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Numerical and experimental analysis of combustion in microchannels with controlled temperature

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ABSTRACT

This paper reports on joint experimental-numerical investigations of flame dynamics in a microchannel of diameter 1.85 mm. Experiments show that decreasing the diameter of the channel helps the arising of the FREI instability. Yet leaning the mixture is found to be a mean to make the flame more stable. The numerical model used is based on two- dimensional thermo-diffusive equations with one-step chemistry, and it is tested against the experimental results without any calibration. The model turns out to reproduce in a satisfactory manner all the features from a qualitative point of view, and most of them from a quantitative point of view, showing robustness not only with respect to geometry but also to equivalence ratio changes. Nonetheless, while the analysis of frequencies of the FREI instability shows a qualitative agreement, a quantitative discrepancy is unfold. The results suggest that instabilities in microcombustion of CH4/air are fundamentally triggered by hydrodynamics.

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1. Introduction

Due to the high energy density of hydrocarbon fuels, the need for miniaturized systems powered by high specific energy devices has oriented the interest of combustion applications towards small-scale technologies. As an illustration, even with an energetic efficiency as low as 10%, a miniaturized liquid-fueled combustor would still have a higher energy density than the most powerful battery currently available (Kaisare and Vlachos, 2012; Fernandez-Pello, 2002). As a result, many studies have been conducted over the past decade in the field of micro-combustion.

Still, combustion at these small scales remains a source of hard-to-solve problems. Large wall heat losses combined with relatively short reactant residence times can especially lead to instabilities or even extinction. Review articles help identify the advances that have been made for the last twenty years in this area of research and provide both a comprehensive understanding of the micro-combustion fundamentals and the gaps that still need to be bridged (Kaisare and Vlachos, 2012; Maruta, 2011a).

Pioneering combustion experiments in a microchannel revealed interesting behaviors, such as the flame repetitive extinction-ignition (FREI) phenomenon (Maruta et al., 2005b), weak flames (Tsuboi et al., 2009b), and recently oscillating phenomena at the transitions between these different régimes (Di Stazio et al., 2016b). However, it must be recognized that the small size of the systems examined does not make it easy to obtain spatially and temporally resolved measurements.

Thus, numerous studies performing numerical simulations of these micro-reactors have been conducted. Of particular interest are those able to reproduce the characteristic dynamics of microchannel flames, e.g. the studies of H2/air flames (Pizza et al., 2008b; Alipoor and Mazaheri, 2014; Alipoor and Mazaheri, 2016; Nair et al., 2015; Jiménez et al., 2015), and those of CH4/air flames (Miyata et al., 2015; Kang et al., 2016; Kang et al., 2017). These different studies have used highly elaborate models, for some even including detailed kinetics. However, it is also important to put forward reduced models which are capable to correctly reproduce the main features of the rich flame dynamics that is typical in such devices. On one hand, reduced models are relevant to engineering applications, since more complete approaches, and especially three-dimensional direct numerical simulations, are computationally too expensive for parametric studies and complex geometries. On the other hand, reduced models are also crucial to unfold the basic mechanisms underlying the phenomena exhibited by experiments, what is the key step towards combustion control. In this respect, while full-resolved models are attractive for their predictive capabilities, handling them to isolate specific

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mechanisms is challenging, since many details possibly blur the governing processes.

Additionally, while recent numerical works together with experiments helped get insights, many issues remain controversial and it is not yet clear which ingredients are essential to describe the complex features of reactive flows in microchannels. For instance, the combined role played by chemistry and hydrodynamics especially is still to be assessed, since many studies use a one-dimensional plug flow with detailed chemistry (Maruta et al., 2005b; Nakamura et al., 2012). Concerning this point, it has been shown that a two-dimensional thermo-diffusive model with a one-step chemistry correctly reproduces the qualitative dynamics of microcombustion flows (Kurdyumov et al., 2009), and in a more recent study it has been showed that such an approach (Bianco et al., 2015) is able to decently reproduce the quantitative dynamics exhibited by CH4/air flames in a tube as revealed in experiments (Tsuboi et al., 2009a), provided a calibration of the free parameters is carefully performed. Furthermore, the same study evidenced that downgrading the initial model to a one-dimensional one leads to the loss of some important features, especially for diameters smaller than 2 mm. Thus, a two-dimensional model seems to be the baseline. It is worth noting that in the same framework a rigorous stability analysis has been performed to clarify the nature of the instability regions (Bucci et al., 2016), notably showing that non-axisymmetric modes are stable in the régimes studied.

That being said, the model was calibrated against a specific experiment taken from literature only at stoichiometric conditions. As a result, the model still needs to be assessed more thoroughly over a wider range of conditions. Another important point is that often numerical simulations are used to offer valuable qualitative insights on the dynamics of the flame (Kurdyumov et al., 2009), but are rarely compared against real experiments to evaluate to which extent results are quantitative. Of course this is a particular tough test, because of the many subtleties present in actual experimental flows.

The purpose of this article is to compare the aforementioned two-dimensional model to show to which extent it is possible to correctly reproduce the flame behaviour in a micro-channel using simplified modelling and a one-step reduced kinetics. The simulations, without any use of free parameters, will be compared directly with new experimental results obtained for a CH4/air mixture in a 1.85 mm tube at varying inlet equivalence ratio. The present experiments complement those obtained in a similar temperature profile configuration with a larger diameter (Di Stazio et al., 2016a; Di Stazio et al., 2016b). The investigation of heterogeneous reactions or the influence of the richness of the mixture is of particular relevance for possible applications and has been received recently attention in the case of micro-combustors (Di Stazio et al., 2016b; Wang et al., 2018a; Wang et al., 2018b; Xiang et al., 2019). Not only spatial but also time-dependent observables will be considered for validation. This extended confrontation will enable to identify the minimal requirements for the correct reproduction of the phenomena, but also to find out which are the limitations of such a model, indicating the way to improve it in the future.

2. Experimental setup

A schematic of the experimental setup is shown in Fig. 1 (left). This device has been described in details in our previous studies (Di Stazio et al., 2016a; Di Stazio et al., 2016b). In brief, CH4/air mixtures were supplied in a quartz tube with an inner diameter of 1.85 mm at atmospheric pressure. The channel was heated externally by three H2/O2 micro blowtorches to ensure a stationary temperature profile from ambient temperature up to about 1600 K (see Fig. 1 on the right). The temperature along the outer wall of the channel was continuously measured by a FLIR A655sc thermal camera. An emissivity correction was carried out, since the emissivity of the fused silica depends on the wavelength and the temperature (Sova et al., 1998). A Princeton Instrument spectroscopy EMCCD camera, equipped with an optical band-pass filter (20BPF10-430), was used to collect the CH^* chemiluminescence indicating the flame position. The acquisition rate was set at 4260 Hz and pixel binning was performed. The spatial resolution was 62 pixels/mm. In order to track the unstable flame propagation, a high-speed camera Phantom V1611, equipped with a teleconverter Teleplus MC7, was employed. A rate of 12,000 fps and an exposure time of 82 μs were adopted as a trade-off between brightness and temporal resolution of the image captured.

3. Theoretical model

Given the symmetry of the problem, the axisymmetric experimental device sketched in Fig. 1 is modeled only in two dimensions with an axisymmetric frame. At the inner wall, the gradient of the temperature $T_w(z)$ is imposed, as done in the experiments. It turns out that the temperature at the wall is different for each flow, although the heating system is unchanged. In particular, the flame heats the tube and changes the temperature profile imposed on the wall. To be consistent in the model, a different temperature profile has been used for each speed. The profiles were experimentally recorded with a thermal camera at intervals of 5 cm/s, and for each speed within the range, the temperature profile was obtained by interpolation. Making the difference between the various temperature profiles, a temperature difference up to 70 K can be observed between the different speeds. As the flames around the pipe are three, the temperature is not perfectly constant over the entire circumference of the pipe in the experiments. The average

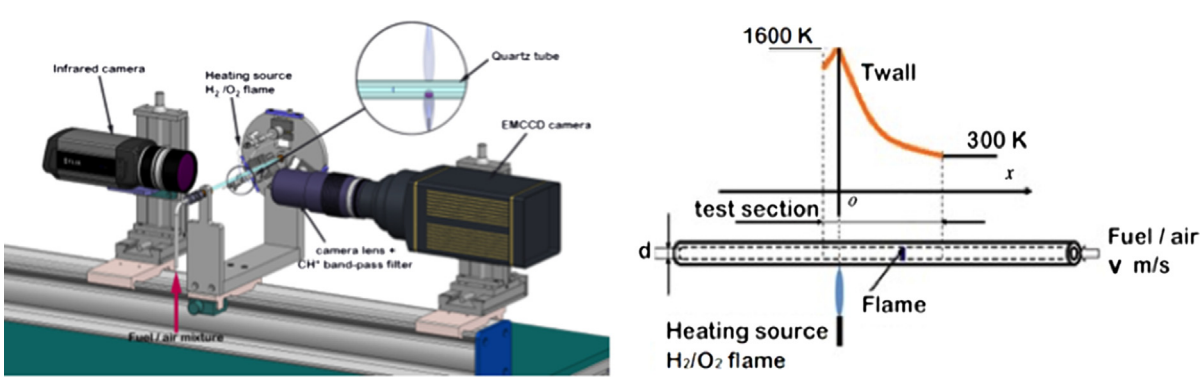

Fig. 1. Left: Schematic of the experimental device; Right: Temperature profile along the channel.

temperature on the circumference has been chosen as representative of the temperature profile at any speed analyzed, in the numerical simulations. In this work, we focus on the reduced model discussed in (Bianco et al., 2015) that has been modified to take into account the equivalence ratio effect. The dynamics is described by only two scalar advection-diffusion-reaction equations, i.e., one for the fuel mass fraction Y_{CH_4} and one for the mixture temperature T, while the mixture density ρ is kept constant:

$$\frac{\partial Y_{CH_4}}{\partial t} + u_z \frac{\partial Y_{CH_4}}{\partial z} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial Y_{CH_4}}{\partial r}\right) + \frac{\partial^2 Y_{CH_4}}{\partial z^2}\right] + S_Y, \tag{1a}$$

$$\frac{\partial T}{\partial t} + u_z \frac{\partial T}{\partial z} = D\left[\frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{\partial^2 T}{\partial z^2}\right] + S_T, \tag{1b}$$

The velocity field $\mathbf{u}$ is an input of the model and is prescribed as follows:

$$\begin{aligned} u_r &= 0 \\ u_z &= -\tfrac{1}{4\eta}\tfrac{\partial p}{\partial z}(R^2 - r^2) = -\tfrac{2U_0}{R^2}(R^2 - r^2); \end{aligned} \tag{2}$$

where U_0 is the mean axial speed, R the radius of the pipe, and D the diffusion coefficient taken to be constant. The production terms are as follows:

$$\begin{aligned} S_Y &= \tfrac{\nu_{CH_4} W_{CH_4}}{\rho} K_f = -A^* Y \exp\left(-\tfrac{T_a}{T}\right) \\ S_T &= -\tfrac{Q}{[(1+\alpha(\phi)]C_p} S_Y \end{aligned} \tag{3}$$

where Q is the heat of combustion, C_p the specific heat at constant pressure, ϕ the equivalence ratio, and ν_{CH_4} the methane molecular coefficient that is taken equal to -1 at stoichiometric conditions (ϕ=1). For $\phi = 1$, the ratio $Q/C_p = 35000$ K is required to match the flame adiabatic temperature at constant pressure ($p_0 = 1$ bar, $T_0 = 300$ K). Finally, a Lewis number equal to unity is assumed. When varying the equivalence ratio, the major effect on the energy balance is attributed to the portion of the preheating from the flame to the fresh stream that will not be used to enable the heat release as hot unburnt reactant will escape together with the hot products. To account for this effect, the correcting factor $(1 + \alpha(\phi))$ has been incorporated to the source term in the temperature equation, see Eq. (3). $\alpha(\phi)$ is such that $\alpha(\phi = 1) = 0$ and $[(1 + \alpha(\phi)]C_p$ is the specific heat at constant pressure of the mixture including the unburnt reactant, i.e., H_2O, CO_2, and N_2, following the computations of transport properties prescribed by Kee et al. (2004).

In the set of Eqs. (1a) and (1b) there are two free parameters D and A^*. Bianco et al. (2015) have shown that the model is able to correctly reproduce the phase-diagram of the flame-position *vs* the flow rate for a particular experiment (Tsuboi et al., 2009a), assuming $D \approx 0.7[\mathrm{cm}^2/\mathrm{s}]$ and $A^* \approx 1.5 \times 10^9[1/\mathrm{s}]$. We use here the same values.

Comments are needed to explain some the hypothesis underlying the model. In particular, keeping the density constant is a strong assumption. As explained in previous works (Pizza et al., 2008a; Pizza et al., 2008b; Kurdyumov et al., 2009; Bianco et al., 2015; Bucci et al., 2016), the purpose of such an approach is to develop a reduced-order model for the flame dynamics yet capable to provide a decent representation of the phenomena in microchannels at varying the physical parameters. We have found that the 2D model previously developed in Bianco et al. (2015) delivers a fine representation of the régimes investigated, even if density is kept constant. In the present work, we assess the robustness of this 2D model changing the equivalent ratio and looking at new observables. As a consequence, we will be able to discriminate among the assumptions those which are too strong to get a satisfactory representation of the aforementioned observables.

Another approximation is to use an axisymmetric model, rather than a full 3D one. This approximation is rather mild, if compared with common models used for microcombustion which are based upon 1D plug-flow yet with detailed chemistry (Maruta, 2011a). However, it has been reported in some experiments (Maruta et al., 2005b) and in direct numerical simulation of a hydrogen-air mixture (Pizza et al., 2010) that spinning-flames and even completely non-axisymmetric flames may appear in some particular régimes, notably for a sufficiently high velocity. For this reason, the present model might appear too restrictive with regard to this issue. However, in the régimes considered in the present study such configurations should not be present, since the diameter is small enough with respect to the velocities considered, and surely they cannot be present in the régime typical of the FREI instability (these non-axisymmetric flames are never observed roughly for $d \lesssim 1.5$ mm and $U \lesssim 1$ m s^{-1}). Moreover, and even more important, in a recent study (Bucci et al., 2016) it has been rigorously demonstrated that such non-axisymmetric flames cannot arise in the present thermo-diffusive framework even in 3D, since all those modes are stable. In summary, there is no bias in using an axisymmetric model within the range of régimes investigated here.

3.1. Numerical method

The inlet/outlet conditions imposed on the temperature and concentration are the following:

$$z = 0 : T(r,0) = T^0 = 300K; \tag{4}$$

$$z = L : \frac{\partial T(r,L)}{\partial z} = 0, \quad \frac{\partial Y_{CH_4}(r,L)}{\partial z} = 0 \tag{5}$$

Symmetry conditions are applied at the channel axis:

$$r = 0 \quad : \quad \frac{\partial T(0,z)}{\partial r} = 0, \quad \frac{\partial Y_{CH_4}(0,z)}{\partial r} = 0 \tag{6}$$

$$r = R \quad : \quad T(R,z) = T_w(z), \quad \frac{\partial Y_{CH_4}(R,z)}{\partial r} = 0 \tag{7}$$

For the initial conditions, $Y_{CH_4}(r,0) = Y^0_{CH_4}$, which depends on ϕ; its value is $Y^0_{CH_4} = 0.055$ at stochiometric conditions ($\phi = 1$). As pointed out by Tsuboi et al. (2009a), it is possible to neglect the influence of the flame temperature on the wall. Yet, possible difference between the diffused temperature near to the wall and T_w represents the heat dissipation. We remark that since radial terms are taken into account, the 2D model includes the exact heat balance, whereas it is necessary to add a supplementary term to represent the heat exchange with walls, in 1D models (Maruta et al., 2005a; Nakamura et al., 2012; Tsuboi et al., 2009a; Bianco et al., 2015).

Like in the experiments, the diameter is $d = 1.85$ mm (see Fig. 1). The length of the numerical domain is set to $L = 10$ cm, beyond which the experimental wall temperature gradient is zero. The numerical domain is discretized with a cartesian grid of $N_z \times N_r$ grid points along the cylinder length and radius respectively, where $z(i) \in [0, L] \quad i = 1, \ldots, N_z$ and $r(j) \in [0, R] \quad j = 1, \ldots, N_r$ are the cylindrical coordinates of the generic grid point (i, j). The mesh must be able to capture the smallest scales without filtering out the solution. Keeping the mesh uniform over the entire domain, the solution turns out to be at convergence, that is not dependent on the grid, with a discretization-size smaller than 0.02 mm in the z direction. A minimum mesh size of $\Delta z = 1.25 \times 10^{-2}$ mm was chosen. Along the r direction, the gradients are weaker. As a result, a coarser grid was used, i.e. $\Delta r = 2.5 \times 10^{-2}$ mm. Following Bianco et al. (2015), to avoid the large number of discretization

points due to an uniform mesh, an adaptive mesh has been adopted. With this method only the region with higher gradients is finely discretized. Away from the flame, the mesh size becomes larger according to a geometric series. The convergence of the adaptive mesh with respect to the uniform one has been duly checked (Bianco et al., 2015). All results were obtained with a relative residual level lower than 10^{-10} with respect to the initial residual. A sixth-order finite difference scheme was used for the spatial gradients. Concerning the numerical integration in time, since oscillatory phenomena have to be captured in our simulations, the choice of an accurate scheme is important. We have chosen an explicit Runge–Kutta fourth-order scheme, which is particularly robust and accurate (Williamson, 1980).

4. Results

4.1. Effect of flow velocity

The numerical results obtained here for a stoichiometric CH_4/air mixture are compared with the experimental ones in Fig. 2. As previously observed (Maruta et al., 2005a; Maruta, 2011b), three flame régimes exist depending on the average inlet velocity, i.e. stable flames at higher velocities (> 0.7 ms^{-1}), Flames with Repetitive Extinction and Ignition (FREI) for intermediate velocities, and weak flames at very low speed (< 0.2 ms^{-1}). For some conditions, oscillatory flames were also observed between the aforementioned régimes, both at the stable/FREI and FREI/weak-flame transition.

Experimental results obtained with the present configuration for $d = 1.85$ mm can be also compared to previous results at a larger diameter 2.15 mm (Di Stazio et al., 2016a). Results are qualitatively similar but display some significant differences. In particular, the present smaller device has been found to be more unstable, since the transition region between the stable flames and the FREI, clearly shown in Fig. 2, reveals around a velocity of 0.41 m/s, whereas in the previous work the same transition appeared for a slower velocity, around 0.33 m/s. In both cases, there is a discontinuity in the evolution corresponding to the 'oscillating FREI', which spans over a range of about 0.2 m/s. The FREI régime appears almost unchanged with respect to experiments made at larger diameter, but the transition to the stable weak flame seems to be possible at even lower velocities, even though measurements in this regions may be affected by significant errors.

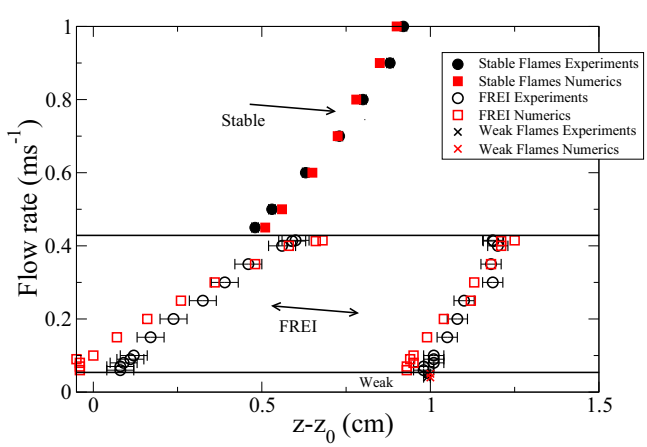

Fig. 2. Phase-diagram at stochiometric conditions $\phi = 1$. Horizontal axis: position z along the tube. The arbitrary offset z_0 has been chosen as in experiments such that the maximum of the wall temperature is located at $z = 1$. Vertical axis: mean inlet flow rate. The filled symbols correspond to the stable flame case. The open symbols indicate FREI régime. Weak flames are represented by crosses. In the FREI régime, the upstream and downstream branches indicate the locations of the ignition and extinction, respectively. Every transition between two régimes is delineated by a horizontal line.

The trends can now be identified in Fig. 2, according to the different régimes observed. First, in the stable régime, the evolution of the stabilization temperature is quasi-linear for the higher velocity régime of $0.7 \div 1$ m/s. Then the dependency on the flow velocity is slightly emphasized and stabilization temperature is reduced with the decreasing velocity ($0.6 \div 0.42$ m/s). This is the region where the convexity of flame front is reversed, as already illustrated by recent experiments (Di Stazio et al., 2016a). In the FREI régime, a weak but clear dependency is observed for the ignition data points with respect to the position in the tube. The trend might be always linear. This evidence slightly differs from recent results obtained at larger diameters (Di Stazio et al., 2016a), yet are in line with experiments performed at similar diameter ($d = 2$ mm) but with another experimental setup (Tsuboi et al., 2009a). With regard to extinction, a stronger temperature dependence of the quenching occurence is observed according to the flow velocity. The lower the inlet velocity, the lower the extinction temperature, given that higher velocity helps thermal quenching, as already investigated numerically (Norton and Vlachos, 2003). Once the diffusive weak flame is then stabilised again, there does not seem to be any dependence on the flow conditions. However, the data concerning this region are probably not sufficient to characterize comprehensively the process.

Considering the numerical results, the agreement is fairly good in all regions. In particular, the stable dynamics appears to be very well captured and possible discrepancies stand within the error bars. The transition between stable flames and FREI is caught quantitatively, further evidencing that the mechanics of the instability recently analysed with the present model (Bucci et al., 2016) corresponds to the actual one. As pointed out in that global stability analysis (Bucci et al., 2016), even the oscillations in the transition region between the stable flame and the FREI régimes are qualitatively captured. Then, the FREI instability is correctly reproduced, with regard to both ignition and extinction points, with a slightly larger discrepancy in the vicinity of the transition with the weak flame régime. From a technical point of view, it is important to remind that the identifiation of the locations of the ignition and extinction points requires some care and actually hides some arbitrariness. Since it is not possible to use a strictly identical procedure to locate those points in numerical simulations and in experiments, some small differences are to be expected just for technical reasons. In particular, from a numerical point of view, we can readily identify the point of maximum heat release (ignition) and that where the flame heating falls below a given threshold (extinction). In contrast, in experiments, measurements result from convoluted information which makes the precise location more difficult to define, especially for the lower range of equivalence ratio where flames appears very diffused.

Finally, the transition to the weak régime turns out to be at the velocity condition met in the experiment.

4.2. Equivalence Ratio

Experiments and numerical simulations have been performed at different equivalence ratios, i.e. $\phi = 0.7 \div 0.9$. Since the two branches of rich and lean mixture are nearly symmetric, we consider here only the lean one that is the most relevant branch from the technological standpoint. The results obtained are shown in Fig. 3. We find that the leaner the mixture, the higher the temperature needed to stabilize the flame. As a result, the position of the stable flame is shifted in the tube. Moreover, the flames fed by leaner mixtures are found to be more stable than those for stoichiometric condition. In particular, the transition to the FREI

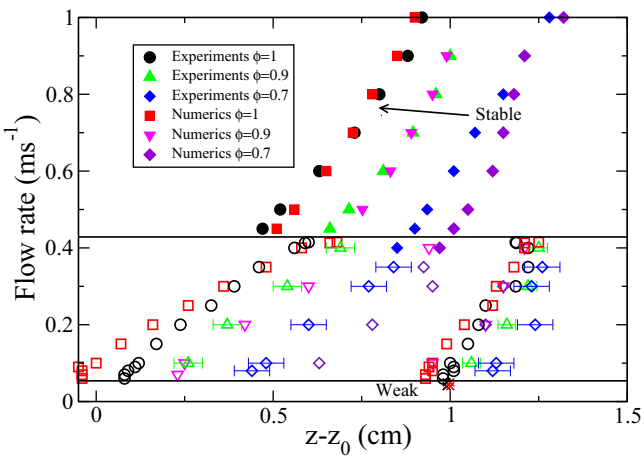

Fig. 3. As in Fig. 2, the solid symbols correspond to the stable flame case, the open symbols indicate FREI régime, and weak flames are represented by crosses. The transitions are clearly highlighted by two lines. For the sake of clarity error bars are not shown for the $\phi = 1$ case, since they are given in Fig. 2.

régime for $\phi = 0.7$ is found at $U = 0.39$ m s^{-1} rather than at $U = 0.41$ m s^{-1} for $\phi = 1$.

The same trend with decreasing flow rate is followed in the FREI régime, but in a different way for extinction and ignition. While the effect is significant and similar to the stable flames for the extinction point, there is a relatively small shift of the ignition point. Yet, at variance with recent experiments (Di Stazio et al., 2016a), the effect seems small but visible also in this region, although the uncertainty in the location of the ignition point is larger for leaner mixtures because of the poor brightness of the flames. Moreover, the transition between stable weak flame and FREI remains more or less always at the same level of flow rate over the range of equivalence ratio investigated, even though the leanest mixture has a wider transition region between the stable flame and the FREI régime.

The overall agreement between experiments and numerical simulations is striking, considering the simplicity of the model and that no free parameters have been used at this stage. Not only the qualitative trend is reproduced, but further the experimental and numerical curves almost collapse for all ϕ, with some small differences exhibited only at $\phi = 0.7$. In this case, it is worth emphasizing that, on one hand, the measurements are more difficult for lean mixtures, because of the lack of brightness, and, on the other hand, the numerical model is based on crude approximations which appears to be less appropriate far from stoichiometric conditions. Notably, for lean mixtures, the transition to the weak régime is slightly anticipated with respect to experiments, so that the numerical model seems to slightly stabilize the system, at least with the parameters chosen here. However, this small discrepancy between numerics and experiments is mostly due to the presence of the oscillatory FREI régime in this region of parameters, which makes the computation of the precise transition less accurate.

4.3. FREI frequencies

In this work, we investigate also the characteristic frequency f of the FREI mode. It is obtained experimentally through the Fourier Transform analysis of the spectral cross-section of the *CH* signal. In the numerical simulations, the same procedure is carried out using the dynamic of the flame, which represents the *CH* signal. This characteristic frequency was determined for each flow rate and for each equivalence ratio considered here. The results are reported in Fig. 4. It appears that the frequency grows with increasing the flow rate and with a leaner mixture. It is clear that the behaviour of such a delicate quantity appears more elusive and there is a stronger discrepancy between numerical simulations and experiments. Some comments are therefore in order. First, it is worth emphasising that at least the order of magnitude of the frequency and the trend with the flow rate are correctly captured by the numerical model. This is far from being trivial as highlighted by numerical experiments with a 1D model with detailed chemistry (Nakamura et al., 2012), which displayed much larger errors. However there is a significant discrepancy in the quantitative value, even at stoichiometric conditions, i.e. $f \in [5hz, 40hz]$ in the numerical simulations, whereas $f \in [10hz, 80hz]$ in the experiments. In particular, the experiments show a higher frequency for all flow rates, except at very low flow-rate. Moreover, the experiments display a strong dependency of the frequency with the flow rate, whereas numerical model predicts a similar but more modest trend, also with respect to a leaner mixture. In this respect, comparison with previous experiments performed at higher diameters (Di Stazio et al., 2016a) shows also a dependency of the frequency with the diameter.

In order to better characterise the equivalence ratio effect, we have also computed the Strouhal number $St = f \times d/v$, where d is the inner diameter, and v is the inlet velocity. This quantity is displayed in Fig. 5 as a function of (a) the flow rate and (b) the equivalence ratio. As in previous experiments (Di Stazio et al., 2016a), we find a minimum at stoichiometric conditions, where $St \approx 0.7$, which is larger than what found at a larger diameter, confirming the dependence of frequency with diameter. Moreover, for both experiments and numerical simulations, the Strouhal number is found to be approximately constant for each equivalence ratio. While this result shows that the trend both with flow rate and equivalence ratio is qualitatively captured by the numerical model, a significant difference in the value of the Strouhal number is found. The discrepancy is more or less the same for all equivalence ratio, meaning that the main error is related to the representation of the frequency already at stoichiometric conditions, and does not depend much on the chemical details related to a lean/rich combustion.

To get more insights on the variation of the frequency, we have calculated experimentally and numerically the characteristic time between ignition and extinction of the flame (τ_{IE}) and the time between the extinction and ignition (τ_{EI}). The frequency is related to these quantities by the expression $f = \frac{1}{\tau_{IE}+\tau_{EI}}$. These times are shown in Fig. 6 as a function of flow rate. Results allow to understand the basic reasons for the discrepancy between numerics and experiments: numerical model overestimates the two characteristic times, and notably the τ_{EI}. Furthermore, while in the

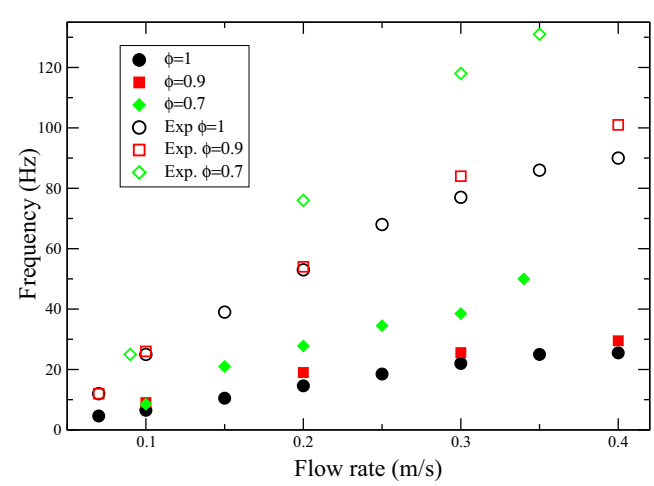

Fig. 4. Frequencies with respect to flow rate for different equivalence ratio. Solid symbols are for numerical simulations, while open symbols are for experiments.

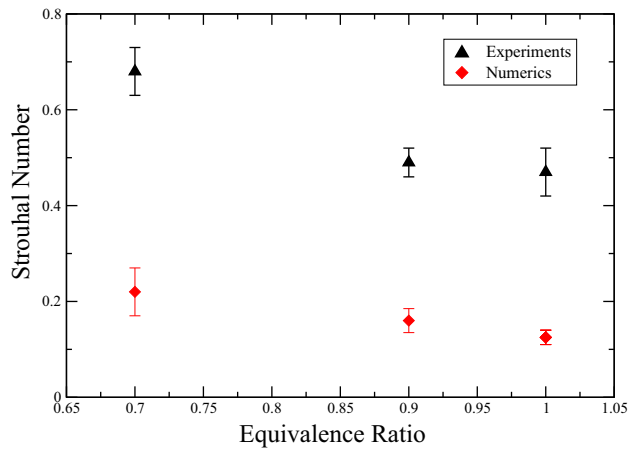

Fig. 5. Strouhal number at different equivalence ratios.

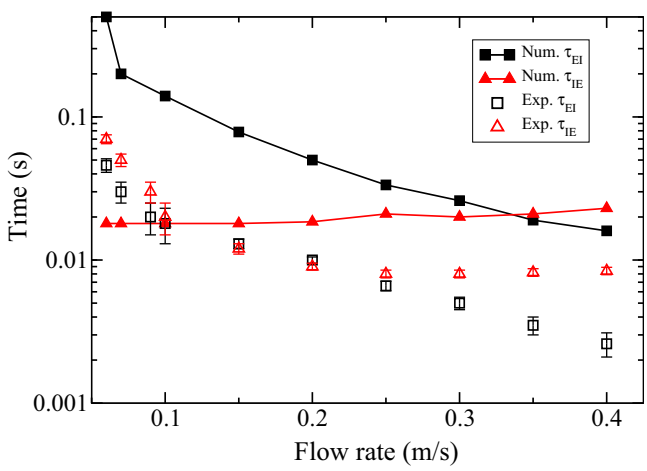

Fig. 6. Characteristic time-scales for the dynamics between the ignition and the extinction points. Numerical simulations are compared against experiments for $\phi = 1$.

experiments both time scales are of the same order of magnitude for lower flow rates, the numerical model displays a large difference between the two. On one hand, the time the flame needs to go from the ignition point to the extinction one is roughly consistent with the experiments at large flow rates displaying a *plateau*. Yet it does not show any clear trend with respect to the velocity for slow flow rate, contrarily to what displayed by experiments. With respect to the hydrodynamic model, the gas expansion, not included in the present study, is expected to play a more significant influence on slower flows. The lack of this effect is identified therefore as one of the main ingredient that prevents capturing quantitatively the frequency of the oscillations. On the other hand, the extinction-ignition time displays a clear dependence on the flow rate with a strong increase in time with decreasing flow velocity, which is found also in the experiments. The trend is qualitatively captured but the overestimation is large, due to a shift in the values at all flow rate. The results for other equivalence ratios display a similar behaviour and are not shown for the sake of clarity.

5. Discussion and conclusion

We have presented new experimental and numerical results about the dynamics of flame in a micro-tube for a diameter of $d = 1.85$ mm and for different equivalence ratios. The experiments have been performed at controlled conditions, using a device which heats the external wall of the tube in a thin region and which almost ensures the axial symmetry. Our main goal was to perform a comprehensive comparison between well-controlled experiments and a 2-D thermo-diffusive model with one-step chemistry for methane to highlight the main mechanisms at play in microcombustion and to assess the predictive capability of such a model. We have chosen a precise model since it has been recently found to get the main features of the combustion in microchannels against experiments performed at different geometry and conditions. In this respect, the present work is aimed also at assessing the robustness of the model to make reliable predictions, that is without test-dependent calibration. For such a reason, the model is used without free parameters. It is important to explain clearly this point in order to emphasise to which extent the robustness has been actually assessed in the present work. The model had been previously calibrated with methane/air mixture in another configuration (Bianco et al., 2015), and no change has been made here. It is worth underlying that the two configurations display important differences, notably concerning the diameter of the tube. While this difference may appear minute (2 mm against 1.85 mm here), it has been shown previously that even such a small change may produce large effects in the dynamics of the flame (Bianco et al., 2015). As an illustration the position of the flame may be shifted of more than two diameters. Furthermore, in the present work we have also changed the temperature profile at the wall, which has been found to have a major influence in experiments (Di Stazio et al., 2016b; Di Stazio et al., 2016a). We believe therefore that present results show already a large degree of robustness, also considering the degree of reduction inherent to the modelling.

To limit possible errors external to the chemical-physical realm due to a difference in geometry or to data acquiring, we stayed numerically as close as possible to the experiments, using all the relevant experimental initial and boundary conditions. That kind of tight comparison has been never done before for such phenomena at our knowledge. We have extensively compared numerical results against experiments at varying flow rate and equivalence ratio. With respect to previous studies, we have also investigated the typical frequencies of the FREI régime, being able to obtain the characteristic time between ignition and extinction as well between extinction and ignition.

Experiments show that using smaller diameters help triggering the FREI instability, whose transition turns out to be at higher flow rate ($U_c = 41$ cm/s) than for a slightly larger diameter, since at $d = 2.15$ mm we found $U_c = 34$ cm/s. On the other hand, using a leaner mixture slightly stabilises the system, and the flame is found stable still for $U = 30$ cm/s at $\phi = 0.5$. The frequency of the FREI mode has been found of the order of 50*hz* with a significant dependency on the flow rate, the higher the flow rate the higher the frequency of the oscillation. Furthermore, the frequency turns out to be larger for leaner mixtures.

Concerning the numerical model, our main findings are the following: (i) The numerical model has been found to reproduce quite well the phase diagram depicting the flow rate against the position of the flame. The agreement is remarkable also for mildly lean mixture and remains decent for poor mixtures. (ii) Concerning frequencies, while the theoretical model well captures the global trend with flow rate and equivalence ratio, it underestimates the value of the frequency. (iii) With respect to the above picture, discrepancy seems to grow near the transition to the weak flame régime. (iv) Most of the discrepancy has been found to be related to the overestimation of the time needed by the front to go from the extinction point to the ignition one.

These results are important to get insights on the dynamics of such reactive flows in small channels. The model has been shown

to be robust in its predictive capabilities with respect to geometry and equivalence ratio changes. From this evidence, we can infer that the dynamics of microcobustion is largely influenced by the hydrodynamicsmechanisms included in the model, at least for CH4/air. That means that the recent refined analysis of the instability dynamics in microchannel based upon the present model (Bucci et al., 2016) should apply to realistic flows, and that reduced models based upon a too crude hydrodynamic description cannot bring quantitative predictions even with detailed chemistry. On the other hand, the discrepancy in the computation of FREI frequencies points to the shortcomings of the present picture. A part of the discrepancy can be surely traced back to the use of a stationary Poiseuille profile for the velocity at each point, without considering the effect of the temperature together with the thermal expansion of the gas. This factor does change precisely the local velocity and thus the time needed by the flame to cross the channel, which has been found to be crucial to predict correctly the frequency of the oscillations. Moreover, this picture is also supported by the fact that this effect is expected to be more significant at slower flowrate, consistently with present results.

Our findings show also that in some conditions a more refined chemistry should be taken into account. In particular, we have found that the model used here describes too crudely the weak flame and more in general the dynamics at very low flow rate. A complete chemistry model is probably not needed, but clearly diffusion is dominant in this régimes and should be better modelled. This appears to be particularly true also for very lean mixtures, which display a more complex behaviour. In order to better understand these issues and also extend the robustness assessment carried out in the present work, it would be important to make available direct numerical simulations of such flows with a reasonable detailed chemistry model. In this way it would be possible to analyse also other observables like the flame temperature and width, which are difficult to access accurately from an experimental point of view. Those simulations are computationally very difficult, and at the moment no such simulations are available, to our knowledge. We plan to sustain the ongoing efforts in the future.

Finally, although future microcombustors are intended to operate at lean conditions to reduce fuel consumption, it would be interesting to assess the performances of the reduced-model also in the rich branch of the configuration.

Declaration of Competing Interest

The authors declare that they have no known competing financial interests or personal relationships that could have appeared to influence the work reported in this paper.

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