2015

Theory of Flame Propagation in Open Obstructed Channels

Jad Sadek

Follow this and additional works at: <https://researchrepository.wvu.edu/etd>

Recommended Citation

Sadek, Jad, "Theory of Flame Propagation in Open Obstructed Channels" (2015). *Graduate Theses, Dissertations, and Problem Reports*. 6554.
<https://researchrepository.wvu.edu/etd/6554>

This Thesis is protected by copyright and/or related rights. It has been brought to you by the The Research Repository @ WVU with permission from the rights-holder(s). You are free to use this Thesis in any way that is permitted by the copyright and related rights legislation that applies to your use. For other uses you must obtain permission from the rights-holder(s) directly, unless additional rights are indicated by a Creative Commons license in the record and/ or on the work itself. This Thesis has been accepted for inclusion in WVU Graduate Theses, Dissertations, and Problem Reports collection by an authorized administrator of The Research Repository @ WVU. For more information, please contact researchrepository@mail.wvu.edu.

Theory of Flame Propagation in Open Obstructed Channels

Jad Sadek

Thesis submitted to the

Benjamin M. Statler College of Engineering and Mineral Resources

at

West Virginia University

in Partial Fulfillment of the Requirements for the Degree of

Master of Science

in

Mechanical Engineering

V'yacheslav Akkerman, Ph.D., Chairperson (WVU-MAE)

Patrick Browning, Ph.D. (WVU-MAE)

Cosmin Dumitrescu, Ph.D. (WVU-MAE)

Department of Mechanical and Aerospace Engineering

Morgantown, West Virginia

(2015)

Keywords: fire safety; mining fire scenario; combustion instability; flame acceleration;
obstacle blockage ratio.

ABSTRACT

Theory of Flame Propagation in Open Obstructed Channels

Jad Sadek

Obstructed pipes constitute one of the most relevant configurations for extremely fast premixed flame acceleration and deflagration-to-detonation transition. While the flame propagation through obstacles is often associated with turbulence and/or shocks, a conceptually-laminar and shockless mechanism of extremely fast flame acceleration in semi-open “tooth-brush”-like obstructed pipes has been developed by Bychkov *et al* [*Phys. Rev. Lett.* 101 (2008) 164501]. Namely, a flame front is ignited at the closed end of a pipe, with the flame propagating towards the open pipe end. This acceleration scenario is devoted to a powerful jet-flow, which is produced by delayed combustion in the spaces between the obstacles. This mechanism is scale-invariant (Reynolds-independent), with turbulence playing only a supplementary role in the flame evolution. In the present work, the Bychkov formulation is extended from semi-open channels and tubes to open or vented ones, for the sake of the industrial needs fulfillment, and in order to describe the recent experiments at Karlsruhe Institute of Technology (KIT), Germany [<http://arxiv.org/abs/1208.6453>]. Both two-dimensional channels and cylindrical tubes are studied. It is demonstrated that flames accelerate extremely fast in open/vented obstructed pipes, with tubes providing stronger acceleration as compared to channels of the same width. The acceleration mechanism is qualitatively the same as that for the semi-open pipes with the ignition at the closed end: namely, it is conceptually-laminar, shockless, and Reynolds-independent, being associated with the delayed burning in pockets between the obstacles. Although the acceleration rate is large enough in open obstructed pipes, it is nevertheless lower than that in the semi-open ones, because the flame-generated flow spreads both upwards and downwards of the flamefront when both pipe ends are open. Starting with obstructed pipes within the inviscid approximation, the analysis subsequently incorporates the viscous forces (hydraulic resistance), comparing their roles with that of the jet-flow driving the acceleration. It is shown that, on the contrary to the common belief, hydraulic resistance is not required to drive the flame acceleration. In contrast, this is a supplementary effect, which actually moderates the acceleration. Besides, hydraulic resistance can be responsible for the initial delay, before the flame acceleration onset, observed in the experiment.

Dedication

I dedicate this thesis to my family, friends and the deceased Dr. Vitaly Bychkov.

Acknowledgements

First and foremost, I would like to express my gratitude to my research advisor, Dr. *V'yacheslav Akkerman*, Assistant Professor of Mechanical and Aerospace Engineering at West Virginia University, for accepting me into his group, funding my research, and providing me with an exceptional learning experience.

Besides, I should mention Dr. *Vitaly Bychkov*, Professor of Physics at Umea University, who extensively consulted my work and offered me a PhD position at his group upon my MS graduation. Unfortunately, Dr. Bychkov unexpectedly passed away in August, 2015, when my work was in progress such that this thesis should be dedicated to his memory.

Let me also thank my MS Thesis Committee Members, Dr. Patrick Browning and Dr. Cosmin Dumitrescu, both Assistant Professors of Mechanical and Aerospace Engineering at West Virginia University, for their referee work, comments, and fruitful suggestions.

I am also thankful to my colleagues from Dr. Akkerman's Analytical and Computational Combustion Research Directions (ACCoRD) group – Orlando Ugarte, Berk Demirgok, Sinan Demir, Ram Chalagalla, Hayri Sezer and Serdar Bilgili – for their support and for the friendly environment they provided.

Finally, I am acknowledging that my graduate research assistant (GRA) position was sponsored, for the entire period, by the Alpha Foundation for the Improvement of Mine Safety and Health, Inc. (ALPHA FOUNDATION) through Grant #AFSTI14-5. The views, opinions and recommendations expressed in this thesis are solely those of the author and do not imply any endorsement by the ALPHA FOUNDATION, its Directors and staff.

Table of Contents

Table of Contents

ABSTRACT	ii
Dedication	iii
Acknowledgements.....	iv
Table of Contents	v
List of Symbols.....	viii
Chapter 1: Introduction.....	1
1.1. Fundamentals of Flame Propagation	1
1.2. Motivation and Objectives.....	6
1.3 Description of the Experiments [11]	7
Chapter 2: Flame Propagation in Semi-Open Channels	9
Chapter 3: Inviscid Formulaiton for Flame Propagation in Open 2D Channel	13
3.1. Open-Channel Configuration and the Tooth-brush Obstacles Set	13
3.2. Derivation of the Theory	13
3.3. Discussion and Results	18
Chapter 4: Viscous Formulation for Flame Propagation in Open 2D Channels	21
4.1. Introduction to the Mechanism Accounting for Viscous Effects	21
4.2. Derivation of the Theory	22
4.3. Discussion and Results	24
Chapter 5: Flame Propagation in Open Cylindrical Tubes.....	31
5.1. Semi-Open Obstructed Cylindrical Tubes.....	31
5.2. Open Obstructed Cylindrical Tubes in the Inviscid Approximation.....	33
5.3. Viscous Formulaiton for Flame Acceleration in Open Obstructed Tubes.....	35
Chapter 6: Summary	37
References:	38

List of Figures

Figure.1.1: Typical internal structure of a planar flame front (a), with the characteristic temperature and density distribution inside it (b), as well as with the profiles of the scaled temperature T/T_b , the local mass fraction of the fresh gas Y and the reaction rate A inside the burning zone (c).

Figure 1.2: Flame acceleration due to wall friction: (a) illustration of the mechanisms; (b) computational snapshots of the process.

Figure 1.3: “Finger” flame acceleration: (a) illustration of the mechanisms; (b) computational snapshots of the process.

Figure 1.4: A schematic of the KIT experiments [11].

Figure 2.1: Illustration of the physical mechanism of ultrafast flame acceleration in semi-open channels with obstacles.

Figure 2.2: Numerical simulation of the toothbrush set of obstacles (snapshot)

Figure 3.1: Schematic of an open-open obstructed channel, neglecting viscosity

Figure 3.2: Comparative plot of Eq. (3.8) and Eq. (3.10) for fixed $\Theta = 3.38$.

Figure 3.3: Comparative plot of Eq. (3.8) and Eq. (3.10) for fixed $\Theta = 5$.

Figure 3.4: Comparative plot of Eq.(3.8) and Eq. (3.10) for fixed $\alpha = 0.5$.

Figure 3.5: Comparative plot of Eq. (3.8) and (3.10) for fixed $\alpha = 0.6$.

Figure 3.6: Time evolution of the flame tip position for $\Theta = 3.38$ and various $\alpha = 0.4 \sim 0.7$.

Figure 3.7: Time evolution of the flame tip position for $\alpha = 0.5$ and various $\Theta = 2.38 - 5.38$.

Figure 3.8: Comparative plot of (3.12) and experimental data

Figure 4.1: Sketch of flame propagation on open obstructed channels with hydraulic forces.

Figure 4.2: Time evolution of the flame tip position for various blockage ratios $\alpha = 0.4 \sim 0.7$.

Figure 4.3: Comparative plot of the exponential acceleration rate versus the flame tip position for various blockage ratios $\alpha = 0.4 \sim 0.7$.

Figure 4.4: Comparative plot of flame propagation position versus time for varied thermal expansion coefficient

Figure 4.5: Comparative plot of scaled acceleration rate versus the flame front position for varied thermal expansion coefficient.

Figure 4.6: Comparative plot of flame propagation position versus time for varied length of the channel

Figure 4.7: Comparative plot of scaled acceleration rate versus the flame front position for varied length of the channel.

Figure 4.8: Comparative plot of flame front position versus time for models developed

Figure 5.1: Comparative plot of flame front position versus time for axisymmetric and two dimensional channels

List of Symbols

LATIN:

Δz	Spacing between obstacles
C_{Π}	Pressure related constant
CJ	Chapman-Jouget
DDT	Deflagration to Detonation Transition
D_{th}	Thermal diffusion coefficient
I_0	Modified Bessel function of order zero
L	Length of the channel
L_y	Channel width in y-direction
P_1	Pressure at entrance of the channel
P_2	Pressure at the exit of the channel
P_b	Pressure of burned fuel
P_f	Pressure of fresh fuel mixture
R	Radius
R_f	Flame radius
Re	Flame propagation Reynolds number
S_L	Laminar flame speed
U_1	Velocity at channel entrance
U_2	Velocity at channel exit
U_f	Laminar flame speed
Z_b	Position of last burning pocket
Z_f	Flame front position
Z_t	Turning point of flame

GREEK:

σ_c	Scaled acceleration in semi-open obstructed channels
σ_o	Scaled acceleration in open obstructed channels
$\sigma_{c,cyl}$	Scaled acceleration in semi-open obstructed tubes
$\sigma_{o,cyl}$	Scaled acceleration in open obstructed tubes
Θ	Thermal expansion coefficient
α	Blockage ratio
η	Dynamic viscosity coefficient
Π	Scaled pressure gradient

ρ_1	Density at the entrance of the channel
ρ_2	Density at the exit of the channel
ρ_b	Burned gas density
ρ_f	Fresh gas mixture density
ν	Viscosity

Chapter 1: Introduction

1.1. Fundamentals of Flame Propagation

Combustion is an exothermal chemical reaction that involves the oxidation of a combustible fuel, and it is considered an essential process in the energy production. In fact, the combustion process has accompanied people for millennia, being simultaneously a friend that protected our ancient forefathers from the darkness, coldness, predators and stomach bacteria; and an enemy that killed them in forest/savanna fires. Applications of combustion-based technologies are found in various branches of the modern transportation and industries such as vehicles, jet planes, metallurgy etc. However, the development and implementation of these new technologies comes along with safety factors as a slightest malfunction or irregularity could cause significant or even fatal damage to personnel, equipment and environment. For example, unwanted combustion in industries dealing with explosive materials, such as the coal mining, often leads to tremendous catastrophes. In order to prevent such incidents from occurring, and with the widening of combustion-related industries, numerous research projects are dedicated to the development of various theories predicting the flame propagation scenarios.

Generally, there are two main regimes of burning – a slow, subsonic *deflagration* (or “flame”), propagating due to thermal conduction, and a fast, supersonic detonation, where the reaction front spreads due to shock waves. A typical deflagration system consists of a region of fresh fuel mixture, where the combustion reaction has not begun yet; a region of burnt matter, where the reaction is completed; and a thin zone called a flamefront separating these two regions. The inner structure of a planar flamefront, commonly known as the simplest structure adapted for studies, is illustrated in Fig. 1.1. It is well known that a forced ignition is necessary to spark the fuel at room temperature, while high temperatures can result in auto-ignition and very high reaction rates. This is due to a strong temperature-dependence of the reaction rate of any burning process. It is noted that the reaction occurs inside a thin active reaction zone, in which the temperature is close to that of the burned matter temperature denoted as T_b . The mechanism of flame propagation can be explained as follows. The thermal energy is transferred from the hot active reaction zone to the cooler layers of the fuel mixture through thermal conduction transports, thereby heating the cool layer, and thus increasing the reaction rate inside it. On the other hand, the exhaustion of the unburnt fuel will cause the reaction rate to go down.

Figure.1.1. Typical internal structure of a planar flame front (a), with the characteristic temperature and density distribution inside it (b), as well as with the profiles of the scaled temperature T/T_b , the local mass fraction of the fresh gas Y and the reaction rate A inside the burning zone (c).

In this light, the flamefront moves continuously from the burnt gas to the fresh pre-mixture. The main flame parameters are: the thermal expansion factor defined as the ratio of the fresh gas density to the burnt gas density, $\Theta \equiv \rho_f / \rho_b$; the unstretched laminar (planar) flame speed, U_f or S_L , as illustrated in Fig. 1.1; and the flamefront thickness, L_f , conventionally defined as $L_f = D_{th} / U_f$, where D_{th} is the thermal diffusivity in the fuel mixture.

It is noted that a sporadic deflagration-to-detonation transition (DDT) may occasionally occur, thereby causing numerous disasters. While DDT is typically a danger that people try to avoid, in principle, this phenomenon can be utilized, constructively, in novel high-efficiency devices such as pulse-detonation engines. In a typical DDT scenario, a flamefront accelerates spontaneously, with the velocity increasing by 3-4 orders of magnitude. This eventually triggers an explosion ahead of the flame front, which converts into a self-sustaining detonation.

Flames in pipes belong to one of the most attractive combustion configurations, combining both the simplicity and the practical relevance. Various mechanisms of flame acceleration in pipes have been identified and quantified – experimentally, computationally and analytically. *Shelkin* [1] proposed the first qualitative explanation of this scenario in combustion tubes, with wall friction and turbulence being the key elements of the process. Also known as the Shelkin mechanism, this study demonstrated the effect of the non-slip boundary condition on the flame-generated flow in a pipe, leading the flow to become non-uniform and corrugated. Specifically, the combustible gas expands with burning, which induces a flow in the fuel mixture. The induced flow is highly non-uniform due to wall friction, and it causes the flamefront shape to corrugate, hence increasing the fuel consumption rate and driving flame acceleration. Turbulence provides an additional distortion of the flamefront, which also compensates for the thermal loss to the walls. Since turbulent combustion is one of the most difficult problems of modern science, there was almost no progress in the quantitative theoretical understanding of the flame acceleration for more than 60 years, since the time of *Shelkin*. However, it was shown in the early 2000s that, at certain conditions, extremely strong flame acceleration and DDT are possible even within the regime of laminar flows, while turbulence plays only a supplementary role [2,3]. Based on such a constructive idea, *Bychkov et al* [4] developed a quantitative theory of flame acceleration and DDT, due to wall friction, in *unobstructed* smooth-walled channels and tubes

[4,5], which was certified by extensive numerical simulations as well as experiments on DDT in micro-pipes [6], thereby validating the key stages and characteristics of the flame dynamics, quantified by the theory of flame acceleration and DDT. The theory and modeling of flame acceleration due to wall friction in semi-open channels [4] and tubes [5] has described the acceleration manner of the flame as well as the evolution of the flame shape and position in a pipe. This acceleration mechanism, along with the color temperature snapshots of the process, is illustrated in Fig. 1.2. It was shown that due to wall friction, a flamefront accelerates in an exponential manner before compressibility effects come to play. The acceleration rate depends strongly on the flame propagation Reynolds number $Re = S_L R / \nu = R / L_f Pr$: indeed the effect of wall friction weakens in wide conduits. Consequently, while the wall-friction-based flame acceleration is unlimited in time, it is viable in micro-pipes only because of its Re -dependence.

Figure 1.2: Flame acceleration due to wall friction:
(a) illustration of the mechanisms; (b) computational snapshots of the process.

Another acceleration mechanism, incorporating smooth wall and known as the so-called finger flame model demonstrated a strong but short acceleration at the initial stages of the flame propagation. The experiments conducted by Clanet and Searby [7] showed that a flamefront propagating in a semi-open tube, with the ignition at the intersection of the tube axis and the closed end, approaches a finger shape as seen in Fig. 1.3. The analytical formulation of this finger flame model, developed by Bychkov *et al* [8], agreed with the observations in [7] as the acceleration phase described by the flame propagation proved to be short in time, vanishing as soon as the flame contacts the pipe wall.

Figure 1.3: “Finger” flame acceleration:
 (a) illustration of the mechanisms; (b) computational snapshots of the process.

As a result, the wall friction mechanism of the flame acceleration is unlimited in time, but weak in realistic tunnels and pipes. In contrast, the finger-flame acceleration mechanism is strong, but short in time. Could the benefits of both mechanisms be combined into a single scenario? Yes, such a possibility has been recently revealed by *Bychkov et al* [9], by placing a “tooth-brush” array of obstacles into a DDT pipe. As a result, a Reynolds-independent model, where turbulence is not necessary for the flame propagation, has been developed. The study [9] emphasized the role of obstacle spacing in the flame propagation leading to DDT. The formulation [9] was validated by numerical simulations, and it has later been extended to axisymmetric geometry by *Valiev et al* [10]. While the studies mentioned so far dealt with semi-open channels, where the ignition takes place at the closed end, other works in the literature, including experiments, deal with different conditions on this configuration.

1.2. Motivation and Objectives

Many technologies in the modern era have been based on combustion as the main source of energy. Nowadays, the demand for effective and clean energy production implies development and optimization of traditional combustion technologies, such as combustion schemes employed in car engines, gas turbines and power plants, as well as advanced combustion technologies like pulse-detonation engines, rotation-detonation engines, scramjets, micro- and nano-combustion devices. As previously mentioned, combustion may proceed in two distinct regimes, namely, the deflagration – a slow subsonic regime, with typical propagation velocities of about 1m/s, and the detonation – a supersonic regime with usual speeds of about 2000 m/s. Traditional combustors such as car engines or gas turbines operate in the deflagration regime in which the flame converts the chemical energy of the fuel mixture into the mechanical motion and/or electrical power. However, under certain conditions, a flame can spontaneously accelerate to super-sonic speed triggering detonation and leading to catastrophes. On the other hand, advanced combustion devices utilize the detonation regime. In particular, detonation provides the highest possible burning efficiency with a short cycle time and high pressures. In pulse-detonation engines, the detonation is employed to create thrust allowing aircrafts to fly at high speeds up to Mach 5. However, most advanced combustion devices are not energy efficient at the current stage of development, as they require a large energy input in the form of a spark to trigger detonation. The transition from a deflagration to detonation event, commonly known as the deflagration-to-detonation-transition, or DDT, is an energy efficient alternative that can be implied in advanced combustion regimes in order to trigger detonation making the system more efficient and in the case of the pulse-detonation engine it decreases the weight as well.

In this study, we extend the formulation by *Bychkov et al* [9], for planar 2D channels, and *Valiev et al* [10], for axisymmetric tubes, from semi-open to open-open obstructed pipes. This new configuration will shed the light on a new mechanism that can serve as a basis for further research and interpretation. To be specific, we have developed equations describing the flame acceleration in the open-open obstructed channel for the slip boundary condition. The derivations follow a similar approach [9], with similar approximations adopted. However, being initially inviscid, the formulation has been subsequently extended to account for the hydraulic resistance due to wall friction. The basis of this extension will permit us to compare our results to the ongoing experiments at the Karlsruhe Institute of Technology (KIT), Germany [11], where the

combustion tube of a square cross-section was open in both ends and had obstacles at the walls. Given that the viscous effects are unavoidable in the practical reality, our model also had to be extended to incorporate viscosity into the formulation – in order to allow enabling a direct comparison to the experiment and validate the theory.

1.3 Description of the experiments [11]

Experiments conducted by Dr. Kuznetsov's team at the Karlsruhe Institute of Technology observed surprisingly powerful flame acceleration in open vented obstructed channels. Their unique setup consisted of a 12.2 m long vented channel with a square cross section and obstacles as seen in Fig. 1.4, with the venting ratio varying between 0% (fully closed end) and 100% (fully open end). The implemented obstacles obstructed 50% of the tube width, characterized by the blockage ratio of 0.5 with respect to the tube radius.

Figure 1.4: A schematic of the KIT experiments [11].

The stoichiometry of the mixture employed by KIT was characterized by the thermal expansion rate, which was set to 3.38 for the data provided. Changes in a blockage ratio would imply changes in the obstructed part of the experimental tube radius, while changes in the thermal expansion rate would imply a change in the stoichiometry of the fuel mixture used in the experiments. Such geometry is characteristic for energy safety problems in particular for problems relevant to mining accidents. Depending on the venting ratio, the almost laminar flamefront spread through a considerable fraction of the channel, up to $\frac{1}{4}$, and only then the powerful flame acceleration is observed. The present analysis shows the mechanism of flame acceleration in open channels with obstacles to be similar to the ultra-fast acceleration identified by *Bychkov et al* [9], with both mechanisms being conceptually independent of the Reynolds number and potentially being equally effective for both macro and micro-channels. The flame acceleration rate in open channels is somewhat smaller than that in semi-open channels: in the

former case the acceleration is reduced approximately by a factor of 3.5 for hydrogen-air flames, with the reduction factor depending on the density ratio. The purpose of this research is to explain the experimental delay, being the initial stages after ignition, where a flame propagates in a laminar regime; prior to the acceleration in open obstructed channels.

The present thesis is organized as follows. Chapter 2 recalls the basics of the flame acceleration in semi-open obstructed pipes. Chapter 3 presents the inviscid formulation for open-open two-dimensional (2D) obstructed channels with non-slip adiabatic walls. The viscous effects at the walls are incorporated in Chapter 4, thereby allowing a more accurate comparison to the experiments. Finally, Chapter 5 extends the 2D formulation to the cylindrical configuration. The overall findings of this study are summarized in Chapter 6. The parametric study involves varying a set of key parameters such as the obstacle blockage ratio (given by the obstacle height as compared to the pipe width) the thermal expansion coefficient (given by the density drop at the flamefront), the unstretched laminar flame speed, and the length of the tube.

Chapter 2: Flame Propagation in Semi-Open Channels

First of all, let me briefly recall the inviscid formulation of the physical mechanism of ultrafast flame acceleration in 2D semi-open obstructed channels, initially developed by *Bychkov et al* [9], illustrated in Fig. 2.1. The numerical simulation is presented in Fig. 2.2.

Figure 2.1: Illustration of the physical mechanism of ultrafast flame acceleration in semi-open channels with obstacles.

Figure 2.2: Numerical simulations of the toothbrush set of obstacles (snapshot)

The “tooth-brush” obstacles array illustrated in Figs. 2.1 & 2.2 consists of thin plates, parallel to each other, with the spacing Δz . Here R designates the half-width of the channel and αR the length of the obstacle, such that α is the blockage ratio – the part of the channel blocked by the obstacles. The unobstructed part of the channel is referred to as the free part of the channel. In this particular problem, small obstacle spacing and deep pockets, $\Delta z \ll \alpha R$, are considered.

However, according to the numerical simulations [10], large spacing Δz would not conceptually change the mechanism of flame acceleration although it would lead to noticeable complications such as turbulent flow pulsations, which may conceal the main physical mechanism of flame acceleration. Still, after time averaging, the turbulent pulsations provide a minor (if any) income to the acceleration mechanism [10]. By neglecting turbulence generated by the obstacles, the latter is considered as a key parameter for the flame propagation.

The theory implemented a common model of infinitely thin flame propagating locally with the laminar flame speed S_L (the Landau limit). When ignited at a point at the closed end of a channel (at a centerline), the flame propagates fast along the free part of the channel leaving unburnt fuel mixture trapped in the “pockets” between the obstacles. Delayed burning in the pockets produces extra gas volume, which flows out of the pockets with the velocity $(\Theta - 1)S_L$, where $\Theta = \rho_f / \rho_b$ is the fuel mixture to burnt matter density ratio and S_L is the unstretched laminar flame speed. The flow out of the numerous pockets is deflected in the free part of the channel, accumulated into a strong jet flow along the channel axis, which drives the flame tip and produces new pockets. The positive feedback between the flame and the flow leads to a powerful, extremely fast flame acceleration.

Due to the symmetry, only the upper half of the channel is taken into consideration, $x > 0$. Let the velocity components in z - and x -directions be $\mathbf{u} = (u; w)$. Delayed burning out of the pockets sets the boundary condition $w = -(\Theta - 1)S_L$ in the burnt gas for $x = (1 - \alpha)R$, $z < Z_f$, where $Z_f(t)$ is the position of the flame tip (the curved shape of the flame tip provides a really minor contribution to the acceleration mechanism and may be neglected as compared to the effect of obstacles-based acceleration). We next solve the incompressible continuity equation in the burnt gas

$$\nabla \cdot \mathbf{u} = 0, \quad \text{or} \quad \frac{\partial u}{\partial z} + \frac{\partial w}{\partial x} = 0, \quad (2.1)$$

to obtain the velocity distribution in the free part of the channel in the form

$$u = \frac{(\Theta - 1)S_L}{(1 - \alpha)R} z, \quad w = -\frac{(\Theta - 1)S_L}{(1 - \alpha)R} x, \quad (2.2)$$

which satisfies the boundary condition at the closed channel end, $u|_{z=0}=0$. Then the flow velocity in the burnt gas just at (behind) the flame tip position is

$$u = \frac{(\Theta - 1)S_L}{(1 - \alpha)R} Z_f \quad \text{at} \quad z = Z_f, \quad (2.3)$$

which specifies the differential equation for the flame tip (written with respect the burnt gas)

$$\frac{dZ_f}{dt} = \frac{(\Theta - 1)S_L}{(1 - \alpha)R} Z_f + \Theta S_L. \quad (2.4)$$

We next solve Eq. (2.4) with the initial condition $Z_f(0) = 0$, to find

$$Z_f = \Theta \frac{R}{\sigma_c} [\exp(\sigma_c S_L t / R) - 1], \quad (2.5)$$

with the scaled acceleration rate

$$\sigma_c = \frac{\Theta - 1}{1 - \alpha}. \quad (2.6)$$

Here, the label “c” indicates a semi-closed channel. Equation (2.5) is used to retrieve the initial flame propagation speed from the closed tube end $dZ_f / dt = \Theta S_L$. It is emphasized that the scaled acceleration rate is quite large. For a density ratio $\Theta = 3.38$ (employed in the KIT experiments) and the blockage ratio $\alpha = 1/2$, we find $\sigma_c = 4.45$. If a flame accelerated in the isobaric regime all the time, then such a growth rate would imply the velocity increase by a factor of $\exp(2 \cdot 4.56) \approx 10^4$ (!) during the characteristic laminar burning time $2R/S_L$. Such a huge velocity rise, of course, does not happen in the practical reality, because the compressibility effects moderate the flame acceleration at the developed stages, with the eventual saturation to the CJ deflagration speed [10]. With turbulence and wall friction playing only a supplementary role, and only pockets between the obstacles really contributing into the flame propagation, the obstacles-based acceleration obviously gets stronger with the increase in the blockage ratio α as well as that in the thermal expansion coefficient Θ ; see Eq. (2.6). An important feature of this mechanism is that it conceptually does not involve viscous forces, and hence it is independent of the Reynolds number. This mechanism is unlimited in time, which makes it similar to that due to wall friction [4]. However, being Re-independent, the Bychkov mechanism [9] is typically much stronger than the Shelkin (wall friction) scenario, because the latter becomes extremely weak in smooth tubes at high Reynolds numbers. While the obstacles-based acceleration resembles,

physically, the finger flame acceleration [7], exhibiting a finger flame shape, the pockets filled with the fresh fuel separates the free part of the channel from the walls enabling the acceleration to last longer than that of the finger flame model, where the acceleration dies when the flame reaches the wall.

Chapter 3: Flame propagation in open 2D channels neglecting viscous effects

3.1. Open channel configuration and the toothbrush obstacle set

Figure 3.1: Schematic of an open-open obstructed channel, neglecting viscosity.

The configuration of an open obstructed channel is similar to that of semi-open one, discussed in the previous chapter, as illustrated in Fig. 3.1. Here, a 2D channel of half-width R , with both ends open is considered. In order to distinguish the role of the obstacles in the flame dynamics, the walls of the channel are assumed to be adiabatic. Similar to semi-open channels, here α denotes the blocked fraction of the channel, or the blockage ratio, such that the height of the obstacle is αR . The obstacle set adopted for this configuration is referred to as the tooth-brush obstacles, illustrated in Figs. 2.2, and consists of infinitely thin obstacles set, stacked parallel to each other, and perpendicular the walls of the channel. It is generally believed that obstacles generate stronger turbulence and promoting flame acceleration and DDT due to turbulence. However, by implementing tightly placed obstacles, with $\Delta z \ll \alpha R$, turbulence can be neglected as laminar burning in the obstacles pockets will go slowly with the normal velocity in the free part of the channel. Similar to the previous chapter, a flamefront will be approximated as an infinitely thin discontinuity surface, which – if planar – would spread normally to itself with a laminar speed S_L with respect to the fuel mixture.

3.2. Derivation of the theory

When ignited from one channel end, a laminar flamefront will propagate fast in the free part of the channel leaving unburnt fuel mixture trapped in the pocket between the obstacles. Delayed burning in the pockets produces extra gas volume, and the burned gas flows to the free part of

the channel where it splits into two flows, namely: (i) that of the exhaust gas out of the channel entrance at $z = 0$ and (ii) that of the fuel mixture out of the channel exit at $z = L$. The velocity in the free part of the channel, going out of the channel exit, is expressed as $(\Theta - 1)S_L$. Here U_1 and U_2 denote the velocities of the exhaust gas at the channel entrance, and that of the fuel mixture at the channel exit, respectively, with Z_t being a turning point in the flow and Z_f the flamefront position as illustrated in Fig. 3.1. The inviscid approximation adopted in this chapter serves to simplify the derivations as well as to provide a comparable model to that developed in Chapter 2, where slip boundary conditions were implemented making the system Re-independent as it would not show up in the calculations. The momentum flux balance at the channel entrance and exit (zero net force on the gas in the channel) reads

$$P_1 + \rho_1 U_1^2 = P_2 + \rho_2 U_2^2. \quad (3.1)$$

On the other hand, the pressure difference in the fuel mixture and the burnt gas is

$$P_b = P_f - (\Theta - 1)\rho_f S_L^2. \quad (3.2)$$

The inviscid approach then yields

$$U_1^2 = \Theta U_2^2 + \Theta(\Theta - 1)S_L^2. \quad (3.3)$$

With the jump of the normal velocity at the flamefront, the velocity of the burnt gas just behind the flamefront is $u(Z_f) = U_2 - (\Theta - 1)S_L$. Then the relation between U_1 and $u(Z_f)$ reads

$$U_1^2 = \Theta \left[u(Z_f) + (\Theta - 1)S_L \right]^2 + \Theta(\Theta - 1)S_L^2 \rightarrow \Theta U_2^2 \approx \Theta u^2(Z_f) \quad (3.4)$$

in the limit of strong flame acceleration, $U_{1,2} \gg (\Theta - 1)S_L$. The boundary conditions are

$$u = u(Z_f) \text{ at } z = Z_f; \quad u = -U_1 \text{ at } z = 0, \quad u = 0 \text{ at } z = Z_t. \quad (3.5)$$

For the initial stages of flame propagation, the flow may be treated as an incompressible such that the continuity equation in the burnt gas reads $\nabla \cdot \mathbf{u} = 0$, with the solution

$$u = \frac{(\Theta - 1)S_L}{(1 - \alpha)R}(z - Z_t), \quad w = -\frac{(\Theta - 1)S_L}{(1 - \alpha)R}x. \quad (3.6)$$

Together, Eqs. (3.5) and (3.6) yield

$$\frac{(\Theta - 1)S_L}{(1 - \alpha)R} Z_t = \frac{(\Theta - 1)S_L}{(1 - \alpha)R} Z_f - u(Z_f), \quad (3.7)$$

$$\sqrt{\Theta[u(Z_f) + (\Theta - 1)S_L]^2 + \Theta(\Theta - 1)S_L^2} = \frac{(\Theta - 1)S_L}{(1 - \alpha)R} Z_f - u(Z_f). \quad (3.8)$$

The system of equations (3.7) – (3.8) determines the flow z -velocity component as a function of the flame tip position, $u = u(Z_f)$. As soon as such a function is known, the flame tip evolution equation reads

$$\frac{dZ_f}{dt} = u(Z_f) + \Theta S_L. \quad (3.9)$$

In the limit of strong flame acceleration, $u(Z_f) \gg (\Theta - 1)S_L$, Eqs (3.8) and (3.9) are reduced to

$$u(Z_f) = \frac{(\Theta - 1)S_L}{(1 - \alpha)R} \frac{Z_f}{\sqrt{\Theta + 1}}, \quad (3.10)$$

$$\frac{dZ_f}{dt} = \frac{(\Theta - 1)S_L}{(1 - \alpha)R} \frac{Z_f}{\sqrt{\Theta + 1}} + \Theta S_L, \quad (3.11)$$

with the solution

$$Z_f = \frac{\Theta R}{\sigma_o} [\exp(\sigma_o S_L t / R) - 1], \quad (3.12)$$

$$\sigma_o = \frac{\Theta - 1}{(\sqrt{\Theta + 1})(1 - \alpha)} = \frac{\sigma_c}{\sqrt{\Theta + 1}}, \quad (3.13)$$

where the labels “ o ” and “ c ” stand for the open and semi-open channels, respectively. The reduction of Eq. (3.8) into Eq. (3.10), based on the approach of strong flame acceleration, is validated in Figs. 3.2 – 3.5, where both Eqs. (3.8) and (3.10) were solved numerically and compared. Specifically, Figs. 3.2 and 3.3 show the scaled flame tip position, Z_f / R , versus the scaled flow velocity at the flamefront, $u(Z_f) / S_L$, at the fixed $\Theta = 3.38$ (like that in the KIT experiments; Fig. 3.2) and $\Theta = 5$ (Fig. 3.3), and various $\alpha = 0.4; 0.5; 0.6$ in each figure. Figures 3.4 and 3.5 are their counterparts, but with the fixed $\alpha = 0.5$ (Fig. 3.4) and $\alpha = 0.6$ (Fig. 3.5) and various $\Theta = 3.38; 5; 8$ in each case. It is seen that Figs. 3.2 – 3.5 justify the transition from Eq. (3.8) to (3.10) for realistic hydrocarbons $\Theta = 3 \sim 10$ and typical $1/3 < \alpha < 2/3$.

Figure 3.2: Comparative plot of Eq. (3.8) and Eq. (3.10) for fixed $\Theta=3.38$.

Figure 3.3: Comparative plot of Eq. (3.8) and Eq. (3.10) for fixed $\Theta = 5$.

Figure 3.4: Comparative plot of Eq. (3.8) and Eq. (3.10) for fixed $\alpha = 0.5$.

Figure 3.5: Comparative plot of Eq. (3.8) and (3.10) for fixed $\alpha = 0.6$.

3.3. Discussion and results

The derivation performed in the previous subsection allowed us identifying the flame spreading velocity, Eq. (3.11), and its instantaneous position, Eq. (3.12). The equations show the same exponential form as the homologous equations in the previous chapter, namely, Eqs. (2.4) and (2.5), respectively. For the open channels, the flamefront accelerates immediately from the ignition point at the open entrance of the channel, with the acceleration rate σ_o being smaller by a factor of $\sqrt{\Theta} + 1$ as compared to the acceleration rate $\sigma_c = (\Theta - 1)/(1 - \alpha)$ for semi-open channels. Even though the acceleration rate in the open channels is smaller than that in the semi-open ones, such acceleration remains quite strong and, foremost, Re-independent. By using the same parameters as in Chapter 2, i.e. from the ongoing KIT experiments [11], such as $\Theta = 3.38$, $\alpha = 1/2$, $R = 8.7\text{cm}$ and $S_L \approx 3.5\text{m/s}$, and employing them in Eq. (3.13), we obtain $\sigma_o \approx 1.8$, which implies a 25 times velocity increase during the characteristic laminar burning time $2R/S_L$ if a flame accelerates in the isobaric regime all the time, which is the case. In other words, this implies a powerful flame acceleration during ~ 0.015 sec.

Figure 3.6: Time evolution of the flame tip position for $\Theta = 3.38$ and various $\alpha = 0.4 \sim 0.7$.

In order to understand better the model employed, the blockage ratio α was varied in Eq. (3.12) while keeping the other parameters at the given (KIT) values such as $\Theta = 3.38$. The outcome is

presented in Fig. 3.6, thereby demonstrating the influence of the blockage ratio on the flame propagation. It is seen that the decrease in α leads to a noticeable delay prior to sudden flame acceleration. This delay did not occur in the semi-open channels, but it happens in the KIT experiments [11] in an open-open pipe, and now the theory presented here shows it as well – at least, qualitatively. The same delay is observed in Fig. 10, where the time evolution of the flame tip position is shown for fixed $\alpha = 1/2$ and various thermal expansion factors $\Theta = 2.38 - 5.38$. Indeed, the expansion factor is essential to the burning time in the pockets, and thereby to the jet flow that will be diverted toward the center of the channel. According to Fig. 3.7, the increase in the thermal expansion coefficient makes such acceleration sudden at the initial stages of the flame propagation, with no delay observed. However, a decrease in the expansion coefficient will lead to a delay before strong flame acceleration. Nevertheless, this delay is still far away from the experimental delay observed; however, it is relevant on its own scale. Sudden acceleration of the flamefront is associated with the increase in the blockage ratio: indeed, large blockage ratios reduce the free part of the channel $(1 - \alpha)R$. It is worth noting that the length of the tube does not influence the flame propagation since viscous effects are neglected so far.

Figure 3.7: Time evolution of the flame tip position for $\alpha = 0.5$ and various $\Theta = 2.38 - 5.38$.

Figure 3.8: Comparative plot of Eq. (3.12) and the experimental data.

The same parameters are used to plot the flame tip position, Eq. (3.12), with respect to time, represented by the blue line in Fig. 3.8. The theoretical evolution of the flamefront position is compared to the experimental data [11], and a significant delay is observed in the experimental curve that is not exhibited by the theoretical one. Such a delay indicates that the flame does not suddenly accelerate starting from the ignition instant, unlike the present theoretical approach. However, this delay can be justifiable by the non-slip boundary condition implied, as viscous forces are definitely present in the experiments. Another potential contributor to this delay observed is the square configuration implemented in the experimental setup as opposed to the two dimensional configuration implemented in the theory.

Chapter 4: Viscous Formulation for Flame Propagation in Open 2D Channels.

4.1. Introduction to the mechanism accounting for viscous effects

In this chapter, the formulation of Chapter 3 is extended to account for viscous effect. Similar to the model employed in Chapter 3, the new model is illustrated in Fig. 4.1, and it consists of a 2D channel of half-width R , with a “tooth-brush” array of obstacle implemented at the adiabatic channel walls. Again, the obstacles are placed close to each other, with deep pockets, as it was demonstrated and mentioned in the previous chapter, because larger spacing would lead to turbulence in the flow and conceal the main physical mechanism in promoting the flame propagation. Let U_1 to be the velocity of the exhaust gas at the channel entrance and U_2 to be that of the fuel mixture at the channel exit, with Z_t being a turning point in the flow. Although, conceptually, viscous forces are not required to drive the acceleration, they even may hinder flame acceleration at the initial stages of flame propagation. This chapter investigates the effect of hydraulic resistance on flame propagation in the open obstructed channels in order to justify the delay observed in the experiments [11]. According to Ref. [11], right after ignition at the open pipe end, the flame propagates in an almost stationary quasi-isobaric regime with the speed $S_{L,eff} \approx 3.5 \text{ m/s}$ for about (1-2) s, and then sudden acceleration starts. We stress that during the initial delay, the flamefront propagates through the distance of about (3-7) m, which corresponds to a considerable fraction, say, $\frac{1}{4}$ to $\frac{1}{2}$, of the total tube length. The main purpose of this chapter is therefore to find out the reason for the delay, and to incorporate it quantitatively into the model of flame acceleration developed in the previous subsection.

Figure 4.1: Sketch of flame propagation on open obstructed channels with hydraulic forces.

4.2. Derivation of the theory

Since a flame may propagate rather slowly at the initial stages of the process, then we have to remember about the finite length of the delayed burning zone. Here Z_b designates the position of the last burning pocket, see Fig. 4.1. In the case of quasi-steady flame propagation, this position lags only slightly behind the flame tip $Z_f - Z_b \approx \alpha R$ if we assume that the flame in the pockets propagates with the laminar flame speed S_L , and hence the time interval $\Delta t = \alpha R / S_L$ is required to burn one pocket. However, in the case of considerable flame acceleration, the lag may be quite large, namely:

$$Z_f - Z_b \approx \frac{\Theta R}{\sigma_o} \exp(\sigma_o S_L t / R) [1 - \exp(-\alpha \sigma_o)] = \left[Z_f + \frac{R}{\sigma_o} \right] [1 - \exp(-\alpha \sigma_o)]. \quad (4.1)$$

It is noted that Eq. (4.1) covers both limits of strong and weak fame acceleration. The former, for which extra volume of the burning gas is mostly produced by delayed burning in the pockets, was considered in Chapter 3. Here, we deal, in particular, with the latter one, accounting for the contribution of the extra volume produced by burning at the flamefront in the free channel part. Then the total volume produced by flame per unit time is given by

$$\frac{dV}{dt} = (\Theta - 1) S_L [Z_f - Z_b + (1 - \alpha) R] L_y, \quad (4.2)$$

where L_y is the channel width in y-direction, i.e. perpendicular to the plane of Fig. 4.1. The next step is to identify the viscous force (hydraulic resistance) produced by an accelerating flame. Generally speaking, three viscous flows have to be considered, namely, two flows to the right, $u > 0$, (i) in the fuel mixture ($z > Z_f$) and (ii) in the burnt matter ($Z_t < z < Z_f$), where Z_t is the turning point; and (iii) one flow to the left, $u < 0$, in the burnt matter, $z < Z_t$. Nevertheless, to simplify the theoretical model, it is recalled that hydraulic resistance is needed to describe the initial stage of the flame propagation only. In that regime, $Z_b \approx Z_t \approx Z_f$, and the difference between Z_f and Z_t may be neglected. In the other opposite limit, of strong acceleration, the effect of hydraulic resistance should be negligible, along with a difference between Z_f and Z_t . As such, only two viscous flows are distinguished, for $z > Z_f$ and $z < Z_f$.

We next employ the classical model of plane-parallel shear flows, $u(x, t)$, both in the fuel mixture, $z > Z_f$, and burnt matter, $z < Z_f$. The shear flows are described by the Navier-Stokes equation

$$\frac{\partial u}{\partial t} = -\Pi(t) + \nu \frac{\partial^2 u}{\partial x^2}, \quad (4.3)$$

where we take for simplicity the same dynamic viscosity coefficient, $\eta = \rho\nu$, both for the unburnt and burnt gases. In Eq. (4.3), $\Pi(t) = \rho^{-1} dP/dz$ stands for the scaled pressure gradient along the channel axis, which depends only on time in a shear flow. In the flow driven by flame acceleration, we have $u \propto \Pi \propto \exp(\alpha S_L t / R)$, and Eq. (4.3) reduces to

$$\frac{\alpha S_L}{R\nu} u = -C_\Pi + \frac{d^2 u}{dx^2}, \quad (4.4)$$

with the boundary conditions $u = 0$ at $x = (1 - \alpha)R$, the constant C_Π coupled to the pressure gradient, and the solution

$$u = \pm \frac{U_{1,2}}{\cosh \mu_{1,2} - 1} \left[\cosh \mu_{1,2} - \cosh \left(\frac{\mu_{1,2} x}{(1 - \alpha)R} \right) \right], \quad (4.5)$$

where

$$\mu_1 = (1 - \alpha)\sqrt{\sigma \text{Re} / \Theta}, \quad \mu_2 = (1 - \alpha)\sqrt{\sigma \text{Re}}, \quad \text{Re} = \rho_f S_L R / \eta. \quad (4.6)$$

The amplitudes $U_{1,2}(t) \propto \exp(\alpha S_L t / R)$ in Eq. (4.5) stand for the maximal gas velocities in the flows attained at the channel axis, $x = 0$. Then the total volumetric flow rate is given by

$$\left(\frac{dV}{dt} \right)_{1,2} = L_y \int_0^{(1-\alpha)R} u \, dx = L_y \exp(\alpha S_L t / R) (1 - \alpha) R U_{1,2} \frac{\cosh \mu_{1,2} - \mu_{1,2}^{-1} \sinh \mu_{1,2}}{\cosh \mu_{1,2} - 1}. \quad (4.7)$$

Along with the continuity condition, Eqs. (4.1) and (4.7) yield

$$(\Theta - 1) S_L \left\{ \frac{Z_f + R/\sigma}{(1 - \alpha)R} [1 - \exp(-\alpha\sigma)] + 1 \right\} = U_1 \frac{\cosh \mu_1 - \mu_1^{-1} \sinh \mu_1}{\cosh \mu_1 - 1} + U_2 \frac{\cosh \mu_2 - \mu_2^{-1} \sinh \mu_2}{\cosh \mu_2 - 1}. \quad (4.8)$$

Equation (4.8) provides the maximal flow velocities $U_{1,2}$ out of the channel entrance and exit to the flamefront position Z_f . The other relation between these quantities follows from the momentum flux balance. Specifically, in the inviscid approximation, integrating a modified Eq. (3.1) over the channel free path cross-section, $(1 - \alpha)RL_y$, and adopting the approximation

$$\int_0^{(1-\alpha)R} u^2 dx \approx U_{1,2}^2 (1-\alpha)R, \quad (4.9)$$

we find

$$\left[\frac{\rho_f}{\Theta} U_1^2 - (\Theta - 1) \rho_f S_L^2 \right] (1-\alpha)RL_y = \rho_f U_2^2 (1-\alpha)RL_y. \quad (4.10)$$

It is recognized that, generally speaking, the integral in the left-hand-side of Eq. (4.9) had to be taken rigorously – analytically or numerically. Nevertheless, the present formulation employed the approximation (4.9). Equation (4.10) is subsequently updated to incorporate the viscous forces into the consideration. The absolute values of viscous stresses in the unburned (index “1”) and burnt (index “2”) gases, at the level of obstacle edges, $x = (1-\alpha)R$, are given by

$$\xi_{1,2} = \left| \eta \frac{du}{dx} \right|_{x=(1-\alpha)R} = \frac{\mu_{1,2} \sinh \mu_{1,2}}{\cosh \mu_{1,2} - 1} \frac{\eta U_{1,2}}{(1-\alpha)R}, \quad (4.11)$$

which yields the respective viscous forces ahead and behind the flame to be

$$F_1 = \frac{\mu_1 \sinh \mu_1}{\cosh \mu_1 - 1} \frac{\eta U_1}{(1-\alpha)R} \frac{Z_f}{(1-\alpha)R} L_y (1-\alpha)R, \quad (4.12)$$

$$F_2 = \frac{\mu_2 \sinh \mu_2}{\cosh \mu_2 - 1} \frac{\eta U_2}{(1-\alpha)R} \frac{L - Z_f}{(1-\alpha)R} L_y (1-\alpha)R. \quad (4.13)$$

The viscous counterpart of Eq. (4.10) then reads

$$\frac{U_1^2}{\Theta S_L^2} + \frac{\mu_1 \sinh \mu_1}{\cosh \mu_1 - 1} \frac{U_1 Z_f}{(1-\alpha)^2 \text{Re } S_L R} = \frac{U_2^2}{S_L^2} + \Theta - 1 + \frac{\mu_2 \sinh \mu_2}{\cosh \mu_2 - 1} \frac{U_2 (L - Z_f)}{(1-\alpha)^2 \text{Re } S_L R}. \quad (4.14)$$

Eventually, the evolution equation for the flame tip (the counterpart of Eq. (3.9)) becomes

$$\frac{dZ_f}{dt} \approx \frac{\sigma S_L}{R} [Z_f + R/\sigma] = U_2(Z_f, \text{Re}) + S_L. \quad (4.15)$$

Altogether, Eqs. (4.8), (4.14) and (4.15) describe the flame acceleration in open obstructed channels accounting for the viscous effects.

4.3. Discussion and Results

By solving the set of equations obtained in the previous section, namely, Eqs. (4.8), (4.14) and (4.15), the relevant parametric study is undertaken in order to better understand the effect of each of these parameters on the flame propagation. In Chapter 3, the flame acceleration rate σ was a constant throughout the process as viscous effects were neglected. However, in this section, the

viscous effects at the boundaries were accounted for such that the acceleration rate cannot be treated as a constant anymore, and it will therefore be treated as a variable that will be assigned a range varying from 0.5 to 2.5 for the purpose of solving the relevant equations. Next, the effect of the blockage ratio on the flame tip position and the acceleration rate was investigated through the parametric study.

Numerical solution to the set of Eqs. (4.8), (4.14) and (4.15) for the most of the parameters employed in the experiments [11] and various blockage ratios is shown in Fig. 4.2, which demonstrates a delay prior to extremely fast acceleration for all values of the blockage ratio α . This delay can be attributed to the viscous effects. It is noted that the delay varies significantly with α , and the increase in α reduces the delay, thereby promoting the onset of the extremely fast acceleration trend. The same effect is also seen in Fig. 4.3, where the exponential acceleration rate is plotted versus the flame tip position, $\sigma = \sigma(Z_f)$. In this respect, it is recalled one more time that, unlike the inviscid formulation of Chapter 3 with constant σ , here the acceleration rate σ depends on the flame tip position Z_f and thereby varies with time. Figure 4.3 shows that the acceleration intensifies (σ increases) with the flame propagation; and the larger the blockage ratio is (i.e. the larger the obstacle size) – the larger σ and the stronger acceleration.

Figure 4.2: Time evolution of the flame tip position for various blockage ratios $\alpha = 0.4 \sim 0.7$.

Figure 4.3: Comparative plot of the exponential acceleration rate versus the flame tip position for various blockage ratios $\alpha = 0.4 \sim 0.7$.

Next, the effect of thermal expansion coefficient Θ on the flame propagation was investigated. Namely, Figs. 4.4 and 4.5 are the counterparts of Figs. 4.2 and 4.3, but this time the blockage ratio is fixed, $\alpha = 1/2$, while the expansion factor is varied as $\Theta = 2.38; 3.38; 4.38; 5.38$. The channel length was taken to be $L = 12.2$ m in all cases, similar to the experiments [11]. Figure 4.4 presents the time evolution of the flame tip position for various Θ . A delay is observed prior to extremely fast acceleration for all values of Θ , which was not always the case in the inviscid approximation of Chapter 3. Therefore, this delay can be devoted to the presence of hydraulic forces. However, the magnitude of the delay seems to be related to the changes in the thermal expansion coefficient Θ , as even the slightest change in Θ will lead to a significant change in the delay observed. An increase in Θ will lead to a decrease in the delay and thereby enable strong flame acceleration shortly after ignition, as opposed to a decrease in Θ that leads to an increase in the delay before sudden acceleration takes place. The latter hypothesis is also certified by Fig. 4.5, where the exponential acceleration rate σ is plotted as a function of the flame tip position Z_f . Indeed, it is seen that the larger Θ , the stronger the jet flow generated in

the pockets between the obstacles, and thereby the stronger flame acceleration is as indicated by the larger values of σ .

Figure 4.4: Comparative plot of flame propagation position versus time for varied thermal expansion coefficient.

Figure 4.5: Comparative plot of scaled acceleration rate versus the flame front position for varied thermal expansion coefficient.

The channel length L is one more parameter that that is expected to influence the flame propagation dynamics. This quantity was not included in the inviscid formulation of Chapter 3

(as well as that of Chapter 2 for semi-open pipes), but it is involved in Eq. (4.14), and thus appears a parameter of the problem as soon as the viscous effects are accounted for (and it is obviously a parameter in the practical reality). For this reason, one more set of counterparts of Figs. 4.2 – 4.5 was generated. This time, the thermal expansion and the blockage ratio are fixed at the values $\Theta = 3.38$ and $\alpha = 1/2$ (similar to those in the KIT experiments), and the channel length varies within the range $L = 10.2\text{ m}; 11.2\text{ m}; 12.2\text{ m}; 13.2\text{ m}; 14.2\text{ m}$. The outcomes are shown in Figs. 4.6 and 4.7. Specifically, Fig. 4.6 presents the time evolution of the flame tip position for various L . It is seen that the increase in the channel length promotes the delay associated with the inclusion of viscous forces into account. This is also certified by Fig. 4.7, where the acceleration rate σ is plotted versus the flame tip position Z_f for various L ; and the larger L the longer the delay prior to fast flame acceleration is. However, the slope of the sudden acceleration rates in Fig. 4.7 seems to be the same for different lengths.

Figure 4.6: Comparative plot of flame propagation position versus time for varied length of the channel.

Figure 4.7: Comparative plot of scaled acceleration rate versus the flame front position for varied length of the channel.

It is recalled that the development of the present viscous formulation, Chapter 4, was caused by a hypothesis that inclusion of the viscous effects should improve the inviscid formulation of Chapter 3 in terms of providing some better quantitative and qualitative agreement with the KIT experiments and, particularly, showing a delay prior to extremely fast flame acceleration. It is a good time now to validate if this is the case indeed. For this purpose, the inviscid theory of Chapter 3, Eq. (3.12), the present viscous formulation of Chapter 4, i.e. the numerical solution to Eqs. (4.8), (4.14) and (4.15), and the KIT experimental results are compared altogether in Fig. 4.8. Here, the time evolution of the flame tip position is plotted, with pink, blue and red curves corresponding to the inviscid theory, viscous model and experiments, respectively. It is clearly seen from Fig. 4.8 that the viscous formulation of Chapter 4 shows perfect qualitative and good quantitative agreement with the experiments; and it is much better than that of inviscid theory of Chapter 3. This thereby justifies the present work well. Regarding quantitative agreement between the blue and red curves in Fig. 4.8, the delay is predicted well indeed, still, it is a little shorter than that in the experiments. Such small deviation (of the order of 0.1s) can be attributed to the 2D geometry implemented in the theory as opposed to a 3D pipe of square cross-section employed in the experiments. In other words, the theoretical model agrees well with the

experimental data, on a quantitative level, and manages to validate the experimental delay observed associated with the hydraulic forces involved in the mechanism.

Figure 4.8: Comparative plot of flame front position versus time for models developed.

Chapter 5: Flame Propagation in Open Cylindrical Tubes

Accounting for the fact that cylindrical tubes are closer to practical applications in laboratory and industrial setups than 2D channels, in this chapter we extend the formulation of Chapters 2-4 to the cylindrical axisymmetric geometry. Specifically, the counterparts of Chapter 2, for semi-open pipes, Chapter 3, for open-open pipes in the inviscid approximation, and Chapter 4, accounting for the viscous effects, are presented in subsections 5.1, 5.2 and 5.3, respectively. The general logic flow of the 2D formulations is thus replicated to accommodate the axisymmetric configuration, and the same assumptions regarding the inviscid or viscous cases are investigated in this chapter. In other words, the axisymmetric model will combine an inviscid model, where hydraulic resistance is neglected, and a viscous model accounting for hydraulic resistance.

5.1. Semi-open obstructed cylindrical tubes

Similar to Chapter 2, the tooth-brush array of obstacles is considered, Fig. 2.2, but now in a cylindrical axisymmetric geometry. Then the incompressible continuity equation reads

$$\frac{\partial u_z}{\partial z} + \frac{1}{r} \frac{\partial}{\partial r} (r u_r) = 0, \quad (5.1)$$

with the solution

$$u_z = 2 \frac{(\Theta - 1) S_L}{(1 - \alpha) R} r, \quad u_r = - \frac{(\Theta - 1) S_L}{(1 - \alpha) R} r \quad (5.2)$$

instead of Eq. (2.2). The counterpart of Eq. (2.4) then becomes

$$\frac{dZ_f}{dt} = \sigma_{c,cyl} \frac{S_L}{R} Z_f + \Theta S_L, \quad (5.3)$$

with the solution

$$Z_f = \Theta \frac{R}{\sigma_{c,cyl}} \left[\exp(\sigma_{c,cyl} S_L t / R) - 1 \right], \quad (5.4)$$

where

$$\sigma_{c,cyl} = 2 \frac{\Theta - 1}{1 - \alpha}. \quad (5.5)$$

It is noted that the acceleration is even stronger because of the additional increase in the flame surface area in the pockets between the obstacles, as compared to the pocket entrances, simply because of the increase in the flame radius. Namely, the flame surface area in the pockets

actually appears $\propto 2\pi R_f \Delta z$ as compared to $\propto 2\pi(1-\alpha)R\Delta z$. Obviously, the effect was absent in a 2D geometry, which makes the formulation conceptually different. Even the theory of this effect is not well founded; in line with the logic of Ref. [10] the following evaluative strategy is proposed. A pocket between the obstacles at the position z starts burning at the instant, $t_f(z)$ with $t_f(z)$ being the inverted function $Z_f(t)$. Then the flame expands in the axisymmetric pockets with the radius growing as

$$R_f = (1-\alpha)R + S_L(t - t_f(z)). \quad (5.6)$$

The radial velocity at the exit of a pocket for an incompressible flow at $r = (1-\alpha)R$ is given by

$$(\Theta - 1)R_f S_L = -(1-\alpha)R u_r, \quad (5.7)$$

from which the boundary condition at the border of the unobstructed part of the tube reads

$$u_r = -(\Theta - 1)S_L \left(1 + \frac{S_L}{(1-\alpha)R} [t - t_f(z)] \right). \quad (5.8)$$

In the event of exponential or near-exponential flame acceleration, the flamefront position has been demonstrated to take the form

$$Z_f = Z_0 [\exp(\sigma S_L t / R) - 1] \quad \Rightarrow \quad t_f = \frac{R}{\sigma S_L} \ln(z / Z_0 + 1), \quad (5.9)$$

with Z_0 being some amplitude. Then the equation for the flame tip evolution becomes

$$u_z(Z_f) = 2 \frac{(\Theta - 1)}{(1-\alpha)} \frac{S_L}{R} Z_f \left(1 + \frac{S_L}{(1-\alpha)R} \langle t - t_f(z) \rangle \right). \quad (5.10)$$

Valiev et al [10] approximated the time-related term in Eq. (5.10) as

$$\langle t - t_f(z) \rangle = t - Z_f^{-1} \int_0^{Z_f} t_f(z) dz \rightarrow t \quad (5.11)$$

(though later this approach will be argued, especially for open pipes). With Eq. (5.11), Eq. (5.10) leads to the solution (5.4), $Z_f = (\Theta R / \sigma_{c2,cyl}) \{ \exp(\sigma_{c2,cyl} t / R) - 1 \}$, but with a modified $\sigma_{c2,cyl}$,

$$\sigma_{c2,cyl} = 2 \frac{\Theta - 1}{1 - \alpha} \left(1 + \frac{1}{2(\Theta - 1)} \right) \quad (5.12)$$

instead of Eq. (5.5). It is seen that the result (5.6) exceeds the 2D exponential acceleration rate, Eq. (2.6), more than twice, thereby providing much stronger acceleration (because this is in the exponent!). Indeed, it is recalled that in a 2D configuration, for the KIT values of $\Theta = 3.38$ and

$\alpha = 1/2$, $\sigma_c = 4.45$ which implies that the velocity increased by a factor of $\exp(2 \cdot 4.56) \approx 10^4$ during the characteristic laminar burning time $2R/S_L$. Here, for the same parameters, Eq. (5.6) yields $\sigma_{c,cyl} \approx 2.72 \sigma_c \approx 12.42$, which would imply a velocity increase by a factor of $\exp(2 \cdot 12.42) \approx 10^{12}$ during the characteristic laminar burning time $2R/S_L$. Again, such a huge velocity increase, of course, does not happen because compressibility effects moderate flame acceleration at the developed stages with eventual saturation to the CJ deflagration speed [10].

5.2. Open obstructed cylindrical tubes in the inviscid approximation

This subsection the derivation performed in Chapter 3 will be extended to an axisymmetric configuration. Similar to Eq. (3.6), the solution to Eq. (5.1) in an open cylinder acquires the form

$$u_z = \frac{2(\Theta - 1)S_L}{(1 - \alpha)R}(z - Z_f), \quad u_r = -\frac{(\Theta - 1)S_L}{(1 - \alpha)R}r. \quad (5.13)$$

with the same boundary conditions, $u = u(Z_f)$ at $z = Z_f$, $u = -U_1$ at $z = 0$, $u = 0$ at $z = Z_f$.

Then

$$\frac{dZ_f}{dt} = u(Z_f) + \Theta S_L = 2 \frac{(\Theta - 1)S_L}{(1 - \alpha)R} \frac{Z_f}{\sqrt{\Theta} + 1} + \Theta S_L, \quad (5.14)$$

with the solution

$$Z_f = \frac{\Theta R}{\sigma_{o,cyl}} \left[\exp(\sigma_{o,cyl} S_L t / R) - 1 \right], \quad (5.15)$$

where

$$\sigma_{o,cyl} = \frac{2(\Theta - 1)}{(\sqrt{\Theta} + 1)(1 - \alpha)} = \frac{\sigma_{c,cyl}}{\sqrt{\Theta} + 1}. \quad (5.16)$$

Accounting for the flame surface area increase in the pockets, associated with a growth of the flame radius R_f , will modify Eq. (5.10), assuming the same effects as semi-open channels (5.12)

$$\sigma_{o2,cyl} = \frac{2(\Theta - 1)}{(\sqrt{\Theta} + 1)(1 - \alpha)} \left(1 + \frac{1}{2(\Theta - 1)} \right) = \frac{\sigma_{c,cyl}}{\sqrt{\Theta} + 1}. \quad (5.17)$$

Again, the labels “o” and “c” stand for the open and semi-open tubes, respectively. It is seen that Eq. (5.16) predicts twice larger acceleration exponent as compared to that in 2D channels, Eq. (3.13). The result (5.17) is even larger. Meanwhile, both in Eqs. (5.16) and (5.17), the ratio $\sigma_{c,cyl} / \sigma_{o,cyl} = \sqrt{\Theta} + 1$ proves to be the same as that in the 2D case. To better apprehend the difference between the two configurations, Eqs. (3.12), (5.16) and (5.17) are compared in Fig.

5.1. It is seen that the axisymmetric configuration demonstrates much faster acceleration than the 2D model. The axisymmetric case seemed to diminish the small delay observed in the two dimensional case as the flame accelerate suddenly at ignition.

Figure 5.1: Comparative plot of flamefront position versus time for axisymmetric and two dimensional channels.

Finally, it should be noted that the approach (5.11), which was employed from the semi-open configuration [10] and led to the result (5.17), is not fully satisfied. Generally speaking, the integral in Eq. (5.11) should be accounted for. Then an “open-open” counterpart of Eq. (5.10) would be

$$u_z(Z_f) = 2 \frac{(\Theta - 1)S_L}{(\sqrt{\Theta} + 1)(1 - \alpha)R} Z_f \left(1 + \frac{(\sqrt{\Theta} + 1)}{2(\Theta - 1)} \ln\left(\frac{\sigma_0 Z_f}{\Theta R} + 1\right) - \frac{(\sqrt{\Theta} + 1)}{2(\Theta - 1)} \frac{Z_0}{Z_f} \ln\left(\frac{Z_0 + Z_f}{Z_0 + \frac{\sqrt{\Theta} Z_f}{\sqrt{\Theta} + 1}}\right) - \frac{(\sqrt{\Theta} + 1)}{2(\Theta - 1)} \ln\left(\frac{Z_f}{Z_0} + 1\right) + \frac{\sqrt{\Theta}}{2(\Theta - 1)} \ln\left(\frac{Z_f}{Z_0} \frac{\sqrt{\Theta}}{\sqrt{\Theta} + 1} + 1\right) - \frac{\sqrt{\Theta}}{2(\Theta - 1)} + \frac{\sqrt{\Theta} + 1}{2(\Theta - 1)} \right) \quad (5.18)$$

Solving the latter equation requires comprehensive efforts and constitutes my pending and future work on this topic. This extends beyond a master’s thesis and will be presented elsewhere.

5.3. Viscous formulation for flame acceleration in open obstructed tubes

Similar to Chapter 4, the next aim is to incorporate the effect of hydraulic resistance into the present formulation associated with open-open axisymmetric cylinder configuration. The plane-parallel Navier-Stokes equation in this configuration reads

$$\frac{\partial u}{\partial t} = -\Pi(t) + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right), \quad (5.19)$$

where the term $\Pi(t) = \rho^{-1} dP / dz$ stands for the scaled pressure gradient along the channel axis, which depends only on time in a shear flow. For simplicity, the same dynamic viscosity $\eta = \rho\nu$ is employed for both the fuel mixture and the burnt gas. In a flow driven by flame acceleration we have $u \propto \Pi \propto \exp(\sigma S_L t / R)$ such that Eq. (5.19) reduces to

$$\frac{\sigma S_L}{R\nu} u = -C_\Pi + \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right), \quad (5.20)$$

where C_Π is a constant related to the pressure. With a boundary condition $u = 0$ at $r = (1 - \alpha)R$, the solution to Eq. (5.20), describing the velocity profile generated by the accelerating flame, is

$$u = \pm U_{\max} \frac{I_0(r\sqrt{A}) - I_0((1 - \alpha)R\sqrt{A})}{1 - I_0((1 - \alpha)R\sqrt{A})}, \quad (5.21)$$

where

$$A = \frac{\sigma S_L}{R\nu} = \frac{\sigma}{R^2} \frac{RS_L}{\nu}. \quad (5.22)$$

In is recalled, in this respect, that the flame propagation Reynolds numbers is $\text{Re} = RS_L \rho_f / \rho\nu$. At the entrance of the pipe $\rho = \rho_b$ such that $A_1 = \text{Re} \sigma / R^2 \Theta$. Then Eq. (5.21) in the burnt matter reads

$$u_1 = U_{\max 1} \frac{I_0\left(\frac{r}{R} \sqrt{\frac{\sigma \text{Re}}{\Theta}}\right) - I_0((1 - \alpha) \sqrt{\frac{\sigma \text{Re}}{\Theta}})}{1 - I_0((1 - \alpha) \sqrt{\frac{\sigma \text{Re}}{\Theta}})}. \quad (5.23)$$

Similarly, at the exit of the pipe $\rho = \rho_f$ such that $A_2 = \text{Re} \sigma / R^2$ such that Eq. (5.21) in the fuel is

$$u_2 = U_{\max 2} \frac{I_0\left(\frac{r}{R} \sqrt{\sigma \text{Re}}\right) - I_0((1 - \alpha) \sqrt{\sigma \text{Re}})}{1 - I_0((1 - \alpha) \sqrt{\sigma \text{Re}})}. \quad (5.24)$$

Equation (5.21) represents the axisymmetric counterpart of Eq. (4.5), describing the flame velocity at the entrance (1) and the exit of the channel (2). Unfortunately solving for cylindrical axisymmetric counterparts of Eqs. (4.8), (4.14) and (4.15) would require an approximation to the amplitudes $U_{1,2}$ which generally vary proportionally to the flame front position. The later would require accounting and solving equation also Eq. (5.18) in order for the derivation to proceed.

Chapter 6: Summary

This study ventured into a new geometric configuration of an open obstructed pipe (channel or tube) by establishing understanding of previously founded analytical formulations and numerical simulations. Specifically, on the basis of the studies by *Bychkov et al* [9] and *Valiev et al* [10], the analytical formulation of an extremely fast flame acceleration mechanism was extended from semi-open to open-open pipes. The mechanism demonstrated strong acceleration similar to that observed in semi-open channels in a sense that the open-open acceleration mechanism does not depend on turbulence, shocks or hydraulic resistance. By implementing large obstacles with deep pockets, $\Delta z \ll \alpha R$, the effects of turbulence may be neglected. Therefore, the mechanism obtained is conceptually Reynolds-independent. Even though the exponential acceleration rate in open channels is found to be smaller by a factor of $1 + \sqrt{\Theta}$ than that in semi-open ones, it is nevertheless associated with strong acceleration. Such strong acceleration supports the recent experimental observation [11]. However, the experiments [11] show a noticeable delay before the onset of the acceleration, which was attributed to the hydraulic effects. This was validated in the present thesis. Namely, while the model initially neglected viscosity, Chapter 3, then the analysis was extended to account for viscous forces. It was demonstrated that hydraulic resistance is not required for flame acceleration and may, in fact, hinder the acceleration process. The parametric study solidified the effects of the thermal expansion coefficient and the blockage ratio, with the increase in the blockage ratio contributing into the increase in the acceleration and a decrease in the delay time prior to the acceleration. The same conclusion can be deduced for the thermal expansion coefficient. In addition, the present study concluded that the length of the channel, even being a parameter in the viscid model, plays a relatively minor role in the flame propagation scenario, with a minor influence on the acceleration and the delay observed. Finally, given the industrial utilization of axisymmetric tubes, the model developed in Chapter 4 was extended to an axisymmetric geometry in Chapter 5.

References:

1. K. Shelkin, J. Exp. Teor. Phys. 10 (1940) 823.
2. L. Kagan, & G.I Sivashinsky, 2003. The transition from Deflagration to Detonation in Thin Channels. Combustion and Flame, 134, pp. 389-397.
3. J.D. Ott, E.S. Oran, & J.A. Anderson, 2003. A Mechanism for Flame Acceleration in Narrow Tubes. American Institute of Aeronautics, 41, pp. 1391-1396.
4. V. Bychkov, A. Petchenko, V. Akkerman, L.-E. Eriksson, 2005. Theory and Modeling of Accelerating Flames in Tubes. Phys. Rev. E 72, p. 046307.
5. V. Akkerman, V. Bychkov, A. Petchenko, L.-E. Eriksson, 2006. Accelerating Flames in Cylindrical Tubes with Non-slip at the Walls. Combustion and Flame, 145, pp. 206-219.
6. M. Wu & C. Wang, 2011. Reaction Propagation Modes in Millimeter-Scale Tubes for Ethylene/Oxygen Mixtures. Proc. of the Combustion Institute, 33, pp. 2287-2293.
7. C. Clanet & G. Searby, 1996. On the “Tulip Flame” Phenomenon. Combustion and Flame, 105, pp. 225-238.
8. V. Bychkov, V. Akkerman, G. Fru, A. Petchenko & L.E. Eriksson, 2007. Flame Acceleration at the Early Stages of Burning in Tubes. Combustion and Flame, 150, pp. 263–276.
9. V. Bychkov, D. Valiev & L.E. Eriksson, 2008. Physical Mechanism of Ultra-Fast Flame Acceleration. Physical Review Letters, 101, p. 164501.
10. D. Valiev, V. Bychkov, V. Akkerman, C.K. Law & L.E. Eriksson, 2010. Flame Acceleration in Channels with Obstacles in the Deflagration-to-Detonation Transition. Combustion and Flame, 157, pp. 1012-1021.
11. J. Yanez, M. Kuznetsov, V. Bykov, Sudden acceleration of flames in open channels driven by hydraulic resistance. <http://arxiv.org/abs/1208.64>