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Influence of the Lewis Number and Boundary Conditions on Finger Flame Acceleration

Mohammed Alawi AlKhabbaz

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Influence of the Lewis Number and Boundary Conditions on Finger Flame Acceleration

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**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**

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**Keywords: Premixed flame; Finger flame; Slip walls; Boundary conditions;
Lewis number; Flame acceleration; Computational simulations**

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Abstract

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Mohammed AlKhabbaz

One of the mechanisms of premixed flame acceleration in pipes is devoted to the following scenario: an initially hemispherical flame embryo, ignited at a closed end of a tube or a channel with one end open, at a tube/channel centerline, eventually acquires a convex, finger-like shape. This is accompanied by powerful flame acceleration, which lasts until the flame skirt contacts a side wall of the tube/channel and is followed by flame deceleration and formation of a concave, “tulip” flame shape. While this phenomenon has been observed and studied extensively in the past, experimentally, computationally, and analytically, the previous theoretical and numerical studies employed a set of conventional simplifying assumptions such as equidiffusive burning and ideally-slip, adiabatic walls of the pipe, which are not the cases in the practical reality.

The present work reduces such a gap between the research and practice. Specifically, the impacts of the Lewis number (the thermal-to-mass diffusivities ratio) Le and of the various wall boundary conditions on finger flame acceleration is investigated by means of the computational simulations of the reacting flow equations, with a fully-compressible hydrodynamics, transport properties (thermal conduction, diffusion and viscosity), and an Arrhenius chemical kinetics. The simulation results include the monitoring and analysis of the major flame parameters such as the evolutions of the locus and velocity of the flame tip, the flame surface area and the burning rate.

It is shown that the $Le > 1$ flames are intrinsically thickened and thereby propagate slower than the equidiffusive ($Le = 1$) flames, though the difference is minor. In contrast, the $Le < 1$ flames propagate faster due to the onset of the diffusional-thermal instability. As for the wall conditions, various isothermal (cold/preheated) and mechanistic (slip/non-slip) boundaries are employed and compared. Overall, it appears that side walls provide a minor impact on finger flame acceleration, which is different for another acceleration mechanism where wall friction plays a greater role. The latter result can be explained by the fact that finger acceleration occurs far from the walls, i.e. along the centerline and before the flame skirt contacts the side walls.

Dedication

*I dedicate this work to my family and anyone who has any form of inflammatory bowel diseases,
especially people with crohn's disease.*

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First, I want to thank Allah for everything. Then I want to thank my parents and siblings Wafa, Ghadeer, and Ahmed for their unconditional love and support throughout this journey. I could not have done this work without them. I also would like to express my gratitude to my research advisor, Dr. Akkerman, for his guidance and support. Also, I want to thank my committee members, Dr. Musho and Dr. Li, for giving me sometime out of their busy schedule and for helping me with my thesis work. Lastly, I want to thank my colleagues from Dr. Akkerman's group, namely, Abdulafeez Adebiyi, Furkan Kodakoglu, Olatunde Abidakun, Gideon Udochukwu and Sai Satish Guda for everything they have done for me during my research work.

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Nomenclature

C_p	Heat capacity at constant pressure
C_v	Heat capacity at constant volume
c_s	Speed of sound
DL	Darrius-Landau
DT	Diffusional-thermal
DDT	Deflagration-to-detonation transition
E_a	Activation energy
f	A function describing the flame shape
FA	Flame acceleration
L_f	Flame thickness
Le	Lewis number
m	Molecular weight
Ma	Mach number
P	Pressure
P_f	Fuel pressure
Pr	Prandtl number
Q	Specific energy released
R_p	Universal gas constant
R	Tube radius/half-width
Re	Reynolds number of flame
Sc	Schmidt number
S_w	Flame surface area
T	Temperature
T_w	Wall temperature
T_b	Burnt matter temperature
T_f	Fuel temperature
U_f	Planar flame velocity
U_w	Total burning rate
U_{tip}	Velocity of the flame tip
Y	Fuel mass fraction
Z_{tip}	Position of the flame tip

Greek

γ_{ij}	Stress tensor
q_i	Energy diffusion vector
ε	Specific internal energy
Θ	Thermal expansion factor ($\Theta = \rho_f/\rho_b$)
μ	Dynamic viscosity
ν	Kinematic viscosity
ρ	Density
ρ_f	Fuel density
τ	Scaled time ($\tau = U_f t/R$)
τ_R	Time dimension constant
γ	Adiabatic exponent ($\gamma = C_p/C_v$)
σ	Acceleration rate
ϕ	Equivalence ratio

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Chapter 1: Introduction

Combustion is a sequence of rapid chemical reactions between a fuel and an oxidizer, which is accompanied by the release of thermal energy in the form of heat that makes it exothermic in nature. Combustion science is one of the most complex disciplines requiring solid knowledge in different scientific subjects such as chemistry, physics, thermodynamics and fluid mechanics. Among a wide range of combustion processes in the nature, each process has its own approach and applications, starting with energy production in steam engines and power plants, and ending with the advanced modern technologies such as rotating-detonation engines. When speaking about combustion, two types are known: premixed and non-premixed (diffusion) combustion. In premixed combustion, the reactants are perfectly mixed and delivered concurrently to the reaction zone. An example of premixed combustion is seen in spark-ignition gasoline engines. In the case of diffusion combustion, the combustible gas and the oxidizer are delivered separately to the reaction zone and mixed by diffusion in the combustion chamber. An illustration of a diffusion combustion can be seen in compression ignition engines [1,2].

One of the distinctive features of premixed combustion is formation of self-sustained combustion waves with the ability to propagate through a fresh combustible mixture with a defined velocity, either subsonic or supersonic. The reaction wave is initiated by an increase in the temperature of the pre-mixture and it can propagate through a homogenous pre-mixture in two self-supporting regimes: either in a slow, subsonic regime of deflagration (or flame), or in a fast, supersonic regime of detonation. In deflagration, the energy is transferred from the hot burnt matter to the cold fuel mixture by thermal conduction. The temperature of the cold mixture increases such that another portion of the fuel is burnt, and more energy is released and transferred to the next layer of the cold fuel mixture resulting in further propagation of the combustion wave. On the other hand, a detonation wave is initiated and induced by shock waves that compress and preheat the combustible mixture. The expansion of the burnt matter in this regime is accompanied by localized explosions and thereby detonation initiation. Furthermore, in a subsonic process, a flame may accelerate spontaneously with an increase in its propagation velocity by 2-4 orders of magnitude, which triggers explosions and eventually develops into a self-sustained detonation [3-5].

The dynamics and morphology of premixed flames are influenced by numerous factors such as composition of the fresh gaseous mixture, with certain premixtures moving faster than the others under the same thermal-chemical conditions. In addition, the initial pressure and temperature as well as the boundary conditions and the geometrical configuration of the combustion system may facilitate or mitigate propagation of the reaction wave leading to well-known patterns of corrugated flames, which is accompanied by a considerable increase in the flame velocity. Moreover, planar stationary flames rarely exist in the practical reality; the interaction between the hot burnt matter and the cold fuel-air mixture is subjected to hydrodynamic instabilities that bend a flame front. Similarly, the fronts of spherical flames appear unstable against small perturbations, thus acquiring a fractal structure. One of the known hydrodynamic instabilities is referred as the Darrieus-Landau (DL) instability, and it is caused by the density drop across the flame front due to the gas expansion during the exothermic reaction. Another combustion instability mode is the diffusional-thermal (DT) instability, which is related to the diffusive properties of the reaction wave [2,6]. The dynamics of flame propagation is described by the hydrodynamic equations of mass, momentum, and energy conservations as well as the chemical kinetics and transport properties such as thermal conduction, diffusion and viscosity.

In the present thesis, a computational analysis on the effect of the Lewis number and of the boundary conditions on the dynamics and structure of a finger flame during the early stages of burning is performed by means of solving the hydrodynamic and combustion equations. This thesis is organized as follows. First, a literature review on accelerating flames in two-dimensional (2D) channels and cylindrical tubes as well as the motivation of this work is discussed. Specifically, Chapter 2 summarizes different studies on the finger flame acceleration phenomenon, especially the experiments, theory and modelling [7,8]. The numerical methods of the simulations, the governing equations, the boundary conditions, and the assumptions, employed in this study, are explained in Chapter 3. In Chapter 4, non-equidiffusive finger flame acceleration in the 2D planar channels and cylindrical tubes with ideally-slip, adiabatic walls is presented and discussed in detail, followed by the study of the impact of slip and non-slip walls as well as cold and pre-heated isothermal walls on finger flame acceleration. Finally, Chapter 5 provides a summary of this work.

1.2 Literature review

The dynamics and morphology of propagating flames have been widely studied in a variety of configurations [9], in particular, in pipes or tubes, for their reasonably simple geometry. Also, combustion tubes can be utilized in the foreseeable novel technologies as well as being employed in numerous existing practical applications. Indeed, with a high aspect ratio, such a configuration is favorable for prompt flame propagation with a high possibility of initiating an explosion, which is followed by a detonation. While a deflagration-to-detonation transition (DDT) was observed experimentally [10-14], there has been limited theoretical understanding of this scenario, while one of the most crucial questions in combustion science is how to avoid or initiate the DDT [15].

There are three identified mechanisms of flame acceleration in channels or tubes. The first mechanism of flame propagation was proposed by Shelkin [16], where the non-uniform flame flow due to turbulence and wall friction, with non-slip boundary conditions at the tube walls, bend the flame front, which increases the flame velocity and facilitates flame acceleration until the initiation of shock waves leading to a detonation. A subsequent quantitative analytical and computational study in a 2D planar configuration with non-slip adiabatic walls have been conducted by Bychkov *et al.* [15], which was followed by another analytical formulation and computational simulations by Akkerman *et al.* [17], for the cylindrical geometry. The analytical theories then have been elucidated extensively by the numerical simulations [15,17-20]. However, all these formulations employed a set of conventional simplifications such as equidiffusive burning (i.e. the Lewis number, defined as the thermal-to-mass diffusivity ratio to be unity, $Le = 1$) and the assumption of zero flame front thickness. Later, it was proven that the transport mechanisms within the flame front, including the thermal and mass diffusivities, may influence flame propagation [21]. Figure 1.1 illustrates, schematically, flame propagation with non-slip adiabatic walls.

Fig. 1.1: Flame acceleration with non-slip adiabatic walls [15].

Other analytical and computational studies by Bychkov *et al.* [22,23] demonstrated that the geometrical configuration of the obstructed channels can initiate a DDT even in a laminar environment, while the role of turbulence would be minor and supplementary. The flame front expands toward the unburnt matter in the unobstructed part of the channel, where delayed burning of the trapped fuel between the obstacles produces a strong jet flow that can lead to a DDT event. Figure 1.2 illustrates a flame front propagating in an obstructed channel. Furthermore, according to Zeldovich and Frank-Kamenetsky [24], a flame undergoes five distinctive stages during its transition into a detonation wave. During acceleration of a laminar flame, the combustion wave pushes weak shocks, which then will interact and get merged, thereby forming stronger shock waves, which will compress and heat the unburnt matter to trigger a detonation wave.

Fig. 1.2: Flame evolution in obstructed channels [25].

Moreover, one of the mechanisms of flame propagation is associated with a finger-like shape of the flame front. The finger flame phenomenon has been first studied experimentally, for a flame in a closed cylindrical tube, by Ellis [26], who observed that the flame structure is spontaneously inverted from a pointing forward finger to a backward directed cusp for certain geometrical configurations, namely, for tubes with a high aspect ratio (length/diameter). Later, the backward pointing cusp was given the name of a “tulip flame” by Salamanda *et al.* [27], who conducted an experiment with premixed flame acceleration that resulted in detonation initiation. A typical tulip flame can be seen in Fig. 1.3. The parametric 2D computational study of Gonzalez *et al.* [28] showed that the perturbation of the flame front due to the DL instability, along with the inversion of the velocity gradient, are the main mechanisms of tulip flame formation, with wall friction playing only a supplementary role. Rotman *et al.* [29] concluded that the generation of vorticity in the fresh gaseous mixture is the main cause of the inverted concave flame. On the other hand, Dunn-Rankin *et al.* [30] observed a tulip flame in the absence of vorticity generation. Furthermore,

Markstein [31] observed the appearance of the tulip flame formation in fully-closed tubes as well as in semi-open ones, referring the change in the flame curvature to the initial conditions, the tube aspect ratio, and the equivalence ratio of the fuel mixture. A numerical study by Marra *et al.* [32] demonstrated the importance of wall friction on the inversion of the concave flame front. This mechanism will be discussed and studied briefly in this work.

Fig. 1.3: Tulip flame formation in a cylindrical tube [33].

1.2 Motivation and objectives

The majority of the engineering systems are powered by combustion, and they have a great impact in our daily life. In particular, internal combustion engines have been continuously developed to acquire more power at lower costs, which sheds the light on the advancement of the computational analysis in combustion science. Numerical modeling has grown virtually to play a significant role in engineering since their inception, and it seems to be a relatively cheap and a very promising alternative to more expensive experiments. Additionally, many scientists and engineers are starting to use computational methods in combustion, since these numerical analyses have been successfully implemented in chemical kinetics, laminar and turbulent combustion, and fluid dynamics. Moreover, numerical methods are preferable as they offer prompt assessment of the parametric design. However, these systems and methods are still set to some limiting factors, in which their capability to effectively handle the massive amount of data to utilize different combustion applications is the most significant one. Fortunately, the modern computing techniques are being cultivated rapidly, so the quantitative and qualitative numerical results can be obtained accurately.

The need for energy-efficient devices is continuously increasing over the years as combustion is still the dominant provider of energy worldwide. This implies continuous development of the modern combustion technologies such as gas turbines, pulse and rotation-detonation engines, as well as micro- and nano-combustors. The foundation of the modern combustion science focuses on the optimization of the energy conversion, improving the flame stability, reduction of pollutant formation, and prevention of uncontrolled accidental explosions, which elucidates the importance to study the flame propagation mechanisms. Although the studies of flame acceleration have been stimulated for decades, the theoretical and analytical understanding of this phenomenon is still limited, especially when it comes to DDT [24].

One of the main mechanisms of flame acceleration is that associated with a finger-like shape of the flame front, which describes the early stage of the burning process in pipes. Specifically, a small hemispherical flame strongly expands and experiences a transition into a finger-shaped flame front. A well-known experimental study on finger flame acceleration was conducted by Clanet and Searby [7], followed by the analysis of the tulip flame phenomenon, and then it was studied analytically and numerically by Bychkov *et al.* [8], where the dynamics and morphology along with the other characteristic parameters of finger flame acceleration such as the total acceleration time, the position and velocity of the flame tip, have been identified. However, similar to the multitude of analytical formulations, a set of simplifications and assumptions were adopted in the previous studies on finger flame acceleration. In particular, the approach of an equidiffusive flame was employed such that the Lewis number characterizing the thermal-to-mass diffusivities ratio and defined as:

$$Le = \frac{\text{Thermal diffusivity}}{\text{Mass diffusivity}} = \frac{Sc}{Pr} \quad (1.1)$$

where Sc and Pr are the Schmidt and Prandtl numbers, respectively, was assumed to be $Le = 1$.

Another factor influencing flame acceleration is the boundary conditions of the combustion system such as: mechanistic (slip/non-slip) and thermal (adiabatic/isothermal) boundaries, which are defined as follows:

- Slip boundary condition indicates that the normal velocity of the flow at the wall is zero, $u_n = 0$, while the tangential velocity is not, $u_t \neq 0$.
- Non-slip boundary condition indicates that both the tangential and the normal velocities of the flow are zero at the wall, $\mathbf{u} = 0$.
- Adiabatic processes refer to the nonexistence of the heat and mass transfer into or out of the thermal system; this can be achieved by using highly insulating materials.
- The isothermal boundary condition means a fixed temperature of the combustor surface throughout the combustion process.

This thesis presents a computational analysis of finger flame acceleration at the early stages of burning in pipes. The parametric studies include the Lewis number in the range $0.2 \leq Le \leq 2$ and different temperatures for the isothermal slip and non-slip walls in the range $300\text{ K} \leq T_w \leq 1200\text{ K}$.

Chapter 2: Finger Flame Acceleration

Premixed flame propagation in semi-open channels (one end is closed) has been studied extensively in combustion science. A mechanism associated with the initial stages of burning is finger flame acceleration. Ignition of a hemispherical flame embryo occurs at the closed end at the tube axis, and the flame expands towards the open extreme of the tube, thereby acquiring a shape of a pointing forward finger. This acceleration is strong, yet it is limited in time, being terminated when the flame front contacts a side wall of the tube. Then, if there is no considerable effect of wall friction, the flame will subsequently decelerate, and the flame surface area will decrease. As a result, the shape of the flame front shifts from a convex finger flame to a cusp pointing backward or a tulip flame front. There are several analytical formulations and experimental studies that observed and investigated the finger flame acceleration mechanism within the context of formation of a tulip flame; some of them are related to this work and will be discussed briefly in the following sections. A typical finger flame acceleration scenario is illustrated in Fig. 2.1, with four stages to be distinguished: 1) a hemispherical flame, 2) a pointing forward finger flame, 3) a quasi-planar flame, and 4) a tulip flame.

Fig. 2.1: Finger flame evolution at different time instants.

2.1 Finger flame acceleration: an experimental study

Finger flame propagation in cylindrical tubes was investigated experimentally by Clanet and Searby [7]. Specifically, a semi-open tube made of Pyrex glass of radii 2.5 and 5 cm, with various lengths in the range $0.6 \text{ m} < L < 6 \text{ m}$, was filled with a propane-air mixture of equivalence ratios in the range $0.65 < \phi < 1.3$. The mixture was injected into the burner using an insulating valve and the flame was ignited using a spark igniter at the closed end, with a laminar flame velocity being in the range $20 \text{ cm/s} < U_f < 41 \text{ cm/s}$. The authors of Ref. [7] stated that the flame front undergoes four different stages. The first stage represents an expanding small hemispherical flame that is not affected by the side walls of the tube. The second stage is that when the flame front approaches the side walls and acquires a finger shape, with a time interval for this stage being $t_{\text{sphere}} \leq t \leq t_{\text{wall}}$, where t_{sphere} is the characteristic time when a transition from a hemispherical to a finger shape occurs, $10 \text{ ms} \leq t_{\text{sphere}} \leq 20 \text{ ms}$, and t_{wall} is the time when a flame “skirt” contacts a side wall. Clanet and Searby [7] also identified the exponential increase in the flame tip velocity within the range $30 \text{ m/s} \leq U_{\text{tip}} \leq 50 \text{ m/s}$. The following figures demonstrate the experimental apparatus with an image of the tulip flame formation using high-speed photography.

Fig. 2.2: The experimental apparatus of [7].

Fig. 2.3: An inverted concave “tulip” flame observed in [7].

The third observed stage of this mechanism is defined within a time interval $t_{wall} \leq t \leq t_{tulip}$. In this stage, the flame decelerates, and the flame front undergoes an inversion to a backward pointing cusp, because of the decrease in the flame surface area and the flame tip velocity, where Clanet and Searby [7] also defined a time in which the flame front acquires a tulip shape flame with $t_{tulip} \approx 40$ ms. Finally, the fourth stage of combustion is defined for $t > t_{tulip}$. The authors of Ref. [7] concluded their study suggesting that the acoustic effects and viscosity do not have the dominant influence during the first three stages, especially in formation of a tulip flame, while these factors may have an impact during the latter stages of burning. In addition, Clanet and Searby [7] suggested that the unstretched laminar flame velocity U_f and the geometrical configuration of the combustor as well as the composition of the combustible mixture are the three main factors influencing flame propagation during the early stages of burning. A three-dimensional (3D) design of an experimental apparatus is shown in Fig. 2.4.

Fig. 2.4: 3D design of an experimental setup as in [7].

2.2 Theory of flame acceleration in cylindrical tubes

A theoretical formulation on flame acceleration at the initial stages of burning in semi-open cylindrical pipes has been developed computationally by Bychkov *et al.* [8]. Specifically, the authors of Ref. [8] developed an analytical theory that determines the maximal surface area of the flame front S_w , the total exponential growth rate σ during the finger flame acceleration regime, as well as the total acceleration time, with the flame tip displacement and velocity, Z_{tip} and U_{tip} ,

respectively. The equation for the increased volume of the burnt matter during the burning process reads as [8]

$$dZ_{tip}/dt = 2\theta \frac{U_f}{R} Z_{tip}, \quad (2.1)$$

where U_f is the laminar flame velocity, R is the tube radius and $\theta = \rho_{fuel}/\rho_{burnt}$ is the thermal expansion coefficient. The authors of Ref. [8] also developed an analytical theory for the flame displacement and the timing in cylindrical tubes as:

$$\frac{d\eta_f}{d\tau} - (\theta - 1)(1 - \eta_f^2) = 1, \quad (2.2)$$

$$\tau = \frac{1}{2\alpha} \ln \left(\frac{\theta + \alpha\eta_f}{\theta - \alpha\eta_f} \right), \quad (2.3)$$

where $\tau = U_f t/R$ is the scaled time and $\alpha = \sqrt{\theta(\theta - 1)}$. Furthermore, the time intervals for two stages of burning, specifically, a time instant in which the hemispherical flame expands to acquire a pointing finger flame, τ_{sph} , as well as the characteristic time when the flame skirt contacts the side walls, τ_{wall} , before inverting to a pointing backward cusp, have been found. These intervals, in dimensionless units, are calculated as:

$$\tau_{sph} \approx \frac{1}{2\alpha}, \quad \tau_{wall} \approx \frac{1}{2\alpha} \ln \left(\frac{\theta + \alpha}{\theta - \alpha} \right). \quad (2.4)$$

Using Eq. (2.4), one expects a pointing finger flame at a scaled time instant $\tau_{sph} \approx 0.067$ and the elongated flame to touch the wall at a scaled time instant $\tau_{wall} \approx 0.23$ for a typical propane-air burning with an expansion factor of $\theta = 8$. Additionally, as the flame propagates in the cylindrical tube, the flame tip position can be found as:

$$Z_{tip} = \frac{\theta}{4\alpha} \sinh(2\alpha\tau). \quad (2.5)$$

The flame tip velocity is then given by $U_{tip} = dZ_{tip}/dt$. Moreover, the flame front accelerates exponentially in time, with the exponential growth rate of flame acceleration given by:

$$\sigma = 2\alpha = 2\sqrt{\theta(\theta - 1)}. \quad (2.6)$$

Finally, Bychkov *et al.* [8] expressed the scaled surface area of a curved flame front as

$$S_w / \pi R^2 \approx -2 \int_0^1 \eta \frac{\partial f}{\partial \eta} d\eta = 2 \frac{\theta^2}{\theta + 1}. \quad (2.7)$$

Equation (2.7) can be used to estimate the maximal scaled surface area of the curved flame front. For a typical propane-air burning with the expansion factor $\theta = 8$, the maximal scaled surface is evaluated to be as large as $S_w / \pi R^2 \approx 14.2$. Figure 2.5 demonstrates finger flame acceleration, followed by tulip flame formation, according to the simulation in Ref. [34].

Fig. 2.5: Flame front evolution in a cylindrical tube [34].

Chapter 3: Numerical Analysis

In the present thesis, the impacts of the Lewis number as well as that of the thermal and mechanistic boundary conditions are analyzed computationally, in both the 2D Cartesian and cylindrical axisymmetric coordinate systems, using a Navier-Stokes code for fully-compressible reacting flows. The chemical kinetics is imitated by a first-order one-step irreversible Arrhenius reaction, with both the fuel mixture and the burnt matter assumed to be ideal gases. The numerical scheme of this solver is cell-centered and finite-volume, being second-order accurate in time, and spatially accurate of the fourth-order for the convective terms and second order for the diffusive terms. The code was first implemented by Volvo Aero in 1995 and was developed subsequently for the academic use.

3.1 Governing equations

The governing equations are those for the balance of mass (continuity), momentum, energy, and species, and in the general form for 2D Cartesian and cylindrical axisymmetric flows, they read:

- the continuity equation:

$$\frac{\partial \rho}{\partial t} + \frac{1}{r^\beta} \frac{\partial}{\partial r} (r^\beta \rho u_r) + \frac{\partial}{\partial z} (\rho u_z) = 0, \quad (3.1)$$

- the momentum equations:

$$\frac{\partial}{\partial t} (\rho u_r) + \frac{1}{r^\beta} \frac{\partial}{\partial r} [r^\beta (\rho u_r^2 - \zeta_{r,r})] + \frac{\partial}{\partial z} (\rho u_r u_z - \zeta_{r,z}) + \frac{\partial P}{\partial r} + \Psi_\beta = 0, \quad (3.2)$$

$$\frac{\partial}{\partial t} (\rho u_z) + \frac{1}{r^\beta} \frac{\partial}{\partial r} [r^\beta (\rho u_r u_z - \zeta_{r,z})] + \frac{\partial}{\partial z} (\rho u_z^2 - \zeta_{z,z}) + \frac{\partial P}{\partial z} = 0, \quad (3.3)$$

- the energy equation:

$$\frac{\partial e}{\partial t} + \frac{1}{r^\beta} \frac{\partial}{\partial r} [r^\beta ((e + P) u_r - Z_{r,r} u_r - Z_{r,z} u_z + q_r)] + \frac{\partial}{\partial z} [(e + P) u_z - Z_{z,z} u_z - Z_{r,z} u_r + q_z] = 0, \quad (3.4)$$

- the species equation:

$$\frac{\partial}{\partial t} (\rho Y) + \frac{1}{r^\gamma} \frac{\partial}{\partial r} \left[r^\gamma \left(\rho u_r Y - \frac{\mu}{Sc} \frac{\partial Y}{\partial r} \right) \right] + \frac{\partial}{\partial z} \left(\rho u_z Y - \frac{\mu}{Sc} \frac{\partial Y}{\partial z} \right) = - \frac{\rho Y}{\tau_R} \exp(-E_a/R_p T), \quad (3.5)$$

where $\beta = 0$ and 1 for 2D and cylindrical geometries respectively,

- the total energy equation:

$$\varepsilon = \rho(QY + C_v T) + \frac{\rho}{2}(u_z^2 + u_r^2), \quad (3.6)$$

- the heat diffusion vectors:

$$q_r = -\mu \left(\frac{C_p}{Pr} \frac{\partial T}{\partial r} + \frac{Q}{Sc} \frac{\partial Y}{\partial r} \right), \quad (3.7)$$

$$q_z = -\mu \left(\frac{C_p}{Pr} \frac{\partial T}{\partial z} + \frac{Q}{Sc} \frac{\partial Y}{\partial z} \right), \quad (3.8)$$

- the stress tensor equation for the Cartesian geometry:

$$\zeta_{i,j} = \mu \left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i} - \frac{2}{3} \frac{\partial u_k}{\partial x_k} \delta_{i,j} \right), \quad (3.9)$$

- the stress tensor equations for the cylindrical geometry:

$$\zeta_{r,r} = \frac{2\mu}{3} \left(2 \frac{\partial u_r}{\partial r} - \frac{\partial u_z}{\partial z} - \frac{u_r}{r} \right), \quad (3.10)$$

$$\zeta_{z,z} = \frac{2\mu}{3} \left(2 \frac{\partial u_z}{\partial z} - \frac{\partial u_r}{\partial r} - \frac{u_r}{r} \right), \quad (3.11)$$

$$\zeta_{r,z} = \mu \left(\frac{\partial u_r}{\partial z} + \frac{\partial u_z}{\partial r} \right). \quad (3.12)$$

The last term of Equation (3.2) takes the form

$$\psi_\beta = \frac{2\mu}{3} \left(2 \frac{u_r}{r} - \frac{\partial u_r}{\partial r} - \frac{\partial u_z}{\partial z} \right), \quad (3.13)$$

if $\beta = 1$, and $\psi_\beta = 0$ if $\beta = 0$. We employ the ideal gas equation of state:

$$P = \rho R_p T / m. \quad (3.14)$$

The flame thickness is conventionally defined as:

$$L_f = \frac{\mu}{Pr \rho_f U_f}, \quad (3.15)$$

where Y represents the mass fraction of the fuel, Q is the energy release from the chemical reaction, μ is the dynamic viscosity, $C_v = 5 R_p / 2m$ and $C_p = 7 R_p / 2m$ are the specific heats at constant volume and pressure, respectively, where $R_p = 8.31 \text{ J / (mol K)}$ is the universal gas

constant and m is the molar mass of the fuel-air mixture, assumed to be $m = 2.9 \times 10^{-2} \text{ kg/mol}$. The initial pressure, temperature, and density of the fuel mixture are $P_f = 10^5 \text{ Pa}$, $T_f = 300 \text{ K}$, and $\rho_f = 1.16 \text{ kg/m}^3$, respectively.

The chemical parameters of the fuel-air mixture were chosen to provide a strongly subsonic flame propagation, with initial Mach number, $Ma \equiv U_f/c_s = 10^{-3}$, where $U_f = 34.7 \text{ cm/s}$ is the laminar flame velocity and $c_s = 34700 \text{ cm/s}$ is the speed of sound in the fuel mixture. In this case the flow is almost isobaric at the initial stage of the burning process. Additionally, to initiate a typical propane-air burning, the thermal expansion coefficient was held at $\theta = 8$, and the dynamic viscosity as $\mu = 2.38 \times 10^{-5} \text{ Ns/m}^2$. The activation energy was set as $E_a = 7R_p T_b$ in order to smoothen the reaction zone over less computational cells. Moreover, different tube radii and channel widths were considered in the domain $10 \leq R/L_f \leq 30$, which correlates with a relatively low Reynolds number (Re) associated with the flame propagation, given by:

$$Re = \frac{U_f R}{\nu} = \frac{R}{Pr L_f} = 14 - 30. \quad (3.16)$$

Furthermore, the Lewis number is considered in the domain $0.2 \leq Le \leq 2$ by varying the Schmidt number while the Prandtl number is held constant at $Pr = 0.7$ for the Cartesian configuration, and $Pr = 1$ in the cylindrical coordinates.

3.3 Numerical scheme

This computational platform has been effectively applied in the studies of laminar flame acceleration, flame corrugation, and other related flame propagation mechanisms [34]. In this computational study, the width of the channel in the 2D planar geometry is varied within the range $20L_f \leq R \leq 30L_f$, and the tube diameter in the cylindrical geometry is $2R = 40L_f$ and $60L_f$, respectively. The length of the tube is assumed to be infinitely long such that its effect is neglected. The composition of the dynamic mesh consists of a structured rectangular grid, with the grid walls parallel to each direction in the Cartesian and cylindrical configurations. Additionally, the grid is made uniform in the axial direction for both the 2D planar and cylindrical axisymmetric geometries. A schematic of a typically-used dynamic mesh is shown in Fig. 3.1. The cell size of the adaptive grid is $0.2L_f$, which is quite adequate to simulate the structure, dynamics and

morphology of a strongly corrugated flame front. To check the mesh accuracy, a validation test was also performed with a grid of size $0.1L_f$. Figure 3.2 compares the scaled flame tip positions for two grid sizes.

Fig. 3.1: The dynamic mesh used with different resolutions [35].

Fig. 3.2: A resolution test for the scaled flame tip position Z_{tip}/R , versus the scaled time, $U_f t/R$.

3.2 Boundary conditions

The present thesis consists of two major parts, with different boundary conditions employed for different configurations. The first part is devoted to the effect of non-equidiffusive flames on finger flame acceleration with ideally-slip, adiabatic walls for both 2D planar and cylindrical-axisymmetric geometries, while the second part scrutinizes the role of mechanistic (slip/non-slip)

and isothermal (cold/preheated) wall boundary conditions for equidiffusive flames in 2D channels.

These conditions are implemented as follows:

- Flames propagate in a channel/tube with one end closed, from the closed end to the open one.
- The slip walls are implemented as $\mathbf{n} \cdot \mathbf{u} = 0$, where $\mathbf{n}$ represents the normal vector to the walls
- The non-slip walls are implemented by $\mathbf{u} = 0$.
- The adiabatic walls are represented by $\mathbf{n} \cdot \vec{\nabla}T = 0$.
- The isothermal walls are set by $T_w = \frac{T_{in}+T_{out}}{2}$, where $T_w = \{300\text{ K}, 500\text{ K}, 800\text{ K}, 1200\text{ K}\}$.

Chapter 4: Results and Discussion

In this chapter, the impact of the diffusive properties as well as the mechanistic and thermal boundary conditions on the dynamics and morphology of finger flames in the early stage of the burning process in a semi-open channel/tube (one end of the channel/tube is closed and the other end is open such that the flame propagates toward the open end) are scrutinized using a set of parametric studies by means of the computational simulations. Specifically, the channel/tube is filled with a gaseous pre-mixture; a flame embryo is ignited at the centerline at the closed end of the channel, and then propagates toward the open end as illustrated in Fig. 4.1. The hemispherical flame then experiences a stage of powerful acceleration, acquiring eventually a convex finger shape. This fast acceleration lasts until the flame skirt contacts a side wall of the channel/tube, which is accompanied by flame deceleration and formation of a concave tulip flame shape.

Fig. 4.1: Illustration of the initial geometry and boundary conditions.

The first section of this chapter is devoted to the effect of the Lewis number on finger flame propagation in 2D channels and cylindrical tubes. This section is further divided into three major subsections as follows: the first subsection examines equidiffusive ($Le = 1$) flames propagation for different channel widths/ tube diameters, followed by two subsections for non-equidiffusive finger flames, for $Le < 1$ and $Le > 1$, respectively. The second part of this parametric study will identify the role of the boundary conditions. Here both mechanistic (slip/non-slip) as well as the thermal (adiabatic/isothermal) boundary conditions are employed for equidiffusive flames to clearly examine their roles on the finger flame acceleration scenario. Finally, the third subsection will discuss finger flame acceleration and the deflagration-to-detonation transition.

4.1. Effect of the Lewis number on finger flame acceleration

The Lewis number is one of the major parameters influencing flame propagation in combustion systems. To fully evaluate the effect of the diffusive properties on the flame dynamics and morphology, numerical simulations of finger flame acceleration in 2D channels and cylindrical tubes with slip adiabatic walls are performed at different flow parameters. Specifically, the planar and axisymmetric geometries are employed, and the Reynolds number (Re) associated with the laminar flame is varied in the range $14 \leq Re \leq 30$ by controlling the channel width/tube diameter. Additionally, the Lewis number is varied in the range $0.2 \leq Le \leq 2$.

4.1.1 Equidiffusive flame propagation

In this subsection, we discuss the computational simulations, performed for equidiffusive flames ($Le = 1$). Here, the hemispherical flame expands at an initial stage of burning, it propagates towards the open end of the tube and elongates to acquire a finger-shaped form of the front, followed by formation of a tulip flame. A typical evolution of an equidiffusive flame is shown in Fig. 4.2 for a 2D channel with half-width of $R = 20L_f$.

Fig. 4.2: Flame morphology in the 2D planar geometry for $R = 20L_f$.

At the initial stage of burning, a hemispherical flame front of initial radius $1.5L_f$, as in Fig. 4.2, expands uniformly outwardly. The flow is mainly pushed towards the axial direction because the radial expansion is limited by the side walls. The velocity pattern of the flame front is influenced by the walls such that the flame front elongates to acquire a finger shape; see Fig. 4.2c. Strong expansion of the ignited hemispherical flame leads to strong acceleration of the flow in the

axial direction. As a result, the flame surface area S_w increases and the flame consumes more fuel per unit time. Simultaneously, the flame tip position Z_{tip} becomes much larger than the tube radius because of the elongated flame shape. This regime of flame acceleration is terminated when the flame skirt touches a side wall and, consequently, the flame front decelerates, and the flame surface area decreases considerably, which is followed by formation of a cusp at the center of the flame front, which results in the inversion into a concave tulip flame shape shown in Fig. 4.2f. The flow pattern and the flame shape at different time instants are presented in Fig. 4.3. The flow is mainly directed towards the axial direction as indicated by the arrows.

Fig. 4.3: The flow pattern of a hemispherical flame (a), and a finger flame (b).

In this parametric study, the major characteristic of the described process is the flame surface area scaled by the cross-sectional area of the channel or tube, being S_w/D for the 2D planar geometry and $S_w/\pi R^2$ for the cylindrical tubes. Furthermore, the flame tip velocity, $U_{tip} \equiv dZ_{tip}/dt$, is scaled by the planar flame velocity U_f . Finally, the total burning rate in the 2D planar coordinate system is calculated as in [36]:

$$U_w = \frac{1}{\rho_f R} \int \frac{\rho_Y}{\tau_R} \exp(-E_A/R_u T) dx dz. \quad (4.1)$$

Fig. 4.4: The scaled flame surface area, S_w/D , the scaled total burning rate, U_w/U_f , the scaled flame tip velocity, $U_{tip}/\theta U_f$, and the scaled flame tip position, Z_{tip}/R versus the scaled time, $U_f t/R$ for $R = 10L_f$ in the 2D planar geometry.

The exponential increase in time of the flame surface area, the total burning rate, and the flame tip velocity is illustrated in Fig. 4.4 which demonstrates the finger flame acceleration phenomenon, starting with the expansion of the initially small hemispherical flame, including propagation of the finger flame, and ending with formation of the tulip flame. The sharp peaks of the flame surface area, the burning rate and the flame tip velocity correspond to the maximal values attained when the flame skirt contacts the wall at the scaled time instant $\tau = 0.279$.

Fig. 4.5: The scaled flame surface area, S_w/D , for $R/L_f = 10 - 20$ and $Le = 1$ in the 2D planar geometry.

Fig. 4.6: The scaled total burning rate, U_w / U_f , versus the scaled time, $U_f t / R$, for $R/L_f = 10 - 20$ and $Le = 1$ in the 2D planar geometry.

Fig. 4.7: The scaled flame tip velocity, U_{tip} / U_f , versus the scaled time, $U_f t / R$, for $R/L_f = 10 - 20$ and $Le = 1$ in the 2D planar geometry.

Fig. 4.8: Flame morphology for $R = 10L_f$ and $Le = 1$ at different time instants in the 2D planar geometry.

Fig. 4.9: Flame morphology for $R = 15L_f$ and $Le = 1$ at different time instants in the 2D planar geometry.

Figures 4.5 – 4.7 clearly show that the finger flame acceleration mechanism is practically Reynolds-independent for equidiffusive flames in 2D channels. Additionally, the scaled time instant when the flame skirt touches the wall, τ_{wall} , is almost identical for all equidiffusive flames, which means that the channel width has almost no influence on this acceleration mechanism. We next consider finger flame acceleration for the cylindrical axisymmetric geometry with the tubes of radii $R = 20L_f$ and $30L_f$ respectively. Figure 4.10 shows the scaled flame surface area and the scaled flame tip position versus the scaled time τ for $R = 20L_f$ and $30L_f$. One can see that a flame propagates faster and acquires higher exponential stage of acceleration in the cylindrical tubes than

in the 2D planar channels. These flames are also more corrugated, thus consuming more fresh fuel per unit time. Another distinctive feature of flame acceleration in the cylindrical geometry is that the sharp peak of the maximal scaled surface area is followed by an almost planar flame, which collapses to form a tulip flame after the scaled time of $\tau \approx 0.08$.

Fig. 4.10: The scaled flame surface area, $S_w / \pi R^2$ (a), and the scaled flame tip position, Z_{tip} / R (b), versus the scaled time, $U_f t / R$, in the cylindrical axisymmetric geometry.

Fig. 4.11: Flame morphology for $R = 20L_f$ and $Le = 1$ at different time instants in the cylindrical axisymmetric geometry.

4.1.2 Non-equidiffusive flame propagation ($Le > 1$)

This subsection studies non-equidiffusive flames for the Lewis number exceeding unity, which implies a dominance of the thermal diffusivity over the mass diffusivity. Specifically, the dynamics of non-equidiffusive flames is scrutinized for half-width $R/L_f = 10, 15, 20$ in the 2D geometry and in a tube of radii $R/L_f = 20$ and 30 in the cylindrical axisymmetric configuration with $Le = 1.5$ and $Le = 2$, respectively. Figures 4.12 and 4.13 demonstrate the dynamics and morphology of non-equidiffusive finger flames. One can see that these flames accelerate slower due to the effect of the flame front thickening and the reduction of the flame elasticity. Furthermore, the high thermal diffusivity effect can be seen from the heated localized regions, mainly, at the side walls and then at the flame tip after formation of the tulip flame.

Fig. 4.12: Temperature snapshots of finger flame acceleration for $R = 20L_f$ and $Le = 1.5$ at different time instants in the 2D planar geometry.

Fig. 4.13: Temperature snapshots of finger flame acceleration for $R = 15L_f$ and $Le = 2$ at different time instants in the 2D planar geometry.

Fig. 4.14: The scaled flame surface area, S_w/D (a), the scaled total burning rate, U_w/U_f , (b), the scaled flame tip position, Z_{tip}/R , (c), and the scaled flame tip velocity, U_{tip}/U_f , (d), versus the scaled time, $U_f t/R$, for $Le = 2$ in the 2D planar geometry.

Fig. 4.15: The scaled flame surface area, S_w/D (a), the scaled total burning rate, U_w/U_f (b), the scaled flame tip position, Z_{tip}/R (c), and the scaled flame tip velocity, U_{tip}/U_f , (d) versus the scaled time, $U_f t/R$, for $Le = 1.5$ in the 2D planar geometry.

As shown in Figures 4.12 and 4.13, the channel width for non-equidiffusive flames has an impact on the exponential growth of the flame surface area such that flames in narrower channels acquire less exponential growth of the surface area and the total burning rate as compared to wider channels. These results are associated with the fact that the thickness of the flame front grows as Le increases. On the other hand, for non-equidiffusive flames with $Le > 1$ in the cylindrical axisymmetric geometry, the flame front curvature still acquires some corrugation during the acceleration scenario. In contrast, the acceleration rate is not as high as that for the equidiffusive flame due to the flame front thickening. Figures 4.16 – 4.21 illustrate the finger flame acceleration mechanism for $Le = 1.5$ and $Le = 2$.

Fig. 4.16: Flame morphology for $R = 20L_f$ and $Le = 1.5$ at different time instants in the cylindrical axisymmetric geometry.

Fig. 4.17: Flame morphology for $R = 30L_f$ and $Le = 2$ at different time instants in the cylindrical axisymmetric geometry.

Fig. 4.18: The scaled flame surface area, $S_w/\pi R^2$, versus the scaled time, $U_f t/R$, for $Le = 1.5$ in the cylindrical axisymmetric geometry.

Fig. 4.19: The scaled flame tip positions, Z_{tip}/R , versus the scaled time, $U_f t/R$, for $Le = 1.5$ in the cylindrical axisymmetric geometry.

Fig. 4.20: The scaled flame surface area, $S_w/\pi R^2$, versus the scaled time, $U_f t/R$, for $Le = 2$ in the cylindrical axisymmetric geometry.

Fig. 4.21: The scaled flame tip positions, Z_{tip}/R , versus the scaled time, $U_f t/R$, for $Le = 2$ in the cylindrical axisymmetric geometry.

4.1.2 Non-equidiffusive flame propagation ($Le < 1$)

In this subsection, non-equidiffusive fuel mixtures where the mass diffusivity is higher than the thermal diffusivity, such that $Le < 1$ are examined. Specifically, the cases of $Le = 0.2$ and $Le = 0.5$ are considered. It is observed that such flames accelerate much faster as compared to the $Le \geq 1$ flames. The hemispherical flame expands axially, where the flame surface area, the flame tip velocity, and the total burning rate grow exponentially promoting acceleration. The acceleration regime ends when the flame skirt touches the wall. The flame subsequently decelerates and, eventually, forms a concave, tulip shape where the upper and lower crests almost exhibit flame channeling this time. Another interesting stage of flame acceleration occurs when a secondary finger-like-shaped flame is formed. The latter effect is presumably related to the onset of the diffusional-thermal instability. The following figures demonstrate flame propagation for $R = 10 L_f$ and $R = 15 L_f$ with $Le = 0.2$ and $Le = 0.5$.

Fig. 4.22: Finger flame evolution for $R = 10L_f$ and $Le = 0.2$ at different time instants in the 2D planar geometry.

Fig. 4.23: Finger flame evolution for $R = 15L_f$ and $Le = 0.2$ at different time instants for the 2D planar geometry.

Fig. 4.24: The scaled flame surface area, S_w/D (a), the scaled total burning rate, U_w/U_f (b), the scaled flame tip position, Z_{tip}/R (c), and the scaled flame tip velocity, U_{tip}/U_f (d), versus the scaled time, $U_f t/R$, for $Le = 0.2$ in the 2D planar geometry.

Fig. 4.25: The scaled flame surface area, S_w/D (a), the scaled total burning rate, U_w/U_f (b), the scaled flame tip position, Z_{tip}/R (c), and the scaled flame tip velocity, U_{tip}/U_f (d), versus the scaled time, $U_f t/R$, for $Le = 0.5$ in the 2D planar geometry.

Figures 4.24 and 4.25 illustrate the minor effect of gradually increasing the width of the channel on $Le < 1$ flames. It is further noted that the second stage of finger acceleration might be related to the diffusive properties of the non-equidiffusive flames by means of the thermal and mass diffusivities. Moreover, similar to the first stage, the second stage of finger acceleration is also limited in time with less exponential growth rate of the surface area and the total burning rate.

In summary, the multiple stages of the acceleration scenarios for both equidiffusive and non-equidiffusive hydrocarbon flames have been identified. It is demonstrated that the Lewis number plays a significant role. Specifically, due to a thickening of the flame front for $Le > 1$, such a flame accelerates slower than the respective equidiffusive flame. Additionally, the impact of the flame thickening on flame propagation is coupled to the Reynolds number through the increase of the width in 2D channels. It is shown that $Le > 1$ flames accelerate slower with less exponential growth of the flame surface area and the total burning rate. On the other hand, the $Le < 1$ flames acquire the highest acceleration rate as compared to the $Le \geq 1$. The distortion of the tulip flame is followed by acceleration of an intriguing second phase of a finger-like flame propagation, which may be attributed to the diffusional-thermal instability. Figures 4.26 and 4.27 compare the flame surface area and the total burning rate for the Lewis numbers in the range $0.2 \leq Le \leq 2$ for the half-widths of $R = 10 L_f$ and $R = 15 L_f$. Figure 4.28 presents the scaled flame surface area and the scaled flame tip position for the tube of radius $R/L_f = 30$ for the axisymmetric configuration.

Fig. 4.26: The scaled flame surface area, S_w/D (a), and the scaled total burning rate, U_w/U_f (b), versus the scaled time, $U_f t/R$, for $R = 10 L_f$ in the 2D planar geometry.

Fig. 4.27: The scaled flame surface area, S_w/D (a), and the scaled total burning rate, U_w/U_f (b), versus the scaled time, $U_f t/R$, for $R = 15 L_f$ in the 2D planar geometry.

Fig. 4.28: The scaled flame surface area, $S_w/\pi R^2$ (a) and the scaled flame tip position, Z_{tip}/R (b), versus the scaled time, $U_f t/R$, for $R = 30 L_f$ in the cylindrical axisymmetric geometry.

4.2. Impact of boundary conditions on finger flame acceleration

Thermal and mechanistic boundary conditions belong to the key factors providing a remarkable impact on the dynamics and morphology of a flame front. Specifically, the role of wall heat losses increases with the decrease in the channel size, which makes the effect particularly essential for micro-combustors. Furthermore, both wall friction and the heat transfer through the combustion system directly deform the flame front, thereby the surface area of the flame and the burning rate dramatically increase. Therefore, the flame consumes more fuel per unit time and propagates faster. The following studies examine these parameters under various conditions, to fully identify their effect. Specifically, the wall temperature is held constant with slip and non-slip walls. The channel width is fixed as $R = 20 L_f$ and, unlike section 4.1, the Lewis number is taken to be unity ($Le = 1$) to avoid the diffusional-thermal instability. Finally, the wall temperature is varied in the range $300 K \leq T_w \leq 1200 K$.

4.2.1 Slip and isothermal walls at low temperature

When the combustor walls are maintained at a constant temperature of $300 K$, the heat exchange occurs when the burnt matter expands, and the heat is transferred from the combustor to the environment through the cold walls. The heat loss causes the flame skirt to cool down where the region of the heat is localized in the flame tip. A typical finger flame acceleration scenario in a 2D channel with slip and isothermal walls is shown in Fig. 4.29. It is seen that the hemispherical flame expands whereas its surface area and the total burning rate increase exponentially until the flame skirt touches the side walls and the heat loss cools down the flame, such that the flame front surface area and the total burning rate then decrease dramatically. Formation of the tulip flames is followed by appearance of a quasi-planar flame which then collapses to acquire a curved convex shape of the front, presumably, because of the DL instability [8]. Figure 4.30 illustrates the scaled flame surface area, the scaled total burning rate, as well as the velocity and position of the flame tip versus the scaled time.

Fig. 4.29: Flame evolution for slip isothermal walls at $T_w = 300\text{ K}$.

Fig. 4.30: The scaled flame surface area, S_w/D , and the scaled total burning rate, U_w/U_f , versus the scaled time, $U_f t/R$, at $T_w = 300\text{ K}$.

4.2.2 Slip and nonslip isothermal walls at high temperatures

In this subsection, the finger flame acceleration mechanism is examined for hot isothermal walls at two different wall temperatures, namely, $T_w = 500\text{ K}$ and $T_w = 800\text{ K}$, considering both mechanistic boundary conditions, slip and non-slip. Referring to the flame evolutions shown in Figs. 4.31 and 4.32, typical finger flame acceleration was observed. The flame front exhibits similar behavior for slip and non-slip boundary conditions; thus, the effect of the mechanistic boundary conditions is concluded to be minor and can be neglected in the early stages of burning. This is mainly because a hemispherical flame embryo expands and accelerates to acquire a pointing finger-shaped flame far from the side walls. It is further noted that due to the walls heat loss, the flame skirt will be cooled down after contacting the side walls, while the heat is localized in the flame tip. Moreover, one can point out that the curvature of the flame front is more corrugated for

non-slip walls due to friction between the flame and the side walls, for which the flame surface area and the burning rate are slightly higher than that with freely-slip walls. Figures 4.33 and 4.34 compare the scaled surface area and the scaled total burning rate versus the scaled time τ for the channel half-width $R = 20 L_f$ with slip and non-slip isothermal walls.

Fig. 4.31: Flame evolution for slip isothermal walls at $T_w = 500 \text{ K}$.

Fig. 4.32: Flame evolution for non-slip isothermal walls at $T_w = 800 \text{ K}$.

Fig. 4.33: The scaled flame surface area, S_w/D , versus the scaled time, $U_f t/R$, for slip and non-slip isothermal walls, with $T_w = 500 \text{ K}$ and 800 K .

Fig. 4.34: The scaled total burning rate, U_w / U_f , versus the scaled time $U_f t / R$, for slip and non-slip isothermal walls, with $T_w = 500\text{ K}$ and 800 K .

4.2.3 Nonslip isothermal walls at very high temperature

In this subsection, non-slip isothermal walls at a very high constant wall temperature, $T_w = 1200\text{ K}$, are employed. It is observed that such hot walls provide several interesting features that qualitatively influence the flame dynamics and morphology. Specifically, as soon as the flame embryo is ignited and expands toward the open end of the channel, additional flame front segments are formed at the pre-heated walls. The fundamental cause of this phenomenon is the hot regions near the side wall, which can initiate and facilitate the combustion process. The expansion of the ignited flame at the centerline is accompanied by a formation of a finger-shaped flame, while the flame segments near the walls also propagate with an increase in the acceleration rate and the total burning rate. Once the flame segments merge with the flame tip, the flame surface area and the total burning rate decrease, after which the flame front acquires a corrugated tulip shape. One can also observe that heat is localized at the walls due to wall friction. Also, the flame skirt is cooled down due to the heat loss at the walls. The following figures demonstrate the temperature evolution of the flame front as well as the scaled total burning rate for non-slip, isothermal walls at $T_w = 500\text{ K}$, 800 K , and 1200 K .

Fig. 4.35: Flame evolution for non-slip isothermal walls at $T_w = 1200K$.

Fig. 4.36: The scaled total burning rate, U_w / U_f , versus the scaled time $U_f t / R$, for non-slip isothermal walls at $T_w = 500 K$, $800 K$, and $1200 K$.

In summary, the impact of the mechanistic boundary conditions with the account for isothermal walls is scrutinized and quantified for different scenarios. We started with freely-slip isothermal walls at $T_w = 300\text{ K}$, where the heat loss can be seen clearly as the flame skirt cools down and the heat is mainly localized in the flame tip. Finger flame acceleration can be described here as a sequence of four stages, namely: (i) expansion of a hemispherical flame at the initial stage of burning, (ii) elongation and acceleration of a finger flame, (iii) deceleration of the flame and its convex-to-concave inversion, and finally, (iv) cooling down of the flame skirt due the heat loss to the side walls, while the flame tip accelerates again and acquires a curved shape again. Similar scenarios were observed for slip and non-slip preheated isothermal walls, where the effect of the mechanistic boundary conditions can be negligible, especially at the early stages of burning, and/or until the flame skirt contacts the side walls. Finally, for preheated walls at very high temperatures such as $T_w = 1200\text{ K}$, the flame surface area and the total burning rate grow rapidly as a result of formation of the secondary flame segments at the wall. Then a flame propagates with an “octopus” shape until the segments merge with the flame tip to form a tulip flame.

4.3 Finger flame acceleration and DDT

This supplementary section is devoted to examining finger flames in the case of artificially high laminar flame velocity, U_f . This is because a spontaneous transition from a subsonic deflagration to a supersonic detonation is often observed experimentally for flame propagation in tubes. The following figures demonstrate acceleration of initially hemispherical flames under three different conditions. First, a non-equidiffusive flame ($Le = 0.5$) and non-slip adiabatic walls are chosen; the second condition is for an equidiffusive flame ($Le = 1$) with ideally-slip adiabatic walls; and, lastly, a flame with $Le = 2$ and non-slip adiabatic walls is considered. It is seen that all these flames accelerate fast enough to trigger detonation because of the initially high (artificial) U_f . The hemispherical flame embryo expands spontaneously in these cases and after it touches the wall, the flame then experiences intense distortion of the front, where three crests are formed, in which the upper and lower crests accelerate and take over to acquire a tulip flame with a high acceleration rate such that the accelerating flame pushes the compressed waves and weak shocks into the fresh gaseous mixture where these waves then get stronger to heat the fuel mixture, leading to an explosion that eventually is followed by the detonation initiation.

Fig. 4.37: A DDT for $Le = 0.5$ and $R = 20 L_f$ with non-slip adiabatic walls.

Fig. 4.38: A DDT for $Le = 1$ and $R = 20 L_f$ with slip adiabatic walls.

Fig. 4.39: A DDT for $Le = 2$ and $R = 20 L_f$ with non-slip adiabatic walls.

It is shown that increasing the planar flame velocity such that $U_f \approx 70$ m/s and $Ma = U_f/c_s = 0.2$ will initiate shock waves that trigger detonation for both equidiffusive and non-equidiffusive flames. Also, the boundary conditions do not play a noticeable role, since detonation waves were observed for both slip and non-slip walls. Furthermore, as a flame accelerates and pushes the flow, the fuel mixture is preheated by the shock waves, thus the temperature of the burnt matters increases drastically, which leads to an explosion and, eventually, detonation. The heated zones in Figs. 4.37 – 4.39 demonstrate the localized explosions followed by the detonation.

Chapter 5: Summary and Conclusion

The effect of the Lewis number as well as the impacts of the mechanistic and the thermal boundary conditions on finger flame acceleration have been investigated by performing computational simulations of the reacting flow equations with fully-compressible hydrodynamics, transport properties and one-step Arrhenius chemical kinetics. First, the effect of the Lewis number was investigated in the domain of $0.2 \leq Le \leq 2$ for various channel widths and tube diameters with freely-slip adiabatic walls employed. It is demonstrated that the Lewis number influences flame acceleration substantially. Specifically, due to the flame front thickening, non-equidiffusive flames with $Le > 1$ propagate slower than that $Le = 1$ flames. In contrast, as the Lewis number decreases, the flames acquire stronger distortion such that the flame surface area and, respectively, the total burning rate increase exponentially in the limited time interval lasting until the flame skirt touches the side walls.

Moreover, the impact of the isothermal walls and the mechanistic boundary conditions have been thoroughly studied. Specifically, to identify the effect of wall friction as well as the impact of heat loss through the combustor walls, the slip and non-slip walls were employed, as well as the isothermal walls, with a constant walls temperature in the range $300\text{ K} \leq T_w \leq 1200\text{ K}$. It is observed that the wall boundary conditions have a minor effect on the finger flame acceleration mechanism. This can be explained by the nature of flame propagation, where the flame front expands and propagates away from the side walls. However, once the flame front contacts the side walls, the impact of wall friction can be seen through the slight increase in the flame surface area and the total burning rate as well as from the corrugated tulip flames. Also, the effect of heat transfer can be seen in the latter stages of the burning process when the flame front acquires a pointing backward cusp, where the flame skirt cools down as a result of the heat transfer through the walls. It is further noted that at very high temperatures, the walls will heat the fresh combustible mixture to initiate secondary flame segments. The ignited flame will propagate towards the open end, until the secondary flame segments merge with the flame tip into a unified flame front, which then decelerates to form a tulip flame.

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