Sudden acceleration of flames in open channels driven by hydraulic resistance

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1 Introduction

Deflagration experiments in tubes are usually initiated by a weak source of energy which produces the ignition of the reactive mixture in one of the extremes of the channel. At the beginning the flame propagates slowly with a velocity that may vary between several centimeters and several meters per second. The expansion of the burned gases in presence of obstacles generates turbulence that in turn increases the effective burning rate causing an acceleration of the propagation of the flame to sonic speed and then to detonation. This transition is very sensitive to small perturbations, for instance, for lower reactive mixtures this feedback loop may be countered, or even interrupted, by the tendency of the flame to quench due to stretch and heat losses or through momentum losses due to venting.
The stationary modes of the propagation of a flame in confined obstructed channels can be classified as slow sub-sonic, sonic (choked), fast super-sonic and detonations Certainly, most of the previous investigations, have devoted a special emphasis to the deflagration to detonation transition (DDT) e.g. [1] and [2]. Although for the most important stationary propagation regimes the multiplicity and peculiarities have been studied extensively and understood quite well (see e.g. [3]) the transition between them is still poorly understood and it represents very complex open problem.
The transition of the deflagration to fast sonic flames and then to super-sonic flame is in the focus of this research. In the current study, flames propagating in obstructed channels ignited from its open end are investigated. In such configuration, a prolonged quasi-laminar propagation phase is followed by a sudden and violent shockless flame acceleration that culminates when the sonic regime is reached. The main mechanism causing this sudden acceleration of flames was, in the opinion of the authors, suggested by Brailovsky and Sivashinsky [3] (see also e.g. [4], [5]) who found that the ultimate cause triggering the DDT was the hydraulic resistance. Due to friction forces, a quasi-laminar deflagration wave cannot reach a stationary regime. Nevertheless, the parameters controlling the de/acceleration and the form in which this occurs remains unclear. In order to improve current understanding of the phenomenon, the authors have carried out the analysis presented in this article by combining experimental, numerical and analytical approaches to the problem.

2 Description of the experiments and the numerical simulations

The experiments were performed in the DRIVER facility [6], which is an obstructed combustion tube with a total length of 12.2 m and an internal diameter of 174 mm. Inside the tube, ring shape obstacles

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were positioned in a regular manner and spaced by a tube diameter accounting for a blockage ratio equal to 0.6. A 13% vol. hydrogen-air mixture at ambient conditions was ignited at the open end, directly at the interface between the inflammable mixture and the surrounding air. The instrumentation included photo diodes and pressure gauges installed along the channel. The venting ratio α of the orifice was varied from fully closed to completely open.

Numerical simulations of three significant experiments for venting ratios 0%, 40% and 100%, were carried out with the combustion code COM3D [7] in order to provide an enhanced comprehension of the test and analyze the mechanism of the flame acceleration in presence of end venting. The numerical representation of the problem include the geometry of the tube, the obstacles inside it and a supplementary volume with open-non reflective boundary conditions to simulate the release of the combustion products through the vent area into an unconfined atmosphere. The supplementary volume allows the products of the combustion to be discharged from the tube on an area of the calculation domain in order to make the simulations significant. The total volume and time to be simulated restrict the minimum resolution achievable to 5.8 mm due to the available computational power. This has several implications. Specifically, the Kolmogorov and Taylor turbulent micro-scales, the boundary layers and the laminar flame thickness remain unresolved.
To overcome those restrictions, the KYLCOM combustion model [8], specifically designed for under-resolved calculations, and the standard k-ε turbulence model [9] was utilized. The combustion model was coupled with the turbulent burning velocity correlation proposed by Schmidt et al. [10].
The influence of the resolution in the flame and hydrodynamic instabilities requires further considerations. Until the flame acceleration takes place, the thermo-diffusive instability plays an important role [11]. In open tubes, the quasi-laminar propagation region grows significantly compared with closed ones and the effect of flame wrinkling and folding becomes very important. Thus, to estimate the increase in burning velocity due to this, the Driscoll's relation [12], $\Xi=Le^{-1}$ was utilized, where Ξ is the increase in the burning velocity due to thermal-diffusive effects and Le is the Lewis number of the mixture.

3 Experimental/numerical results. Analysis of the acceleration mechanism

Figure 1 displays a comparison of the flame propagation obtained from the results of simulations and experiments. In the closed channel, the flame accelerates immediately after reaching the first obstacle generating an additional flow motion which steepens into the shock wave. The turbulent flow ahead of the flame created by the thermal expansion of the products supports the flame acceleration within a relatively short time after ignition (~0.1 s). Beyond the run-up distance, of about 1.3 m, the flame reaches the sonic regime and propagates further with a steady velocity of 540 m/s (close to the sound velocity in the product) and with the characteristic pressure of the leading shock wave oscillates from 6 to 11 bar.
In the presence of venting, combustion products are discharged in the atmosphere through the end orifice and do not support flame acceleration. Two regions with different propagation regimes, fast and slow, can be clearly identified. Initially, the flame propagates in a quasi-laminar regime with a stationary velocity of ~3.5 m/s. The experimental records show that during this phase no significant pressure increments exist (≈300 Pa) and, therefore, no relevant flow motion (generating turbulence) appears ahead of the flame. Nevertheless, around 1 s after the ignition, the flame suddenly accelerates from the quasi-laminar to the fast sonic regime within the interval of 3-30 ms (50 ms in the calculations). Both in experiments and simulations after the acceleration, the sonic flame propagates until the end of tube with a constant velocity of ~540 m/s.
The reproducibility of the essays was analyzed repeating the test with 40% of venting twice. The results of the two experiments show significant divergence of the transition location confirming high sensitivity of the transition to the initial conditions. However, the order of magnitude of the transition time and location as well as all properties of the transition (initial deflagration velocity, thickness of

the sharp acceleration region etc.) remains akin. The discrepancies between different experiments should be considered as one of the characteristic inherent to this type of combustion problems. The second test for 40% of venting and the experiment with 100% venting almost superpose and the acceleration of the process suffers a 40% delay (from ~0.6 s to ~1.0 s after the ignition). Significantly, the results of the numerical simulation for 40% of venting appear in the interval between the two experimental curves.

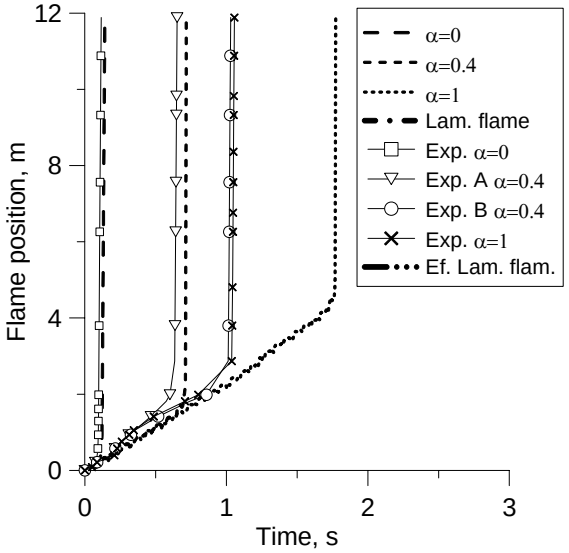

Figure 1 Flame position. Dashed lines calculations. Thin continuous lines with symbols represent the experiments while dashed lines the calculations. Venting ratio is indicated in the legend.

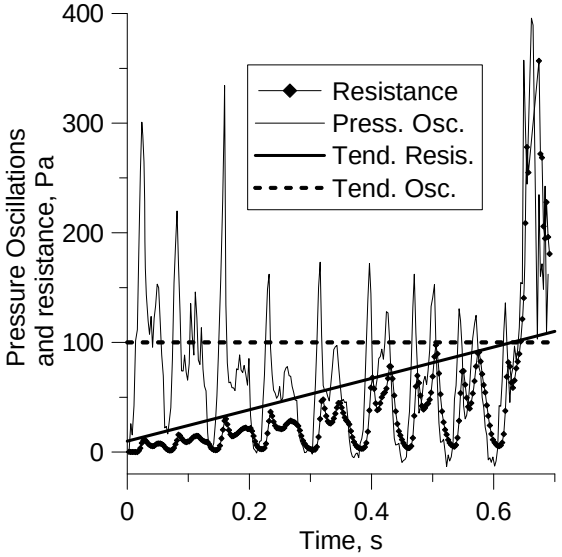

Figure 2 Pressure oscillations near the discharge orifice and resistance obtained for the case α=0.4.

While the flame penetrates in the tube, the combustion products are discharged into the atmosphere via the venting orifice. The propagation of the flame inside the channel implies that combustion products should traverse a longer distance until they are discharged suffering an enhanced *momentum loss*. The hydrodynamic resistance was expressed by Brailovsky et al [3], as $F=-2c_D\rho u^2/d$ in which c_D is the drag force coefficient. The results of the numerical experiments carried out with diverse flow velocities in the range 1-30 m/s allow approximating c_D with the value 0.12. Therefore the total *loss of momentum* can be estimated as $\Delta P=\int F dx$ where integration is taken until the flame front position and the opening of the tube. The existence of obstacles increases the complexity in the flow pattern. For the propagation of the flame in the laminar regime the obstacles produce a change in the total surface of the flame and thus of the total fuel consumption. In first approach this change can be estimated to be of the order of *(1-BR)* being *BR* the Blockage Ratio. As the obstructions are gradually reached, cyclic oscillations in the pressure (order of tens of Pa, peak of ~340 Pa, see Figure 2) as well as in the velocity of the discharge products will appear. Those oscillations will have a frequency $\omega_l=\square_f/d$ where $\square_f$ is the velocity of the flame front and d is the interval between obstacles, which in this problem is equal to the diameter. It is important to underline that no shock waves were developed and observed during the entire quasi-laminar regime.

Figure 2 shows how pressure variations slightly compress and decompress the part of the tube filled by the reactants. This area can be understood as a close cylinder, or a *drum*, in which the flame actuates as an oscillating piston. In order to study the compression/decompression cycle of the reactants the one dimensional Euler's equations of continuity and impulse may be used to model the phenomenon. Performing cross derivatives on them (in t-x) and operating, the wave equation can be obtained supposing the velocity of the oscillations is small and thus the hydrodynamic resistance can be neglected. Additionally, by taking into account the observations performed during the numerical

experiments, the oscillations inside the reactants resulted to be mainly of the first harmonic. The wave equation may thus be simplified to

$$\ddot{p} + \left(0.5\pi c / \left(L - x_f\right)\right)^2 p = 0 \qquad (1)$$

where L is the total length of the tube, c is the local sound velocity in the fresh mixture. Therefore a second cyclic process with a frequency $\omega_2=c/(4(L-x_f))$, is present in our system, as can be seen in Figure 2. The final pressure signal obtained, are the superposition of the two cyclic processes with frequencies ω_1 and ω_2, and the variable peaks of the registered amplitudes results from this superposition.

The resistance of the products grows linearly ($\Delta P=\int F dx=-2c_D\rho u^2 x_f/d$) as the flame penetrates inside the tube (see Figure 2, thick line (trend)). When the resistance is comparable with the pressure peaks created by the flame, the products have difficulties to be discharged and a part of them are accumulated inside the tube. The reactants receive an enhanced compression and thus an increased compression-decompression cycle is triggered. The flame suffers an additional acceleration and traverses an augmented distance per oscillation. Some significant flow appears ahead of the flame. If during this displacement an obstacle is overcome, the burning rate will be enlarged by the turbulence created by the barrier and the flame starts to burn in the turbulent regime. The burning rate, the compression of the reactants and the hydrodynamic resistance are thus enhanced. Next compression-decompression cycle will drive the flame to a very intense acceleration that will ultimately finish in the fast sonic regime.

The coupling between the described phenomena is complex. The small, but predictable, discrepancies between the repeated experiments with 40% of venting (Figure 1) may cause the distinct timing of the flame acceleration (i.e. the flame traverse the same length but only one obstacle is trespassed).

4 One dimensional reduced model

The discussion above opens the possibility to use a one dimensional model of the propagation of the flame in order to figure out critical parameters and to study the acceleration mechanism. In the following a coarse tube is considered to simplify the model and make it treatable analytically, in which the effect of the obstacles is taken into account as an enhanced hydrodynamic resistance. Two separate regions of the tube are considered for the modeling. In the so-called products region, between the flame and the discharge orifice the flow is assumed to be uncompressible. For the reactants, region between the flame and the closed end of the tube, the velocity is considered to be small and the term $u\cdot(\mathrm{grad}\ u)$ can therefore be neglected during the initial flame acceleration stage.

With these considerations, the one dimensional equation of the momentum conservation, $(\rho u)_t+(\rho u^2)_x+p_x=F$, can be simplified for the region of the products (between the flame and the discharge orifice) to be

$$\rho u_t + p_x = F. \qquad (2)$$

Taking into account the open end and typical deflagration velocities before the flame acceleration, uncompressible flow in the products region can be assumed to the leading order. In the case of propagation of the flame in the deflagration laminar regime, and considering the reactants as uncompressible, the velocity of the products can be defined as $u=-(\sigma-1)\dot{x}_f$ with σ expansion ratio. This follows from the mass conservation and from definition of the mean flame surface. Integrating between the open end of the tube and the position of the flame, under the assumptions made, yeilds

$$-\rho(\sigma-1)x_f\ddot{x}_f + p_f - p_0 = -2c_D\rho(\sigma-1)^2\dot{x}_f^2 x_f / d\,. \qquad (3)$$

This equation contains p_f, the pressure at the flame position in the products side, as a free parameter that can be closed with the equation (1) obtained in the reactants area. The increment of pressure between both sides, in the case of a stationary flame front can be estimated applying Rankine-Hugoniot conditions $\Delta p\approx\rho\sigma(\sigma-1)\dot{x}_f^2$. With the help of this equation, the pressure in the reactants, p_f^+

side can be considered. The formulation can be re-written considering over-pressure, *P,* instead of pressure to obtain $P=p_f^+-\sigma(\sigma-1)S_L^2-p_0$. If additionally, $\square_f(0)=S_L$ then (3) can be cast in the form

$$\rho(\sigma-1)x_f\ddot{x}_f = P-\rho\sigma(\sigma-1)\left(\dot{x}_f^2-S_L^2\right)+2c_D\rho(\sigma-1)^2\dot{x}_f^2x_f/d\,. \quad (4)$$

This equation can be coupled with the equation (1) to obtain a closed system. The result of this problem, considering as initial conditions $t=0$, $x_f(0)=0.1$, when walls are reached by the flame with velocity $\square_f(0)=S_L$ are shown in Fig. 3. The initial conditions for the pressure were obtained from the numerical experiments and where $P(0)=0$ and $\square(0)=10\ Pa$. Although there is a good agreement of the results obtained with the one dimensional simplification it has to be underlined that the validity of the analysis is restricted to the initiation stage of the flame acceleration. Moreover, significant divergences obtained in the reproduction of experiments themselves and of numeric simulations (compare critical times shown in Figs. 1 and 3) may then be mathematically expressed through strong dependence of the early flame development.

In order to illustrate this and explain the core mechanism of the flame acceleration let us consider the equation (5) without the overpressure term, namely, $P(t)=0$ is assumed. Thus,

$$\ddot{x}_f x_f = -\sigma\left(\left(\dot{x}_f\right)^2-S_L{}^2\right)+2c_D\left(\sigma-1\right)\left(\dot{x}_f\right)^2x_f/d\,. \quad (5)$$

This equation can be studied in the phase plane by transforming the second order ODE to a plane system of ODEs of the first order via regular transformation, $v=x$, $u=\square$

$$\dot{v}=u,\quad \dot{u}\,v=-\sigma\left(u-S^2{}_L\right)+2c_D\left(\sigma-1\right)u^2\,v/d\,. \quad (6)$$

The most important observation about the system initial behavior, namely, the role of the system isocline of the flame speed equation can be analyzed studying the points $\mathring{u}=0$ that naturally fulfill

$$u^2=2d\,S_L^2c_D\sigma\left(\sigma-1\right)/\left(2c_D\left(\sigma-1\right)\left(d\,\sigma-2vc_D\left(\sigma-1\right)\right)\right)\,. \quad (7)$$

Figure 4 right shows this locus with solid black line that near the origin represents a stable attractor, all trajectories starting nearby converges (fast) to the lower branch of the isocline and follow the detailed solution. Moreover, right after crossing the isocline the system solution trajectories changes the character (speeding up instead of decreasing for initial point above the curve), this make the border line which is asymptotically given by

$$x_f^*=d\,\sigma/\left(2c_D\left(\sigma-1\right)\right)=0.94\,. \quad (8)$$

a very important and crucial property defining the critical behavior. It explains the transition phenomena in terms of the phase plane. One clearly sees that if the initial point is on the right from this curve $v=d\sigma/(2c_D(\sigma-1))$ the vector field demonstrates the exponential increase of the flame speed as a function of the flame distance. Additionally, the form of the isocline dependence on the system parameters and variables (7) predicts the sensitivity of the critical phenomena on the initial pressure perturbation with respect to the time of the transition (critical time equal $t_f^*=1.24$) but the sensitivity is much lower with respect to the location of the transition in the space. A weak sensitivity to the perturbation of the initial pressure and the form of the critical parameter can be explained in more simple way. Namely, in the asymptotic limit considered, the equation (7) physically means that the flame starts rapidly accelerating whenever the pressure jump (drop of the pressure - work of the pressure force) less or equals to the work of the friction forces,

$$\Delta p=\int_0^{x^*_f}F\left(u(t,s)\right)ds\Rightarrow x^*{}_f=d\,\sigma/\left(2c_D\left(\sigma-1\right)\right)\,. \quad (9)$$

Thus, when the work of the friction force starts dominate, the pressure in the reaction front increases triggering the flame acceleration due to the cumulative effect of the pressure diffusion.

It is very important to note that there no regular singularity (reaching infinity in final time or space as a reaction front position) was observed in the solution of the governing equations (6), just very smooth (although exponential , i.e. hyper-geometric) growth of the system solution was found to take place. This might explain an irregular *shockless* character of the flame acceleration observed in the experiments.

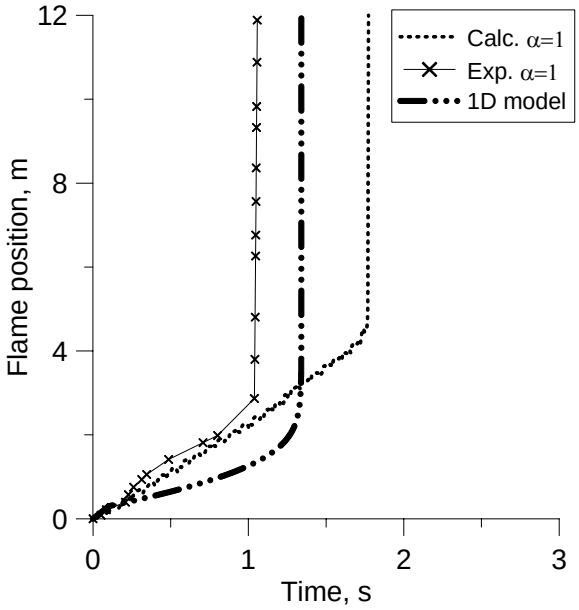

Figure 3 Flame position. Comparison of calculations experiments and one dimensional model.

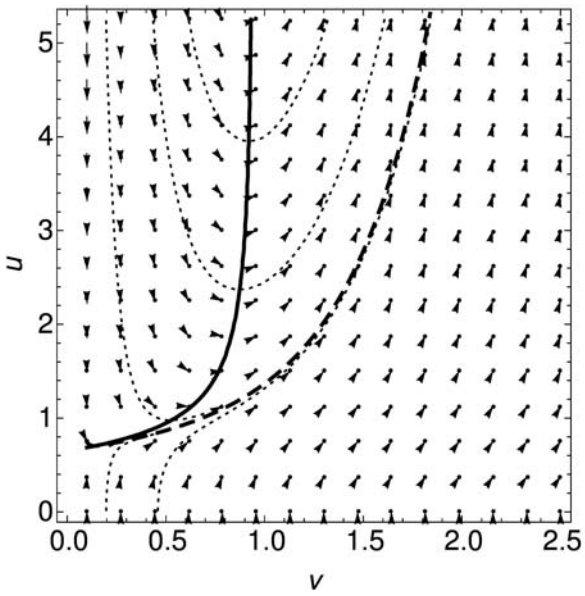

Figure 4 Phase portrait *(x,□)=(v,u)* of the reduced model is shown with system solution trajectories and a vector field. Solid line shows the isoclines of the reaction wave speed showing minimal possible flame velocity for a given initial state x. Arrows are streamlines of the vector field. Dashed line is the solution trajectory of the system.

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