

Three-dimensional simulations of isobaric premixed flames freely propagating in narrow circular channels: breaking of symmetry

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ABSTRACT

In this work we perform three-dimensional simulations to study the breaking of symmetry of lean premixed isobaric flames propagating in narrow channels of circular cross-section subject to an inlet Poiseuille flow. In particular we consider the effects of the flow rate, the channel diameter, wall heat-losses for flames with the Lewis number (Le) equal or less than unity.

Numerical analysis shows that for $Le = 1$ and under adiabatic conditions, a supercritical bifurcation occurs at flow rates exceeding the critical value and the axisymmetric flame becomes unstable, giving rise to a nonaxisymmetric flame. For flames with $Le < 1$, a subcritical bifurcation occurs and we report multiplicity of stable solutions: the flame can be axisymmetric and non-axisymmetric for the same values of parameters. It is important to underline that both types of solutions are stable, and thus can be observed experimentally. In the presence of wall heat-losses, the critical flow rate corresponding to the bifurcation point increases. This indicates a promoting effect of wall heat-losses on flame shape symmetry. We also find that an extinction gap can appear when increasing the flow rate. For the smaller Lewis number ($Le = 0.5$) we observe a complex flame dynamics, showing the coexistence of steady and oscillatory combustion regimes.

KEYWORDS

symmetry breaking, premixed laminar flame, wall-heat losses, Lewis number, three-dimensional circular channel

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1. Introduction

Propagation of laminar premixed flames in channels has been studied for several decades. Early fundamental works focused on quenching phenomena [1, 2], shape and structure of the flame such as the transition from mushroom to tulip flame [3–6], and on the related intrinsic instabilities [7, 8]. More recently, dynamics of propagating flames has been extensively investigated by active research conducted on the development of small-scale combustors [9–11]. Experiments reveal a very rich and complex flame behaviour in which transport, thermodynamics, chemistry and geometry are all influential: mild [12] and excess enthalpy [13] combustions, repetitive ignition/extinction [12, 14], steady symmetric and asymmetric flames [15–19] as well as oscillatory flames [12, 20] were observed. Of particular interest for the present study is the loss of flame shape symmetry reported in some of these experiments under various conditions.

Stability analysis and numerical works focusing on symmetry breaking of a flame propagating in a channel are quite recent. As consequence of the high computational cost required by numerical three-dimensional (3D) simulations, a particular emphasis on the flame symmetry properties in bi-dimensional (2D) planar channels has been given first in [21–27]. These studies provide important information on the parameters (thermal expansion, wall-heat losses, channel height, inlet flow rate, Lewis number) that promote the occurrence of asymmetric flames. Loss of symmetry is shown to be associated with two different instabilities. One of them is the differential-diffusion instability, controlled by the Lewis number (when non-equal to unity) and the other one is the Darrieus-Landau instability which has a purely hydrodynamics character due to thermal expansion. In numerical experiments, effects of these two instabilities can be separated. Making use of a constant density combustion model (hydrodynamic contribution is suppressed), [23, 24] report propagation of non-axisymmetric flames for non-unity Lewis number. On the other hand, [27] shows as well breaking of flame symmetry when considering a variable density model and unity Lewis number (only Darrieus-Landau is accounted for). Occurrence of asymmetric flames is thus a result of a complex non-linear interaction between instabilities that also depends on various flow parameters. Increase of inlet flow rate and/or diameter and decrease of Lewis

number are found to favour asymmetry while wall heat-losses have a stabilizing effect on symmetry. Note as well that gravity effects (neglected in the previous works) may alter the flame shape symmetry. Those were considered for a 2D channel in [28, 29].

Examination of breaking of symmetry in a circular channel is much more restricted as the azimuthal direction has to be accounted for, implying fully 3D calculations. Studies making use of thermo-diffusive (constant density) model [30, 31] and including thermal expansion effects [28, 31–34] report non-axisymmetry for freely propagating flames under adiabatic/cold wall (uniform wall temperature) [28, 30–33] and for stabilized flames with prescribed wall temperature gradient [34]. In particular, numerical works show that multiple stable solutions for flames with Lewis numbers smaller than unity can occur for an identical set of parameters (inlet flow rate, tube diameter, wall temperature condition): the coexistence of steady axisymmetric with steady non-axisymmetric flames was observed in [30, 31, 33] and of steady axisymmetric with spinning flames in [34]. Multiplicity of stable flame solutions was not found in planar channels, revealing in turn the relevance of including the azimuthal mode in the analysis of flame shape dynamics. As mentioned earlier, the flame behaviours reported in the above numerical studies were observed in experiments [15, 16, 18, 19, 29]. However, a systematic analysis of loss of symmetry is difficult to perform experimentally and further 3D numerical simulations are missing to scrutinize the various shapes a flame can take when propagating in a circular channel.

The present work aims to complete previous studies carried out on breaking of flame symmetry in narrow channels. It is a direct continuation of [33] done for low Lewis numbers ($Le < 1$) flames propagating in a circular adiabatic channel. In contrast to [33], here we analyse the loss of symmetry also for flames with Lewis number equal to unity. This allows to consider separately the Darrieus-Landau instability ($Le = 1$) from the thermo-diffusive instability ($Le \neq 1$), both associated with breaking of symmetry. In addition, we also investigate here the effects of wall heat-losses. On the basis of the results reported in [27], we select a range of the critical parameters involved in the emergence of non-symmetric flames and perform 3D numerical simulations of the full set of Navier-Stokes and conservation equations. The flame chemistry is modeled by a one-step overall reaction. This simple model allows to explore an extended range of

the relevant parameters promoting loss of symmetry (inlet flow rate, Lewis number, wall-heat losses and tube diameter) at a reduced computational cost compared to the use of a more detailed chemistry.

The paper is organized as follows. Although the general equations are generally standard, in Section 2 we describe the formulation of the problem, for the sake of completeness. In Section 3 we present the results obtained for the effects of the flow rate, channel diameter and wall heat-losses for flames with unit Lewis number. In this latter case, only the Darrieus-Landau instability takes place. Then, Section 4 reports results that include the thermo-diffusive instability for flames with Lewis numbers smaller than unity. Conclusions are given in Section 6.

2. Mathematical formulation

2.1. Governing equations

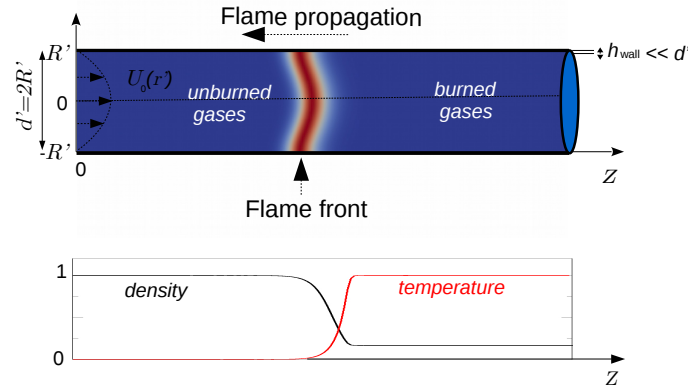


Figure 1. Schematic of the flame propagating in a circular channel of radius R' : the flame propagates towards the inlet boundary of the circular channel where a Poiseuille flow is prescribed; the wall thickness h_{wall} is supposed to be much smaller than the diameter $d' = 2R'$; (top) flame front visualized by isocontours of reaction rate, (bottom) corresponding non-dimensional density and temperature profiles along the axial direction (Oz).

We consider a lean combustible mixture at initial temperature T_0 and density ρ_0 that flows in a circular channel of diameter d' and axial direction (Oz). At the inlet of the channel is imposed a Poiseuille flow, $\mathbf{v}' = 2U_0[1 - (2r'/d')^2]\mathbf{e}_z$, with mean velocity U_0 and where $\mathbf{e}_z$ denotes the unit vector along the channel axis and r' the

radial coordinate. To be specific, the fresh cold mixture is located at the left of the flame while combustion products at its right, as sketched in Fig. 1. Here above and below, primes denote dimensional variables.

A global, one step and irreversible chemistry model with Arrhenius law is used for the reaction rate, $\Omega = \mathcal{B}\rho'^2 Y' \exp(-E/\mathcal{R}T)$, where E is the overall activation energy, $\mathcal{R}$ the universal gas constant, Y' the mass fraction **of the deficient species (fuel) of the lean combustibile mixture** and $\mathcal{B}$ is a pre-exponential factor. Note that, the mixture being lean in fuel, the oxidizer mass fraction is assumed constant and included in $\mathcal{B}$. The transport properties and the specific heat are considered constant. Note that we use a squared-density dependence for Ω which is more realistic for lean mixtures, the rich component consumption being thus neglected.

Similar to [33], the governing equations are made non-dimensional using the burning velocity of the planar flame, S_L , the thermal flame thickness defined as $\delta_T = \mathcal{D}_T/S_L$, the characteristic time $\mathcal{D}_T/S_L^2$, adiabatic flame temperature $T_a = T_0 + QY_0/c_p$, the characteristic pressure value $\rho_0 S_L^2$ and the upstream fuel mass fraction Y_0 . Here $\mathcal{D}_T$ stands for the thermal diffusivity, c_p for the specific heat at constant pressure and T_0 is the fresh mixture temperature.

The dimensionless variables are the coordinates, $(z, r) = (z', r')/\delta_T$, the time, $t = S_L t'/\delta_T$, the velocity, $\mathbf{v} = \mathbf{v}'/S_L$, the density $\rho = \rho'/\rho_0$, the reduced temperature $\theta = (T' - T_0)/(T_a - T_0)$, the mass fraction $Y = Y'/Y_0$ and the pressure deviation from the ambient (atmospheric) pressure, $p = (p' - p_{atm})/\rho_0 S_L^2$.

All calculations presented in this work were performed in a finite domain. In order for the flame not to leave the computational domain and not approach its boundaries, we use a computational framework moving at a speed as close as possible to the flame velocity relative to the wall as done in [25]. **In this way, the channel can be considered as infinitely long.** The (uniform) speed of this reference frame is designated as $\mathbf{w} = w \mathbf{e}_z$.

When applying the low Mach number approximation, the dimensionless equations of continuity, momentum, temperature, mass fraction in the moving reference frame and the equation of state become:

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho[\mathbf{v} + \mathbf{w}]) = 0, \quad (1)$$

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\rho [\mathbf{v} + \mathbf{w}] \cdot \mathbf{v}) = -\nabla p + Pr \nabla (\nabla \cdot \mathbf{v} + \nabla \cdot \mathbf{v}^T), \quad (2)$$

$$\frac{\partial \rho \theta}{\partial t} + \nabla \cdot (\rho \theta [\mathbf{v} + \mathbf{w}]) = \nabla^2 \theta + \omega, \quad (3)$$

$$\frac{\partial \rho Y}{\partial t} + \nabla \cdot (\rho Y [\mathbf{v} + \mathbf{w}]) = Le^{-1} \nabla^2 Y - \omega, \quad (4)$$

$$\rho(1 + q\theta) = 1, \quad (5)$$

This set of equations is solved for $0 < r < d/2$, $0 < z < L_z$, $0 < \varphi < 2\pi$ in terms of the standard cylindrical coordinates. The gas velocity, $\mathbf{v}$, appearing in Eqs. (1)-(4) represents the velocity relative to the wall. The velocity $\mathbf{w}$ is uniform and adjusted to the flame velocity according to Eq. 8 (see below) so that the computational framework moves with the flame. This formulation allows to change the reference frame speed without including non-inertial terms in the momentum equation.

The dimensionless parameters in Eqs. (1)-(5) are the channel diameter $d = d'/\delta_T$, the heat release parameter $q = (T_a - T_0)/T_0$, the Lewis number $Le = \mathcal{D}_T/\mathcal{D}_F$, with $\mathcal{D}_F$ being the molecular diffusivity of the fuel, and the Prandtl number $Pr = \nu/\mathcal{D}_T$, with ν being the kinematic viscosity of the mixture.

The dimensionless reaction rate takes the following form:

$$\omega = \frac{\beta^2}{2Leu_p^2} (1 + q)^2 \rho^2 Y \exp \left\{ \frac{\beta(\theta - 1)}{(1 + q\theta)/(1 + q)} \right\}, \quad (6)$$

where $\beta = E(T_a - T_0)/\mathcal{R}T_a^2$ represents the Zel'dovich number. The factor $u_p = S_L/U_L$ appears in Eq. (6) to account for the difference between the asymptotic value of the planar laminar flame speed obtained at $\beta \rightarrow \infty$ and that at finite β . This makes possible to have the dimensionless planar flame speed equal to unity at finite β .

2.2. Boundary conditions

At the inlet ($z = 0$), exit ($z = L_z$) and wall of the channel, the following boundary conditions are used:

$$\begin{aligned}
 z = 0 : \quad \mathbf{v} &= 2m(1 - (2r/d)^2)\mathbf{e}_z, \quad Y = 1, \theta = 0; \\
 z = L_z : \quad \partial \mathbf{v} / \partial z &= \partial \theta / \partial z = \partial Y / \partial z = 0, \\
 r = d/2 : \quad \mathbf{v} &= \mathbf{0}, \quad \partial Y / \partial r = \partial \theta / \partial r + b\theta = 0,
 \end{aligned} \tag{7}$$

where $m = U_0/S_L$ is the (dimensionless) fresh gas flow rate, $b = \lambda_w \delta_T / \lambda_0 h_{wall}$ is the heat-losses intensity. Here λ_0 and λ_{wall} stands for the conductivity of the unburned gas and of the solid wall, respectively, and are constant while h_{wall} is the wall thickness. The temperature wall boundary condition is identical to that one introduced in [24]. We assume that the wall is thin in comparison with the channel cross-section, $h_{wall} \ll d'$, and that the external temperature is equal to the initial temperature of the mixture. Note that the limit $b \rightarrow \infty$ corresponds to an isothermal wall while the value $b = 0$ to an adiabatic wall. For the outlet boundary conditions, the velocity, temperature and mass fraction have the z -derivative equal to zero. For a sufficiently large domain, the influence of the outlet condition becomes negligible.

For the steady-state flame motion, namely when $\partial/\partial t \equiv 0$ in Eqs. (1)-(4), the reference frame speed, w , should coincide with the flame velocity u_f relative to the channel wall. By integrating Eq. (4) and continuity equation Eq. (1) one can obtain (see details in Appendix A)

$$u_f = u_c - m \tag{8}$$

with the consumption speed u_c defined by

$$u_c = \frac{4}{\pi d^2} \frac{1}{\rho_0(Y_0 - Y_{L_z})} \int_0^{L_z} \int_0^r \int_0^{2\pi} \omega dz r dr d\varphi \tag{9}$$

where Y_{L_z} is the fuel mass fraction averaged in the cross-section of the channel located downstream of the flame at the exit of the channel. In the case of adiabatic wall the fuel is completely consumed ($Y_{L_z} = 0$) while in presence of wall heat-losses, depending on the value of b , fuel may not be totally burned ($Y_{L_z} \neq 0$, see Appendix C). During the simulation, we set $w = u_f$ computed from Eq. (8) and add it to the axial velocity. **Note that the velocity w is iteratively corrected so that its variation during transient state is very small.** In this way, the balance between burning and reactant rates is satisfied and the computational framework moves concomitantly with the flame. The dimensionless velocity u_f is positive when the flame moves to the left while it is negative when it moves to the right. When $u_f = 0$, the flame is motionless (the flash-back point) relative to the channel wall.

For the present configuration, the control parameters are the inlet flow rate m and the wall-heat loss parameter b . The Lewis number Le takes the values $Le = 1, 0.7$ and 0.5 and the channel diameter $d = 6.32$ and 10 . The smaller value $d = 6.32$ has been selected to allow comparisons with our previous study [33] that reports results for this diameter for flames with Lewis number less than unity propagating in adiabatic circular channel (see details in [33]). The other parameters $Pr = 0.7$, $\beta = 10$ and $q = 5$ are fixed. The corresponding numerical values of u_p calculated for $Le = 1, 0.7$ and 0.5 are 1.0546 , 1.0851 and 1.1068 , respectively [27].

2.3. Numerical methodology

The open source Computational Fluid Dynamics (CFD) code OpenFoam [35] is used to resolve the set of equations (1)-(5). This computational code is based on the finite volume method formulated in a collocated grid arrangement. For temporal discretization we use the first order Euler scheme and a second-order scheme for spatial discretization.

We performed simulations for a fully 3D circular channel geometry as well as for a 2D geometry with an axisymmetric frame. These simulations will be referred as to 3D and 2DA simulations, respectively.

In the 2DA simulations, the grid resolution takes the dimensionless values $\Delta_r = 0.1$ for $Le = 1, 0.7$, and $\Delta_r = 0.05$ for $Le = 0.5$. Using of half-grid resolution provided

identical results (see Table B1, in Appendix B).

In the 3D simulations, the grid resolution is similar to the one used in the 2DA simulations for $Le = 1$ and $Le = 0.7$ while it is slightly relaxed to 0.07 for $Le = 0.5$. Two different types of grid mesh were used to discretize the computational domain. One grid mesh consists of a triangular prism decomposition and the other is a block-structured one composed of hexahedra computational cells (see Fig. B1 in Appendix B). These different meshes aim to check grid-mesh cell shape independence on the flame solution. We use a number of 1773360 prism cells and of 1372000 hexahedra cells to discretize the 3D channel geometry. We performed test on the grid resolution for some cases by making use up to 6250000 cells. Details on the tests performed for the grid resolution and cell decomposition are given in Appendix B. The length of the channel varies from $40\delta_T$ to $58\delta_T$ by maintaining the same numerical resolution. The increase of the channel length is required to well resolve the cases of flame highly stretched under large values of the inlet flow rate. It is also important to check that computational length is large enough in case of important wall heat-losses to ensure that temperature and mass fraction are well resolved far downstream of the flame. Tests on computational domain length are reported in Appendix C.

Finally, numerical stability and convergence of the solution were obtained by using a dimensionless time step equal to 5×10^{-5} .

3. Numerical results for flames with $Le = 1$

First, we focus on the cases with unity Lewis number to analyze the effect of channel diameter and wall heat-losses on the flame structure under varying inlet flow rate. All numerical solutions presented in this section are steady-state solutions **in the sense that flame propagates along the channel with a constant velocity as a rigid structure.**

It should be noted that conventional axisymmetric (2DA) solutions always exist, at least as a mathematical object. These solutions may be unstable to non-axisymmetric perturbations. However, they can always be calculated by imposing $\partial/\partial\varphi \equiv 0$ (in terms of standard cylindrical coordinates) in the governing equations. Obviously, when both 3D and 2DA calculations provide the same flame structure, the

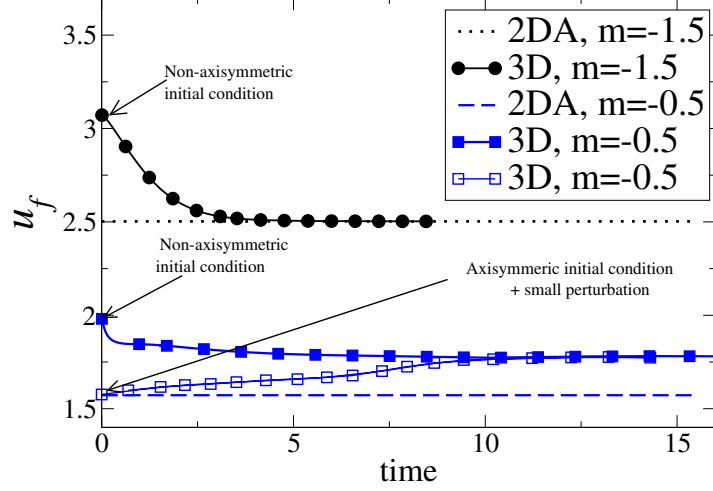


Figure 2. Time history of flame velocity u_f for $Le = 1$, $d = 10$ and adiabatic wall conditions ($b = 0$); comparisons between 2DA and 3D simulations given for different values of the inlet flow rate m . Dashed and dotted lines correspond to 2DA simulation solutions. At time $t = 0$ different initial conditions are used for the 3D simulations to illustrate how they converge to stable axisymmetric or non-axisymmetric solutions. When 2DA and 3D solutions coincide the axisymmetric flame is stable otherwise it is unstable and instead a stable non-axisymmetric solution is obtained.

latter axisymmetric flame solution is stable but otherwise is unstable. Note that, to find the non-axisymmetric flames, a small non-axisymmetric perturbation consisting of a hot spot is initially added to the axisymmetric flame solution. If the hot spot is placed in the upper part of the channel (by respect to the plane (xOz) at $y = 0$ in our simulations), an upper axisymmetric flame is obtained; in the opposite case, that is a hot spot located in the lower part of the channel, a lower non-axisymmetric flame takes place. Evidently, if the flame recovers an axisymmetric shape after being perturbed, this axisymmetric flame is stable. The time evolutions of the flame velocity u_f provided in Fig. 2 show all a stationary convergence after a transition time. They also picture how two different initial conditions (at time $t = 0$) provide identical solutions with 2DA and 3D simulations when the axisymmetric flame is stable ($m = -1.5$) but different ones when the 2DA flame is not stable ($m = -0.5$).

3.1. Effects of channel diameter d for adiabatic flames

Figure 3 shows the flame velocity u_f plotted as a function of the inlet flow rate m obtained from the 2DA and 3D simulations. All cases correspond to $Le = 1$, $b = 0$, and two values of the channel diameter, $d = 6.32$ and $d = 10$. Vertical dashed lines in Fig. 3 indicate the critical values of the flow rate, m_{3D} , above which the non-axisymmetric

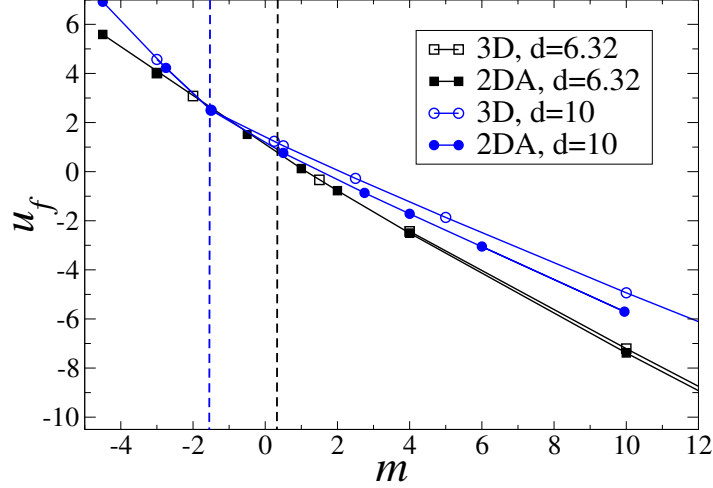


Figure 3. Comparison between 2DA and 3D simulations, $Le = 1$, adiabatic wall ($b = 0$): flame velocity u_f as function of the dimensionless flow rate m obtained for $d = 6.32$ and 10 . Vertical dashed lines indicate the critical value m_{3D} for which only non-axisymmetric (3D) flame solution is obtained; vertical dashed lines are colored according to d values.

(3D) solutions emerge. For $d = 10$ we find $m_{3D} \approx -1.5$ while for $d = 6.32$, $m_{3D} \approx 0.25$. The transition from an axisymmetric solution to a non-axisymmetric one with increasing values of m corresponds to a supercritical bifurcation. The difference between the 2DA and 3D simulations results are used as an indicator of departure from axisymmetry for the stable flame, when $\delta m = m - m_{3D} \gtrless 0$ the degree of axisymmetry loss is small.

Shown in Fig. 4 are the temperature isosurface $\theta = 0.9$ plotted for various m and two values of d . The flame initially axisymmetric for $m = -3$ becomes non-axisymmetric as m is further increased to 4. Note that for the same value of m , the degree of non-axisymmetry is larger at larger values of d .

It is generally accepted [6] to classify the flame shape in channels into mushroom (convex) and tulip (concave) structures (relative to the fresh side of the mixture). Figure 4 exhibits an axisymmetric mushroom-like structure flame for $m = -3$ and both values of the channel diameter. For larger values of m , the flame takes a non-axisymmetric tulip-like shape.

3.2. Effects of wall heat-losses

The influence of the heat-loss parameter b is analyzed for both stable axisymmetric and non-axisymmetric flames previously found under adiabatic conditions. The effect

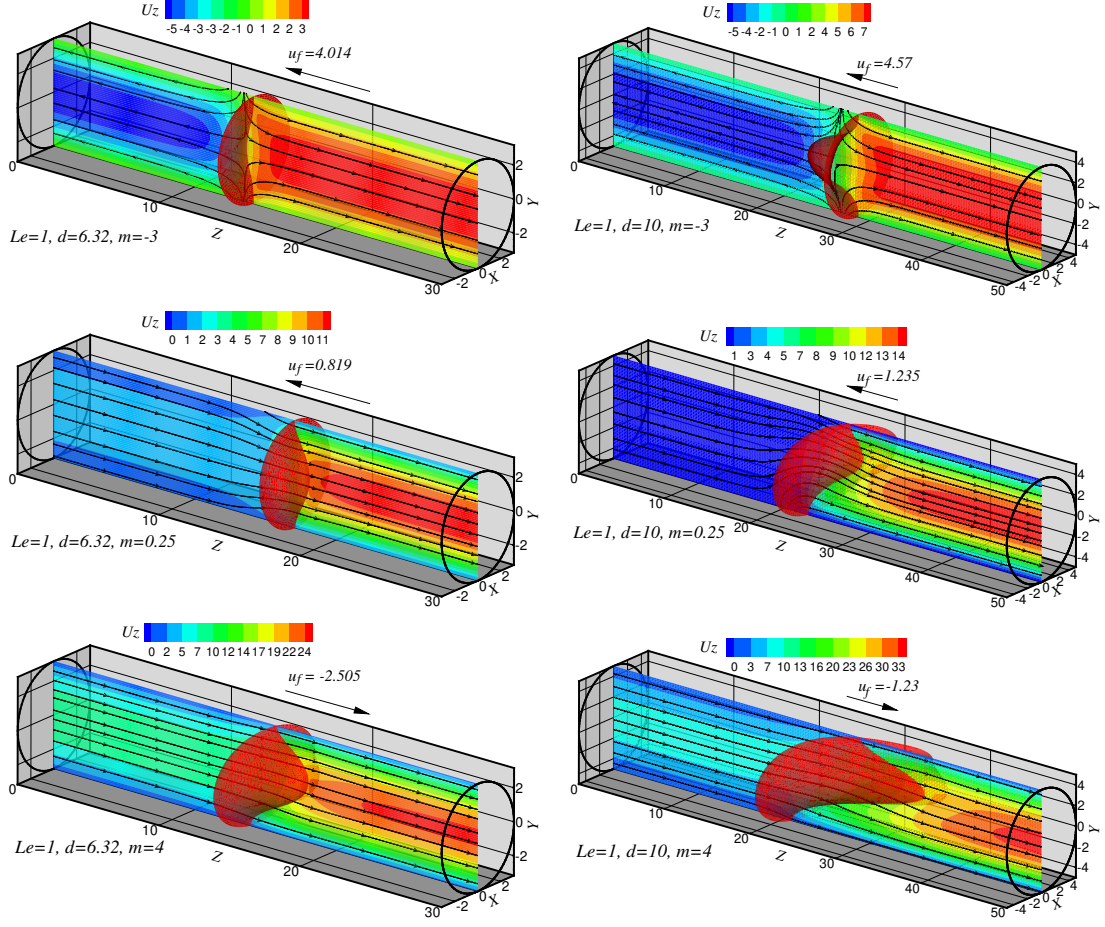


Figure 4. 3D simulations, $Le = 1$, adiabatic wall ($b = 0$): isosurface value $\theta = 0.9$ superimposed with isocontours of axial velocity U_z and streamlines drawn in the transverse plane (yOz) at $x = 0$ for (left column) $d = 6.32$ and (right column) $d = 10$, $m = -3, 0.25$ and 4 . The isocontours of axial velocity U_z are divided into 10 values between the minimum and maximum of U_z value of each case.

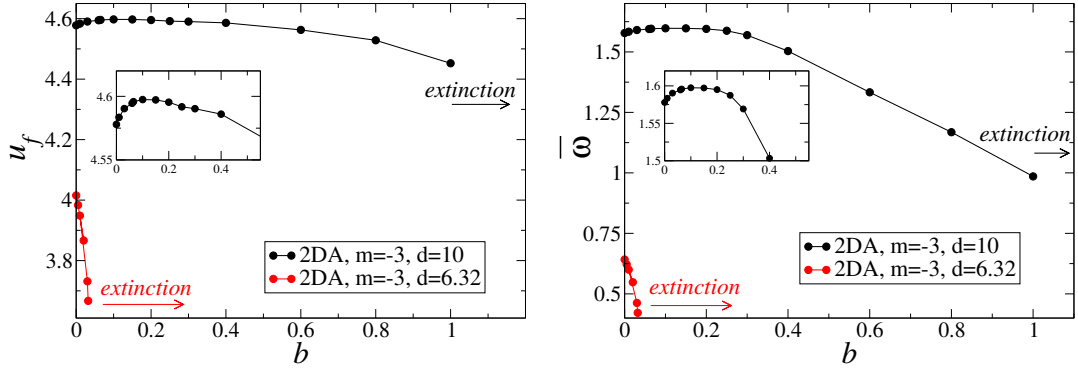


Figure 5. 2DA simulations, $Le = 1$, $m = -3$: influence of wall-heat loss parameter b and channel diameter d on axisymmetric flames; (left) flame velocity u_f and (right) average burning-rate $\bar{\omega} = \frac{4}{\pi d^2} \int_0^{L_z} \int_0^r \int_0^{2\pi} \omega dz dr d\varphi$, as function of b .

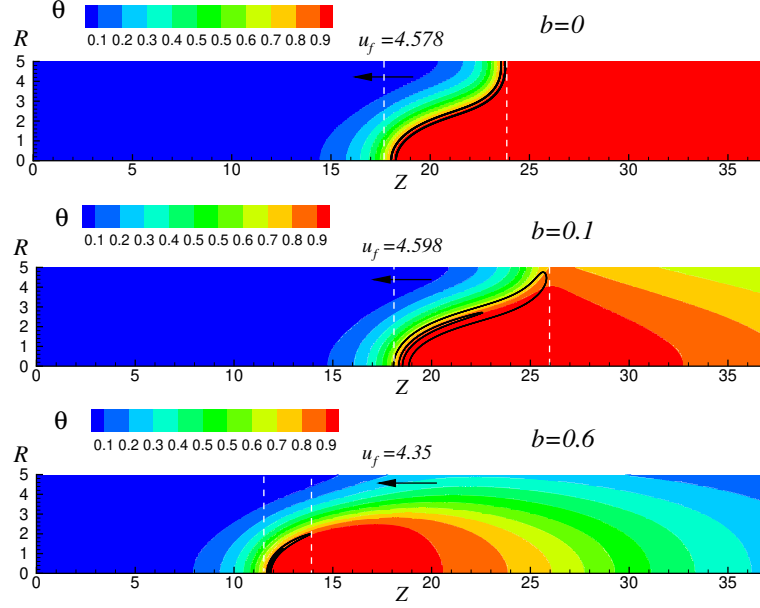


Figure 6. 2DA simulations, $Le = 1$, $m = -3$ and $d = 10$: influence of wall-heat loss parameter b . Colored isocontours correspond to those of reduced temperature Θ and the white dashed lines delimits the flame area. The front flame is pictured by the two black isocontours that delimit the zone of maximum reaction rate values: $\omega = 1.5$ and $\omega = 1.6$. Note that for sake of clarity the original channel length $L_z = 50$ has been reduced to 35 in these illustrations.

of b is shown in Fig. 5 for the axisymmetric flames ($m = -3$ and both values of d) and in Fig. 7 for the non-axisymmetric flames ($d = 10$ and two values of the inlet flow rate, $m = -1$ and 0.25). Note that there exists a critical value of the heat transfer parameter b_c such that the flame extinction occurs for $b > b_c$.

3.2.1. Axisymmetric flames, $m = -3$

For $m = -3$, the flame is axisymmetric for the considered diameters under adiabatic wall conditions. Figure 5 shows that, as expected, the effect of b is stronger as the diameter decreases. For $d = 6.32$ flame extinction occurs at $b_c \approx 0.03$ while in the case $d = 10$, at $b_c \approx 1$. Comparison of flame curvature between both diameters in the adiabatic wall case (see Fig. 4, $m = -3$) shows that major part of the (convex) flame surface is highly curved in the center of the channel for $d = 10$ while the flame is almost flat for $d = 6.32$. Wall heat-losses are thus less effective in the larger channel as main flame curvature is located far from the wall. It is interesting that, for $b \approx 0.1$, the inset plots in Fig. 5 evidence a maximum of u_f and of the average burning rate $\bar{\omega}$ that take values slightly larger than for $b = 0$. This can be explained by Fig. 6

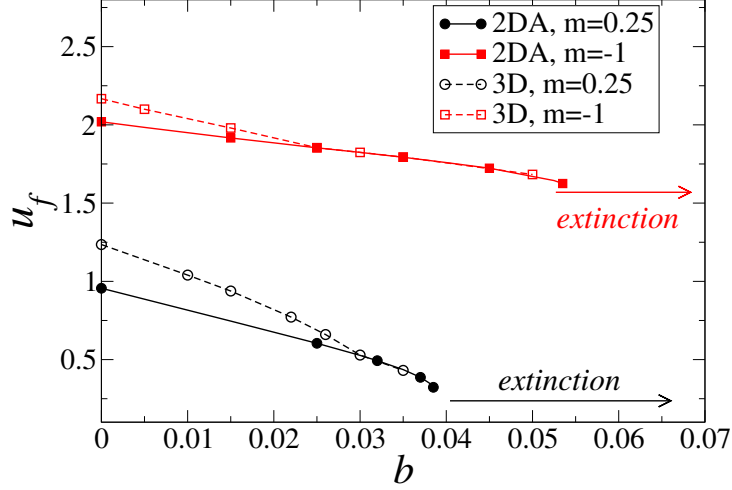


Figure 7. Comparison between 2DA and 3D simulations, $Le = 1$, $d = 10$: influence of wall-heat loss parameter b for inlet flow rates $m = -1$ and $m = 0.25$; flame velocity as function of b . As b is increased symmetrisation is observed before extinction, the 3D simulation branch recovering the 2DA branch.

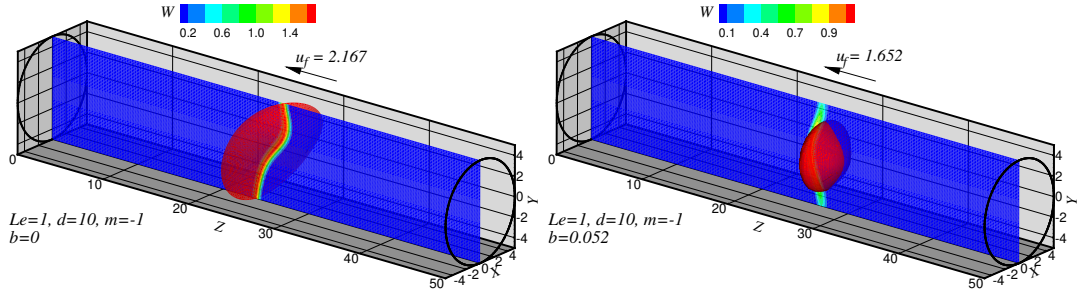


Figure 8. Symmetrisation of non-axisymmetric flame under wall-heat losses, $Le = 1$, $d = 10$, $m = -1$: isosurface of temperature $\theta = 0.9$ superimposed with isocontours of reaction rate w for (left) $b = 0$ and (right) $b = 0.052$.

that displays the flame surface by drawing two isocontours of the reaction rate which values are very close to the maximum one. For the adiabatic condition ($b = 0$), the zero temperature-gradient wall condition gives rise to a less extended flame near the wall when compared to the case with small heat-losses ($b = 0.1$). *In this latter case, heat diffusion due to wall heat-losses clearly manifests downstream of the flame and alters the flame shape.* When further increasing wall heat-losses ($b = 0.6$), the flame curvature reduces and flame velocity decreases as expected. Note that in this latter case the heat-losses are large enough to create a space between the wall and the flame where a non-negligible amount of unburned gas flows downstream of the flame (see Appendix C).

3.2.2. Non-axisymmetric flames, $d = 10$

For $d = 10$, we have shown that the flame is non-axisymmetric if $m > -1.5$ under adiabatic wall conditions ($b = 0$). Figure 7 indicates that extinction of the non-axisymmetric flame occurs at $b_c \approx 0.055$ for $m = -1$ and at $b_c \approx 0.038$ for $m = 0.25$. These extinction values are much smaller than the value $b_c \approx 0.6$ reported for the axisymmetric flame for $m = -3$ and shown in Fig. 5. This result is in agreement with [5] that reported that mushroom-shaped flames were a more robust manifestation than tulip-shaped flames in channels with isothermal walls. We indeed observe that the axisymmetric flame, with a mushroom-like structure, is more resistant than the non-axisymmetric flame with a tulip-like structure as b increases.

It is interesting to note that, under a gradual increase of b towards the critical value b_c , the non-axisymmetric flame can become axisymmetric. This is shown in Fig. 7 where the 3D and 2DA flame solutions recover each other as the parameter b approaches the extinction limit value b_c . The symmetrization of the flame shape is also illustrated for $m = -1$ in Fig. 8: the flame with non-axisymmetric shape found for $b = 0$ turns out axisymmetric when $b \approx 0.052$. Not shown here, we did not observe flame symmetrization for the larger values of the inlet flow rate $m = 2.5$, but instead the non-axisymmetric flame extinguishes at $b_c \approx 0.03$.

An overview of the results presented for $d = 10$ is given in Fig. 9 that provides an approximate map of the different combustion regimes found within the ranges of m and b considered here.

4. Flames with $Le < 1$

For flames with Lewis number smaller than unity we mainly consider only one value of the channel diameter. As the Lewis number decreases, the grid resolution must be finer and this limits 3D simulations. In our previous work [33], the reduced Damköhler number defined as $d_{Dk} = (d'/2\delta_T)^2 = R^2$ was used to analyse the symmetry properties for flames with $Le = 0.7$ and 0.5 propagating in an adiabatic channel ($b = 0$). The value $d_{Dk} = 10$ was examined which is equivalent to the non-dimensional diameter $d = 6.32$ considered here.

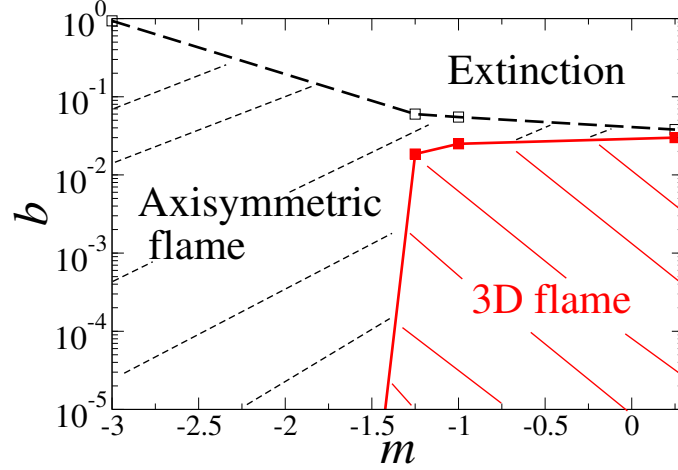


Figure 9. $Le = 1$, $d = 10$: map of axisymmetric and non-axisymmetric (3D) flame combustion regimes as function of b and m . Axis b is in logarithmic scale for sake of clarity.

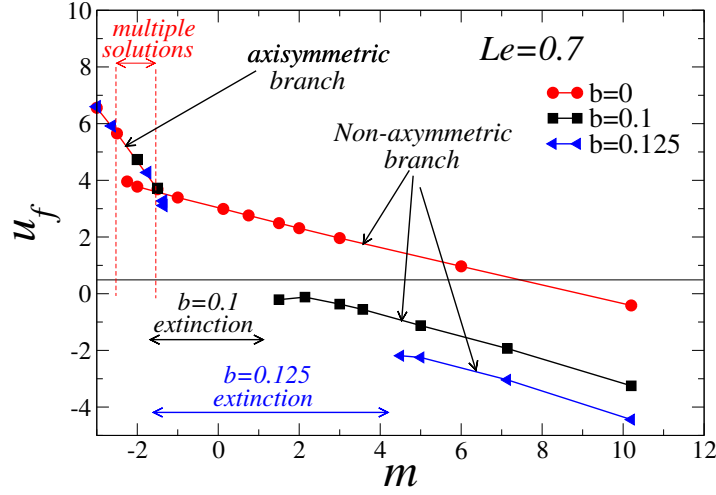


Figure 10. 3D simulations, $Le = 0.7$: flame velocity u_f as a function of the dimensionless flow rate m , obtained for $d = 6.32$. Dashed lines delimit the multiplicity region obtained for $b = 0$. All 3D simulation solutions are obtained from the prism cell decomposition (see Sec. 2.3 and Fig. B1). Results for $b = 0$ were extracted from [33].

The main results reported in [33] are briefly recalled: there exists a region of multiple solutions where both stable axisymmetric and stable non-axisymmetric flames can coexist within an interval of the flow rate $m_{min} < m < m_{max}$. All cases with multiple solutions were obtained by gradually increasing or decreasing the flow rate parameter starting from an already calculated variable field distribution (axisymmetric when increasing m or non-axisymmetric when decreasing m) chosen as initial condition. The hysteresis shape of the response curves shows a multiplicity of modes. We indicate the interval of multiplicity with vertical dash-dot lines in Figs. 10 and 11. This interval

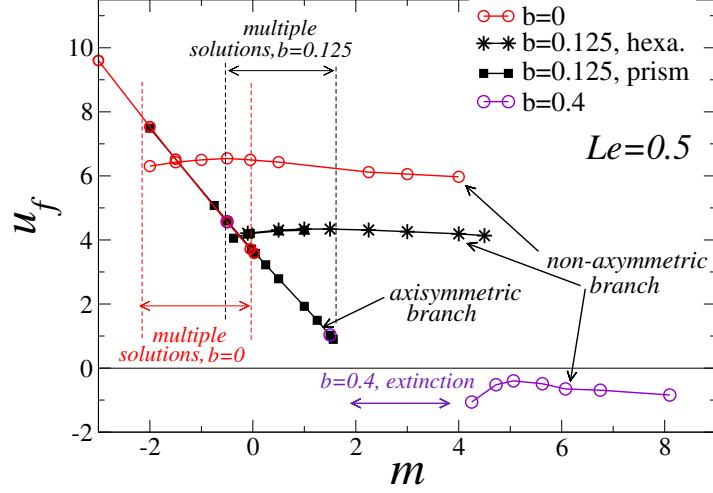


Figure 11. 3D simulations, $Le = 0.5$: flame velocity u_f as a function of the dimensionless flow rate m , obtained for $d = 6.32$. Dashed lines delimit the region of solution multiplicity and are colored according to b values. The solution curves referred to as “prism” and “hexa” indicate those obtained from the prism and hexahedra cell decomposition, respectively (see Sec. 2.3 and Fig. B1). Results for $b = 0$ were extracted from [33].

of m becomes wider for smaller values of Le . The transition from axisymmetric to non-axisymmetric flames is in this case subcritical. Note that the multiplicity of stable solutions seems to be associated with the low Lewis number effect. For flames with $Le = 1$, such a multiplicity was not found and a supercritical transition was observed for the range of parameters considered here.

4.1. Effect of wall heat-losses

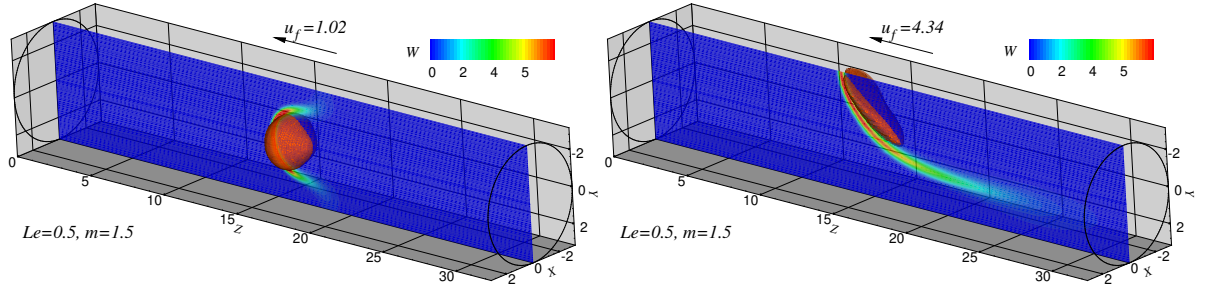


Figure 12. 3D simulations, multiplicity of solutions for $Le = 0.5$, $d = 6.32$ and $m = 1.5$, $b = 0.125$: isosurface value $\theta = 1.16$ superimposed with isocountours of reaction rate ω drawn in the transverse plane (yOz) at $x = 0$ for the axisymmetric flame solution (left) and the non-axisymmetric solution (right).

Figure 10 shows that for $Le = 0.7$, the multiplicity interval of m found for $b = 0$ disappears with increasing values of b . Furthermore, for $b = 0.1$ and 0.125 the

axisymmetric and non-axisymmetric branches do not intersect and are separated by a gap. By contrast, the flame with $Le = 0.5$, illustrated in Fig. 11, still exhibits an interval with multiple stable solutions for $b = 0.125$. Note however that, as b is increased from 0 to 0.125, the multiple solution interval is displaced to higher values of m . The picture of two stable solutions calculated for $Le = 0.5$, $b = 0.125$ and $m = 1.5$ is given in Fig. 12 showing the stable axisymmetric and stable non-axisymmetric flame structures by drawing the temperature isosurface $\theta = 1.16$ and isocontours of the reaction rate ω in the transverse plane (yOz) at $x = 0$.

Figures 10 and 11 indicate that the flame velocity u_f corresponding to the axisymmetric branch is not modified significantly by wall heat-losses. However, the heat-loss effect is notable for the non-axisymmetric flames. This can be explained by considering Fig. 12 that illustrates the flame structure for both axisymmetric and non-axisymmetric flames with $Le = 0.5$. It shows that the maximum of reaction rate ω is located in the center of the channel for the axisymmetric flame while it occurs in the close region to the wall for the non-axisymmetric flame. This latter is thus more altered by wall-heat losses. Not shown here, similar flame structure characteristics as those displayed in Fig. 12 were found for $Le = 0.7$. One also can observe that, taking as reference the left red dotted line delimiting the region of multiple stable solutions for $b = 0$ in Figs. 10 and 11, the axisymmetric flame branch extends further towards larger m in presence of wall heat-losses. This is clearly observed for $Le = 0.5$ in Fig. 11 where the axisymmetric branch ends at $m_{max} \approx 0$ for $b = 0$ while at $m_{max} \approx 1.7$ for $b = 0.125$. This effect is significantly reduced for $Le = 0.7$. These results indicate that the 2D axisymmetric flame structure is more resistant to wall heat-losses as previously reported for $Le = 1$.

By increasing the value of b up to 0.4, the non-axisymmetric branch of $Le = 0.5$ (see Fig. 11) shifts towards larger values of m and a gap appears between both branches, as similarly observed for $Le = 0.7$ but for $b = 0.1$. For large values of m , only the non-axisymmetric flames propagate in the channel. The shape of these non-axisymmetric flames are illustrated in Fig. 13 for $Le = 0.7$ and in Fig. 14 for $Le = 0.5$. It is noteworthy to mention that a similar extinction gap was previously reported for flames propagating in planar channels, in [24] using the constant-density model and

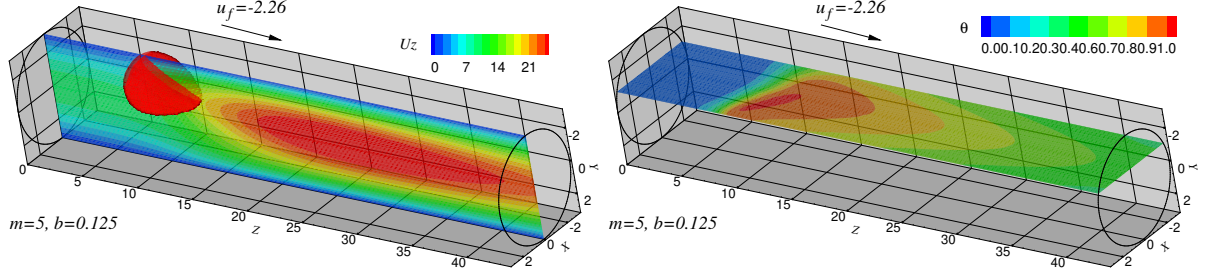


Figure 13. 3D simulations, $Le = 0.7$, $d = 6.32$, $m = 5$ and $b = 0.125$; (left) isosurface temperature value $\theta = 1$ superimposed with the isocountours of the axial velocity given in the transverse plane (yOz) located at $x = 0$; (right) isocontours of θ drawn in the transverse plane (xOz) at $y = -1.16$.

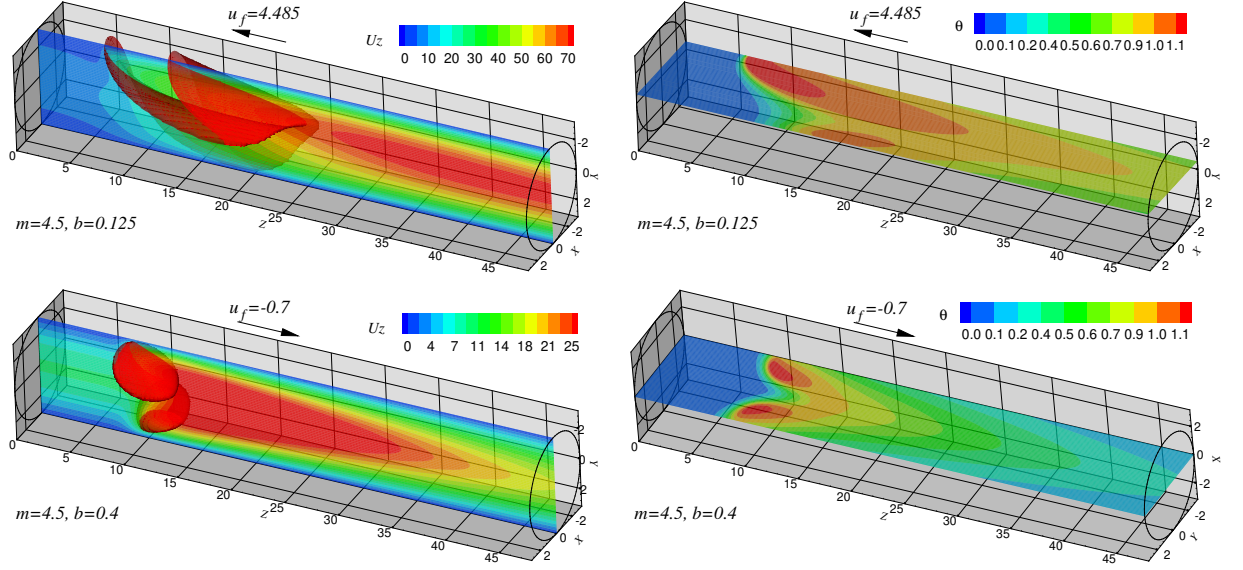


Figure 14. 3D simulations, $Le = 0.5$, $d = 6.32$, $m = 4.5$ with $b = 0.4$ and $b = 0.125$; (left) isosurface temperature value $\theta = 1$ superimposed with the isocountours of the axial velocity given in the transverse plane (yOz) located at $x = 0$; (right) isocontours of θ drawn in the transverse plane (xOz) at $y = 0$.

in [26] for lean hydrogen-air flames calculated with detailed chemistry and full set of Navier-Stokes equations. Rebirth of the flame for large m can be explained by the larger stretch and curvature of the flame resulting in a higher consumption rate as shown by the non-axisymmetric branch of u_c in Fig. 15. This figure also shows that as Le is made smaller, the consumption speed is larger, so that flames with $Le = 0.5$ are more robust to wall-heat losses than flames with $Le = 0.7$. Indeed, for $m = -1$ no flame solution is found for $b = 0.125$ while flame solution exists for $Le = 0.5$.

As given above for $Le = 1$, Fig. 16 provides an overview of the axisymmetric and

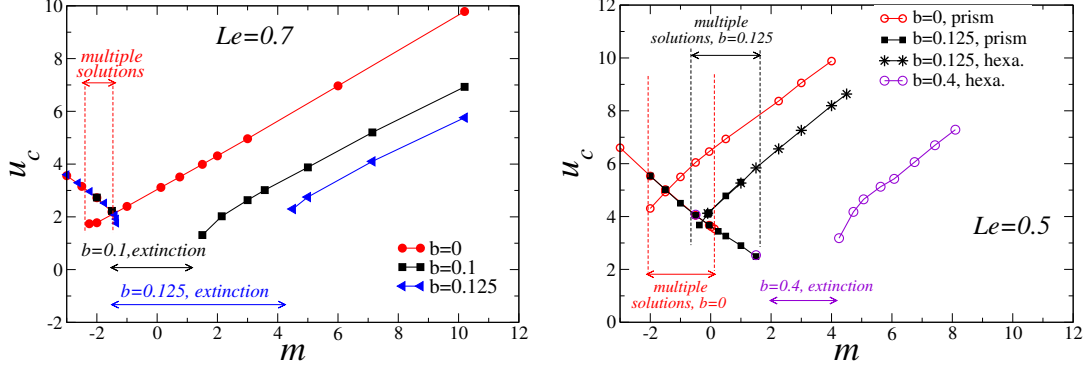


Figure 15. 3D simulations: consumption speed u_c as a function of the dimensionless flow rate m , obtained for $d = 6.32$ with $Le < 1$. Dashed lines delimit the region of solution multiplicity and are colored according to b values. All 3D simulation solutions are obtained from the prism cell decomposition (see Sec. 2.3 and Fig. B1). Results for $b = 0$ were extracted from [33].

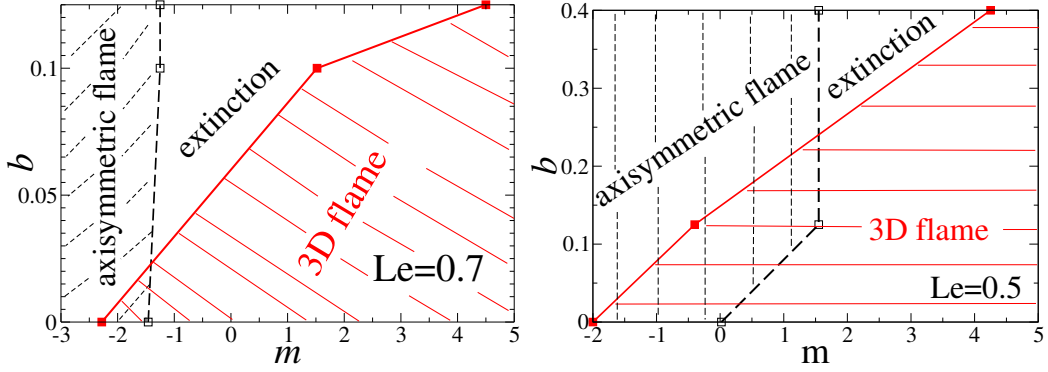


Figure 16. $Le < 1$, $d = 6.32$: map of axisymmetric and non-axisymmetric (3D) flame combustion regimes as function of b and m . (left) $Le = 0.7$, (right) $Le = 0.5$.

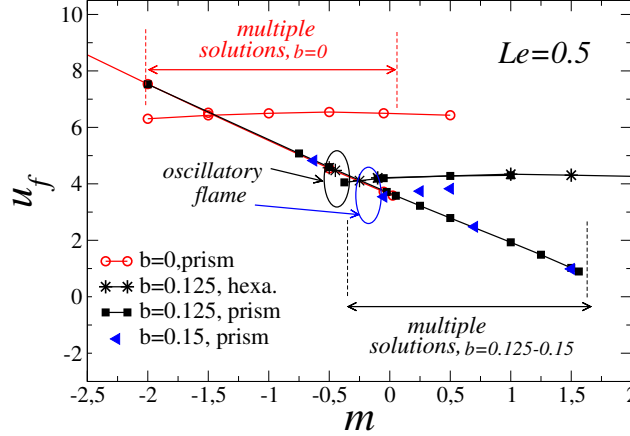


Figure 17. 3D simulations, close view of the regions of multiple solutions: flame velocity u_f as a function of the dimensionless flow rate m , obtained for $d = 6.32$ with $Le = 0.5$. Dashed lines delimit the region of solution multiplicity and are colored according to b values. The solution curves referred to as “prism” and “hexa” indicate those obtained from the prism and hexahedra cell decomposition, respectively (see Sec. 2.3 and Fig. B1). Results for $b = 0$ were extracted from [33].

non-axisymmetric combustion regimes obtained for $Le = 0.7$ and 0.5 in the present range of parameters. The zones of extinction and of solution multiplicity clearly appear.

5. Oscillatory solution for flames with $Le = 0.5$

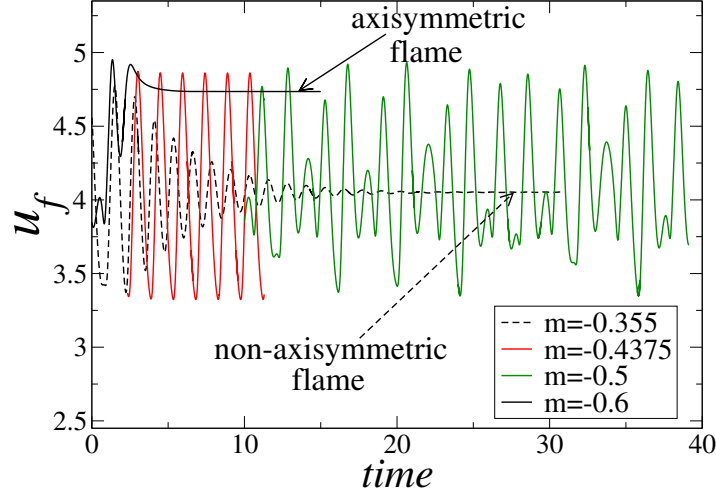


Figure 18. 3D simulations, $Le = 0.5$, $d = 6.32$ and $b = 0.125$: time evolution of flame velocity u_f given for inlet flow rates $-0.6 \leq m \leq -0.5$.

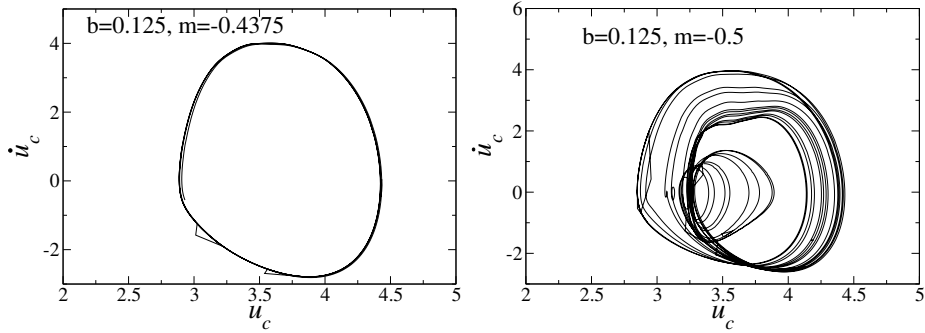


Figure 19. 3D simulations, oscillatory regime combustion, $Le = 0.5$, $d = 6.32$ and $b = 0.125$: phase portraits of consumption speed for $m = -0.4375$ (left) and $m = -0.5$ (right)

This section focuses on the flame dynamics obtained for $Le = 0.5$ in the range of the inlet flow rate for which the axisymmetric branch and non-axisymmetric branch cross each other. This narrow range of flow rate values is delimited by ellipses in Fig. 17. Interestingly, in this region and for $b = 0.125$ and 0.15 , the flame exhibits unsteady dynamics. To ensure that the unsteady regime is not a numerical artifact,

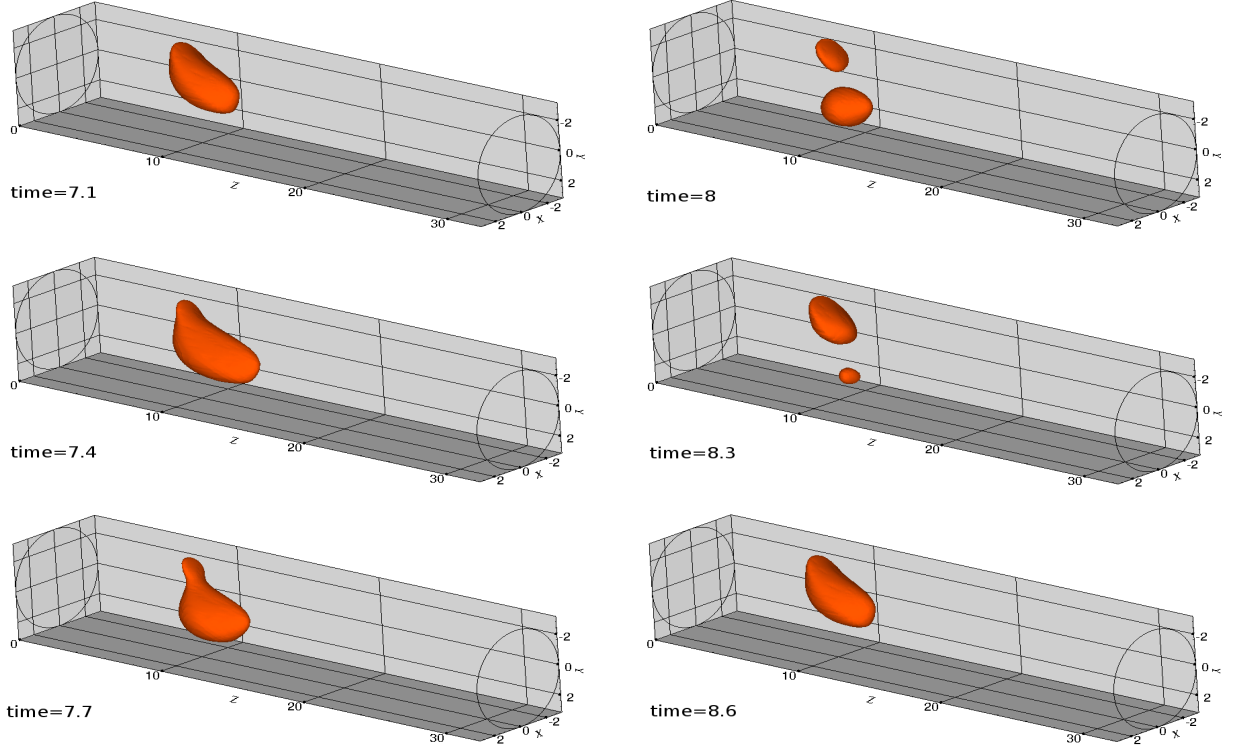


Figure 20. 3D simulations, oscillatory regime combustion: $Le = 0.5$, $d = 6.32$, $m = -0.4375$ and $b = 0.125$; time evolution of the isosurface of temperature $\theta = 1.16$ over a full cycle. The solution at the time $t = 8.6$ is identical to the one at $t = 7.1$ and the cycle repeats.

we have verified that identical dynamics are recovered using the two different grid topologies: the unstructured mesh composed of prism computational cells of identical size and the block-structured grid mesh composed of hexahedra computational cells (see B, Fig. B1).

Figure 18 represents the time evolution of the flame velocity obtained as the value of m is varied from the steady non-axisymmetric solution ($m = -0.355$) to the steady axisymmetric branch ($m = -0.6$). In between these two branches, as m is slightly decreased, the flame performs oscillations for $m = -0.4375$ leading to a more chaotic behaviour for $m = -0.5$ (see corresponding phase diagrams in Fig. 19). A plausible scenario for the onset of unsteadiness is that the flame is performing recurrent transitions from one stationary branch to another, similarly to state transition of dynamical system near bifurcation and resulting from nonlinear interactions that might lead to complicated behaviour [36]. To highlight this point, it is interesting to observe that the oscillations of u_f in Fig. 18 for $m = -0.4375$ range between the

values corresponding to the two stationary branches, its average being close to the non-axisymmetric solution and its maximum value close to that of the axisymmetric branch. The periodic flame dynamics is displayed in Fig. 20 by providing the time evolution of the temperature isosurface $\theta = 1.16$ over one cycle. It shows that a periodic formation of unique and two flame balls occurs over the cycle. Noteworthy to mention that oscillatory flames have been observed for weak flames [37] and flames with repetitive extinction and ignition [38] near the turning (extinction) point but as well for propagating flames [19]. These experimental and numerical studies show that flame oscillation phenomena can occur under various conditions and are an outcome of high non-linear coupling between hydrodynamics, heat release and thermal effects. Up to our knowledge, the physical mechanisms underlying flame oscillations are still an open question. A detailed analysis of these mechanisms is outside the scope of the present study.

6. Conclusions

In this work we analyze the structure and dynamics of premixed flames propagating in narrow circular channels submitted to inlet Poiseuille flow rate. Notably, compared to our recent study [27] which was carried out for a planar channel, we include azimuthal (3D) effects here.

The present study confirms the general trends identified in the appearance of asymmetry reported previously for flames propagating in 2D planar channels. We unveil the existence of two flame solution branches: an axisymmetric (2DA) and a non-axisymmetric (3D) one. In general, the 2DA solution becomes unstable if the inlet flow rate, m , is made larger than a critical value, $m > m_{3D}$, leading to a 3D structured flame. The value of m_{3D} increases with enhancing the heat-loss parameter b . This means that wall heat-losses prompt the formation of axisymmetric flames. For instance, for $Le = 1$, we observed that a non-axisymmetric (3D) flame under adiabatic wall conditions ($b = 0$) takes an axisymmetric shape as b is increased. In the case of $Le < 1$, the effects of wall heat-losses are much more stronger on the non-axisymmetric branch solution than on the axisymmetric branch. However, as channel

diameter increases or Lewis number decreases, non-axisymmetry is more likely to occur.

Interestingly, while for $Le = 1$ the axisymmetric flame branch solution becomes unstable giving rise to a non-axisymmetric branch as the inlet flow rate m is increased, two types of flames, axisymmetric and non-axisymmetric, can be simultaneously stable over an interval of m for $Le < 1$. This interval widens as the Lewis number decreases. In the language of bifurcations, the bifurcation from axisymmetric to non-axisymmetric solution is supercritical for $Le = 1$, while subcritical for $Le < 1$.

As the wall heat-loss parameter b increases, this multiplicity region disappears. Instead, an extinction gap appears between both branches, which enlarges as b is further enhanced. Outside this gap, the axisymmetric branch remains roughly the same, but the non-axisymmetric branch is shifted towards larger values of the inlet flow rate.

An interesting behaviour is displayed by the numerical simulations performed for flames with $Le = 0.5$. A non-axisymmetric oscillatory flame regime is found at relatively low heat losses. This oscillatory regime occurs over a small range of the inlet flow m , precisely where the two stationary branches cross each other. As m is slightly decreased, the non-axisymmetric oscillatory flame transits from a periodic to a chaotic state before recovering the axisymmetric solution, suggesting a non-linear interaction between the two axisymmetric and non-axisymmetric steady modes.

The present study shows that flames with complex 3D structures and dynamics might appear in narrow circular channels. These solutions are stable, can have very different characteristics (for example, the propagation speed), fade out and then revive with an increase in the flow rate, have non-uniqueness and even have oscillatory dynamics. **The manifold flame structure stems from a complex interplay between intrinsic instabilities that depends on flow parameters.** Some of these properties have already been observed in experiments. However, the obvious difficulties of their exhaustive experimental study indicate the importance and usefulness of numerical simulation of flames.

Acknowledgments

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References

- [1] D. B. Spalding, A theory of inflammability limits and flame-quenching, *Proc. Roy. Soc. London A* 240, (1957) 83–100.
- [2] J. Buckmaster, The quenching of deflagration waves, *Combust. Flame* 26 (1960) 151–162.
- [3] D. Dunn-Rankin, P. K. Barr, R. F. Sawyer, Numerical and experimental study of “tulip” flame formation in a closed vessel, *Twenty-first Symposium (International) on Combustion*, The Combustion Institute, Pittsburg (1986) 1291–1301.
- [4] C. Clanet, G. Searby, On the “Tulip Flame” Phenomenon, *Combust. Flame*, 105 (1996) 225–238.
- [5] S. T. Lee, C. H. Tsai, Numerical investigation of steady laminar flame propagation in circular tube, *Combust. Flame* 99 (1994) 484–490.
- [6] C. L. Hackert, J. L. Elisey, A. Ezekoye, Effect of thermal boundary conditions on flame shape and quenching in ducts, *Combust. Flame* 112 (1998) 73–84.
- [7] C. Clanet, G. Searby, First experimental study of the Darrieus-Landau instability, *Phys. Rev. Lett.* 27 (1998), 3867–3870.
- [8] G. Searby, Experimental studies of instabilities of laminar premixed flames, *International Conference on Combustion and Detonation, Zel’dovich Memorial II*, Moscou, (2004).
- [9] C. Fernández-Pello, Micropower generation using combustion: issues and approaches, *Proc. Combust. Inst.* 29(1) (2002) 883–899.
- [10] D. C. Walther, J. Ahn, Advances and challenges in the development of power-generation systems at small scales, *Prog. Energy Combust. Sci.* 37(5) (2011) 583–610.
- [11] Y. Ju, K. Maruta, Microscale combustion: technology development and fundamental research, *Prog. Energy Combust. Sci.* 37(6) (2011) 669–715.
- [12] K. Maruta, T. Kataoka, N. I. Kim, S. Minaev, R. Fursenko, A. Arnold, Characteristics of combustion in a narrow channel with temperature gradient, *Proc. Combust. Inst.* 30(2) (2005) 2429–2436.
- [13] V. Zamashchikov, Experimental investigation of gas combustion regimes in narrow tubes, *Combust. Flames* 108 (1997) 357–359.
- [14] F. Richecoeur, D. Kyritsis, Experimental study of flame stabilization in low Reynolds and Dean number flows in curved mesoscale ducts. *Proc. Combust. Inst.* 30 (2005) 2419–2427.

- [15] U. Dogwiler, J. Mantzaras, P. Benz, B. Kaeppli, R. Bombach, A. Arnold, Homogeneous ignition of methane-air mixture over platinum: comparison of measurements and detailed numerical predictions, *Proc. Combust. Inst.* 27(2) (1998) 2275–2282.
- [16] N. I. Kim, T. Kataoka, S. Maruyama, K. Maruta, Flammability limits of stationary flames in tubes at low pressure, *Combust. Flame* 141(2) (2005) 78–88.
- [17] V. N. Kurdyumov, E. Fernández-Tarrazo, J. M. Truffaut, J. Quinard, A. Wangher, G. Searby, Experimental and numerical study of premixed flame flashback, *Proc. Combust. Inst.* 31(1) (2007) 1275–1282.
- [18] C. J. Evans, D. C Kyritsis, Experimental investigation of the effects of flame phenomenology on the wall temperature distribution of mesoscale nonadiabatic ducts, *Combust. Sci. and Tech.* 183(9) (2011) 847–867.
- [19] T. A. Connely, D. C Kyritsis, Experimental investigation of flame propagation in long, narrow and open tubes, *J. Energy Eng.* 141(2) (2015) C4014016-1-7.
- [20] V. N. Kurdyumov, J. M. Truffaut, J. Quinard, A. Wangher, G. Searby, Oscillations of premixed flames in tubes near the flashback condition, *Combust. Sci. Technol.* 180 (2008) 731–742.
- [21] V.N. Kurdyumov, G. Pizza, C.E. Frouzakis, J. Mantzaras, Dynamics of premixed flames in a narrow channel with a step-wise wall temperature, *Combust. Flame* 156 (2009) 2190-2200.
- [22] G. Pizza, C.E. Frouzakis, J. Mantzaras, A.G. Tomboulides, K. Boulouchos, Dynamics of premixed hydrogen/air flames in microchannels, *Combust. Flame* 152 (2008) 433-450.
- [23] V. Kurdyumov, Lewis number effect on the propagation of premixed flames in narrow adiabatic channels: Symmetric and non-symmetric flames and their linear stability analysis, *Combust. Flame* 158 (7) (2011) 1307–1317.
- [24] V. Kurdyumov, C. Jiménez, Propagation of symmetric and non-symmetric premixed flames in narrow channels: Influence of conductive heat-losses, *Combust. Flame* 161 (4) (2014) 927–936.
- [25] C. Jiménez, D. Fernández-Galisteo, V. Kurdyumov, DNS study of the propagation and flashback conditions of lean hydrogen-air flames in narrow channels: Symmetric and non-symmetric solutions, *Int. J. Hydrogen Energy* 40 (2015) 12541–12549.
- [26] C. Jiménez, V. Kurdyumov, Propagation of symmetric and non-symmetric lean hydrogen-air flames in narrow channels: Influence of heat losses, *Proc. Combust. Inst.* 36(1) (2017) 1559–1567.

- [27] A. Dejoan, C. Jiménez, V. Kurdyumov, Critical conditions for non-symmetric flame propagation in narrow channels: influence of the flow rate, the thermal expansion, the Lewis number and heat-losses. *Combust. Flame* 209 (2019) 430–440.
- [28] C.-H. Tsai, The asymmetric behavior of steady laminar flame propagation in ducts, *Combust. Sci. Tech.* 180 (2008) 533–545.
- [29] K. Bioche, A. Pieyre, G. Ribert, F. Richecoeur, L. Vervisch, The role of gravity in the asymmetry of flames in narrow combustion chambers, *Combust. Flame* 203 (2019) 238–246.
- [30] V. Kurdyumov, E. Fernández-Tarrazo, Lewis number effects on the propagation of premixed laminar flames in narrow open ducts. *Combust. Flame* 128 (2002) 382–394.
- [31] V. Kurdyumov, C. Jiménez, Structure and stability of premixed flames propagating in narrow channels of circular cross-section: Non-axisymmetric, pulsating and rotating flames, *Combust. Flame* 167 (2016) 149–163.
- [32] A. Petchenko, V. Bychkov, Axisymmetric versus non-axisymmetric flames in cylindrical tubes, *Combust. Flame* 136 (2004) 429–439.
- [33] A. Dejoan, V. Kurdyumov, Thermal expansion effect on the propagation of premixed flames in narrow channels of circular cross-section: multiplicity of solutions, axisymmetry and non-axisymmetry, *Proc. Combust. Inst.* 37 (2019) 1927–1935
- [34] G. Pizza, C. E. Frouzakis, J. Mantzaras, A. G. Tomboulides, K. Boulouchos, Three-dimensional simulations of premixed hydrogen/air flames in microtubes, *J. Fluid Mech.* 658 (2010) 463–491.
- [35] User, P. G. T. Report, <http://www.openfoam.com>.
- [36] M. Golubitsky, I. Stewart, D.G Schaeffer, Singularities and groups of bifurcation theory: volume II, Applied Mathematical Science, Springer, 1st ed. (1988)
- [37] A. Di Stazio, C. Chaveau, G. Dayma, P. Dagaut, Oscillating flames in micro-combustion, *Combust. Flame* 167 (2016) 392–394.
- [38] M.A. Bucci, A. Di Stazio, C. Chaveau, G. Dayma, G. Legros, P. Dagaut, S. Chibbaro Numerical and experimental analysis of combustion in microchannels with controlled temperature, *Chem. Eng. Science*:X 4 (2019) 100034.

Appendix A. Evaluation of flame velocity u_f

In a computational moving with a flame propagating at constant velocity u_f in an infinite channel of circular cross-section, volume integration of Eq. (4) (with $w = u_f$) writes as follow:

$$\int_{\mathcal{V}} \nabla \cdot (\rho Y [\mathbf{v} + \mathbf{u}_f]) dv = \int_{\mathcal{V}} \frac{1}{L_e} \nabla^2 Y dv - \int_{\mathcal{V}} \omega dv \quad (\text{A1})$$

and volume integration of continuity equation (Eq. (1) with $w = u_f$) as:

$$\int_{\mathcal{V}} \nabla \cdot (\rho [\mathbf{v} + \mathbf{u}_f]) dv = 0 \quad (\text{A2})$$

Making use of Gauss theorem, volume integrals convert to surface integrals, so that Eq. (A1) and Eq. (A2) respectively write as:

$$\int_S \nabla \cdot (\rho Y [\mathbf{v} + \mathbf{u}_f]) \cdot \hat{n} ds = \int_S \frac{1}{L_e} \nabla Y \cdot \hat{n} ds - \int_{\mathcal{V}} \omega dv \quad (\text{A3})$$

and

$$\int_S \nabla \cdot (\rho [\mathbf{v} + \mathbf{u}_f]) \cdot \hat{n} ds = 0 \quad (\text{A4})$$

Surface integrals are written as following:

$$\int_S \nabla \cdot (\rho Y [\mathbf{v} + \mathbf{u}_f]) \cdot \hat{n} ds = \frac{4}{\pi d^2} [\rho_+ Y_+ (U_+ + u_f) - \rho_- Y_- (U_- + u_f)] \quad (\text{A5})$$

$$\int_S \frac{1}{L_e} \nabla Y \cdot \hat{n} ds = \frac{4}{\pi d^2} [\nabla Y_+ - \nabla Y_-] \quad (\text{A6})$$

$$\int_S \nabla \cdot (\rho [\mathbf{v} + \mathbf{u}_f]) \cdot \hat{n} ds = \rho_+ (U_+ + u_f) - \rho_- (U_- + u_f) = 0 \quad (\text{A7})$$

where subindices + and - refer to channel cross section average quantities at $z_- = -\infty$ (fresh gas) and $z_+ = \infty$ (burnt gas), respectively. No-gradient boundary conditions being imposed at the inlet and outlet of the channel for Y , we have $[\nabla Y_+ - \nabla Y_-] = 0$. Note that, the computational length L_z being finite, we checked that L_z was large enough to minimize gradient effects if present (see Appendix C).

Combining Eqs. (A5)-(A7) and designating $z_- = 0$ and $z_+ = L_z$, we obtain:

$$\rho_0(m + u_f)(Y_{L_z} - Y_0) = -\frac{4}{\pi d^2} \int_{z=0}^{z=L_z} \int_0^r \int_0^{2\pi} \omega dz r dr d\varphi \quad (\text{A8})$$

defining $u_c = \frac{4}{\pi d^2} \frac{1}{(Y_0 - Y_{L_z})} \int_{z=0}^{z=L_z} \int_0^r \int_0^{2\pi} \omega dz r dr d\varphi$, and recalling that m denominates the inlet flow rate, we finally have:

$$u_f = u_c - m \quad (\text{A9})$$

Appendix B. Numerical grid resolution and mesh decomposition

	$d = 6.32, b = 0$				$d = 10, b = 0.06$		
	2DA	2DA	3D Hex.	3D Prism	2DA	3D Hex.	3D Hex.
L_z	40	30	50	40	40	50	50
N_{cell}	12800	37950	1372000	1773360	80000	1372000	6250000
Δ_r	0.1	0.05	0.1	0.1	0.05	0.1	0.05
u_f	4.0150	4.0152	4.0143	4.0145	4.5955	4.5924	4.5951

Table B1. Effect of numerical resolution and grid mesh decomposition on the propagation flame velocity u_f for different axisymmetric solutions obtained for $Le = 1$ and $m = -3$; L_z is the non-dimensionalized channel length, N_{cell} is the total number of computational cells, Δ_r the non-dimensional numerical solution. See Fig. B1 for the hexahedra (Hex.) and prism (Prism) 3D grid mesh decompositions. Note that 2DA refers to simulations performed with an axisymmetric frame.

This appendix details the tests performed on the grid mesh resolution and computational cell shape. The solution selected for the numerical tests is the stable axisymmetric flame with $Le = 1$ obtained for $m = -3$. The two grid-cell decompositions used in the 3D simulations are represented in Fig. B1. Table B1 shows that both prism and hexahedra cell decompositions provide similar results (the difference not exceeding

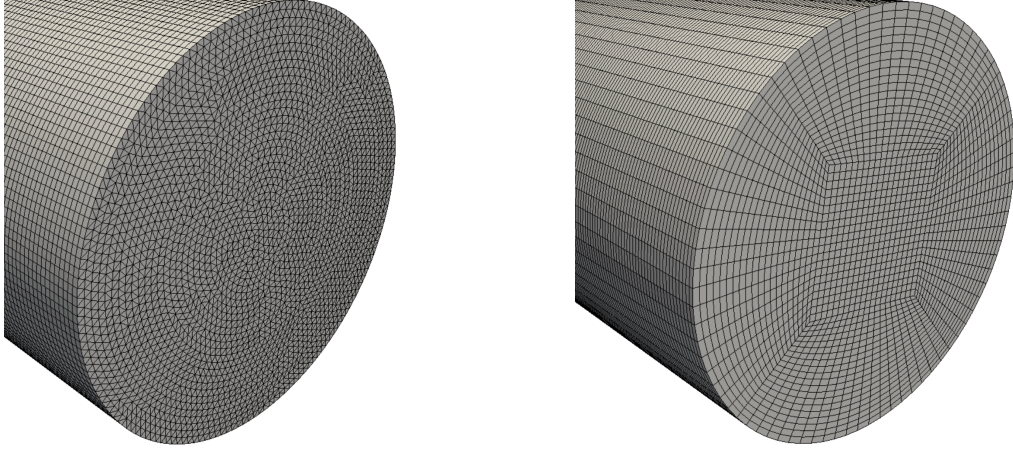


Figure B1. 3D simulation grid-mesh: (left) unstructured prism cell decomposition and (right) block-structured hexahedra cell decomposition

0.01% between the results for the flame velocity). The axisymmetric flame solutions given by the 3D and 2DA simulations are very close, with a maximum difference of 0.02% between the computed flame velocities. Table B1 also displays that increasing the number of cells to 6250000 provides a small difference of about 0.06% with the results obtained with the coarser grid resolution.

Appendix C. Effects of channel length

The effects of channel length L_z is examined in Table C1 for the circular channel with non-dimensional diameter $d = 10$, Lewis number $Le = 1$ and inlet flow rate $m = -3$. In this case, the flame has a stable axisymmetric flame. We have performed 2DA simulations for two values of the length channel, $L_z = 50$ and 80 and various values of the wall heat-loss parameter b . As wall heat-losses increase, fuel may not be fully burned downstream of the flame. It is thus important to check that the computational length domain along the flame propagation direction is large enough to correctly resolve the temperature and mass fraction of gases which gradients must vanish far downstream of the flame. Table C1 shows very small differences (of order 10^{-4}) between $L_z = 50$ and 80. Figure C1 shows how the mass fraction Y_{L_z} averaged over the exit section channel varies with b for $d = 10$, in the case $Le = 1$ and $m = -3$. Not shown, for $d = 6.32$, the mass fraction far downstream of the flame front was found very close to

zero for all cases considered.

	$L_z = 50\delta_T$		$L_z = 80\delta_T$	
b	$\frac{1}{\pi d^2} \int_0^{L_z} \int_{-r}^r \int_0^{2\pi} \omega dz dr d\varphi$	u_f	$\frac{1}{\pi d^2} \int_0^{L_z} \int_{-r}^r \int_0^{2\pi} \omega dz dr d\varphi$	u_f
0.15	1.59722	4.59720	1.59715	4.59715
0.3	1.56917	4.59030	1.56901	4.59011
0.4	1.50333	4.58601	1.50123	4.58587
0.6	1.33301	4.56281	1.33012	4.56237

Table C1. Effect of channel length on average reaction rate and flame velocity u_f with wall heat-loss parameter b : $Le = 1$, $d = 10$ and $m = -3$.

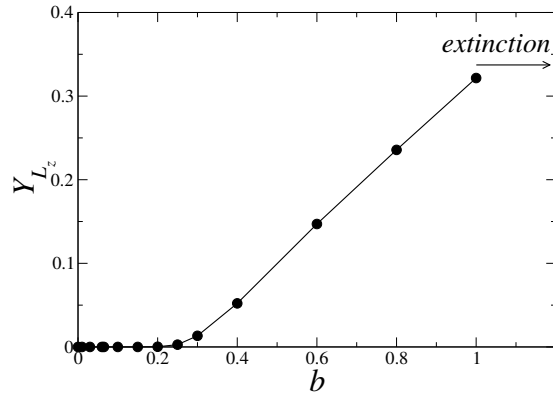


Figure C1. 2DA simulations, $Le = 1$, $d = 10$ and $m = -3$: evolution of mass fraction Y_{L_z} downstream of the flame as a function of wall heat-loss parameter b .