^4 - T_{env}^4) \quad (7)$$

where σ is the Stefan–Boltzmann constant, T_{env} is the environment temperature and a_p is the Planck mean absorption coefficient.

The equations described above were implemented in the laminarSMOKE code by Cuoci et al. [26], according to the numerical procedure presented in Figure 1. A detailed kinetic mechanism consisted of 32 species and 173 reactions are used in this work to take the chemical reaction pathways of premixed hydrogen combustion into account [27]. This mechanism was developed and validated by CRECK Modelling Group in Polytechnic University of Milan, and more details can be found in [27]. The mathematical and physical models implemented in the laminarSMOKE were validated at microscale in previous studies of [17,18,28], and the results were able to capture the reaction pathways with good accuracy.

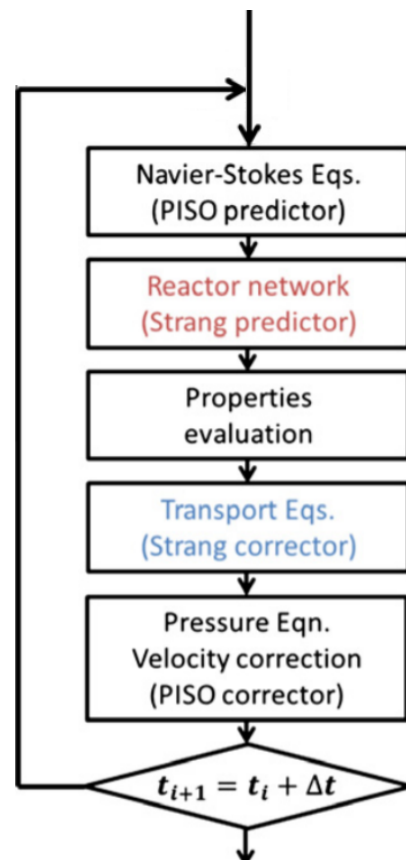


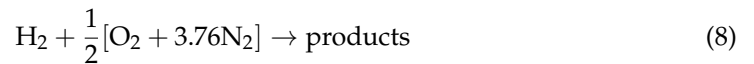
Figure 1. Numerical algorithm, adapted from Cuoci et al. [26].

3. Problem Description and Computational Domain

As reported previously, in order to verify if the flammability at microscales can be improved by designing non-straight microchannels, here we proposed an undulate symmetric microchannel burner, as represented in Figure 2a. The undulated microchannel

presents 10 mm length and minimum/maximum height of 0.30/1.28 mm in the center of the chamber, where the inlet and outlet keep the same height of 0.8 mm for 2 mm length.

For all simulations, the equivalence ratio and inlet temperature are the same, $\phi = 1.0$ and $T_{in} = 300$ K, respectively, at atmospheric pressure. The reaction composition of the H_2 /air mixture for $\phi = 1.0$ is given by Equation (8). The remaining boundary conditions are represented in the schematic illustration of the case setup (Figure 2a).



In all simulations, the temperature profile at the wall remained constant during each simulation. A hyperbolic temperature profile was imposed at the burner walls in which the wall temperature increases from 300 K at the inlet to 1300 K at 2/10 of the channel length, remaining constant at 1300 K afterward. This temperature distribution profile is extensively used to mimic the experimental profiles and was used in several works [12,28–30].

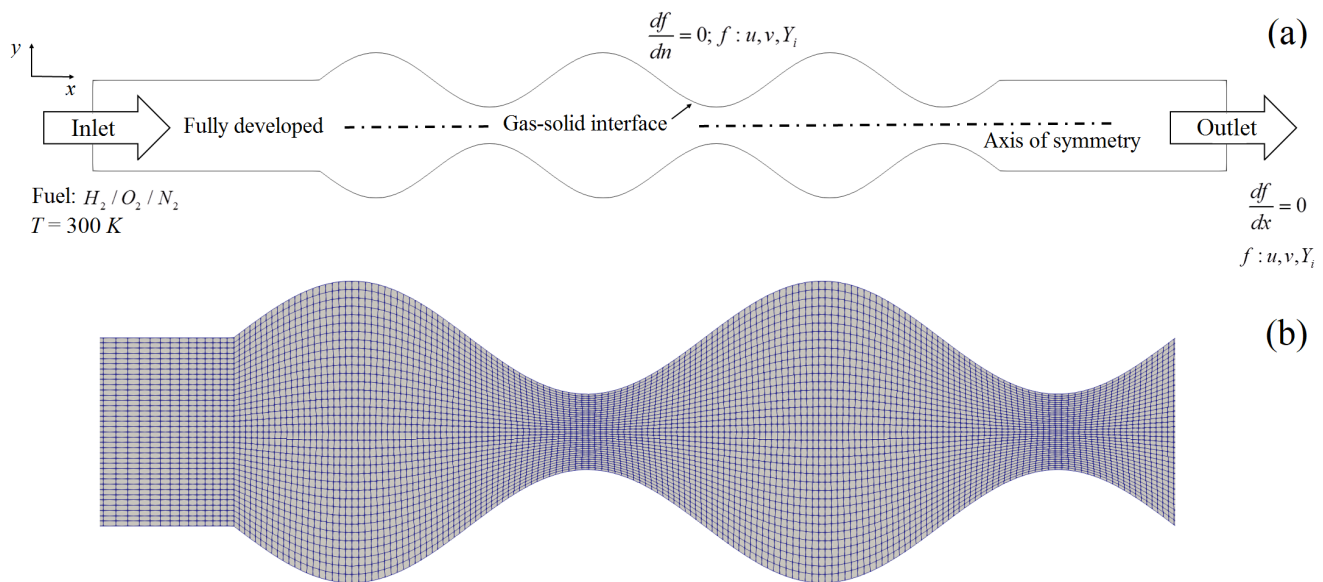


Figure 2. Schematic illustration of the (a) undulated geometry and (b) mesh resolution.

In order to verify the effect of the inlet velocity, U_{in} , on the flame structure, combustion dynamics and emissions, we performed a set of simulations for different inlet velocities, ranging from 4 to 22 m/s, as described in detail in Table 1.

Table 1. Summary of the simulated cases in this study.

Description	U_{in} (m/s)
C1	4
C2	8
C3	10
C4	14
C5	18
C6	22

Two distinct mesh resolutions were used in order to verify the independence of the results. The smaller computational domain comprises 10,836 total volume cells, with equidistant space cell in the center, resulting in a refinement of the smaller width zones (Figure 2b). The refined mesh has 21,672 total volume cells, similar to the mesh resolution

used in previous works while studying the effect of N_2 dilution on a H_2 and air combustion in a microchannel by Resende et al. [17,18]. Figure 3 presents the temperature profiles obtained with both computational domains using the conditions of case C1, Table 1, and it can be observed that the results presented a good agreement for both mesh resolutions.

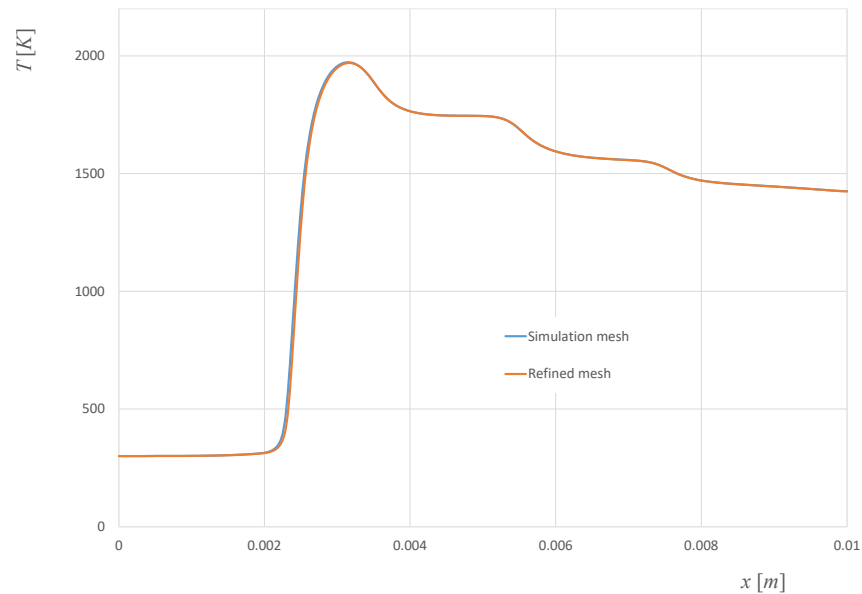


Figure 3. Temperature profile obtained in the mesh independence study using the conditions of case C1.

4. Results

In this section, the results for the flame dynamics, NO_x emissions, temperatures and heat release rates are discussed in detail for different inlet velocities. The dynamics of the flame structure are analyzed by comparing with other cases carried out in previous works. The comparison with experimental data is not possible due to the difficulty in measuring the combustion characteristics at this scale and because, to the authors' best knowledge, there are no experimental results for these and similar geometries.

The impact of the inlet velocity on the flame structure for the stable cases can be observed in Figure 4, presenting the contour maps of the heat release rate distribution Q and the streamlines of the flow field. Regardless of the inlet velocity, the flame becomes stable with the location of the maximum values of Q distribution, shifting downstream up to case C3, for $U_{in} = 10$ m/s. For higher inlet velocities, the heat release rate is divided into two different regions that are further stretched for higher inlet velocities. Another interesting observation is the effect of the vortices on the Q distribution for higher inlet velocities due to geometry of the burner that narrows the heat release into the middle of the burner, even in the convex zones.

Figure 5 presents the contour maps of the elevated temperature T^* which represents the temperature difference between the gas temperature (T) and the maximum wall temperature, defined here as $T^* = T - \max(T_{wall})$ (if $T < T_{wall,max}$, $T^* = 0$), allowing a better comprehension of the results by eliminating the wall temperature effects. The elevated temperature is higher for lower inlet velocity, for C1 case, located at the first contraction of the burner. As the inlet velocity increases, the flame is stretched downstream and the maximum T^* values decrease. For inlet velocities between 10 and 14 m/s, C3 and C4, the flame splits into the two first cavity regions at the burner entrance. For velocities above 18 m/s, cases C5 and C6, the flame is divided into the three cavity regions of the undulated microchannel.

Due to the detailed kinetic mechanism used in the simulations, it is possible to study the different species of the combustion reaction. Figure 6 presents the contour maps

of OH species. Here, the OH is used to identify the front of the flame. The OH mass fraction distribution shows the flame structure becoming more stretched as the inlet velocity increases with the maximum OH concentrations located more further downstream in the microcombustion chamber. For higher inlet velocities, above 14 m/s, case C4, there are two distinct OH concentrations regions, one at the entrance and the other downstream of the microchannel, with a reduction in the maximum OH value and the maximum flame temperature as the energy release becomes more dispersed. However, the energy dispersion, consequence of the Q stretching downstream (Figure 7), allows to maintain a higher flame temperature along the burner centerline, as observed in Figure 8.

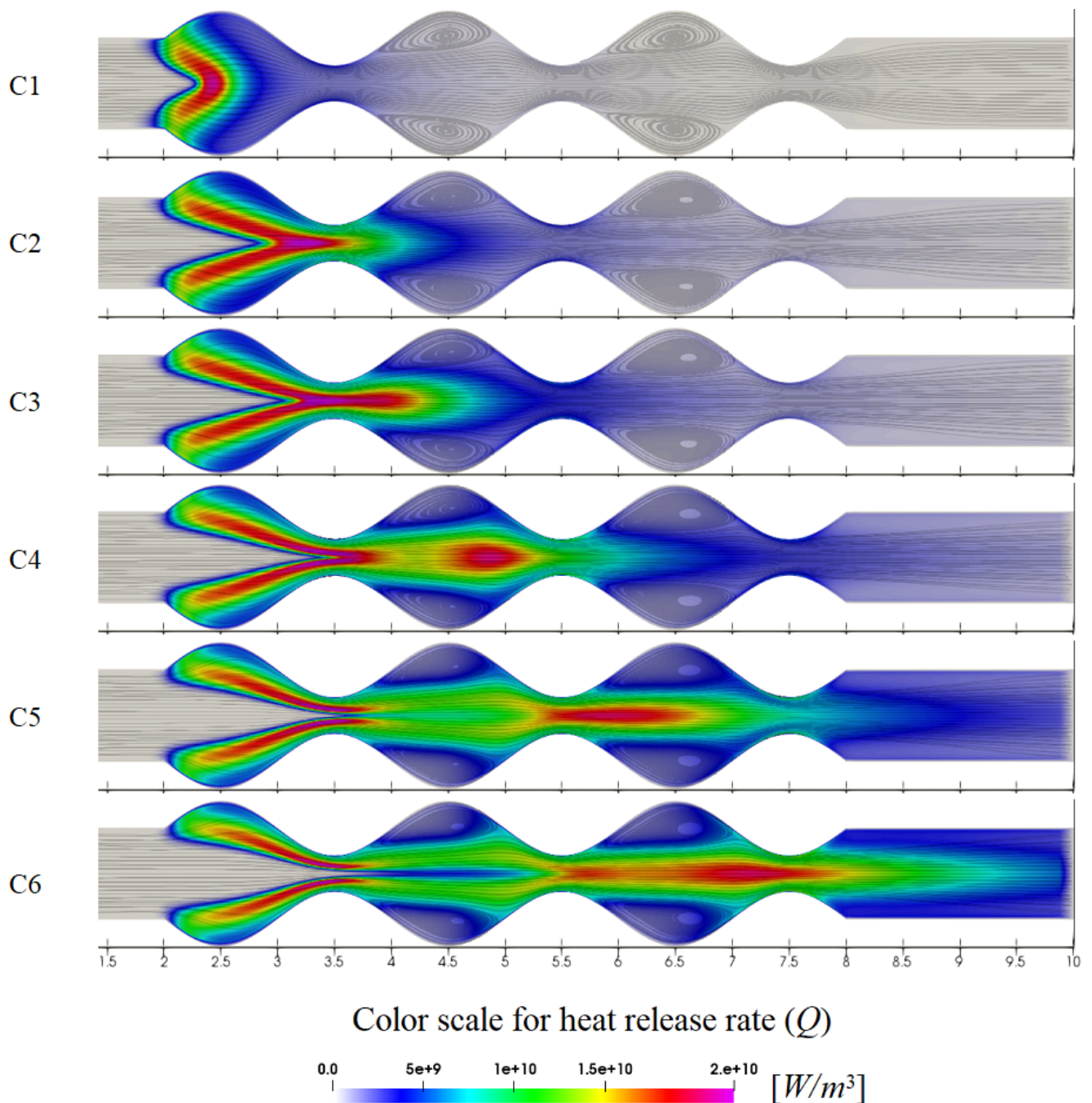


Figure 4. Contour maps for the streamlines superimposed on heat release rate distribution for different cases.

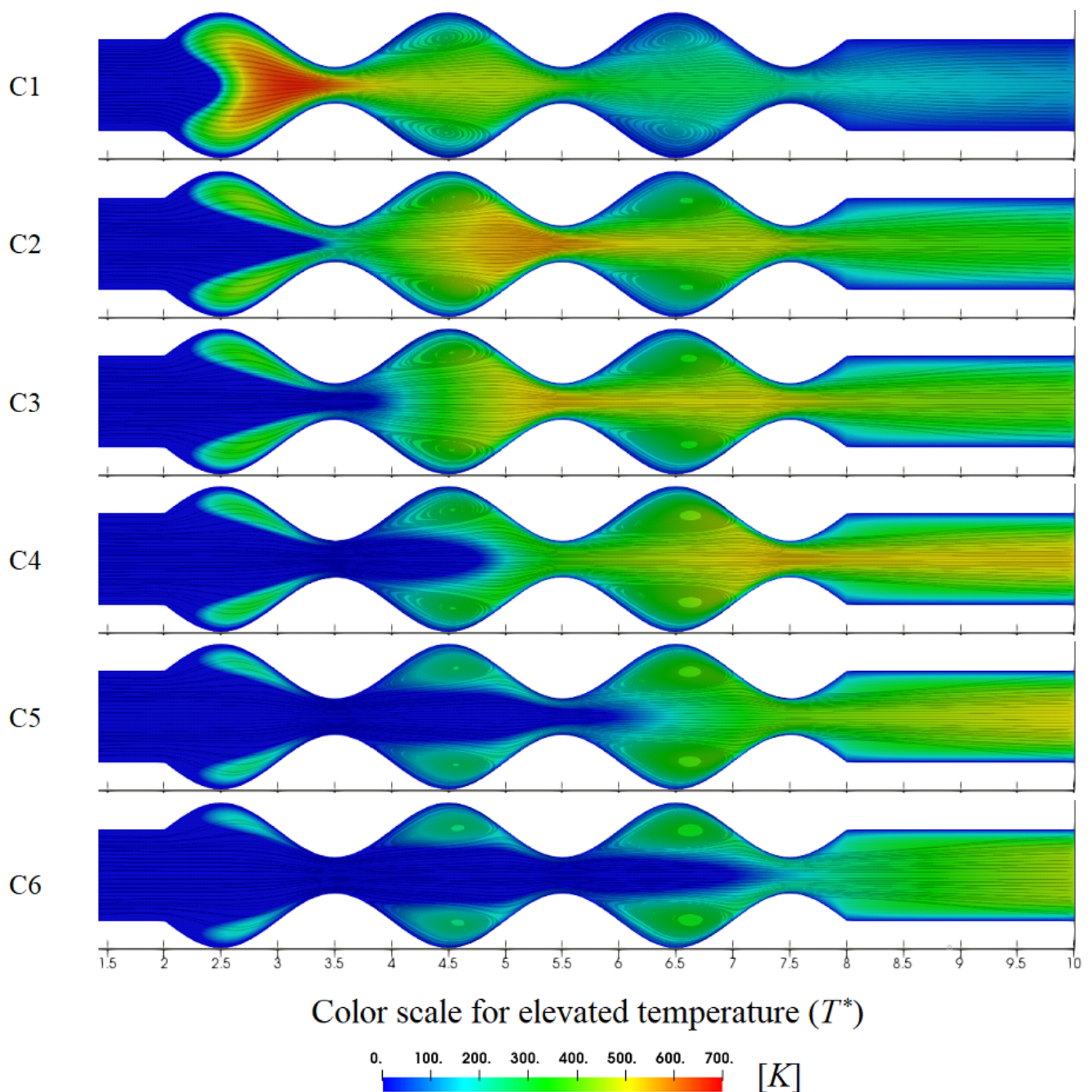


Figure 5. Contour maps for the streamlines superimposed on elevated temperature distribution for different cases.

Figure 7 presents heat release rate profiles along the centerline axis for different inlet velocities. For lower inlet velocity, cases C1 and C2, one can observe the typical profile observed in microchannel combustion with the heat release rate peak near the flame location, while the energy peak shifting downstream with the increase in the inlet velocity. Increasing the inlet flow rate for C3, the heat release profile presents a maximum value of Q , higher than the other cases, and non-monotonic decay is observed after the heat release peak. For the remaining cases, the Q profiles become broader due to the convective effect of the inlet velocity, and the non-monotonic behavior is more pronounced while the magnitude of the maximum values of Q remains similar to C1.

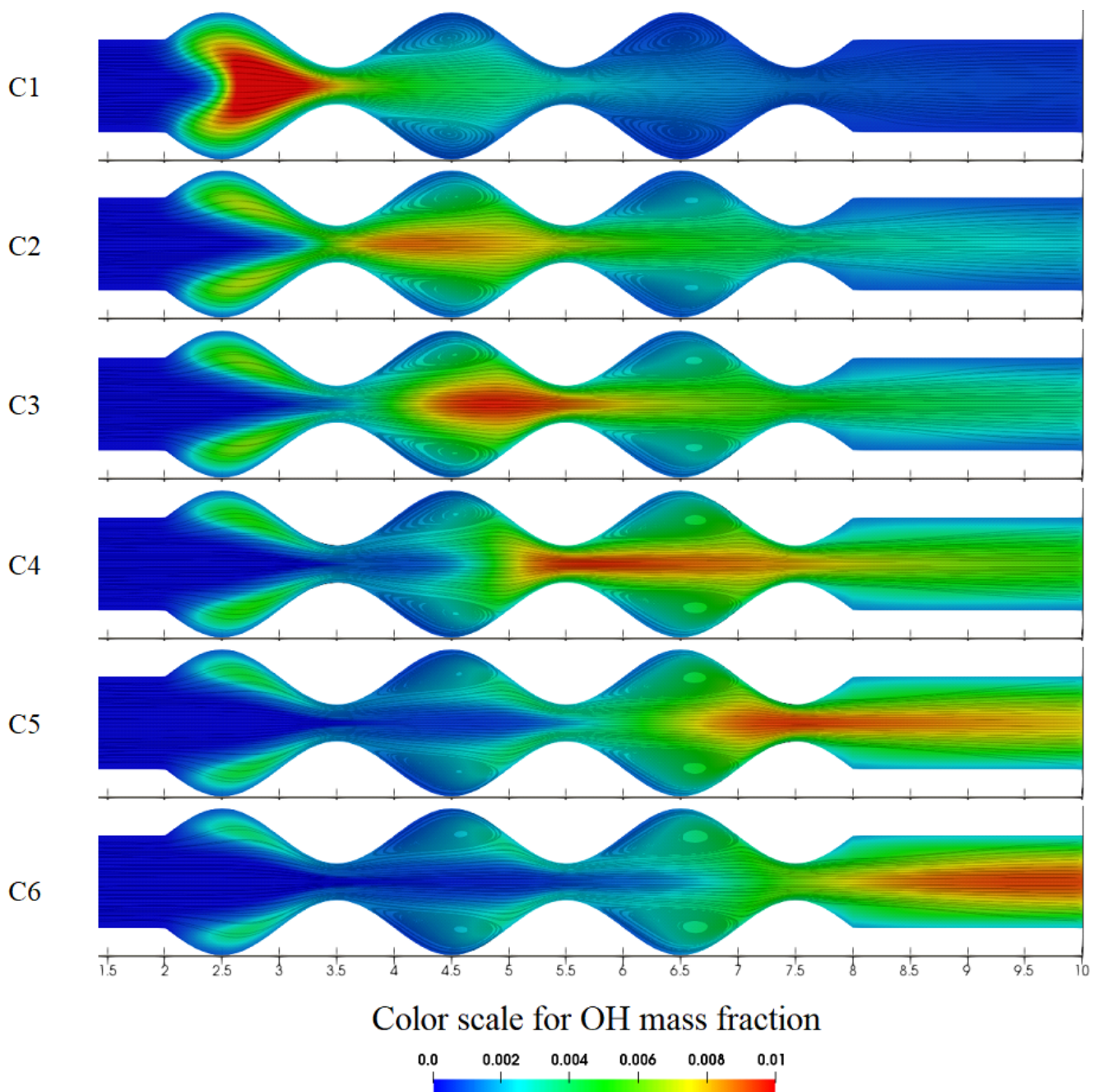


Figure 6. Contour maps for the streamlines superimposed on OH mass fraction distribution for different cases.

It should be noted that the increase in the maximum values of Q are not sufficient to increase the flame temperature, as can be observed in Figure 8, presenting the temperature profiles along the centerline axis for different inlet velocities. Figure 8 also presents the hyperbolic temperature profile imposed at the microburner walls. It can be observed that, as the inlet velocity increases, the loci of the maximum value for the temperature at the centerline shifts downstream in the microchannel. For the lower inlet velocity, case C1, it can be observed that the undulated walls of the microchannel impacts the temperature profile at the centerline, reflected in a stepping temperature profile along the microchannel.

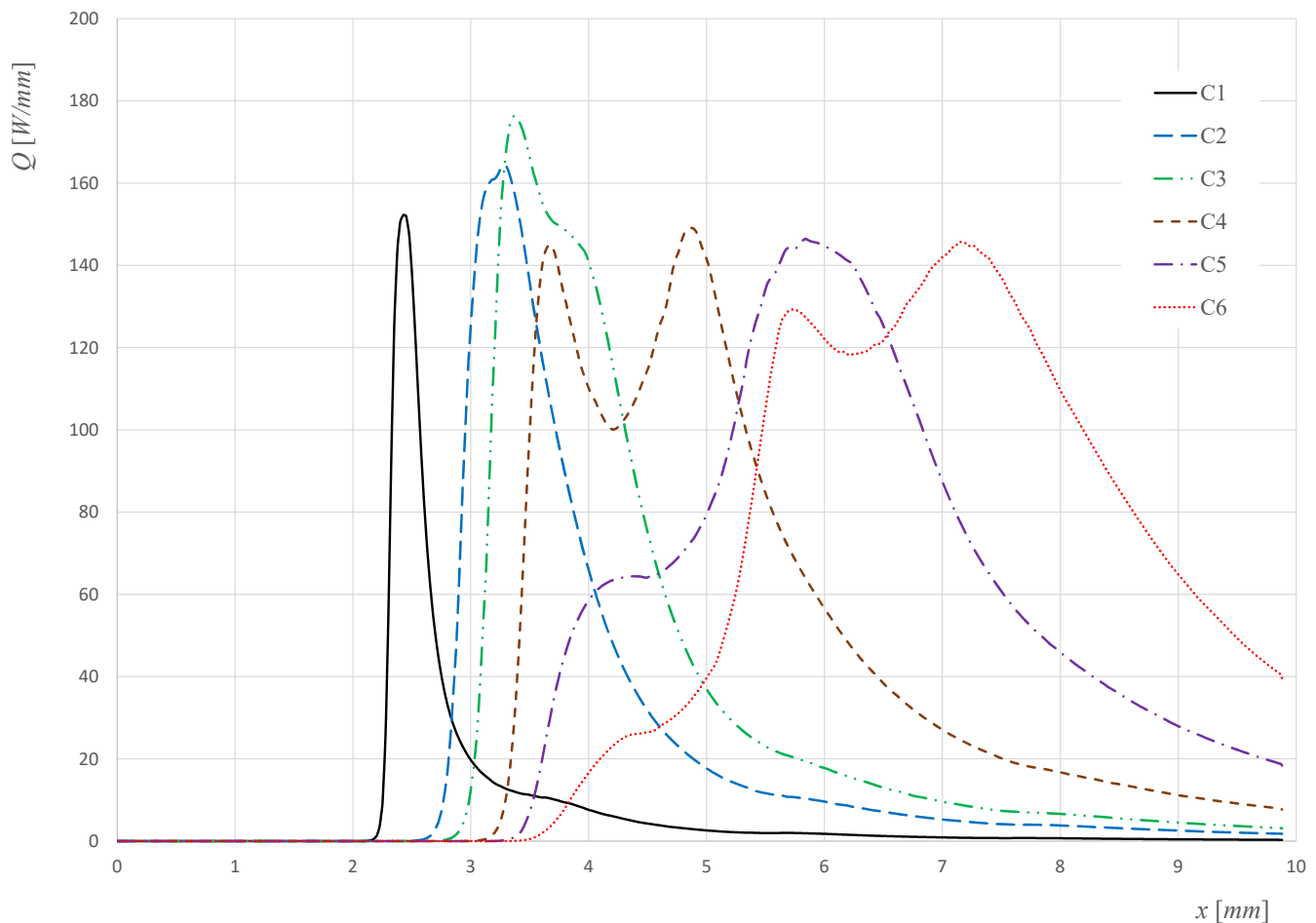


Figure 7. Heat release rate profiles along the centerline axis for different inlet velocities.

In order to better understand the effect of the geometric non-uniform microchannel walls, a new case was included, referred to as R1 in Figure 8, presenting the predictions of a premixed H_2 /air combustion in a uniform axisymmetric channel burner performed by Resende et al. [17], for the same boundary conditions of equivalence ratio, $\phi = 1.0$, and inlet velocity, 4 m/s, (equivalent to the case C1). Note that, in order to facilitate the comparison, the loci of the flame/temperature sharp increase for the uniform wall case, R1, was shifted to the respective loci of undulate microchannel, case C1, as can be verified in Figure 8.

Typically, in channel burners, the temperature reduction evolution along the centerline, after reaching the maximum value, is accomplished by a smooth variation, case R1, but here is made by steps caused by the heat losses through the walls. As the distance from the wall increases, there is a reduction in heat losses, consequence of the mass gas mixture/reaction products present between the flame and the wall, which acts as resistance to the heat flux and the temperature stabilizes. This effect can be visualized by the presence of the vortices for the case C1 at $x = 4.5$ and 6.5 mm, in Figure 5, and as the vortex becomes larger, the resistance to the heat flux increases and consequently causes the temperature stabilization. In other cases, the recirculation effect leads to a small reduction in temperature in the centerline after reaching the maximum flame temperature as, for example, cases C2 and C3. Comparing both cases at $x = 6.5$ mm, it is possible to visualize that the temperature reduction is smaller in case C3 when compared to C2. In the first, the temperature reduces to 1790 K and, in the second, to 1756 K, consequence of the vortex size at that location, where the vortex of C3 is higher than the C2 due to the higher inlet velocity of C3.

In addition, another phenomenon occurs before the flame, specially for highest inlet velocities, which could be considered as a pre-combustion effect caused by the stretching of the flame combined with the vortices size and the burner geometry, as mentioned before,

when referring to the presence of different structures of the heat release rate. This can be seen in Figure 8, through the linear temperature evolution along the chamber where, as the inlet velocity increases, the temperature increases more slowly and the maximum value is reached downstream of the channel.

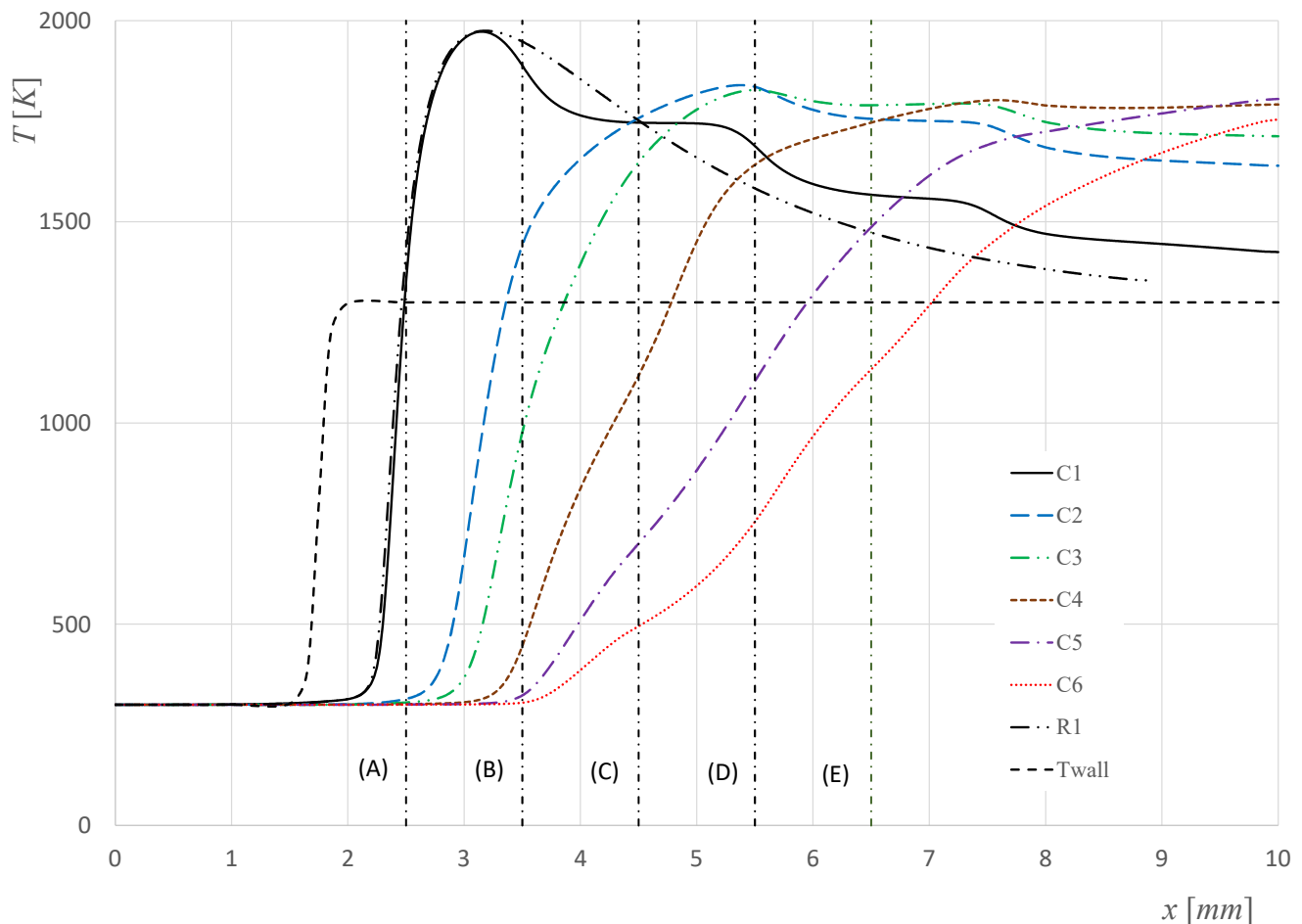


Figure 8. Temperature profiles along the centerline axis for different inlet velocities.

Figure 9 shows temperature profiles along the cross-sectional direction of the burner at several channel locations, $x = 2.5, 3.5, 4.5, 5.5$ and 6.5 mm, referred to in Figure 8 through the letters (A) to (E). These locations correspond to the consecutive middle of the convex and the contraction zones of the burner. Note that temperatures above the wall temperature represent a combustion reaction zone; therefore, it is possible to identify the extension of a single or separated flame.

For the case C1, for all locations across the burner, the temperatures are above T_{wall} , which means that the flame is continuous, starting with a V shape at the entrance of the burner and, after reaching the maximum temperature value at $x = 3.15$ mm, it decreases with the maximum values across the burner, occurring always in the center.

As the inlet velocity increases, the flames becomes weaker in the first convex zone (Figure 9A), while presenting a decrease in temperature. In all cases, the maximum flame temperature occurs at the center of the burner.

The mass fraction distribution of the main species for the C1 and R1 cases, along the centerline of the burner, can be visualized in Figure 10. To compare both cases, the referred location adjustment was performed, keeping the same flame front location for both cases. In the C1 case, the hydrogen and the oxygen are completely consumed, but in the R1 case, the H_2 fraction reduces in front of the flame and then increases. As a consequence, the N_2 and OH species are lower when compared with the C1 case. The mass fraction of water, H_2O

stabilizes at 0.25 for both cases; however, in the C1 case, it presents a shorter augmentation due to the effect of the velocity increase caused by the presence of the contraction.

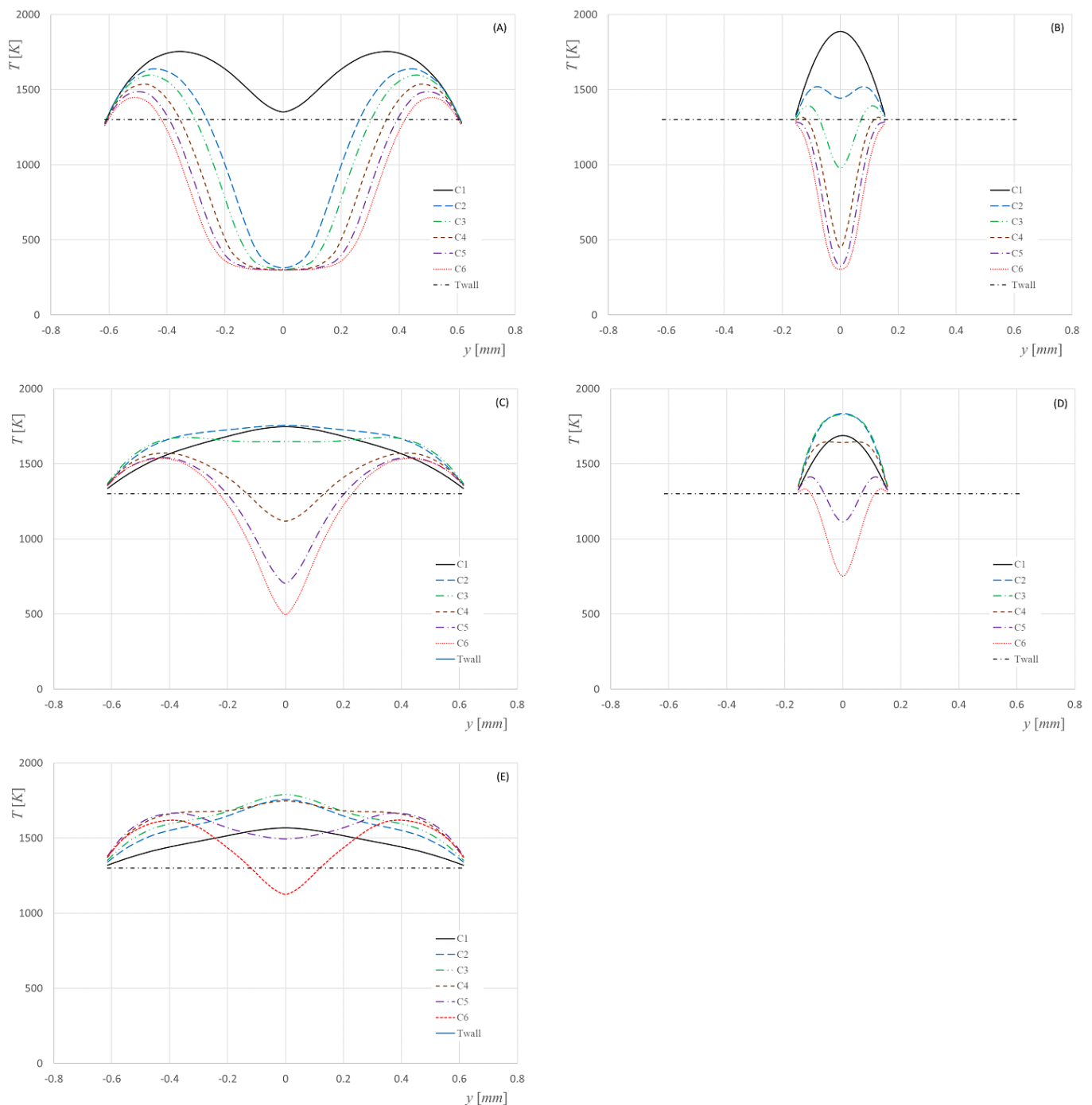


Figure 9. Temperature profiles across the burner for all cases. (A): $x = 2.5$ mm; (B): $x = 3.5$ mm; (C): $x = 4.5$ mm; (D): $x = 5.5$ mm; (E): $x = 6.5$ mm.

In terms of pollutant emissions, C1 presented a higher NO_x value of 4.25 ppm versus 3.32 ppm for case R1, due to the complete consumption of hydrogen in the combustion.

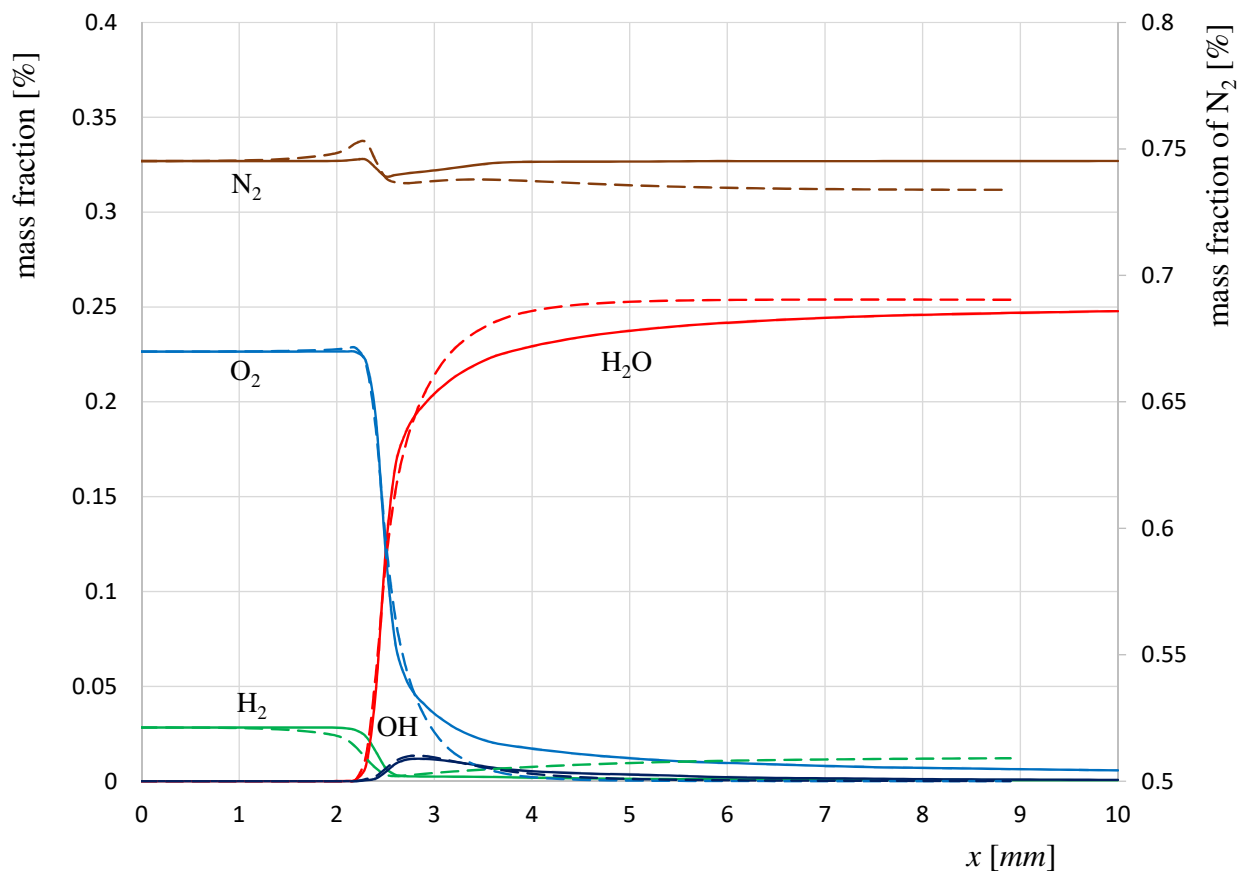


Figure 10. Comparison between the cases CH1 (continuum lines) and R1 (dashed lines) of the main species mass fractions in axial direction along the centerline.

5. Conclusions

A numerical study of a premixed H_2 /air combustion in an undulated microchannel was performed to analyze the effects of geometry impact on the flame structure and dynamics using different inlet velocities, from 4 to 22 m/s, with an equivalence ratio of $\phi = 1.0$. In all the tested cases, a hyperbolic temperature profile at the wall was imposed to mimic the heat external losses occurred in experimental setups. Due to the non-linear geometry of the burner, the increase in the inlet velocity defines a flame that extends along the burner, and although the instabilities appear at velocities above 8 m/s for all cases, the flame stabilizes regardless of the inlet velocity. However, the flame is stretched and divided into two parts for velocities above 14 m/s. Here, the evolution of the temperature along the axis, after reaching the maximum value, decreases by steps, instead of a smooth variation as occurs with the typical combustion in a channel burner. This effect is caused by the mass gas of the mixture/reaction products present in the vortices located in the convex regions, which acts as a resistance to the flux of heat losses. The larger the vortex size is, the higher the resistance to the heat flux. This also imposes smaller temperature decreases along the axis, consequence of the flame stretch combined with the heat flux resistance. This reduction in heat transfer to the walls is quite important in the flame stability in microcombustion and allows the development of new geometries based on the undulate or other non-uniform shapes as an alternative to existing burners.

Author Contributions: Investigation, P.R.R.; Validation, L.C.M., C.P. and A.M.A.; Data curation, P.R.R.; Writing—original draft, P.R.R.; Writing—review and editing, L.C.M., C.P. and A.M.A.; supervision, A.M.A. All authors have read and agreed to the published version of the manuscript.

Funding: This research received external funding by FAPESP through Project No. 2015/26842-3. A.M. Afonso was supported by Project UID/EMS/00532/2019 of CEFT (Centro de Estudos de Fenómenos de Transporte) and through Project PTDC/EMS-ENE/3362/2014-funded by FEDER funds.

Data Availability Statement: The data will be made available at reasonable request from the corresponding author.

Acknowledgments: P. R. Resende acknowledges the funding by FAPESP through Project No. 2015/26842-3. A. M. Afonso acknowledges the FCT for financial support through Project UID/EMS/00532/2019 of CEFT (Centro de Estudos de Fenómenos de Transporte) and through Project PTDC/EMS-ENE/3362/2014-funded by FEDER funds through COMPETE2020-Programa Operacional Competitividade e Internacionalização (POCI) and by national funds through FCT-Fundação para a Ciência e a Tecnologia.

Conflicts of Interest: The authors declare no conflict of interest.

Nomenclature

a_p	Planck mean absorption coefficient
C_p	Specific heat coefficients
D_k	Mixture-averaged diffusion coefficient of species k
$\mathbf{g}$	Gravity acceleration vector
h_k	Enthalpy
N_C	Total number of species
p	Pressure
$\mathbf{q}$	Heat flux vector
$\mathbf{q}_{rad}$	Radiative heat transfer
$\dot{R}_k$	Formation rate
t	Time
T	Temperature
T_{env}	Environment temperature
$\mathbf{u}$	Mixture velocity vector
$\mathbf{V}_k$	Diffusion velocity
X_k	Mole fraction of species k
Y_k	Mass fraction
Θ_k	Thermal diffusion of species k
$\boldsymbol{\sigma}$	Fluid stress tensor
λ	Mixture thermal conductivity
ρ	Mixture density
σ	Stefan–Boltzmann constant
$\dot{\Omega}_k$	Net production rate of the k^{th} species

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