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Stabilisation of Laminar Premixed Methane/Air Flames

R.M.M. Mallens
Stabilisation of Laminar Premixed Methane/Air Flames

PROEFSCHRIFT

ter verkrijging van de graad van doctor aan de Technische Universiteit Eindhoven, op gezag van de Rector Magnificus, prof.dr. M. Rem, voor een commissie aangewezen door het College van Dekanen in het openbaar te verdedigen op vrijdag 13 december 1996 om 16.00 uur

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Chapter 1

Introduction

1.1 Prologue

Laminar flame stabilisation in small-scale combustion equipment has become an important issue of study in the past decades. Up to some years ago the fuel/air mixture in small-scale combustion equipment was only partially premixed at the burner ports, i.e. the mixture flowing through the burner ports contains not enough oxygen to burn all the fuel. The partially unburnt hydrocarbons still present in the mixture after the primary premixed flame are burnt with oxygen from the ambient air in a secondary diffusion flame. The mixing rate of the oxygen in the ambient air with the partially unburnt hydrocarbons, which determines the burning rate of the diffusion flame, increases with the outflow velocity from the burner. This minimises the danger of blow-off of such flames. Flash-back is also very unlikely to occur because the mixture flowing out of the burner is fuel rich and, therefore, has a low burning velocity. Thus the flames are relatively stable. Another important advantage of these burners is their simple (and cheap) construction. The burners, however, operate at atmospheric pressure which hampers their application in modern domestic high-efficiency boilers with a relatively high flow resistance of the large heat exchangers.

The introduction of high efficiency boilers led to a need for burners with a forced air supply (forced draft burners), operating at slightly over-atmospheric pressures. The mixture composition is controllable because the amount of air which is premixed with the fuel can be adjusted. This facilitates the reduction of $NO_x$ and $CO$ emissions. Generally, lean fuel/air mixtures are used in modern boilers. The use of lean mixtures results in a complete combustion (low $CO$-emission) at a relatively low flame temperature (low $NO_x$-emission). The burning rate of the fuel-lean flames is determined by chemical reaction kinetics with much smaller time scales than the mixing processes which determine the mass burning rate of diffusion flames, like the secondary flame on atmospheric burners. This results in higher burning velocities and a higher sensitivity for flash-back for the premixed flames. Compared to diffusion flames, the mixing with ambient air at high burner exit velocities leads to lower fuel concentrations in the (partially) unburnt mixture. The lower fuel concentration causes lower mass burning rates. This means that lean premixed flames tend to blow-off at lower mixture velocities than diffusion flames. Therefore, the changes in burner design used to meet the emission reduction demands can endanger the stabilisation of
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the premixed flames.

Fully premixed flames can show various kinds of instabilities. The flame front can show oscillatory motions induced by, for example, hydrodynamic and/or diffusional-thermal instabilities (see e.g. Clavin (1985) or Law (1988)). These instabilities may lead for instance to cellular flames. The oscillating flame fronts can also generate noise, which is unwanted in modern heating equipment.

Steady flames may also show stabilisation problems, such as quenching, flash-back and blow-off. As explained above, premixed flames are much more sensitive to flash-back and blow-off than diffusion - or partially premixed flames. The stabilisation of steady premixed laminar flames is complex because it is affected by numerous physical processes, such as cooling by the burner wall and the surrounding, mixing of the combustible mixture with surrounding gases, flame stretch, flame curvature and local flow straining. It is, however, not well known to what extent the various processes affect the stabilisation of laminar flames and what their relative importance is. To answer these questions detailed investigations of the local flow field and flame structure are necessary. Another area which requires further investigation is the difference between the stabilisation of flames on slit burners as compared to the stabilisation on tube burners.

The aim of the research described in this thesis is to formulate a description and explanation of the effects of various phenomena on steady laminar premixed flames and their stabilisation on slit burners as well as on tube burners. The contents of this thesis will be restricted to the stabilisation, flash-back and blow-off behaviour of steady two-dimensional methane/air flames. Numerical simulations are used to facilitate a detailed and systematical investigation of the various
1.2. Stabilisation of One-Dimensional Flames

Phenomena.

Fig. 1.2: A scheme of a burner stabilised flat flame. The velocity and temperature in the unburnt mixture are \( u_u \) and \( T_u \), respectively; the burning velocity and flame temperature are equal to \( S_L \) and \( T_b \), respectively. Both \( S_L \) and \( T_b \) are smaller than their adiabatic values \( (S_{L,ad} \) and \( T_{ad} \).

In the remainder of this chapter we will first discuss some basic mechanisms of steady flame stabilisation described in the literature. The aim of these sections is not to give a full review of the work on flame stabilisation described in the literature. We will limit ourselves to the theories or quantities which are most important within the scope of this thesis. Relevant work done by other researchers will be treated in the appropriate chapters of this thesis. An outline of the thesis will be given in the last section.

1.2 Stabilisation of One-Dimensional Flames

One-dimensional flames are discussed in detail by de Lange (1992) and Somers (1994). We will therefore focus only on some properties of one-dimensional flames which are useful for the understanding of the stabilisation of two-dimensional flames.

A scheme of an adiabatic one-dimensional flame is given in figure 1.1. Figure 1.1 also shows the schematic profiles of the fuel and oxygen mass fractions \( Y_{fu}, Y_{ox} \) and the temperature \( T \). The mixture upstream of the reaction zone is heated by conduction in the preheat zone. The reactants fuel and oxygen are transported to the reaction zone by convection and diffusion. The burning velocity of the flame in figure 1.1 with respect to the unburnt mixture, the adiabatic burning velocity \( S_{L,ad} \), only depends on the type of fuel, the unburnt mixture composition, the temperature and the pressure. The flame is at rest with respect to a fixed reference frame if the mixture velocity \( u_u = S_{L,ad} \). Now consider figure 1.2 where a cold porous or perforated plate is
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Fig. 1.3: A photograph of a laminar Bunsen flame on a tube burner with particle tracks indicating the stream lines. The equivalence ratio is 0.9 and the velocity profile at the burner exit is parabolic with a maximum velocity of 0.9 m/s.

Put upstream of the flame. The flame can now also stabilise when \( u_u < S_{L,ad} \) due to heat loss to the burner surface. The heat loss to the burner results in a lower flame temperature \( T_b \) and thus in a lower burning velocity \( S_L \). The heat produced by the flame is transported to the burner surface by conduction. The stabilisation mechanism for this flame is based on flame cooling. The flame in figure 1.2 is referred to as a burner-stabilised flame. Note that the flame blows off when \( u_u > S_{L,ad} \).

1.3 Stabilisation of Two-Dimensional Bunsen Flames

In this section theories and quantities developed or defined by other authors will be used to explain the basic principles of the stabilisation of two-dimensional flames. Only the theories and quantities which are most important in the context of this work will be discussed in this section.

\(^1\)Note that axisymmetrical (cylindrical) flames can also be described as two-dimensional flames (from a mathematical point of view) because they can be described by two independent coordinates.
1.3. Stabilisation of Two-Dimensional Bunsen Flames

fig. 1.4: A schematical view of a burner wall with the profiles of the mixture velocity ($u_\delta$) and burning velocity ($S_L$). Three flame positions (1, 2 and 3) relative to the burner are depicted.

We refer to the appropriate chapters of this thesis (see section 1.5) for further discussion about these theories and the assumptions they contain.

1.3.1 The Gradient Theory.

One of the first extensive theoretical and experimental investigations of the stabilisation and structure of laminar natural gas flames on tube burners was carried out by Lewis and von Elbe (1943). Methane and propane flames on tube burners were studied subsequently by Harris et al. (1949). These investigations mainly focus on the stabilisation of the flame base on a burner wall. A picture of a Bunsen flame on a tube burner is given in figure 1.3.

First, a short description will be given of the stabilisation theory developed by Lewis and von Elbe, the so-called gradient theory (see fig. 1.4). This theory starts with the assumption that the mixture velocity ($u_\delta$) profile near the wall is linear, which is valid for large burners (see chapter 4). The wall not only reduces the mixture velocity by friction, also the burning velocity near the wall is reduced by the destruction of chain carriers and cooling, especially for cold burner walls. The burning velocity is zero near the wall and then gradually increases to its undisturbed value. The profiles of the mixture velocity and the burning velocity are given in figure 1.4 for three flame positions. When the mixture velocity exceeds the burning velocity everywhere (position (1)) the flame moves upward, out of the burner. This decreases the quenching effect of the wall which causes the flame to move towards the wall (position (2)) until $S_L$ equals the mixture velocity $u_\delta$ in a point near the wall. A flame position (at the same mixture velocity) somewhat higher above the burner (position (3)) leads to a further decrease of the quenching effect near the wall and a subsequent increase of the burning velocity near the wall. The burning velocity now exceeds the mixture velocity somewhere near the wall. This causes a downward movement of the flame, again until the stable position (2) is reached.

The mixture velocity at larger distances from the wall, however, still exceeds the maximum burning velocity at distances from the wall which are larger than $\delta_q$. In this area the flame is able to stabilise by tilting until the magnitude of the component of the mixture velocity perpendicular
Chapter 1. Introduction

fig. 1.5: Flame stabilisation at the flame sides through flame tilting. The mixture velocity \( u_g \) is shown with its components parallel and perpendicular to the local flame front. The dotted lines denote the flame; the drawn lines with arrows indicate stream lines which bend near the flame front due to thermal expansion.

to the local flame front is equal to the burning velocity \( S_L \) (see fig. 1.5). This implies that the burning velocity of a two-dimensional flame can be defined as a vector perpendicular to the local flame front (directed towards the unburnt mixture) with a magnitude \( S_L \). This explains the typical cone-shaped structure of Bunsen-type flames on rectangular slit burners and tube burners.

1.3.2 Flame Stretch and Curvature

In the gradient theory it is assumed that changing stream tube areas or velocity gradients in the unburnt mixture have no effect on the local burning velocity, which is justified when changes in the mass flux or stream tube area near the flame front can be neglected. It is, however, apparent from figure 1.3 and 1.5 that the stream tube area does change through the flame front. Several authors conducted theoretical investigations of the effect of varying stream tube areas on the propagation velocity of premixed flames. The most important results of these investigations will be discussed in this subsection to show which quantities can affect the stream tube area and the propagation velocity. A detailed analysis of the effects mentioned above is given in chapter 6 and 7. For the adiabatic one-dimensional flame described in the previous section, the mass flux perpendicular to the flame front is equal to \( \rho_u S_{L,ad} \) with \( \rho_u \) the density in the unburnt mixture. Note that \( S_{L,ad} \) is the maximum burning velocity for the one-dimensional flame. A changing stream tube area can be caused by velocity gradients along the flame front. The effect of a velocity gradient on the burning velocity of an adiabatic flame has been investigated by Karlovitz (1953). He showed that the burning velocity for a flame stretched by a velocity gradient can be higher than \( S_{L,ad} \), thus enabling the flame to stabilise for higher velocities upstream of the flame. Karlovitz investigated a flat flame in a flow with a uniform velocity gradient \( \partial u / \partial y \) (figure 1.6) and a reference velocity
1.3. Stabilisation of Two-Dimensional Bunsen Flames

fig. 1.6: A flame front in a flow field with a uniform velocity gradient, as used by Karlovitz. The position where \( y = \eta = 0 \) is situated at the ignition point. The velocity \( u \) as a function of \( y \) is given in the lower left corner.

\( U \) at the ignition point \((y = \eta = 0)\). The mass flux perpendicular to the flame just ahead of the preheat zone (with \( u(y) = U + (\partial u/\partial y)y \) and \( y = \eta \cos \alpha \)) is then equal to:

\[
\rho_u u_\eta = \rho_u u \sin \alpha = \rho_u U \sin \alpha + \rho_u \frac{\partial u}{\partial y} \eta \cos \alpha \sin \alpha.
\]

With the angle of the flame front with the \( x \) axis very small \((\cos \alpha \approx 1)\) and \( \sin \alpha = S_{L,ad}/U \), it can be shown that the local mass flux perpendicular to the flame \( \rho_u u_\eta \) is equal to:

\[
\rho_u u_\eta = \rho_u S_{L,ad} \left[ 1 + \frac{K_A \eta}{S_{L,ad}} \right], \tag{1.1}
\]

with:

\[
K_A = \frac{S_{L,ad}}{U} \frac{\partial u}{\partial y}. \tag{1.2}
\]

Note that, in the description of Karlovitz, the mass flux at the ignition point \((\eta = 0)\) is equal to \( \rho_u S_{L,ad} \). Just upstream of the preheat zone \((\eta > \eta_p)\) the mass flux is larger than its adiabatic value (for the configuration shown in figure 1.6) which implies that the mass burning rate \( \rho_u u_\eta \) defined in the unburnt mixture is larger than \( \rho_u S_{L,ad} \).
Karlovitz also showed that the so-called stretch factor $K_A$ (the subscript $A$ refers to the definition by Karlovitz) can be interpreted as the relative change $dA$ of the stream tube area $A$ through the flame:

$$K_A \equiv \frac{1}{A} \frac{dA}{dt} = \frac{\partial u}{\partial \xi},$$

(1.3)

with $dt$ the time in which the area $A$ moves through the flame front. $K_A$ can be interpreted as the derivative with respect to $\xi$ of the velocity component parallel to the flame front ($\partial u_\xi/\partial \xi$) for $\cos \alpha \approx 1$ (this implies $u \approx u_\xi$).

An important assumption in the work of Karlovitz is the neglect of flame curvature and the observation that the burning velocity of a flame can only be modified by velocity gradients parallel to the flame. From a phenomenological point of view it can be argued that flame curvature also modifies the burning velocity, as it also leads to a change of stream tube area. This was shown by Markstein (1951), who assumed that only flame curvature is responsible for the modification of the local burning velocity. The different views of Markstein (1951) and Karlovitz were reconciled by Matalon and Matkowsky (1982) and Clavin and Joulin (1983) who showed that the local burning velocity is controlled by both curvature and velocity gradients. It can, in fact, be shown that the gradient $\partial u_\xi/\partial \xi$ contains a velocity gradient and a curvature part for a curved flame in a non-uniform flow (also see chapter 6 and 7).

In the previous subsection the stabilisation of a Bunsen flame on a burner wall and at the flame sides was explained with the gradient theory. The stabilisation of a Bunsen flame at the tip, however, cannot be explained with the gradient theory because the flame front is not tilted in the tip and the upstream mixture velocity is much higher than $S_{L,ad}$. The flame front in the tip (see fig. 1.3) is strongly curved and stretched. The theory discussed above may explain the stabilisation of the flame in the tip because the curvature of the tip may lead to much higher burning velocities. This might enable the stabilisation of the tip.

The investigations by Clavin and Joulin (1983) and Matalon and Matkowsky (1982) (based on large activation energy asymptotics) only yield linearised expressions for weak stretch. Chung and Law (1988) present a physically more transparent analysis in which equations for stretch and curvature effects on the local burning velocity (defined both on the burnt and the unburnt side) are derived by using an integral analysis on a flame with a finite thickness. The effects of stretch and curvature on the stabilisation of the tip of a Bunsen flame and on the stabilisation of a V-shaped flame is investigated in chapter 6 and 7.

1.3.3 The effect of preferential diffusion

The effects of stretch on the burning velocity described in the previous subsection are caused by stream tube area changes. The burning velocity of a stretched flame can also be modified by the diffusion processes of heat and species in the preheat zone, or more specifically by the misalignment of the diffusive and convective transport processes. This is illustrated in figure 1.7. The area of the stream tube is increasing in flow direction which results in a positive stretch. The arrows indicating the diffusion of reactants (upstream) and heat (downstream) show that there is diffusion of heat and mass in and out of the stream tube, respectively. When the diffusivities of heat ($D_T$) and mass ($D_M$) are not equal, the stream tube (and the flame) will lose or gain energy
and this, in turn, will modify the flame temperature and the burning velocity. This effect is referred to as preferential diffusion. The Lewis number (equal to $D_T/D_M$) can be used to quantify the effect of preferential diffusion. For the mass diffusivity the diffusivity of the deficient reactant can be taken, as the concentration of this reactant is rate-limiting.

1.4 Flash-back and blow-off

Part of the research described in this thesis concerns flash-back and blow-off of premixed Bunsen flames. In this section the most important physical phenomena involved in flash-back and blow-off of Bunsen flames will be discussed to clarify the various research topics which are treated in this thesis. We will use the gradient theory to explain the processes of flash-back and blow-off.

Flash-back occurs at low mixture velocities. When, starting from situation (2) in figure 1.4, the mixture velocity is decreased so much that the burning velocity becomes higher than the mixture velocity near the wall, the flame will move into the burner (towards position (1)) and the cooling rate by the burner wall will increase. The flame will eventually flash-back into the burner port if the mixture velocity becomes so low that the burning velocity exceeds the mixture velocity somewhere near the wall where the flame is less influenced by cooling. The velocity gradient $\partial u_b/\partial x$ at the wall at which this happens is referred to as the critical flash-back gradient $g_f$. If the burner width or diameter is smaller than twice the quenching distance ($2\delta_q$) the flame will be quenched by the burner wall before it flashes back. In practice, the burner ports are often made smaller than twice the quenching distance so that flash-back can't occur.

The flame will move away from the burner when, again starting from situation (2), the mixture velocity is increased. This leads to an increasing burning velocity, caused by the decreased cooling
by the burner wall, until a new equilibrium position is reached. This, however, cannot be continued indefinitely because the burning velocity still decreases to zero at the boundary of the mixture stream flowing from the burner, especially if the surrounding gas acts as a diluent. Therefore, at some mixture velocity the flame will blow-off. When the surrounding gas enriches the mixture (e.g. fuel rich flames burning in air) the burning velocity at the boundary of the mixture stream becomes higher which leads to a higher blow-off velocity.

The velocity gradient at the burner wall corresponding to the blow-off velocity is referred to as the critical blow-off gradient $g_b$. Blow-off is more complex than flash-back because it is governed by more phenomena. Beside the effects of the surrounding atmosphere, flame stretch and curvature effects may play an important role because of the high velocities and velocity gradients which are involved.

1.5 Outline

In this section the contents of the thesis will be discussed. Much of the research described in the thesis is performed by numerical modelling. The model used for the numerical investigations will be discussed in chapter 2.

The presence of a surrounding atmosphere is important when investigating the stabilisation of laminar flames. The rate of cooling by and mixing with the surrounding atmosphere is especially important near blow-off. The degree of confinement caused by the surrounding also influences the stabilisation through its effect on the flow field near the flame zone. In chapter 3 a model for two-dimensional Bunsen flames on slit burners and on tube burners burning in an atmosphere of cold air and an investigation of the effects of confinement is presented. The model will be validated by comparing modelling results for flames burning in an atmosphere of cold air with experimental results. The discussion of the stabilisation mechanisms in section 1.2 and 1.3 indicates the importance of energy transport in the preheat and reaction zone for the stabilisation of premixed flames. The effects of a surrounding atmosphere on the energy transport in two-dimensional flames will, therefore, also be investigated in chapter 3. First, the energy transport in a one-dimensional flame described by our global chemical model is compared with results obtained with skeletal chemistry by Smooke (1991) to determine how the energy transport predicted by our chemical model relates to the energy transport predicted by a more complex chemical scheme. The modelling results for the two-dimensional flames are then used for an investigation of the effects of confinement on the flame shape, the mass flux along the centreline and the energy transport.

Flash-back of flames on slit and tube burners is investigated in chapter 4. Numerical results for the velocity gradient at the burner wall at the point of flash-back are compared with experimental results. Differences between tube and slit burners and the effects of burner size are also investigated.

M-shaped and V-shaped flames and their blow-off behaviour are investigated in chapter 5. Photographs of an M- and a V-shaped flame are given in figure 1.8. The investigation of blow-off is started with V-shaped flames because the mixing with and cooling by the surrounding air is not important for their blow-off behaviour. The velocity gradients at the transition from an M- to a V-shaped flame and at blow-off of the V-shaped flame predicted by the model will be compared
1.5. Outline

fig. 1.8: Photographs of an M-shaped flame (*top*, mean burner exit velocity 0.53 m/s) and a V-shaped flame (*bottom*, mean burner exit velocity 0.73 m/s) for $\phi = 0.7$. 

with experimental values. Furthermore, velocity profiles measured with Laser Doppler velocimetry are compared with numerical profiles.

In chapter 6 we will investigate flame stretch and curvature and the effects of these quantities on the local value of the burning velocity. The existing expressions for flame stretch and for the effects of flame stretch and - curvature on the local burning velocity are not directly applicable to a numerical flame. This has several reasons, such as the absence of flame thickness variation effects in the existing stretch expressions and the assumption in existing theories of small stretch rates and an infinitesimal reaction zone. Therefore, a new expression for flame stretch in a flame with a finite thickness will be derived which gives additional contributions to the flame stretch due to e.g. flame thickness variations. The separate contributions are calculated in the tip of a flame on a slit burner at various inlet velocities. These calculations are used to investigate the effects of various quantities on the stabilisation mechanism of the flame tip and to calculate the effective burning velocity in the tip.

The stabilisation mechanism of V-shaped flames will be investigated in chapter 7. The relative importance of e.g. flame stretch and - curvature and cooling by the burner on the stabilisation
of V-shaped flames is still obscure. Calculations of the contributions to the flame stretch and the effective burning velocity for different flames will, therefore, be used to unravel the importance of various quantities on the stabilisation of V-shaped flames.
Chapter 2

Combustion Model

The modelling of two-dimensional flames with complex chemistry (N species) is very difficult. Beside the mixture-averaged mass -, energy - and momentum conservation equations in two directions, \( N - 1 \) conservation equations must be solved for the \( N \) species in the mixture, which results in \( N + 3 \) equations at every node of the computational domain. Calculations with many species (the combustion of methane with air involves more than 35 species) therefore require a huge memory and much computing time and is thus necessarily limited to one-dimensional or simple two-dimensional systems with a small number of grid points. For instance, two-dimensional diffusion flames with multi-step chemistry as were modelled by Smooke (1989, 1992) and Coelho (1993) take about 15 hours computing time on a Cray-2. The modelling of premixed flames is even more complex than the modelling of diffusion flames, because the burning velocity of premixed flames is determined by the details of the chemical kinetics (Somers (1993)) in the relatively thin premixed flame front. A small premixed two-dimensional methane/air flame was computed recently employing skeletal chemistry (25 reactions among 15 species, Smooke (1989)) by Somers (1995) and took about 100 hours on a Silicon Graphics Power Challenge.

Most of the results presented in this thesis are obtained with a one-step reaction mechanism. This reduces the computation times and enables us to use larger domains with more complex boundary conditions. It is shown in the following chapters that the global flame properties (such as flame shape and the flow field) and the flame stabilisation are described sufficiently accurate by this chemical model for most cases of interest. The results obtained by Somers (1995) show that the flame shape predicted by the one-step reaction mechanism doesn’t deviate more from experimental results than the flame shape predicted by the skeletal chemistry model. For a one-dimensional flame the one-step chemistry results are compared with skeletal chemistry results in chapter 3. In this way the effects of chemical kinetics on the flame structure and stabilisation can be estimated.

In the following section the physical model is discussed. In the second section the numerical method is discussed.
2.1 The physical model

In this section we will first discuss the model equations, the one-step chemical model used for most of the flame calculations and the calculation of the physical properties of the mixture. Then, the boundary conditions used in the numerical model will be presented.

2.1.1 The governing equations.

The equations describing a stationary combustion process are the conservation equations of mass, momentum, species and energy, combined with the equation of state of the system. In this section a 'coordinate free' description of the model equations is given, which is valid for both a two-dimensional cartesian \((x, y)\) and a two-dimensional cylindrical system \((r, z)\) with \(r = x\) and \(z = y\). Only relevant differences between these systems will be indicated. The stationary mass conservation equation is given by

\[
\nabla \cdot (\rho \vec{v}) = 0,
\]

with \(\rho\) the mass density of the mixture and \(\vec{v}\) the mixture velocity. The density of the mixture is defined as the summation of the densities of the \(N\) species \(i\) present in the mixture: \(\rho = \sum_{i=1}^{N} \rho_i\), while the mass averaged flow velocity is defined by

\[
\rho \vec{u} = \sum_{i=1}^{N} \rho_i \vec{v}_i,
\]

with \(\vec{v}_i\) the velocity of species \(i\) in the mixture. The \(N\) conservation equations for species \(i\) can now be formulated as

\[
\nabla \cdot (\rho_i \vec{v}_i) = \dot{\rho}_i,
\]

with \(\dot{\rho}_i\) denoting the rate of production of mass of species \(i\) due to chemical reactions. Usually a diffusion velocity \(\vec{V}_i = \vec{v}_i - \vec{v}\) and the mass fraction of species \(i\) \((Y_i = \rho_i/\rho)\) is introduced for convenience. The conservation equation for species \(i\) then becomes

\[
\nabla \cdot (\rho Y_i \vec{v}) + \nabla \cdot (\rho Y_i \vec{V}_i) = \dot{\rho}_i.
\]

The diffusion velocity of species \(i\), \(\vec{V}_i\), is determined by pressure gradients, concentration gradients of the species, temperature gradients (the so-called Soret effect) and differences in external forces (see, e.g., Bird (1960) and Williams (1988)). If, however, one component is abundant like nitrogen in the case of combustion with air, \(\vec{V}_i\) may be assumed to be proportional with the gradient of species \(i\), leading to Fick’s law. In laminar atmospheric combustion processes the diffusion due to pressure gradients, external forces and temperature gradients is small (see e.g. Somers (1994)) and is, therefore, neglected. With the above assumptions the expression for \(\vec{V}_i\) becomes

\[
Y_i \vec{V}_i = -D_{im} \nabla Y_i,
\]

with \(D_{im}\) the binary diffusion coefficient of species \(i\) in mixture \(m\) (Bird, 1960). Combining equations (2.4) and (2.5) leads to the species conservation equation which is used in this thesis

\[
\nabla \cdot (\rho Y_i \vec{v}) - \nabla \cdot (\rho D_{im} \nabla Y_i) = \dot{\rho}_i.
\]
Momentum conservation is described by the Navier-Stokes equation, given by e.g. Bird (1960). The stationary Navier-Stokes equation is given by

\[ \nabla \cdot [\rho \mathbf{v} \mathbf{v}] - \nabla \cdot \mathbf{\tau} = -\nabla p + \rho \mathbf{g}, \tag{2.7} \]

in which \( \mathbf{\tau} \) denotes the viscous stress tensor, \( p \) denotes the static pressure and \( \mathbf{g} \) denotes the gravitational acceleration vector. The use of dynamic grid refinement in our numerical method (see the following section) hampers the application of staggered grids. The numerical solution of the Navier-Stokes equations on non-staggered grids can cause checkerboard-like solutions (see e.g. Patankar (1980)). Checkerboard solutions on non-staggered grids can be avoided by pressure-gradient-correction methods (Tan (1988)). De Lange (1992), however, found that this method is not useful to simulate flows with varying density on locally refined grids. To avoid the above complications, it was decided to use a vorticity-stream function formulation (Smooke (1989), de Lange (1992)) for the flow field. This formulation consists of a convection-diffusion equation for the vorticity vector \( \omega \) and a Poisson-like equation for the stream function \( \phi \). Xu (1993) has shown that, with the correct boundary conditions for the vorticity, the vorticity-stream function formulation gives the same results for the flow field as a primitive variable solver. We use the same boundary condition for \( \omega \) at the inlet as Xu (1993); see section 2.1.4. Here, we define the vorticity \( \omega \) by

\[ \omega = -\nabla \times \mathbf{v}. \tag{2.8} \]

In two-dimensional problems only the component perpendicular to the \( (x, y) \) plane is non-zero. We will denote this component by the scalar \( \omega \) for convenience

\[ \omega = \frac{\partial u}{\partial y} - \frac{\partial v}{\partial x}, \tag{2.9} \]

with \( u \) and \( v \) the \( x \) and \( y \) components of the mixture velocity \( \mathbf{v} \), respectively. The conservation equation for \( \omega \) is derived by taking the negative rotation of the Navier-Stokes equations (cf. eqn. (2.9)). The resulting equation can be written in a convection-diffusion form

\[ [\rho \mathbf{v} \cdot \nabla] \omega - \nabla \cdot [\mu \nabla \omega] = S_\omega. \tag{2.10} \]

Terms arising from density and viscosity variations are included in the source term \( S_\omega \) (de Lange (1992)). Expressions for the source term \( S_\omega \) are given by de Lange (1992) and Smooke (1989) for the cartesian and cylindrical system, respectively. The stream function \( \phi \) is defined as

\[ \frac{\partial \phi}{\partial y} \equiv \rho u; \quad \frac{\partial \phi}{\partial x} \equiv -\rho v \quad \text{and} \]

\[ \frac{\partial \phi}{\partial y} \equiv \rho u x; \quad \frac{\partial \phi}{\partial x} \equiv -\rho v x, \tag{2.11} \]

for a cartesian and a cylindrical system, respectively. Note that this formulation satisfies the stationary continuity equation (2.1) automatically. A Poisson-like equation for the stream function
can be derived by substituting the stream function definition (2.11) in equation (2.9)

\[
\frac{\partial}{\partial x} \left( \frac{1}{\rho} \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{1}{\rho} \frac{\partial \phi}{\partial y} \right) = -\omega \quad \text{and} \\
\frac{\partial}{\partial x} \left( \frac{1}{\rho} \frac{\partial \phi}{\partial x} \right) + \frac{\partial}{\partial y} \left( \frac{1}{\rho} \frac{\partial \phi}{\partial y} \right) = -\omega,
\]

(2.12)

for a cartesian and a cylindrical system, respectively. After solving equations (2.12) and (2.10) for \( \phi \) and \( \omega \) the flow velocity \( \vec{v} = (u, v) \) can be calculated from (2.11).

The energy transport due to viscous forces and pressure gradients is small compared to the conductive and convective energy transport in near-atmospheric combustion of hydrocarbons with air (de Lange (1992)). Smooke (1991) shows that the enthalpy transport due to diffusive fluxes (the Dufour effect) is also small for methane/air flames. When the energy transport due to viscous forces, pressure gradients and diffusive fluxes is neglected the energy equation becomes

\[
c_p \vec{\nabla} \cdot (\rho \vec{v} T) - \vec{\nabla} \cdot \left( \lambda \vec{\nabla} T \right) = - \sum_{i=1}^{N} h_i \dot{\rho}_i.
\]

(2.13)

In equation (2.13), \( T \) denotes the fluid temperature and \( c_p \) and \( \lambda \) denote the specific heat and the thermal conductivity of the mixture, respectively. The source term on the right hand side, with \( h_i \) the enthalpy of species \( i \) and \( \dot{\rho}_i \) the mass change of species \( i \) due to chemical reactions, denotes the net enthalpy change due to chemical reactions.

The ideal gas law has been chosen as the equation of state

\[
p = \frac{\rho RT}{\bar{M}},
\]

(2.14)

with \( R \) the molar gas constant and \( \bar{M} \) the mean molar mass of the mixture. In atmospheric combustion the atmospheric pressure \( (O(10^5)) \) usually is large compared to the pressure variations arising from equation (2.7). It is therefore justified to approximate the pressure \( p \) in equation (2.14) by the, constant, atmospheric pressure. Furthermore, the temperature gradients are much larger than the pressure gradients which implies that the effect of the pressure gradients on the density can be neglected compared to the effect of the temperature gradients. This is the so-called 'combustion approximation'. Note that the pressure gradients in the Navier-Stokes equations (2.7) are not neglected. When it is further assumed that the number of particles remains unchanged during the combustion the mass density depends on temperature only

\[
\frac{\rho}{\rho_u} = \frac{T}{T_u},
\]

(2.15)

with \( \rho_u \) and \( T_u \) prescribed.

### 2.1.2 The chemical model

The one-step chemical model used in this thesis has been developed by de Lange (1992). Other one-step reaction models are described by e.g. Coffee (1983), Williams (1985) and Westbrook
2.1. The physical model

The one-step model departs from an irreversible reaction between the fuel \( C_{n1}H_{n2}O_{n3} \) and the oxidiser \( O_2 \), given by

\[
C_{n1}H_{n2}O_{n3} + mO_2 \rightarrow n_1CO_2 + \frac{1}{2}n_2H_2O + [m - \nu]O_2 \quad \text{and},
\]
\[
C_{n1}H_{n2}O_{n3} + mO_2 \rightarrow [n_1 - 2\nu + 2m]CO_2 + [2\nu - 2m]CO + \frac{1}{2}n_2H_2O
\]

for equivalence ratios \( \phi \leq 1 \) and \( \phi > 1 \), respectively, with \( \nu = n_1 + \frac{1}{4}n_2 - \frac{1}{2}n_3 \). The equivalence ratio \( \phi \) and \( m \) are related by

\[
\phi = \frac{\nu}{m}.
\]

Note that an equivalence ratio \( \phi = 1 \) coincides with a stoichiometric mixture in which both fuel and oxygen are fully transformed into products. Equivalence ratios \( \phi < 1 \) and \( \phi > 1 \) indicate a fuel-lean and a fuel-rich mixture, respectively.

The products are treated as one species, so that only \( Y_{fu}, Y_{ox} \) and \( Y_{pr} \) have to be considered. The rate of mass production of species \( i \) (\( \dot{\rho}_i \)) in equations (2.6) and (2.13) due to the reaction (2.16) can be expressed in terms of \( \dot{\rho}_{fu} \) as follows

\[
\dot{\rho}_{ox} = \nu \frac{M_{ox}}{M_{fu}} \dot{\rho}_{fu} \quad \text{and} \quad \dot{\rho}_{pr} = -\left[1 + \nu \frac{M_{ox}}{M_{fu}}\right] \dot{\rho}_{fu} \quad \text{for} \quad \phi \leq 1
\]

and

\[
\dot{\rho}_{ox} = m \frac{M_{ox}}{M_{fu}} \dot{\rho}_{fu} \quad \text{and} \quad \dot{\rho}_{pr} = -\left[1 + m \frac{M_{ox}}{M_{fu}}\right] \dot{\rho}_{fu} \quad \text{for} \quad \phi > 1.
\]

The factor \( s_i \) is now introduced as the mass of species \( i \) consumed per unit mass fuel. This implies that \( s_{fu} = 1 \) and \( s_{ox} = \nu M_{ox}/M_{fu} \). For the fuel mass consumption rate \( \dot{\rho}_{fu} \) an Arrhenius-type form is chosen

\[
\dot{\rho}_{fu}(T, \rho, Y_{fu}, Y_{ox}) = -A\rho^{\alpha+\beta}(Y_{fu})^\alpha(Y_{ox})^\beta e^{-Ta/T}.
\]

Here \( A, \alpha, \beta \) and \( T_a \) are reaction rate parameters and \( Y_i \) (\( i = fu, ox, pr \)) are the mass fractions of fuel, oxidiser and products, respectively. The reaction rate parameters are determined in such a way that the dependence of the burning velocity on temperature, computed for flat burner-stabilised methane/air flames, deviates no more that 10% from experimental results of Andrews (1972), Kaskan (1967) and van Maaren et al. (1994) in the range of equivalence ratios \( 0.8 \leq \phi \leq 1.2 \) (see de Lange (1992) and van Maaren (1994) for more details). The method is similar to that of Coffee et al. (1984), who determined \( \phi \)-dependent one-step reaction parameters, using detailed numerical chemistry data for comparison. For most of the calculations in this thesis the parameters determined by de Lange (1992) are used. These parameters are given by: \( \alpha = 2.8, \beta = 1.2, A = 2.6\cdot10^{15} \text{[kgm}^{-3}]^{-3}\text{s}^{-1} \) and \( T_a = 16900 \text{ K} \). Note that these values are not physical as they are the results of a fitting procedure. Also, some results obtained with the parameters determined by van Maaren (1994) will be discussed.

\(^1\)For methane: \( n_1 = 1, n_2 = 4 \) and \( n_3 = 0 \)
Chapter 2. Combustion Model

The use of equation (2.19) ensures the correct reproduction of the local values of the burning velocity on the flame temperature $T_b$. The reproduction of the correct adiabatic flame temperature is ensured by using the following equations for $\Delta H$, $T_b$ and the mean specific heat $\bar{c}_p$, respectively (also see de Lange (1992))

$$
\Delta H \equiv \sum_i h_i^0 \frac{(Y_{i,b} - Y_{i,u})}{Y_{fu,b} - Y_{fu,u}}, \quad (2.20)
$$

$$
\sum_i h_i^0 [Y_{i,b} - Y_{i,u}] = - \sum_i \left[ Y_{i,b} \int_{T_{ref}}^{T_b} c_{p,i}(t) dt - Y_{i,u} \int_{T_{ref}}^{T_u} c_{p,i}(t) dt \right], \quad (2.21)
$$

and

$$
\sum_i \left[ Y_{i,b} \int_{T_{ref}}^{T_b} c_{p,i}(t) dt - Y_{i,u} \int_{T_{ref}}^{T_u} c_{p,i}(t) dt \right] \equiv \bar{c}_p [T_b - T_u], \quad (2.22)
$$

with $T_{ref}$ the reference temperature. In the above equations the counter $i$ runs over the set of species occurring in the reactions (2.16). The definition of $\Delta H$ in equation (2.20) results in a considerable simplification of the source term of the energy equation (2.13)

$$
\sum_{i=1}^{N} h_{0,i} \dot{\rho}_i = \Delta H \dot{\rho}_i \quad (2.23)
$$

### 2.1.3 Physical properties

The relevant physical properties of the mixture are the density $\rho$, the specific heat $c_p$, the thermal conductivity $\lambda$, the viscosity $\mu$ and the binary diffusion coefficient $D_{lm}$. The density $\rho$ and the specific heat $c_p$ are calculated according to equations (2.15) and (2.22), respectively. The other properties are supposed to be governed by the abundant nitrogen part of the mixture. The expressions used for $\lambda$ and $\mu$ are (de Lange (1992))

$$
\lambda(T) = 0.092 \left[ \frac{T}{1500} \right]^{0.77}, \quad (2.24)
$$

and

$$
\mu = 0.71 \frac{\lambda}{c_p}, \quad (2.25)
$$

respectively. The binary diffusion coefficients $D_{lm}$ are calculated using the kinetic theory according to Bird (1960).

### 2.1.4 The boundary conditions

An example of a computational domain containing all types of boundaries which will be considered is given in figure 2.1. These boundaries are

- The inlet (I);
- The burner wall (normal direction $y$ and $x$; (II) and (II')).
2.1. The physical model

- The outlet (III);
- In/outstream boundaries (normal direction $y$ and $x$; (IV) and (IV'));
- The symmetry boundary (V).

In this subsection the boundary conditions are specified in terms of the primitive variables $(u, v, T, Y_i)$. The boundary conditions for the velocity components $u$ and $v$ are not used in the model, they are only given to clarify some physical backgrounds of the boundary conditions for $\varphi$ and $\omega$ which are discussed in the following section where the discretisation method is presented.

- The Inlet (I)

At the inlet the values of the primitive variables are specified according to the conditions in the unburnt mixture upstream of the burner port. It is assumed that the mixture has a uniform temperature and that it is perfectly mixed. Furthermore, mostly the assumption is made that the flow is a fully developed Poiseuille flow with a parabolic velocity profile with the maximum velocity at $(0, 0)$. The boundary conditions at the inlet can be summarised as follows

$$
\begin{align*}
Y_i(x, 0) &= Y_{i,u}; \\
T(x, 0) &= T_u; \\
u(x, 0) &= 0; \\
v(x, 0) &= v(0, 0) \left\{ 1 - \left( \frac{x}{b} \right)^2 \right\};
\end{align*}
$$
for $0 \leq x \leq b$, $b$ being the width of the burner inlet. The mass fractions in the unburnt mixture are given by

$$Y_{f_{u,u}} = \frac{M_{fu}}{M_{fu} + \frac{m}{Y_{ox,air}}};$$

$$Y_{ox,u} = Y_{ox,air}[1 - Y_{f_{u,u}}];$$

where $Y_{ox,air}$ denotes the mass fraction of oxygen in air.

- **The burner wall (II) and (II')**

Heterogeneous chemical reactions at the wall (such as destruction of radicals) are neglected. Their effect is small compared to the effect of cooling on the chemical reactions near the wall. This implies that the diffusive flux of the mass fractions is zero at the wall, i.e. the derivative of the mass fractions perpendicular to the wall is zero. The wall material is also assumed to be impermeable with a large conductivity and cooling capacity so that the wall temperature $T_w$ is constant. The boundary conditions for wall (II) then become

$$\frac{\partial Y_i(x, H)}{\partial y} = 0;$$

$$T(x, H) = T_w;$$

$$u(x, H) = 0;$$

$$v(x, H) = 0.$$  

with $b \leq x \leq B$. For wall (II') these conditions become

$$\frac{\partial Y_i(x, y)}{\partial x} = 0;$$

$$T(x, y) = T_w;$$

$$u(x, y) = 0;$$

$$v(x, y) = 0.$$  

for $x = b$ or $x = B$ and $0 \leq y \leq H$.

- **The outlet (III)**

The prescription of the boundary conditions at the outlet starts from the assumption that the boundary is placed in a region where the primitive variables are (nearly) constant so that the gradients perpendicular to the boundary can be set to zero

$$\frac{\partial O(x, L_y)}{\partial y} = 0,$$  

(2.30)
2.1. The physical model

for \( 0 \leq x \leq L_x \) and with \( O \) denoting any one of the primitive variables \((u, T, Y_i)\). The velocity perpendicular to the outlet, \( v \), is calculated from the stream function, see section 2.2.1. It is not possible to give a boundary condition for \( v \) which does not involve \( \phi \) or \( \omega \). Note that the boundary condition given by equation (2.30) implies that it should be checked afterwards if the domain size \((L_x, L_y)\) influences the solution, especially for the flow field.

- The in/outstream boundaries (IV) and (IV)’

The boundary conditions for the velocities \((u, v)\) on the in/outstream boundary (IV) are identical to those prescribed at the outlet with \( B \leq x \leq L_x \) and \( y = 0 \). The velocity boundary conditions for (IV)’ become

\[
\frac{\partial v}{\partial x}(L_x, y) = 0, \tag{2.31}
\]

with \( 0 \leq y \leq L_y \). The perpendicular velocity component (in this case \( u \)) is, again, calculated from the stream function. The boundary conditions for \( T \) and \( Y_i \) are different from the boundary conditions at the outlet. The in/outstream boundaries are used in the next chapter for the modelling of flames burning in an atmosphere of cold air. The idea behind the modelling of these flames is that the flow field around the flame, resulting from the flow from the burner, induces a coflow in its surrounding. This coflow, in turn, induces a flow into the domain at the in/outstream boundaries which should adapt the properties of cold air. The temperature and mass fractions at the in/outstream boundaries are, therefore, prescribed for cold air with a temperature \( T_s \)

\[
Y_{fu}(x, y) = 0; \tag{2.32}
\]
\[
Y_{ox}(x, y) = Y_{ox, air};
\]
\[
T(x, y) = T_s;
\]

with \( x \) and \( y \) equal to the values given above.

- The symmetry boundary (V)

The boundary conditions at the symmetry boundary consist of zero derivatives perpendicular to the wall for the scalar variables \( T \) and \( Y_i \) and the parallel velocity \( v \). The velocity component perpendicular to the boundary \((u)\) is zero. This results in the following boundary conditions for the symmetry boundary (V)

\[
\frac{\partial Y_i}{\partial x}(0, y) = 0; \tag{2.33}
\]
\[
\frac{\partial T}{\partial x}(0, y) = 0;
\]
\[
\frac{\partial u}{\partial x}(0, y) = 0;
\]
\[
u(0, y) = 0;
\]

with \( 0 \leq y \leq L_y \).
2.2 The numerical method

The description of the numerical method (de Lange (1992), Mallens (1995c)) is split up in three parts

- Discretisation of the differential equations and boundary conditions;
- The mesh generation;
- The solution procedure.

In this section the discretisation of the differential equations and their boundary conditions is discussed. The mesh generation and the refinement technique will be discussed in section 2.3. Finally, in section 2.4, the procedure followed to solve the set of discretised equations will be treated.

2.2.1 The discretisation of the differential equations

The discretisation method used for the differential equations is based on the method developed by Thiart (1990). The method has already been used in two-dimensional problems by de Lange (1992) and Somers (1994). We will, therefore, limit ourselves to a short discussion of the discretisation of the equations for $T$ (2.13), $Y_i$ (2.6), $\omega$ (2.10) and $\phi$ (2.12) in a cartesian and a cylindrical system. In the next subsection the implementation and discretisation of the boundary conditions will be discussed.

Suppose that we have a grid point $P$ in a rectangular mesh (see fig. 2.2), with four neighbouring points $N, S, E, W$ which denote the north, south, east and west neighbours of point $P$, respectively. The quantities $\delta_i$ ($i=n, e, s, w$) denote the distances from point $P$ to its neighbours, as indicated in figure 2.2. The mesh is assumed to be non-equidistant, i.e. the distances $\delta_i$ are not equal. The conservation equations for the scalar variables $T$, $Y_i$ and $\omega$ can be written as

\[ [\rho \bar{v} \cdot \bar{\nabla}] f - \bar{\nabla} \cdot [\Gamma \bar{\nabla} f] = S_f, \]  

with $f$ equal to $T$, $Y_i$ or $\omega$. The diffusivity $\Gamma$ and the source term $S_f$ depend on the variable considered. The same discretisation is used as in de Lange (1992) and Somers (1994). The discretisation is similar to the second-order power-law discretisation given by Patankar (1980) or to the discretisation scheme given by Thiart (1990) without source term weighting. The discretised convection-diffusion equation can be written as

\[ \psi_P f_P - \psi_N f_N - \psi_S f_S - \psi_E f_E - \psi_W f_W = S_P, \]

with the coefficients $\psi_i$ ($i=N, S, E, W$) equal to

\[ \psi_N = \frac{2 \Gamma_n}{\delta_n(\delta_n + \delta_s)} A(P_N), P_N = \frac{(\rho u)_n \delta_n}{\Gamma_n} \]
\[ \psi_E = \frac{2 \Gamma_e}{\delta_e(\delta_e + \delta_w)} A(P_E), P_E = \frac{(\rho u)_e \delta_e}{\Gamma_e} \]
2.2. The numerical method

![Figure 2.2: A mesh point P with its four neighbours and the length scales of the finite-difference cell.]

\[ \psi_S = \frac{2\Gamma_s}{\delta_s(\delta_n + \delta_s)}A(P_S), \quad P_S = \frac{(\rho u)_s\delta_s}{\Gamma_s} \]
\[ \psi_W = \frac{2\Gamma_w}{\delta_w(\delta_e + \delta_w)}A(P_W), \quad P_W = \frac{(\rho u)_w\delta_w}{\Gamma_w} \]
\[ \psi_P = \psi_N + \psi_S + \psi_E + \psi_W, \]

and \( S_P \) is the source term evaluated at point \( P \). The function \( A(P) \) is given by (Patankar (1980))

\[ A(P) = \max(0, 1 - \frac{1}{10} P^5) + \max(0, -P). \]  (2.37)

The extension of the one-dimensional schemes given by Patankar and Thiart to two dimensions is not straightforward. Thiart does give correction terms for the two-dimensional fluxes, but these are very costly to calculate and are, therefore, not included in the discretisation scheme. The loss of accuracy caused by omitting the correction terms is expected to be largest in regions with large gradients. In these regions the accuracy is improved by using local grid refinement which leads to small grid sizes and small cell Peclet numbers \( P_e \) (2.36) in these regions.

In a cylindrical system (with the radial direction in \( z \) direction) the east and west coefficients become

\[ \psi_E = \frac{x_e}{x_p \delta_e(\delta_e + \delta_w)}A(P_E), \quad P_E = \frac{(\rho u)_e\delta_e}{\Gamma_e} \]
\[ \psi_W = \frac{x_w}{x_p \delta_w(\delta_e + \delta_w)}A(P_W), \quad P_W = \frac{(\rho u)_w\delta_w}{\Gamma_w}. \]  (2.38)
Chapter 2. Combustion Model

The other coefficients are the same as for the cartesian system. The values for \( \Gamma_i \) are determined by taking the harmonic mean of the values of \( \Gamma_i \) at the adjacent grid points. Patankar (1980) has shown that the harmonic mean gives a good representation of the diffusive fluxes between the adjacent grid points. Application of the harmonic mean to \( \Gamma_e \) leads to

\[
\Gamma_e = \frac{2\Gamma_E\Gamma_P}{\Gamma_E + \Gamma_P}.
\] (2.39)

The mass fluxes at the interfaces \( n, e, s, w \) are determined by linear interpolation between the adjacent grid points, which is second-order accurate if the interfaces are placed midway between the adjacent grid points.

The stream function is solved from equation (2.12). The velocities are calculated from the stream function afterwards, using equation (2.11). The discretisation of equation (2.12) should be in accordance with the discretisation of (2.11) because this ensures that the velocity field satisfies mass conservation. The equidistant discretisation of (2.12) and (2.11) used by de Lange (1992) is extended to a non-equidistant, but equally accurate, discretisation. The discretisation of equations (2.12) is third-order accurate. This higher accuracy is chosen because the velocities are determined from the stream function through numerical integration which leads to an expression which is one order less accurate. The resulting discretised form of equation (2.12) can be written as equation (2.35) with the following coefficients

\[
\begin{align*}
\psi_N &= \frac{1}{\gamma_y(\delta_n + \delta_s)} \left[ \frac{1}{4\rho_n} - \frac{\gamma_y^2}{4\rho_s} \right] (\rho v)_N \\
\psi_E &= \frac{1}{\gamma_x(\delta_e + \delta_w)} \left[ \frac{1}{4\rho_e} - \frac{\gamma_x^2}{4\rho_w} \right] (\rho v)_E \\
\psi_S &= \frac{1}{\gamma_y(\delta_n + \delta_s)} \left[ \frac{1}{4\rho_n} - \frac{\gamma_y^2}{4\rho_s} \right] (\rho v)_S \\
\psi_W &= \frac{1}{\gamma_x(\delta_e + \delta_w)} \left[ \frac{1}{4\rho_e} - \frac{\gamma_x^2}{4\rho_w} \right] (\rho v)_W \\
\psi_P &= \psi_N + \psi_S + \psi_E + \psi_W \\
S_P &= \omega_P - \frac{1}{\gamma_x(\delta_e + \delta_w)} \left[ \frac{1}{4\rho_e} + \frac{\gamma_x^2}{4\rho_w} - 1 \right] (\rho v)_P \\
&\quad - \frac{1}{\gamma_y(\delta_n + \delta_s)} \left[ \frac{1}{4\rho_n} - \frac{\gamma_y^2}{4\rho_s} \right] (\rho v)_N \\
&\quad - \frac{1}{\gamma_x(\delta_e + \delta_w)} (\rho v)_E - \frac{\gamma_x^2}{4\rho_w} (\rho v)_W \\
&\quad - \frac{1}{\gamma_y(\delta_n + \delta_s)} (\rho v)_S \\
&\quad - \frac{1}{\gamma_y(\delta_n + \delta_s)} (\rho v)_N - \frac{\gamma_y^2}{4\rho_s} (\rho v)_S
\end{align*}
\] (2.40)

with \( \gamma_x = \delta_e/\delta_w \) and \( \gamma_y = \delta_n/\delta_s \). The cylindrical equivalent of equation (2.40) can be obtained by multiplying \( \rho_i, v_i \) and \( u_i \) by \( x_i \). The finite-difference expressions used for the calculation of the
2.2. The numerical method

Velocities are given by

\[
\begin{align*}
 u_P &= \frac{1}{\rho P (\gamma_x + 1)} \left[ \frac{3}{\gamma_x \delta w} \left( \varphi_E + (\gamma_x^2 - 1) \varphi_P - \gamma_x^2 \varphi_W \right) - (\rho u)_E - \gamma_x (\rho u)_W \right], \\
 v_P &= \frac{1}{\rho P (\gamma_y + 1)} \left[ \frac{-3}{\gamma_y \delta s} \left( \varphi_N + (\gamma_y^2 - 1) \varphi_P - \gamma_y^2 \varphi_S \right) - (\rho v)_N - \gamma_y (\rho v)_S \right].
\end{align*}
\]

Expressions for \((\rho u x)_P\) and \((\rho v x)_P\) in the cylindrical system can be obtained by replacing \((\rho u)_i\) and \((\rho v)_i\) by \((\rho u)_ix_i\) and \((\rho v)_ix_i\) in the right hand side of equations (2.41).

2.2.2 The discretisation of the boundary conditions

In this subsection the discretisation of the Neumann boundary conditions for \(T\) and \(Y\), and the discretisation of the boundary conditions for \(\varphi\) and \(\omega\) will be treated. In the discretisation of the Neumann boundary conditions for \(T\) and \(Y\), at the burner walls and symmetry boundaries a fictitious neighbour node \(B\) (figure 2.3) is used. The velocity at point \(B\) is chosen so that there is no mass flux through the wall. The value of \(T\) or \(Y\) in the fictitious neighbour \(B\) is set equal to the values in the neighbour \(D\). It can be shown by symmetry arguments that the flux through the east interface \(b\), \(J_b\), is related to the flux through the west interface \(J_d\) by

\[ J_b = -J_d. \]

fig. 2.3: Illustration of the discretisation of the zero-flux boundary conditions. \(\vec{n}\) denotes the local normal vector to the boundary and \(\vec{v}\) denotes the local flow velocity. Also see Somers (1994).
Chapter 2. Combustion Model

The Peclet number in the fictitious neighbour $B$, $P_B$, is equal to $-P_D$. The mass fraction or temperature in the boundary node $P$ can then be calculated from equation (2.35) with $\psi_B f_B = \psi_D f_D$ and $S_P$ equal to zero

$$\psi_P f_P = \psi_A f_A + \psi_C f_C + 2\psi_D f_D.$$

Equation (2.42) effectively is a second-order accurate discretisation of the Neumann boundary conditions for $T$ and $Y_t$ given in section 2.1.4. Applying the above approach to the corners of the burner wall leads to equation (2.35) with the coefficients given by equations (2.36) and (2.38) and $S_P$ equal to zero.

The boundary conditions for $\overline{V}$ given in section 2.1.4 have to be translated to boundary conditions for the stream function $\varphi$ and the vorticity $\omega$. The stream function on the burner wall, the symmetry boundary and the inlet is determined analytically from the mass flux perpendicular to the boundary, according to its definition (eqn. (2.11))

$$\varphi(x_1, y_w) = \varphi(x_0, y_w) + \int_{x_0}^{x_1} \rho u dx \text{ and}$$

$$\varphi(x_w, y_1) = \varphi(x_w, y_0) + \int_{y_0}^{y_1} \rho u dy,$$

for boundaries in $x$-direction at $y_w$ and in $y$-direction at $x_w$, respectively. Similar expressions are used for the cylindrical case. The above integrals lead to a constant stream function on the burner wall and the symmetry boundary. At the inlet the velocity profile given in equation (2.26) is integrated which yields the following expression for the stream function at the inlet in figure 2.1 for the cartesian case

$$\varphi(x, 0) = \varphi(0, 0) + \rho v(0, 0)x \left\{ 1 - \frac{1}{3} \left( \frac{x}{b} \right)^2 \right\}.$$

Again, a similar expression is easily derived for the cylindrical case. The stream function at the outlet and the in/outstream boundaries is calculated by setting its second derivative perpendicular to the wall equal to zero, which yields the following second-order accurate expression for the cartesian case (see figure 2.4 for the neighbour definitions)

$$\varphi_P = 2\varphi_P - \varphi_Q - (y_P - y_P') \cdot (\rho u_P - 2\rho u_P' + \rho u_Q)$$

$$\varphi_P = 2\varphi_P - \varphi_Q + (x_P - x_P') \cdot (\rho v_P - 2\rho v_P' + \rho v_Q),$$

for the boundary $AB$ in $y$ and $x$-direction, respectively. The mass flux perpendicular to the boundary is calculated from the stream function at the boundary points using equations (2.42). The mass flux along the outlet and in/outstream boundaries is calculated by setting its first derivative perpendicular to the boundary equal to zero, according to equations (2.31) and (2.30).

We now turn to the vorticity boundary conditions. The vorticity at a symmetry boundary is equal to zero. The vorticity at the other boundaries is calculated by approximating the vorticity at a point $X$ halfway between $P$ and $P'$ (figure 2.4) by $\omega_X = (\omega_P + \omega_P')/2$. A similar approximation is used by Dennis (1979) for zero velocities normal to the boundary. With non-zero velocities
2.3 The mesh generation technique

A major difficulty in the numerical modelling of two-dimensional laminar flames on relatively large burners ($O(10^{-2})$ m) is the large difference in typical length scales between the burner size and the grid spacing needed to resolve the processes inside the flame front (of $O(10^{-4})$ m). An equidistant grid which can resolve all relevant length-scales adequately would then lead to a huge number of points which gives rise to very time consuming computations and large memory sizes. To avoid this de Lange (1992) developed an adaptive local refinement technique which adds points to the grid in the flame region and removes points in regions where they are not necessary anymore.

To determine where the refinements should be added or removed a certain criterion has to be defined which indicates if a cell should be refined or not. In principle any local quantity at point $P$, $Q_{P}$, can be used which is large near and inside the flame front and small outside the flame region. Usually, the gradient of a certain variable is most suitable because it is a measure...
for the truncation error of the discretised conservation equation. In figure 2.5 point $P$ on the coarse base grid (situation $I$) is shown with three neighbours $N$, $NE$ and $E$. The refinement procedure consists of adding a point in the middle of the rectangle $P - N - NE - E$. Therefore, the refinement criterion is averaged over these four nodes. The rectangle $P - N - NE - E$ should be refined when this quantity exceeds a preset critical value $Q_{\text{crit}}$

$$Q_P + Q_N + Q_{NE} + Q_E > 4Q_{\text{crit}}.$$  (2.48)

As indicated above, gradients of several quantities can be used for the refinement criterion. Examples are gradients of, for instance, the temperature, one of the major species or the fuel mass consumption rate. The discretised form of the one-dimensional energy equation can be written as

$$J_e - J_w = \Delta H \dot{\rho}_{fu} + \frac{\Delta x^2 \partial^3 J_p}{6 \partial x^3} + O(\Delta x^4).$$  (2.49)

The discretisation error can be rewritten in terms of $\dot{\rho}_{fu}$

$$\frac{\partial J_P}{\partial x} = \Delta H \dot{\rho}_{fu} \rightarrow \frac{\partial^3 J_P}{\partial x^3} = \Delta H \frac{\partial^3 \dot{\rho}_{fu}}{\partial x^2}.$$  (2.50)

The above shows that the one-dimensional discretisation error is approximately proportional to the second derivative of $\dot{\rho}_{fu}$, multiplied by $\Delta x^2$. If cross-derivatives are neglected, the discretisation error for the two-dimensional case can be estimated by

$$Q_i = \frac{\Delta x^2 \partial^2 \dot{\rho}_{fu}}{6 \partial x^2} + \frac{\Delta y^2 \partial^2 \dot{\rho}_{fu}}{6 \partial y^2}.$$  (2.51)
The quantity $Q_i$ can be used to determine whether the grid should be refined or not. After the calculation of $Q_i$ at every point for which the rectangle $P - N - NE - E$ exists a grid point is added in every rectangle for which equation (2.48) is satisfied. Grid points are added in the middle of the rectangles, as indicated in figure 2.5 by situation $II$. When this first refinement layer is complete the criterion can be recalculated on the refined grid and the procedure described above can start again, resulting in a second refinement layer (situation $III$). This is repeated until the desired number of layers is reached.

\[
\begin{align*}
\frac{f_P^{n+1} - f_P^n}{\xi/\psi_P^n} &= S_P^n - \psi_P^n f_P^n + \sum_{j=N,S,E,W} \psi_j^n f_j^n. 
\end{align*}
\]

In equation (2.52) the superscripts $n$ and $n+1$ denote the value at, respectively, the $n^{th}$ and the $n+1^{th}$ iteration. Equation (2.52) is solved by using the Alternate Direction Implicit (ADI)
method, in two stages
\[
- \frac{\xi}{\xi + 1} \psi^n f_{S}^{n+\frac{1}{2}} + \psi^n f_{P}^{n+\frac{1}{2}} - \frac{\xi}{\xi + 1} \psi^n f_{N}^{n+\frac{1}{2}} = \frac{\xi}{\xi + 1} \left( S_{P}^{n} + \sum_{j=E,W} \psi^n f_{j}^{n} \right) \\
+ \frac{\psi^n}{\xi + 1} f_{P}^{n} \quad \text{and,} \quad (2.53)
\]
\[
- \frac{\xi}{\xi + 1} \psi^n f_{W}^{n+1} + \psi^n f_{P}^{n+1} - \frac{\xi}{\xi + 1} \psi^n f_{E}^{n+1} = \frac{\xi}{\xi + 1} \left( S_{P}^{n} + \sum_{j=S,N} \psi^n f_{j}^{n+\frac{1}{2}} \right) \\
+ \frac{\psi^n}{\xi + 1} f_{P}^{n+\frac{1}{2}}. \quad (2.54)
\]

The advantage of the latter formulation is that it can be written as a matrix equation \( A \mathbf{f} = \mathbf{b} \) where \( A \) is a tri-diagonal matrix. This property of \( A \) renders a system of equations which is easy and cheap to solve.
Chapter 3

Premixed flame stabilisation and the environment

The effect of a surrounding atmosphere on flame stabilisation is quite complex. The surrounding atmosphere affects the stabilisation in three ways:

- The surrounding may affect the degree in which the flue gases expand perpendicular to the main flow direction. This will be referred to as the 'degree of confinement' caused by the surrounding. The surrounding can, for example, consist of cold air or the flames can be surrounded by similar flames (see figure 3.1);

- The surrounding may cool the flame base by conduction of heat and by mixing of cold gases with hot flue gases;

- The mixing of the surrounding gases with the (partially) unburnt mixture flowing from the burner may change the equivalence ratio of the mixture at the base of the flame.

The effect of the surrounding on the stabilisation of the flame tip and the flame sides will be investigated in this chapter. We first present a comparison between experimental and modelling results of unconfined flames on rectangular slit burners and cylindrical (tube) burners (see fig. 3.2). Then, the effects of the surrounding and the confinement on various flame properties which are important for flame stabilisation, such as the flame shape, the mass flux through the tip and the energy transport at the tip and the side of the flame, will be studied. The effect of the surrounding and the confinement is investigated by considering two limiting cases: flames burning in a surrounding atmosphere (figure 3.2c and 3.2d) and flames confined between similar flames (figure 3.2a and 3.2b), both on a tube burner and on a slit burner.

Experimental studies of Bunsen flames on slit and tube burners with a surrounding atmosphere (referred to as 'unconfined flames') have been performed by many authors, e.g. Echekki (1990), Hertzberg (1990), Lewis (1961) and Wagner (1985). These studies mainly focus on the effects of the surrounding atmosphere on the blow-off or flash-back behaviour and on the effects of the curvature of the flame front at the tip. The results show that these effects are related to the convective and diffusive transport of heat and mass near the flame front.
Two-dimensional (2D) methane air Bunsen flames have been studied numerically by several authors. Smooke et al. (1989) and Coelho (1993) consider two-dimensional diffusion flames. A surrounding environment is incorporated by defining a fixed co-flowing air stream surrounding the fuel jet. Fukutani (1993) studied the transport of mass and energy between lean 2D premixed flames surrounded by stoichiometric flames with complex chemistry. In the present investigation, the surrounding atmosphere is not incorporated by means of a co-flowing air stream with a given velocity but by means of 'free' in/outstream boundaries (see chapter 2).

The computational domains used to study the effects of confinement are shown in figure 3.3. Note that the confined tube burner (figure 3.2a) does not have an experimental equivalent, due to the fact that the interface between two coaxial flames at $x = B$ is not an exact symmetry boundary. The chosen domain and boundary conditions are, however, introduced to investigate the effects of the burner geometry on the mass and energy transport in flames surrounded by similar flames.
We will start with a brief discussion of the experimental set-up in section 3.1. In section 3.2, numerical results for a Bunsen flame on a 4.2 mm single-slit burner \((b = 2.1 \text{ mm})\) and a Bunsen flame on a 9.6 mm tube burner \((b = 4.8 \text{ mm})\) will be discussed. The computed velocity field near and within the flame cone on the single-slit burner will be compared with Laser Doppler Velocimetry (LDV) measurements. The predicted shape of the flame on the tube burner will also be compared with its experimental equivalent. Typical flow field characteristics reported in other references (Echekki (1990), Hertzberg (1990), Lewis (1961), Mungal (1994)) will be considered as well.

The effects of the burner geometry on Bunsen flames confined between similar flames is investigated in section 3.3 by comparing differences in flame shape and mass flow through the tip for a tube (fig. 3.2a) and a slit burner (3.2b). Then, the effect of a surrounding atmosphere on the flame shape and the mass flux through the tip is studied.

The energy transport in the tip and sides of confined and unconfined flames is investigated in section 3.4. This section starts with a comparison between the energy transport in a one-
dimensional flame modelled with our one-step chemical model and with skeletal chemistry (Smooke (1991)). After this an investigation of the effects of burner geometry and confinement on the energy transport in the tip and the sides of methane/air flames is presented.

3.1 Experimental set-up

In this section a short description will be given of the experimental set-up used in this chapter to validate the model. The methane and air flows are controlled separately by electronic mass flow controllers. Then the methane and the air is mixed in a large buffer, which also eliminates pressure fluctuations. The length of the rectangular slit burner in \( z \) direction (see figure 3.4) is equal to 55 mm. The slit width in \( x \)-direction can be varied. A detailed cross-section of the burner is given in figure 3.5. The narrow slit (1.5 mm) between the rectangular channel and the round buffers in figure 3.5 prevents flashback into the buffers. The rectangular channel is 400 mm long in \( y \)-direction to obtain a developed flow profile at the burner exit in \( x \) and \( z \) direction. The burner rim and the rectangular channel are cooled separately. The channel is kept at room temperature to prevent heating of the mixture. The burner rim is kept at 50 °C during the experiments to
3.2 Experimental and numerical results for unconfined flames.

A qualitative study of de Lange (1993) showed that the combustion model presented in chapter 2 predicts the flame length and flame shape of confined premixed methane/air flames on slit bur-
Chapter 3. Premixed flame stabilisation and the environment

fig. 3.5: A cross-section of the slit burner in the xy-plane; the slit width 2b is adjustable.

fig. 3.6: Profiles of the burner exit velocity in z-direction in the yz plane (top) and in the xy-plane (bottom). The solid triangles denote Laser Doppler velocimetry measurements; the solid line in the lower graph denote the theoretical profile according to Shah (1978).

ners within 10% accuracy. In this section we present numerical results and a more quantitative validation of the model applied on atmospheric methane/air flames ($T_a = 298$ K, $\phi = 1$) in an open atmosphere ($Y_{air} = 0$, $Y_{ox} = 0.232$). We consider a flame on a slit and a flame on a tube burner. The tube burner flame is discussed first. The flame shape and the flow field produced by the model are compared qualitatively with the visible flame front and flow field on a photograph including particle tracks (see figure 1.3). For the slit burner flame, presented subsequently, we compare the computed profiles of the vertical velocity component $v$ with Laser-Doppler Velocimetry (LDV) measurements.
3.2. Experimental and numerical results for unconfined flames.

Table 3.1: The domain measures for the flames discussed in section 3.2.

<table>
<thead>
<tr>
<th>Burner</th>
<th>slit</th>
<th>tube</th>
</tr>
</thead>
<tbody>
<tr>
<td>b [mm]</td>
<td>2.1</td>
<td>4.8</td>
</tr>
<tr>
<td>B [mm]</td>
<td>4.8</td>
<td>6.0</td>
</tr>
<tr>
<td>( L_x ) [mm]</td>
<td>15.0</td>
<td>24.0</td>
</tr>
<tr>
<td>( L_y ) [mm]</td>
<td>15.0</td>
<td>30.0</td>
</tr>
<tr>
<td>( V_{\text{max}} ) [m/s]</td>
<td>1.1</td>
<td>0.9</td>
</tr>
<tr>
<td>( \phi ) [-]</td>
<td>1.0</td>
<td>0.9</td>
</tr>
<tr>
<td>( \Delta )</td>
<td>0.3</td>
<td>0.3</td>
</tr>
</tbody>
</table>

The computational domain is given in figure 3.3b. The magnitude of the domain, the maximum inlet velocity \( V_{\text{max}} \), the equivalence ratio \( \phi \) and the base grid spacing \( \Delta \) are listed in table 3.1 for the tube and the slit burner. The calculations are performed on a coarse base grid with three adaptive refinement layers.

![Computational grid for the unconfined cylindrical flame (case c). The domain used for the calculation is given in figure 3.3b.](image)

3.2.1 Results for the tube burner.

The computed grid with three refinement levels is presented in figure 3.7. The contours of the stream function and temperature are given in figure 3.8. A qualitative comparison of the stream lines given by the model and the particle tracks visible on the photograph shows that the flow field near the flame cone is reproduced by the code. The stream lines above the experimental
Chapter 3. Premixed flame stabilisation and the environment

Fig. 3.8: Contours of the stream function (left) and the temperature (right) for the unconfined cylindrical flame (case c). The numbers in the contour lines denote the contour value in [kg/ms] and [K], respectively.

Flame \((y \geq 0.01 \text{ m})\) bend back towards the central axis due to acceleration of the hot combustion products by gravitational forces between the hot combustion products and the cold gases in the surrounding atmosphere. This effect is also present in the modelled flow field. A more detailed validation of the flow field inside and near the flame produced by the model is given in the next subsection.

The flow field in the surrounding atmosphere (at \(x\) values larger than 0.007 m) produced by the model cannot be validated because it is not visible on the particle track photograph. Computations with different domain sizes and grid spacings \(\Delta\) did not lead to significant variations in the flow field near and inside the flame. The other flame properties such as the flame shape and temperature were not affected by the domain size and \(\Delta\).

The shape of the flame is reproduced by the model. The numerical flame front is defined as the location of the maximum heat release. For the experimental flame the flame front is defined as the middle of the luminous zone. The sides of the modelled flame are almost parallel to the flame front in the photograph. The deviation is largest in the tip. The length of the modelled flame is about 7.6 mm, while the length of the experimental flame is roughly equal to 8.6 mm. Part of the observed discrepancies (of the order of the thickness of the flame front, which is about 0.9 mm) are probably caused by differences in the flame front definitions. From the results we may conclude that the model reproduces the flame shape and the flow field near the flame well. A more quantitative validation of the model will be given in the next subsection.
3.2. Experimental and numerical results for unconfined flames.

The contours of the stream function and temperature for the modelled flame on the 4.2 mm slit burner are given in figure 3.9. The most striking difference with the modelled flow field for the tube burner (see previous subsection) lies in the flow field downstream of the flame cone. The stream lines for the tube burner converge at larger \( y \) values whereas the stream lines for the slit burner do not show this behaviour; at least not inside the computational domain. Flow fields above slit burners given by Lewis (1961) also show a non-converging behaviour. This leads to the conclusion that the converging behaviour of the stream lines for the tube burner is caused by lower velocities in the radial direction and by the larger gravitational forces on the hot flow near the symmetry axis. The results for \( v \) found with the model and LDV measurements on the slit burner are given in figure 3.10. The vertical velocity component \( v(x, y = H) \) is given as a function of \( x \) for some heights \( H \) above the burner rim. The shape of the profiles is well captured by the model. The values of the measured velocities differ no more than 15% from the velocities produced by the model. These differences are mainly caused by small differences in flame shape. Small variations in the flame position can lead to the observed differences because the profiles change rapidly in \( y \) direction near the flame front. The differences are of the same order of magnitude as the accuracy of the measurements because LDV measurements give errors of 10-15% in the flame tip region (Wagner, 1985). These inaccuracies are mainly caused by the large velocity gradients and by Taylor instabilities. In view of the above we may conclude that the model gives a good representation of the velocity field near the two-dimensional flame on the slit burner.

The profiles at \( H = 3.5 \) mm show a minimum on the central axis. The minimum is caused by the pressure drop over the flame tip which is larger than the pressure drop over the sides (see Poinset, 1992). The minimum is more pronounced in the predicted profile. This could, however, be due
Chapter 3. Premixed flame stabilisation and the environment

to small differences in flame position. The minimum in the velocity profile above the flame tip at the central axis is also reported by Mungal (1994) who performed Particle Image Velocimetry measurements in cylindrical Bunsen flames. The minimum at the central axis is present in all modelled flames.

The measured and modelled vertical velocity \( v \) at the centreline \( (x = 0) \) both decrease slightly with increasing \( y \) in the lower part of the flame cone. The decreasing velocity is a result of the diverging flow field in the lower part of the flame cone. This is in accordance with results for slit burners given by Lewis (1961). The divergent flow field in the lower part of the flame was not found by Echekki (1990) who performed Particle Tracking Velocimetry measurements in flames on slit burners. Echekki (1990), however, considered flames with much higher burner exit velocities (mean velocities of 1.5 to 2.5 m/s) whereas we consider much lower mean burner exit velocities (0.8 m/s). Other computations have shown that the divergence of the flow field in the lower part of the flame is not present for higher inlet velocities. Apparently the pressure drop over the flame sides increases with increasing burner exit velocities. The increasing pressure drop over the flame sides can be explained by the decreasing angle between the main flow direction and the flame front. This, in turn, leads to increasing flow bending, higher velocity gradients and higher pressure gradients.

fig. 3.10: Comparison of the velocity component in \( y \) direction predicted by the model (case d) with LDV measurements.
3.3 Effects of burner geometry and surrounding atmosphere

The effects of burner wall curvature and confinement will be studied in this section. We will first discuss the differences in flame shape and mass flux through the flame tip between Bunsen flames on slit and tube burners surrounded by similar flames. The effects of confinement on the flame shape, the flow field and the mass flux $\rho v$ through the tip will be investigated subsequently.

Table 3.2: The domain measures for the flames used in the investigation of the effects of the burner geometry and surrounding atmosphere (section 3.3).

<table>
<thead>
<tr>
<th>Confined</th>
<th>yes</th>
<th>no</th>
</tr>
</thead>
<tbody>
<tr>
<td>Burner</td>
<td>slit</td>
<td>tube slit</td>
</tr>
<tr>
<td>$b$ [mm]</td>
<td>2.1</td>
<td>2.1 2.1 2.1</td>
</tr>
<tr>
<td>$B$ [mm]</td>
<td>2.4</td>
<td>2.4 4.8 4.8</td>
</tr>
<tr>
<td>$L_x$ [mm]</td>
<td>2.4</td>
<td>2.4 15.0 9.0</td>
</tr>
<tr>
<td>$L_y$ [mm]</td>
<td>10.0</td>
<td>10.0 15.0 15.0</td>
</tr>
</tbody>
</table>

The computational domain for the unconfined flames is given in figure 3.3a; the domain for the confined flames is given figure 3.3b. The domain measures are given in the table 3.2. The equivalence ratio $\phi = 1.0$, $V_{\text{max}} = 1.2$ m/s and $\Delta = 0.3$ mm for all cases.

3.3.1 Flames Confined between Similar Flames

The computed shapes of the flames confined between similar flames are given by the full lines in figure 3.11. These lines represent the maximum locus of the chemical source term $\rho f_u$ (in eq.(2.19)). There is a significant difference in flame length between the slit burner case ($\approx 3.0$ mm) and the tube burner case ($\approx 2.5$ mm). The cylindrical flame is shorter because this flame has more space to expand in radial direction. This can be shown by evaluating the radial term of the continuity equation: $\frac{1}{x} \frac{\partial}{\partial x} (\rho u x) = \frac{\partial u}{\partial x} + \frac{\partial}{\partial x} (\rho u) = 2 \frac{\partial}{\partial x} (\rho u)$ for $x \to 0$, which implies that the total mass flow rate in $x$ direction for the cylindrical case is twice as large as the mass flow in $x$ direction for the slit burner flame, when the mass fluxes $\rho u$ are equal. This has important consequences for the flame stabilisation and flame length. The large mass flow rate on the central axis $\rho V_{\text{max}}$ in the upstream part of the flame has to decrease to values near $\rho^* s_L$, $s_L$ being the adiabatic burning velocity ($\approx 0.4 m/s$ for a stoichiometric methane/air flame) at the flame tip to guarantee stable flame propagation in the tip (at $x = 0$). Note that this leads to values for $u$ at the tip which are almost an order of magnitude larger than $s_L$ (which is also reported by Ehgiki (1990)), because of the decrease of the density of the mixture. The surplus of mass has to be transported in $x$-direction through $\rho u$. It is easier to transport this mass away from the axis in the cylindrical case because of the larger expansion space. As a result, the flame tip on
Chapter 3. Premixed flame stabilisation and the environment

The multiple-slit geometry is longer and has a larger curvature to induce larger convective (and diffusive) transport in \( x \)-direction. This phenomenon is increased further by the confinement of the flames. The modelled flow fields for the slit burner (de Lange, 1993) and the tube burner show converging stream lines in the upstream part of the flame, especially near the tip. This convergence is caused by the restriction of the lateral expansion due to the symmetry boundaries at \( x=B \). This is visible in figure 3.12, where the convective mass flux \( pv \) along the centreline is shown for both geometries. The mass flux \( pv \) in the upstream part of the flame increases less in the cylindrical flame, again due to the larger expansion space in \( x \) direction. The mass flux suddenly decreases to values close to the adiabatic mass burning rate near the flame front for stabilisation reasons, as already mentioned.

Note that the final value of \( pv \) at the flame tip is approximately equal to 0.6 \( kg/m^2s \) for the slit burner flame and \( pv \approx 0.5 \ kg/m^2s \) for the cylindrical flame, indicating that the burning velocity defined in the burnt mixture is roughly equal to 0.5 \( m/s \) for the multiple-slit burner and 0.4 \( m/s \) for the coaxial burner. The relatively large burning velocity of the slit burner flame is caused by the larger curvature and stretch of the flame tip in combination with preferential diffusion effects (see chapter 6).
3.3. Effects of burner geometry and surrounding atmosphere

Note also that the distance along the center line between the maximum mass flux $\rho v$ and the minimum value is considerably smaller for the cylindrical flame than for the slit burner flame, implying that the flame thickness of the tip is smaller in the cylindrical case. This observation is related to the fact that the slit burner flame needs more time and space to dispose of the excess of mass on the central axis.

**3.3.2 The Effect of a Surrounding Atmosphere**

The influence of a surrounding atmosphere on the flame shape and the mass flux $\rho v$ through the tip is also of importance. The markers in figure 3.11 represent the position of the numerical flame front of the flames with a surrounding atmosphere. The flames with the surrounding atmosphere are less curved, because the flow is less confined. This on its turn has consequences for the flame length. For the cylindrical flame, the inclusion of a surrounding atmosphere leads to a smaller flame length (≈ 10%). The change in flame length for the slit burner is negligible. The mass flux $\rho v$ along the centreline for the cylindrical flame with a surrounding atmosphere is shown in figure 3.13. The effect of the surrounding atmosphere on the mass flux $\rho v$ through the tip was similar.
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for the slit burner case. Instead of increasing, the mass flux now initially decreases in the lower part of the flame cone, because the stream lines near the centreline diverge slightly. This is also visible in photographs given by Lewis (1961). This diverging flow field is caused by the pressure drop over the sides of the flame (Poinsot, 1992) and the absence of confining (symmetry) walls near the flame. The flames now have less problems to get rid of the mass surplus on the central axis. Furthermore, the pressure drop over the tip is larger than the pressure drop over the sides of the flame (see e.g. Poinsot (1992)), which might cause the slight convergence of the flow field just ahead of the tip.

The result of these effects is that the mass flux just ahead of the flame tip is only 70% of the mass flux ahead of the flame tip confined between symmetry boundaries. In the final part of the flame (at a distance larger than 4 mm) the mass flux decreases rapidly in the flame front for stabilisation reasons. Now the final mass flow rate is less than \( \rho u s_L \) due to the larger expansion in \( x \)-direction and the absence of confining walls.

The temperature after the tip of a cylindrical flame with a surrounding atmosphere (figure 3.13) decreases slowly which is caused by the cooling effect of the cold surrounding air. A smaller temperature decrease was found after the flame cone on a slot burner which is caused by the limited cooling effect of the cold surrounding gases and the limited length of the computational domain downstream of the flame.
3.4 Energy transport in one- and two-dimensional flames

In this section a numerical analysis is presented of the energy transport in the tip and the side of $CH_4/air$ Bunsen flames. Three geometries will be considered: a confined flame on a slit burner (fig. 3.2b), a confined flame on a cylindrical burner (fig. 3.2a) and an unconfined flame on a cylindrical burner (fig. 3.2c). The analysis will concentrate on the magnitude of the energy transport along the local flame front versus the magnitude of the energy transport perpendicular to the local flame front and on the differences between the geometries mentioned above. The energy transport will be analysed by computation of the contributions to the energy equation in directions along and perpendicular to the local flame front. The analysis is comparable to the analysis performed by Smooke (1991) for one-dimensional flames with detailed transport and skeletal chemistry. Results given by Smooke (1991) show that the general behaviour and relative magnitude of the terms in the energy equation is not affected significantly by the equivalence ratio of the mixture, at least for lean to stoichiometric mixtures. We will, therefore, limit ourselves to stoichiometric flames.

The terms of the energy equation in a one-dimensional flame will be compared with results given by Smooke (1991). The energy transport in two-dimensional flames will be considered subsequently. We will first study the influence of variations in burner geometry on the energy transport in the tip and the side of confined Bunsen flames on a slit and a cylindrical burner. The effect of the confinement on the energy transport will be considered section 3.4.2.

3.4.1 Energy transport in a one-dimensional flame

The terms in the energy equation calculated for a stoichiometric and adiabatic one-dimensional $CH_4/air$ flame with the one-step chemical model are compared with the terms of the energy equation given by Smooke (1991) and Somers (1994) for a similar flame computed with the skeletal mechanism for methane oxidation figure 3.14a.

When the enthalpy transport by diffusive fluxes (which is small in methane/air flames (see Smooke (1991))) is neglected, the one-dimensional energy equation is given by:

$$\frac{\partial}{\partial x} (\rho u c_p T) - \frac{\partial}{\partial x} \left( \lambda \frac{\partial T}{\partial x} \right) = -\sum_i h_i \dot{\rho}_i .$$  \hspace{1cm} (3.1)

Equation (3.1) consists of a convective term, a conductive term and the source term. The terms of the energy equation for the flame calculated with the one-step mechanism are given in Fig. 3.14b. A comparison between the separate contributions in this figure and terms of the energy equation given by Smooke (1991) and Somers (1994) (Fig. 3.14a) shows that the behaviour of the terms is similar throughout the flame. The thickness of the flame (preheat and reaction zone) given in Fig. 3.14b differs no more than a few percent from the thickness of the flame given in Fig. 3.14a. The peak values of the terms are, however, considerably higher than those of Smooke (1991). The difference is mainly caused by the difference in the adiabatic burning velocity $S_L$ (42 cm/s for our case and 38 cm/s for the skeletal chemistry flame).

These one-dimensional results show that the one step model is capable of describing the behaviour of the energy transport in the flame front reasonably well.
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fig. 3.14: The separate contributions to the energy equation in an adiabatic one-dimensional CH₄/air flame calculated with skeletal chemistry (Smooke 1991), Somers (1994)) (a) and with the one-step chemical model (b).

3.4.2 Energy transport in two-dimensional flames

We will consider three flames in this section: a flame on a multiple-slit burner and a flame on a coaxial cylindrical burner, both confined between symmetry boundaries, and an unconfined flame on a cylindrical burner burning in an open atmosphere. We will not treat the case of an unconfined flame on a slit burner because the effect of the confinement is similar for slit and cylindrical burners. We start with the assumption that the local flame contours coincide with the local isotherms. The terms of the energy equation are calculated in a coordinate system \((x', y')\) (which is obtained by rotating and translating the system \((x, y)\)) with \(x'\) perpendicular to the local isotherms and \(y'\) along the local isotherms (see Fig. 3.15). The energy equation for the cartesian case can now be written as:

\[
\frac{\partial}{\partial x'} (\rho u' c_p T) + \frac{\partial}{\partial y'} (\rho v' c_p T) - \frac{\partial}{\partial x'} \left( \lambda \frac{\partial T}{\partial x'} \right) - \frac{\partial}{\partial y'} \left( \lambda \frac{\partial T}{\partial y'} \right) = - \sum_i h_i \hat{\rho}_i \tag{3.2}
\]

with \((u', v')\) the velocities in the \((x', y')\) system. The energy equation in the cylindrical system (with the radial direction in \(x\) direction) is given by:

\[
\frac{\partial}{\partial x'} (\rho u' c_p T) + \frac{\partial}{\partial y'} (\rho v' c_p T) - \frac{\partial}{\partial x'} \left( \lambda \frac{\partial T}{\partial x'} \right) - \frac{\partial}{\partial y'} \left( \lambda \frac{\partial T}{\partial y'} \right) + \frac{\rho u c_p T}{x} - \frac{\lambda \partial T}{x} = - \sum_i h_i \hat{\rho}_i \tag{3.3}
\]

Note that both the convective and conductive parts of eq. (3.2) are extended with an extra term in eq. (3.3). These extra terms denote the transport along the cylindrical flame contour due
3.4. *Energy transport in one- and two-dimensional flames*

The conductive and convective energy transport at the side \( x = b/2 \); see Fig. 3.3) and the tip of the flames mentioned above will be studied in the remainder of this section.

**Confined Flames**

The terms of the energy equation (eq. (3.2) and eq. (3.3)) are given in Fig. 3.16 for the confined flame on the multiple-slit burner and in Fig. 3.17 for the confined flame on the cylindrical burner. The terms at the side of the flame are plotted versus the distance along a grid line in \( y \) direction. It is clear that the energy transport along the isotherms is much smaller than the energy transport perpendicular to the isotherms at the side of the flame cone for both cases. For the flame on the slit burner the conductive (convective) term in \( y' \) direction is maximal 12 \% (9 \%) of the conductive (convective) term in \( x' \) direction; for its cylindrical equivalent this is 10 \% (8 \%). The convective and conductive transport in \( y' \) direction is, however, considerably smaller (8 and 15 \%, respectively) in the cylindrical flame (note that the transport perpendicular to the \( x' - y' \) plane is added to the transport in \( y' \) direction in Fig. 3.17 and Fig. 3.18). The smaller transport in \( y' \) direction at the side of the cylindrical flame is caused by the larger curvature of the flame front on the slit burner. The above implies that the energy transport at the side of the flame is more or less one-dimensional, especially for the cylindrical flame. The behaviour of the terms of the energy equation perpendicular to the isotherms at the side of the flame is comparable with the behaviour in the 1D flame. The thickness of the cartesian flame at the side is about 0.85 mm, the thickness of the cylindrical flames at the side is about 0.70 mm. The smaller flame thickness for the cylindrical flames is probably due to the additional convective mass and energy transport in angular direction (perpendicular to the \( x' - y' \) plane) for axisymmetrical flames. The terms are added to the other corresponding transport terms along the flame in \( y' \) direction in Fig. 3.17 and Fig. 3.18 to keep the figures surveyable.
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fig. 3.16: The terms of the energy equation in the \( (x', y') \) system for the confined flame on a multiple-slit burner in the side (a) and the tip of the flame (b).

We will now consider the energy transport through the flame tip at the centreline. The energy removal by convection parallel to the isotherms in the tip, induced by flow divergence in the tip area, and the energy transport towards the centreline by parallel conduction, caused by curvature effects, almost add up to zero for all cases considered. This leads to the conclusion that the total energy transport is almost quasi one-dimensional in the tip. Note that the above also implies that the tip is nearly adiabatic, i.e. the net heat loss of the flame tip is almost equal to zero. This is sustained by experimental results for stoichiometric methane/air flames (Law (1988)). The almost zero heat loss of the stretched and curved tip is attributed to the nearly diffusional neutrality of the mixture (Chung (1988), Matalon (1982) and Law (1988)). The separate contributions to the energy transport parallel to the isotherms, however, are very important because the terms in parallel \( (y') \) direction are of the same order of magnitude or larger than the energy transport in \( x' \) direction, which is caused by the large curvature of the isotherms in the tip.

The analysis of the mass flux \( \rho v \) along the centreline of the flames confined between symmetry boundaries showed that the cylindrical tip has a smaller thickness (about 0.7 mm) than the tip of the flame on the slit burner (about 1.0 mm); the thickness of the reaction zone (the area where the source term is large) is, however, comparable for both flames. The mass burning rate for

\[ \text{Terms of the energy equation [GJ/m}^2\text{s]} \]

Distance \( y \) along grid line at \( x = b/2 \text{ mm} \) [mm]  
Distance \( y \) along center axis [mm]

- Perpendicular Convection term
- Parallel Convection term
- Perpendicular Conduction term
- Parallel Conduction term
- Source term
3.4. Energy transport in one- and two-dimensional flames

The terms of the energy equation in the $(x', y')$ system for the confined flame on a cylindrical burner in the side (a) and the tip of the flame (b).

![Graph showing terms of the energy equation](image)

Both flames is approximately equal in the tip. The sharper temperature gradients perpendicular to the flame front in the cylindrical tip induced by the smaller flame thickness results in about 20-25% higher convective and conductive transport terms in the cylindrical case (see Fig. 3.16 and Fig.3.17). The larger transport parallel to the flame front in the cylindrical flame is caused by the additional contributions to the transport parallel to the flame by the last two terms in the left hand side of eq. (3.3).

Unconfined Flames

The influence of confinement on the energy transport is investigated by comparing an unconfined cylindrical flame (Fig. 3.18) with the confined cylindrical flame (Fig.3.17). The energy terms in $y'$ direction (along the isotherms) at the side of the unconfined flame are about 10-15% smaller than the comparable parts in the confined cylindrical flame. This implies that the sides of the unconfined flame are less curved than the sides of the confined flame which is also directly visible from the isotherms. The total transport parallel to the local flame front does not differ significantly for the confined and the unconfined flame because the transport perpendicular to the $x' - y'$ plane (which is much larger than the transport in $y'$ direction) is almost equal for both flames.
Chapter 3. Premixed flame stabilisation and the environment

The most significant differences between the energy terms of the confined flames and the unconfined flame are present in the tip. The flame thickness and the energy transport perpendicular to the local isotherms in the tip is not affected significantly by the confinement. The effect of confinement mainly manifests itself in the relative magnitude of the energy transport along and perpendicular to the isotherms. The energy transport along the isotherms in the tip is approximately 35% smaller in the unconfined flame (Fig. 3.18). This is mainly caused by a smaller curvature (which causes smaller conductive transport along the isotherms) and flow divergence (which causes smaller convective transport along the isotherms) in the tip of the unconfined flame.

3.5 Conclusions

Numerical results for laminar Bunsen flames burning in a cold surrounding atmosphere are presented in this chapter. The global flow field and the flame shape of a flame on a tube burner in air have been compared with numerical results. It is shown that the flame shape and global flow field near the experimental flame is well reproduced by the model. Velocity profiles (measured...
3.5. Conclusions

with LDV) at various heights above the edge of a single-slit burner in an open atmosphere are compared with numerical data. The comparison shows that the model gives a good representation of the velocity field near the flame. The velocities given by the model differ no more than 10-15 \% from the measured velocities.

A numerical investigation of the effects of variations in burner curvature and the presence of a surrounding atmosphere on the flame shape and the mass flux through the tip has been carried out. The influence of burner geometry is studied by comparing flames on slit and on tube burners, confined between similar flames. The cylindrical flames are less curved, especially in the tip, and have a smaller mass flow rate on the central axis just ahead of the flame tip. These differences may be ascribed to the extra ability of the cylindrical flame to expand in radial direction. It has also been shown that a surrounding atmosphere has a significant effect on the flame shape, the mass flux through the flame tip and the curvature of the flame tip. The flames in an open environment can dispose of the excess of mass on the central axis more easily, due to the absence of confining objects near the burners. The investigations show that differences in expansion space near premixed Bunsen flames may lead to significant differences in flame shape, flow field and curvature.

The investigation of the energy transport has shown that the energy transport in the sides of the two-dimensional flames is more or less one-dimensional for all cases considered. The magnitude of the convective and conductive terms along the flame contours is, however, affected by the burner geometry and the direct environment. The transport along the flame contours is largest in the confined flame on the slit burner and smallest in the unconfined cylindrical flame. This can be explained by the different ability to expand in directions normal to the main flow direction and the curvature of the flame sides.

The energy transport parallel to the flame contours in the tip is of the same order of magnitude or larger than the energy transport normal to the flame contours. The energy removal by convection parallel to the flame contours is almost compensated by the energy transport due to conduction towards the centreline. The energy transport perpendicular to the flame contours is higher in the cylindrical flames. This is caused by the smaller flame thickness of the cylindrical tip (compared to the flame on the slit burner).

The investigation has resulted in a clear and quantitative insight in the effects of burner geometry and confinement on the energy transport in two-dimensional flames.
Chapter 3. Premixed flame stabilisation and the environment
In this chapter flame stabilisation of laminar methane/air flames near flash-back will be investigated. The main purpose of the investigation is to quantify several phenomena (such as flame cooling by the burner wall) which affect flame stabilisation near flash-back. Another goal of the investigation is the quantification of the effect of burner wall curvature on the stabilisation of laminar flames and their flash-back behaviour.

A numerical and experimental investigation of flash-back (a condition in which a flame moves into the burner) of laminar Bunsen flames on cylindrical and on slit burners with a diameter/width of less than 9 mm is presented in section 4.1. The investigation in section 4.1 gives more insight in the behaviour of the critical flash-back gradients $g_f$ of flames on small cylindrical burners and slit burners. We will also look at the effects of burner size and the equivalence ratio on the critical gradient. The effect of the burner geometry on flame cooling by the burner wall is studied in section 4.2 by analysing the effect of the curvature of the burner wall on the cooling rate by the burner. The aim of this investigation is to provide more physical background for the results given in section 4.1 and to gain more insight in the importance of the processes governing flame stabilisation at low velocities. The results of the investigation in section 4.2 will be used in section 4.3 to investigate the dependence of $g_f$ on burner size. The effect of burner wall curvature on the critical gradient is also investigated in section 4.3.

### 4.1 Flash-back of flames on tube and slit burners

Flash-back of laminar Bunsen flames on cylindrical burners has been investigated experimentally by Lewis et al. (1943) for natural gas/air mixtures and by Harris et al. (1949) for methane/nitrogen/oxygen mixtures. Lewis et al. (1943) consider flash-back in tubes with diameters ranging from 3.9 to 15.5 mm. The gradient theory and the concept of the critical gradient, discussed in chapter 1, was first introduced by Lewis et al. The work of Harris et al. (1949) for methane/air mixtures is limited to relatively large cylindrical burners. The flash-back behaviour of flames on slit burners is, however, different, due to the difference in burner geometry. Therefore, we will also study flames on slit burners, and compare the behaviour with results for cylindrical burners.

The experimental method will be described in subsection 4.1.1. Subsequently, the calculation
Chapter 4. Flame stabilisation near flash-back

of the critical gradients will be discussed in subsection 4.1.2. Then, in subsection 4.1.3 the experimental and numerical results for the critical gradient as a function of burner size and equivalence ratio will be discussed.

4.1.1 Experimental method

The flow rate and the equivalence ratio of the mixture are controlled with electronic mass-flow controllers with an absolute accuracy of 1 % of their full capacity. This implies that the largest errors occur at the lowest flow rates which, in turn, means that the largest errors can be expected for the small cylindrical burners. An investigation of the error in the mass flow rate (the critical gradient is proportional to the flow rate) and the equivalence ratio has shown that the error in the flow rate is about 10 to 15 % while the error in the equivalence ratio is equal to about 5 % for small cylindrical burners. The error in the mass flow rate decreases to about 5 % for the larger cylindrical burners and the slit burners.

The experiments are performed with a rectangular slit burner (see figures 3.4 and 3.5) with a variable slit width (in $x$ direction) and with pyrex tube burners of various diameters. The burners are described in the previous chapter. The flow rate at which flash-back occurs is determined by gradually decreasing the flow rate of the mixture until flash-back occurs, i.e. the flame keeps moving downwards into the burner. The flow rate at which flash-back occurs is then used to calculate the theoretical velocity profile (Shah (1978) and chapter 3) and the velocity gradient at the burner wall, which is referred to as the critical gradient $g_l$. For slit burners, we refer to flash-back as the point when the flame clearly flashes back in the 2D area (the $xy$ plane in figure 3.4) and doesn't stabilise at the burner top anymore.

fig. 4.1: The computational domain.
The flames (especially the slit burner flames) generally become unstable at a flow rate above the flow rate at which actual flash-back occurs. These instabilities, induced by local disturbances in the flow rate or the flame position near the burner wall, may lead to partial flash-back. In this condition the flame base (the part of the flame near the burner wall) partially moves into the burner and partially stabilizes on top of the burner rim (Lewis, 1943).

A difficulty with the slit burner measurements is that the velocity gradient in the $yz$-plane (at the short sides of the burner) is only $50-80\%$ of the velocity gradients in the 2D area, depending on the flow rate. This means that the flames tend to flash-back when the gradient in the 2D area is still much higher than the critical value. This problem has been solved by increasing the gradient at the short sides of the burner with thin wires. Then, the flow rate at which flash-back occurs $\Phi_{v,f}$ is determined (the flame then clearly flashes back in the 2D area). After this the wires are removed and the flame is lit with the same flow rate $\Phi_{v,f}$. It is then judged visually if the flame still flashes back in the 2D area.

### 4.1.2 Numerical Calculation of the Critical Gradient

The computational domain is given in figure 4.1. The height of the wall $H$ is 3 mm for all cases studied. The values for $L_x$ and $L_y$ depend on the burner width or diameter $2b$. They are chosen such that the boundary conditions at $x = L_x$ and at $y = L_y$ do not affect the obtained value for $g_f$.

![A flow diagram of the numerical calculation of the critical gradient.](image)

\[ g_f = \frac{\partial \bar{v}}{\partial x}_{x=b} = \frac{2V_{max,f}}{b} \]

$g_f$. The domain length in $x$-direction, $L_x$, then varies between 10 and 20 mm for the cylindrical
Chapter 4. Flame stabilisation near flash-back

fig. 4.3: An illustration of numerical flash-back: contours of temperature (K) for a stable flame (left) and a flame which keeps moving into the burner (right) for a cylindrical burner.

burners and between 20 to 50 mm for the slit burners. \(L_y\) is equal to 16 and 30 mm for cylindrical and slit burners, respectively. The calculation of the critical gradients is shown schematically in figure 4.2. First a stationary flame is modelled with the domain given in figure 4.1. Then, the inlet velocity \(V_{\text{max}} = v(x, 0)\) (see equation (2.27)) is reduced and the calculation process is resumed. When the flame still stabilises the velocity is reduced again. This sequence is repeated (with velocity reduction steps of 5%) until the velocity is too low for (numerical) flame stabilisation at \(y = H\) (say, at \(V_{\text{max}} = V_{\text{max},f}\)). The critical gradient is then defined as the gradient of the parabolic velocity profile at the burner wall

\[
g_f = \frac{2V_{\text{max},f}}{b} \tag{4.1}
\]

Note that the reduction steps of 5% lead to an uncertainty in \(g_f\). Smaller reduction steps are, of course, possible but result in much larger computation times. Furthermore, model assumptions and experimental errors give errors of the same order of magnitude. A numerical result of a stable flame and of a flame which does not stabilise at the top of the burner rim anymore is given in figure 4.3.

4.1.3 Results

The numerical results with respect to the critical gradient for the slit burners and the cylindrical burners are compared with experimental data in this subsection. The physical picture behind the influence of the burner size and geometry on the behaviour of the critical gradients is discussed in the subsequent sections.
4.1. Flash-back of flames on tube and slit burners

The critical gradients calculated numerically are compared with experimental results in figure 4.4 and 4.5. Figure 4.4 shows that the deviations between the numerical and the experimental results are not larger than about 10% in the full range of burner widths. The deviations are largest for the cylindrical burners. This is mainly due to the low volumetric flow rates at which flash-back occurs which introduces uncertainties in the flow rate of approximately 10-15%.

An important difference between the small cylindrical and slit burners is the curvature of the burner wall. The burner wall curvature of the cylindrical burners enhances the cooling effect (Putnam, 1949). Figure 4.4 shows that the numerical critical gradients for cylindrical and slit burners do not differ significantly (less than 5%) from each other for diameters larger than 6 mm. However, there is a systematic difference between the numerical gradient for flames on slit and tube burners for diameters or widths smaller than 5 mm. The experimental critical gradients do not show a systematical difference which is probably due to experimental errors. The relative magnitude of the critical gradients of flames on slit and cylindrical burners will be investigated further in the next section.

The dependence of $g_f$ on the equivalence ratio is given in figure 4.5 for a 5 mm tube burner. We will only consider this burner because the dependence of $g_f$ on the equivalence ratio is more or less independent of burner size or - geometry. Figure 4.5 shows that the critical gradient is maximal near $\phi=1$. This is due to the fact that the burning velocity is maximal around $\phi=1$. The dependence of $g_f$ on $\phi$ in figure 4.5 shows much resemblance with the dependence given by Harris (1949). The numerical model describes $g_f$ well between equivalence ratios of 0.9 and 1.1. Outside this area the difference between the experimental and the numerical results become larger which
is probably due to larger deviations of the predicted burning velocity by the one-step chemistry model (see chapter 2).

Figure 4.4 clearly shows that the critical gradient decreases with burner size. A slight decrease was also found by Lewis et al. (1943) for natural gas/air flames. The decrease is caused by the assumption of a linear velocity profile in the gradient theory (see figure 4.6), as will be explained below. In the gradient theory flash-back occurs if the mixture velocity is lower than the burning velocity $S_L$ at $x = b - \delta_f$ when the stand-off distance $\delta_f$ is maximal. The velocity gradient for a linear velocity profile at which this occurs ($\approx S_L/\delta_q$) is independent of the burner size. However, the velocity profile at the burner outflow for the burners studied in this thesis is parabolic. The gradient at the burner wall of a parabolic velocity profile decreases with increasing burner size when $v(x = b - \delta_q = S_L$ is constant. This effect causes the decrease of $g_f$ with the burner size and it is undesired because, for engineering applications, an independent measure for flash-back is desired. This decrease requires further investigation to determine whether or not the decrease of $g_f$ is solely due to the curvature of the velocity profile.

Therefore, an alternative critical gradient will be introduced which is insensitive for the curvature of the parabolic velocity profile $v(x)$. The stabilisation theory of Lewis et al. (1943) states that the mixture velocity $v(x)$ for stable flames is equal to the maximum burning velocity $S_L$ at a distance $\delta_q$ from the burner wall (we assume, for the time being, that $\delta_q$ is equal to half the quenching diameter or distance; see Harris (1949) for experimental values). Then, the following equation for $V_{\text{max}}$ can be deduced

$$V_{\text{max}} = \frac{b^2 S_L}{2b d_q - \delta_q^2}. \quad (4.2)$$

When this expression is substituted in equation (4.1) with $V_{\text{max}} = V_{\text{max},f}$ the following expression
4.1. Flash-back of flames on tube and slit burners

fig. 4.6: Illustration of the increase of the critical gradient for small burners. The dashed line illustrates the gradient at the wall for the parabolic profile.

fig. 4.7: The critical gradients for a linear velocity profile for slit burners (solid line) and cylindrical burners (dashed line).

for $g_f$ is obtained

$$g_f = \frac{2b}{2b - \delta_q} \cdot \frac{S_L}{\delta_q}. \quad (4.3)$$

Note that $S_L/\delta_q$ is the value of the gradient of the linear profile at flash-back ($= g_{f,\text{lin}}$). This implies that the gradient $g_{f,\text{lin}}$ of the linear profile that intersects the parabolic profile at $x = b - \delta_q$ is given by:

$$g_{f,\text{lin}} = \frac{2b - \delta_q}{2b} \cdot g_f, \quad (4.4)$$

where we chose $\delta_q$ equal to half the measured quenching distance or the measured quenching radius $R_d$ according to Harris (1949). This results in $\delta_q = R_{d,\text{car}} = 1.2 \text{ mm}$ for the slit burner and $\delta_q = R_{d,\text{cyl}} = 1.6 \text{ mm}$ for cylindrical burners. The gradient $g_{f,\text{lin}}$ is plotted versus the burner size in figure 4.7. It is clear that the variation with the burner size is much less pronounced now,
especially for the slit burner gradients. The slit burner gradients vary about 15% now; before the correction this was 60%. This implies that other effects (such as different convective velocities in the quenching layer) on the critical gradient are relatively small for slit burner. The larger variation for the cylindrical burners is probably caused by the assumption that \( \delta_q \) is constant with increasing burner size. In reality, \( \delta_q \) decreases with increasing burner radius for cylindrical burners due to the decreasing curvature of the burner wall. This implies that the quenching distance and \( g_{f,\text{lin}} \) of slit and cylindrical burners should approach each other for large burners. From figure 4.7 it follows that \( g_{f,\text{lin}} \) for cylindrical and slit burners do not approach each other for large burners. This is probably also due to the assumption of a constant \( \delta_f \) for the cylindrical burners because a lower value of \( \delta_q \) for larger cylindrical burners results in higher values for \( g_{f,\text{lin}} \).

4.1.4 Conclusions

The dependence of \( g_f \) on the burner size predicted by the numerical model agrees well with the experimental results. This shows that the stabilisation of laminar flames near flashback is dominated by flame cooling because other phenomena, such as chain termination processes near the burner wall, are not incorporated in the model. The results for the dependence on the equivalence ratio show larger deviations, especially for very lean and rich flames. This is most likely caused by the worse prediction of the burning velocity by the one-step chemical model.

A calculation of the critical gradient based on a linear velocity profile shows that the decrease of the critical gradient with burner size is mainly caused by the curvature of the velocity profile near the wall. The critical gradients \( g_{f,\text{lin}} \) for slit and cylindrical burners become approximately equal for burners larger than about 6 mm. The effect of the curvature of the burner wall seems to become very small for burners larger than about 6 mm. The difference between \( g_{f,\text{lin}} \) for slit and cylindrical burners larger than about 7 mm is probably caused by the assumption that \( \delta_q \) for cylindrical burners is constant. However, the observation that burner wall curvature doesn’t affect \( g_{f,\text{lin}} \) for burners larger than 6 mm requires further investigation. To clarify the uncertainties in the results for \( g_{f,\text{lin}} \) an analytical analysis of the effects of burner wall curvature on several quantities (e.g. the temperature \( T \) in the quenching layer and \( \delta_f \)) is presented in the following section.

4.2 Flame cooling by the burner wall

In this section we present an analysis of the differences between slit and cylindrical burners with respect to the cooling rate of the burner. The main goal of the analysis is to provide explanations for and to sustain the systematic difference between the flash-back gradients of flames on small slit and cylindrical burners presented in the previous section by analysing the effect of burner wall curvature on the behaviour of \( T \) and \( Y_{fu} \) in the quenching layer and on the stand-off distance \( \delta_q \).

The analysis is an extension of the analytical treatment performed by de Goey (1994) for slit burners. The extension basically consists of the introduction of a burner wall with a curvature \( 1/R_0 \) and of the use of cylindrical coordinates \((r, \theta)\) instead of cartesian coordinates. Note that \( 2R_0 \) is equal to the burner width \( 2b \) for cylindrical burners and that slit burners coincide with \( R_0 \to \infty \).
4.2. Flame cooling by the burner wall

The mass fractions in the quenching layer has been investigated by de Goey (1994). It was shown that the general behaviour of the temperature and the mass fractions in the quenching layer and the quenching layer thickness are not affected significantly by the assumptions. Basic issues of the model are discussed in subsection 4.2.1. The solutions for the temperature $T$, the mass fractions $Y_i$ and the Shvab-Zel'dovich variables are presented in subsections 4.2.2, 4.2.3 and 4.2.4, respectively. In subsection 4.2.5, the energy balance is verified. Then, the effect of the burner wall curvature on the thickness of the quenching layer will be investigated (subsection 4.2.6) and the behaviour of $T$ and the fuel mass fraction $Y_{fu}$ in the quenching layer is discussed (subsection 4.2.7).

4.2.1 Two-dimensional analysis

The burner geometry is the same as the geometry used by de Goey (1994) (see figure 4.8a). The only difference is that the burner wall has a non-zero curvature $1/R_0$. Two coordinate systems are given in figure 4.8a. One system $(x, y)$ that was used by de Goey (1994) and the $(r, y)$ system that will be used in the present study. The coordinate system $(x, y)$ is given because the
results will be compared with the results obtained by de Goey (1994). We will now introduce the basic assumptions used in the analytical model. It is assumed that there is no lateral velocity component \((u = 0)\). Note that this assumption reduces the continuity equation to \(\rho v = \rho^u v^u\), where the superscripts \(u\) refer to the conditions at in the unburnt mixture \(y \rightarrow -\infty\). The ideal gas law \((P = \rho R_y T)\) is used as the equation of state, where \(P\) is the pressure and \(R_y\) the specific gas constant of the mixture. The deflagration process considered here is a low Mach number flow which implies that the pressure can be assumed to be constant. Furthermore, the constant \(R_y\) is assumed to be independent of the mixture composition. These assumptions lead to a density which depends on temperature only: \(\rho T = \rho^u T^u\).

The thermal conductivity \(\lambda\) and the specific heat \(c_p\) are both taken to be constant. For the Lewis numbers of fuel and oxygen we use \(Le_i = 1\). These assumptions are introduced to make the analytical treatment possible.

As chemical model the one-step irreversible reaction \(\text{fuel} + \text{oxygen} \rightarrow \text{products}\) is used with an Arrhenius-type source term (see chapter 2; equation 2.19). The conservation equations for the temperature \(T\) and mass fraction of species \(i\), \(Y_i\) with \(i = (\text{fuel}, \text{oxygen}, \text{products})\), now become

\[
\frac{1}{L} \frac{\partial T}{\partial y} - \frac{\partial^2 T}{\partial y^2} - \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial T}{\partial r} \right) = \Delta H \dot{\rho}_{fu}, \tag{4.5}
\]

and

\[
\frac{1}{L} \frac{\partial Y_i}{\partial y} - \frac{\partial^2 Y_i}{\partial y^2} - \frac{1}{r} \frac{\partial}{\partial r} \left( r \frac{\partial Y_i}{\partial r} \right) = s_i \dot{\rho}_{fu}, \tag{4.6}
\]

with \(\Delta H\) the combustion enthalpy and \(s_i\) the stoichiometric factor of species \(i\). The values of the physical parameters, such as \(\lambda\), \(c_p\), \(\Delta H\) and the unburnt and burnt values of \(T\) and \(Y_{fu}\), are given in table 4.1. The equivalence ratio \(\phi\) is equal to one. The length scale \(L\) is defined by

\[
L = \frac{\lambda}{\rho^u v^u c_p}. \tag{4.7}
\]

Table 4.1: The physical parameters and the temperature and mass fractions of fuel in the burnt and the unburnt mixture.

<table>
<thead>
<tr>
<th>Parameter</th>
<th>Value</th>
<th>Dimension</th>
</tr>
</thead>
<tbody>
<tr>
<td>(\rho_u)</td>
<td>1.13</td>
<td>[kg m(^{-3})]</td>
</tr>
<tr>
<td>(T_u)</td>
<td>300</td>
<td>[K]</td>
</tr>
<tr>
<td>(T_b)</td>
<td>2250</td>
<td>[K]</td>
</tr>
<tr>
<td>(\lambda)</td>
<td>0.092</td>
<td>[J m(^{-1}) K(^{-1}) s(^{-1})]</td>
</tr>
<tr>
<td>(c_p)</td>
<td>1365</td>
<td>[J kg(^{-1}) K(^{-1})]</td>
</tr>
<tr>
<td>(\Delta H)</td>
<td>(4.813 \times 10^7)</td>
<td>[J kg(^{-1})]</td>
</tr>
</tbody>
</table>

In the remainder of this subsection the behaviour of \(T\) and \(Y_i\) in the quenching layer will be discussed to clarify some additional assumptions in the analysis. Profiles of the Shvab-Zel'dovich
variable

\[ J_{fu,ox} = \frac{c_p T}{\Delta H} + \frac{Y_{fu,ox}}{s_{fu,ox}} \]  

(4.8)

will be treated as well. The conservation equation for \( J_i \) can be derived by substituting the conservation equations for \( T \) and \( Y_i \) into equation (4.8). We assume that the flame is flat near the stabilisation point (parallel to the \( r \)-axis) and that the flame flashes back if the velocity \( v^u \) is decreased. This implies that the cooling near the burner wall and the quenching distance \( \delta_q \) are maximal. The flat flame is assumed to be stabilised at \( y=0 \) for \( r < R_0 - \delta_q \) and is extinguished due to the cooling rate by the burner wall for \( R_0 - \delta_q < r < R_0 \). This means that the fuel mass consumption rate \( \dot{\rho}_{fu} \) is almost zero in the latter area (see figure 4.8b). We will, therefore, assume that \( \dot{\rho}_{fu} = 0 \) for \( R_0 - \delta_q < r < R_0 \). The zero fuel mass consumption implies that the mass fractions only change due to diffusion and convection. This, in turn, leads to constant mass fractions in a thin layer of thickness \( \eta \) at the wall \( (R_0 - \eta < r < R_0) \) because there is no diffusion flux through the wall. The Shvab-Zel'dovich variables \( J_i \) are not affected by the presence of the flame because the differential equation for \( J_i \) has no chemical source term. The decrease of the mass fractions in the region \( R_0 - \delta_q < r < R_0 - \eta \), therefore, has to be proportional to the increase of \( T \) in the region, i.e. the heat loss by cooling is compensated by a chemical enthalpy flux caused by diffusion of fuel and oxygen. The Shvab-Zel'dovich variables will decrease for \( R_0 - \eta < r < R_0 \) because the diffusion of fuel and oxygen is zero in this area (see fig. 4.8b).

4.2.2 The thermal boundary layer

In this subsection an approximate solution of the energy equation for the temperature will be presented. The domain is divided into two regions: a region \( R_0 - \delta_q < r < R_0 \) where the cooling is important and a region \( r < R_0 - \delta_q \) in which the profiles of \( Y_i, T, \) and \( J_i \) are independent of the distance from the burner wall. The temperature profile as a function of \( y \) for \( r < R_0 - \delta_q \) is given by the solution for a flat flame which is independent of \( r \)

\[ T(r, y) = T^u + \Delta T e^\frac{y}{\eta} \text{ for } r < R_0 - \delta_q, \ y \leq 0, \]

\[ T(r, y) = T^\phi \text{ for } y > 0 \]

This means that the reaction sheet at \( y = 0 \) is considered to be infinitely thin, which is related to the large value of the activation energy (Bush (1970)). \( \Delta T = T_\phi - T_u \) denotes the difference between the flame and the unburnt temperature. The boundary conditions for the area \( R_0 - \delta_q \leq r \leq R_0 \) where cooling is important then become

\[ y \leq 0; \ r = R_0 : T = T^u \]

\[ y \leq 0; \ r = R_0 - \delta_q : T \rightarrow T^u + \Delta T e^\frac{y}{\eta} \]

and

\[ y \rightarrow -\infty; \ R_0 - \delta_q \leq r \leq R_0 : T = T^u \]
The fuel mass consumption rate \( \dot{\rho}_{fu} \) is assumed to be zero in the cooling layer. This assumption, the shape of the boundary conditions and the assumption of a unidirectional flow imply that a separation of directions may be applied. This leads to the trial solution

\[
T(r, y) = T^u + t_1(y) \cdot t_2(r).
\]

(4.9)

The separation of directions makes it possible to give an exact solution of the energy equation for the given boundary conditions. Substitution of equation (4.9) into the energy equation (4.5) with \( \dot{\rho}_{fu} = 0 \) gives

\[
\frac{1}{t_1} \left[ \frac{1}{L} \frac{dt_1}{dy} - \frac{d^2t_1}{dy^2} \right] = \frac{1}{rt_2} \frac{d}{dr} \left( \frac{dt_2}{dr} \right) = c^2,
\]

(4.10)

with \( c^2 \) the separation constant. Two different solution types for \( t_1(y) \) and \( t_2(r) \) are taken into account

for \( c^2 = 0 \) : \( t_1 = k_1 e^{\nu r}; t_2 = k_2 \ln(r) + k_3 \)

(4.11)

and

for \( c^2 > 0 \) : \( t_1 = k_4 e^{\nu r}; t_2 = k_5 I_0(\nu r) + k_6 K_0(\nu r) \)

(4.12)

with \( \Gamma_{\pm} = \frac{1}{2L} \left[ 1 \pm \sqrt{1 - (2cL)^2} \right] \). The functions \( I_0(\nu r) \) and \( K_0(\nu r) \) are modified Bessel functions of zeroth order. The \( c^2 < 0 \) solution type is not taken into account because it shows an oscillatory behaviour which is not in accordance with the flat flame solution for \( r < R_0 - \delta_q \) and the solutions for \( c^2 \geq 0 \) are sufficient to describe the desired solution. Note that the solution given above also holds for the mass fractions and the Shvab-Zel'dovich variables as long as they are described by the same type of conservation equations.

The solution given by equation (4.11) for \( c^2 = 0 \) satisfies all the boundary conditions for the energy equation (4.5)

\[
T(r, y) = T^u + \Delta T \frac{\ln \left( \frac{r}{R_0} \right)}{\ln \left( 1 - \frac{\delta_q}{R_0} \right)} e^{y \frac{x}{\delta_q}} \text{ for } R_0 - \delta_q < r < R_0
\]

(4.13)

The solution found for a burner wall with no curvature (\( 1/R_0 = 0 \)) by de Goey (1994) should be recovered if the limit for \( R_0 \to \infty \) is taken in equation (4.13). The solution found by de Goey (1994) reads

\[
T(x, y) = T^u + \Delta T \frac{x}{\delta_q} e^{y \frac{x}{\delta_q}}
\]

(4.14)

When \( r = R_0 - x \) is substituted into equation (4.13), it can be shown that equations (4.13) and (4.14) become equal for \( R_0 \to \infty \) by using the expansion \( \ln(1 + \epsilon) = \epsilon + O(\epsilon^2) \) for \( \epsilon \to 0 \).

The resulting profiles \( T(r, y = 0) \) are shown in figure 4.9 for different values of \( R_0 \). The influence of \( R_0 \) on the behaviour of the temperature in the quenching layer will be discussed after the subsection in which the thickness of the thermal boundary layer is discussed.
4.2. Flame cooling by the burner wall

![Graph showing temperature and fuel mass fraction profiles](image)

fig. 4.9: The profiles of $T$ and $Y_{fu}$ for various values of $R_0$. The horizontal distance from the wall is normalised with the quenching distance.

### 4.2.3 The diffusive boundary layer

The mass fractions of fuel and oxygen are described by the same type of differential equation as the temperature $T$. This means that the solutions given in equations (4.11) and (4.12) are also valid for $Y_i$. The boundary conditions for $Y_i$ are:

$$ y \leq 0; \quad r = R_0 : \quad \frac{\partial Y_i}{\partial r} = 0, $$

$$ y \leq 0; \quad r = R_0 - \delta_q : \quad Y_i \rightarrow Y_i^u + \Delta Y_i e^{\frac{y}{\delta_q}}, $$

$$ y \rightarrow -\infty; \quad R_0 - \delta_q \leq r : \quad Y_i = Y_i^u. $$

with $\Delta Y_i$ equal to $Y_i^u - Y_i(R_0 - \delta_q, 0)$ ($\Delta Y_i$ will be calculated furtheron). Note that the boundary condition at $r = R_0$ is of a different type than the boundary condition for $T$. This implies that a solution analogous to equation (4.13) does not describe the solution for $Y_i$ near the burner wall. The correct shape of the mass fraction profiles is found by adding the $c^2 > 0$ solutions to the $c^2 = 0$ solution. The inclusion of the $c^2 = 0$ solution is necessary to ensure that the Shvab-Zel'dovich variables are not influenced by the presence of the flame at $r = R_0 - \delta_q$. The solution for $Y_i$ is, therefore, given by

$$ Y_i(r, y) = Y_i^u + \frac{\Delta Y_i}{\ln \left( 1 - \frac{\delta_q}{R_0} \right)} \left[ \ln \left( \frac{r}{R_0} \right) e^{\frac{y}{\delta_q}} + \bar{Y}_i(r, y) \right], $$

with

$$ \bar{Y}_i(r, y) = \int_0^\infty I_0(c r) \left[ F(c) \exp \left( \frac{y}{2L} \left[ 1 + \sqrt{1 - 4c^2 L^2} \right] \right) \right] \, dc. $$
Chapter 4. Flame stabilisation near flash-back

\[ G(c) \exp \left( \frac{c}{2L} \left[ 1 - \sqrt{1 - 4c^2 L^2} \right] \right) \]  \hspace{1cm} (4.16)

The modified Bessel function \( K_0(cr) \) is not included in equation (4.16) because \( K_0(cr) \) decreases with increasing \( cr \) while \( \tilde{Y}_i(r, y) \) should increase with increasing \( r \). The amplitudes \( F(c) \) and \( G(c) \) indicate the contribution of solutions with length scale \( 1/c \) in \( r \) direction. Note that solutions with \( c < 0 \) do not contribute because \( J_0(cr) \) is symmetrical around \( cr = 0 \). The procedure for obtaining expressions for \( F(c) \) and \( G(c) \) is the same as in de Goey (1994) and will not be repeated here. The resulting expression for \( \tilde{Y}(r, y) \) reads

\[ \tilde{Y}_i(r, y) = -\frac{1}{R_0} \frac{2L}{\pi} \int_0^\infty dk \frac{I_0 \left( \sqrt{1+k^2} \right) r}{I_1 \left( \sqrt{1+k^2} R_0 \right)} \left[ \frac{1}{\sqrt{1+k^2}} e^{\frac{k}{2} y} \right]^{3} \cos(k \frac{y}{2L}) e^{-\frac{k}{2}} \]  \hspace{1cm} (4.17)

with \( ik \equiv \sqrt{1 - 4c^2 L^2} \). \( \Delta Y_i \) can be calculated by setting \( Y_i \) equal to the burnt value \( Y^b_i \) in the flame attachment point \((r, y) = (R_0 - \delta_q, 0)\). This leads to the following expression for \( \Delta Y_i \)

\[ \Delta Y_i = \frac{(Y^b_i - \tilde{Y}_i)}{\ln \left( \frac{1}{1 - \delta_q / R_0} \right)} + \tilde{Y}_i \left( R_0 - \delta_q, 0 \right). \]  \hspace{1cm} (4.18)

A similar expression for \( \Delta T \) is derived in the following subsection. The above solution is verified by determining the limit for \( R_0 \to \infty \). The cartesian solution found by de Goey (1994) has to be recovered then. The latter solution is equal to

\[ Y_i(x, y) = Y_i^u + \Delta Y_i \delta_q \left[ \frac{x}{\delta_q} e^{k \frac{y}{2L}} + \tilde{Y}_i(x, y) \right], \]  \hspace{1cm} (4.19)

with

\[ \tilde{Y}_i(x, y) = -\frac{1}{\delta_q} \frac{2L}{\pi} \int_0^\infty dk \exp \left( -\frac{\sqrt{1+k^2} x}{2L} \right) \left[ \frac{1}{\sqrt{1+k^2}} \right]^{3} \cos(\frac{ky}{2L}) e^{-\frac{k}{2}}. \]  \hspace{1cm} (4.20)

First note that the factor \( 1/R_0 \) in equation (4.17) together with the factor \( 1/\ln(1-\delta_q/R_0) \) becomes equal to the factor \( 1/\delta_q \) in equation (4.20) for \( R_0 \to \infty \). Furthermore, when \( r = R_0 - x \) is substituted in equation (4.15) it can be shown that equation (4.15) becomes equal to equation (4.19) for \( R_0 \to \infty \) if

\[ \lim_{R_0 \to \infty} \left[ \frac{I_0 \left( \sqrt{1+k^2} (R_0 - x) \right)}{I_1 \left( \sqrt{1+k^2} R_0 \right)} \right] = \exp \left( -\frac{\sqrt{1+k^2} x}{2L} \right) \]  \hspace{1cm} (4.21)

which follows from the following property of a modified Bessel function of order \( \nu \)

\[ \lim_{y \to \infty} I_\nu(y) \propto \frac{e^y}{\sqrt{2\pi y}}. \]  \hspace{1cm} (4.22)

The profiles of the mass fractions \( Y_i(r, y = 0) \) given by equation (4.15) are also given in figure 4.9 for various values of \( R_0 \). They will be discussed after the subsection with the discussion of the thickness of the thermal boundary layer.
4.2. Flame cooling by the burner wall

4.2.4 The solution of the Shvab-Zel'dovich variables

The expression for $\Delta T$ in equation (4.13) has to be reconsidered before we turn to the solution for the Shvab-Zel'dovich variables. This is necessary because the solution given in equation (4.13) gives rise to a discontinuous derivative of $J_i(r, y)$ at $r = R_0 - \delta_q$. The derivative becomes continuous if the decline of the mass fractions is proportional to the increase of $T$ in the quenching layer. We will, therefore, redefine the solution for $T$ as

$$T(r, y) = T^u + \Delta T \frac{\ln \left( \frac{r}{R_0} \right)}{\ln \left( 1 - \frac{\delta_q}{R_0} \right)} e^{\frac{y}{T}},$$

(4.23)

for $R_0 - \delta_q < r < R_0$ and with $\Delta T$ defined as

$$\Delta T = \frac{(T^b - T^u) \ln \left( 1 - \frac{\delta_q}{R_0} \right)}{\ln \left( 1 - \frac{\delta_q}{R_0} \right) + \bar{Y}_i \left( R_0 - \delta_q, 0 \right)}.$$  

(4.24)

The solution for $J_i$ can be found by substitution of the solution for $T$ and $Y_i$ in equation (4.8)

$$J_i(r, y) = J_i^u + \frac{\Delta Y_i}{s_i \ln \left( 1 - \frac{\delta_q}{R_0} \right)} \bar{Y}_i(r, y).$$

(4.25)

Note that the solution given above approaches $J_i^u$ for $r \to R_0 - \delta_q$ which implies that the Shvab-Zel'dovich variables are indeed not influenced by the presence of the flame at $r = R_0 - \delta_q$.

![Graph](image)

fig. 4.10: The profiles of $J_{fu}(r, y = 0)$ for various values of $R_0$.

The solution for the Shvab-Zel'dovich variables for $y = 0$ is given in figure 4.10 for various values of $R_0$. The effect of the burner radius $R_0$ is negligible for $R_0 > 3$ mm. This indicates that the difference between cylindrical burners and slit burners (with respect to the behaviour of $J_i$) becomes negligible for burners with a diameter or width larger than 6 mm.
4.2.5 The energy balance

The overall energy conservation in the region upstream of the flame can be verified by using the solution for \( J_i(r, y) \) and \( T(r, y) \). The total cooling rate by the wall can be calculated by using equation (4.13)

\[
Q_w = 2\pi R_0 \int_{-\infty}^{0} dy \lambda \frac{\partial T}{\partial r} \bigg|_{r=R_0} = 2\pi R_0 \int_{-\infty}^{0} dy \frac{e^{y/L} \lambda \Delta T}{R_0 \ln \left( 1 - \frac{\delta_q}{R_0} \right)} = \frac{2\pi \lambda \Delta T L}{\ln \left( 1 - \frac{\delta_q}{R_0} \right)}.
\]  
(4.26)

The total energy loss at the outflow of the tube \((y = 0)\) can be calculated as follows

\[
Q_r = 2\pi \rho u^u \Delta H \int_{0}^{R_0} r dr \left[ J_i^u - J_i(r, y = 0) \right] = 2\pi \rho u^u \Delta H \int_{0}^{R_0} r dr \frac{\Delta Y_i}{s_i \ln \left( 1 - \frac{\delta_q}{R_0} \right)} \tilde{Y_i}(r, 0),
\]  
(4.27)

which, after substitution of equation (4.17), becomes

\[
Q_r = \frac{-4\pi \rho u^u \Delta H \Delta Y_i L}{s_i \pi R_0 \ln \left( 1 - \frac{\delta_q}{R_0} \right)} \int_{0}^{R_0} r dr \int_{0}^{\infty} dk \frac{I_0 \left( \frac{\sqrt{1+k^2} r}{2L} \right)}{I_1 \left( \frac{\sqrt{1+k^2} R_0}{2L} \right)} \left[ \frac{1}{1+k^2} \right]^3.
\]  
(4.28)

The integral in the previous equation can be rewritten by substituting \( \alpha = r/L \) and the constant \( \alpha_0 = R_0/L \). Then the integral over the Bessel function \( I_0 \) can be calculated which results in a Bessel function \( I_1 \). Calculation of the integral over \( k \) then leads to the following expression for the heat loss at the burner outflow

\[
Q_r = \frac{2\pi \lambda \Delta T L}{\ln \left( 1 - \frac{\delta_q}{R_0} \right)},
\]  
(4.29)

where we used

\[
\frac{\Delta H \Delta Y_i}{s_i \delta_q} = \frac{c_p \Delta T}{\delta_q} \quad \text{and} \quad L = \frac{\lambda}{\rho u^u c_p}.
\]

The fact that (4.26) and (4.29) lead to the same result proves that the solutions for \( T, Y_i \) and \( J_i \) in the quenching layer satisfy energy conservation.

4.2.6 The thickness of the thermal boundary layer

In this subsection the effect of the burner wall curvature \( R_0 \) on the thickness of the thermal boundary layer \( \delta_q \) will be estimated. The estimate is based on the local balance of the burning velocity and the mixture velocity in the attachment point \((r, y) = (R_0 - \delta_q, 0)\) (de Goey (1994)).

The solution for the Shvab-Zel’dovich variables indicates that the maximum temperature and burning velocity are only reached for \( \delta_q \rightarrow \infty \). This means that \( \delta_q \) has to be so large that the flame temperature and burning velocity in the attachment point are close to their maximum values (denoted by \( T_b \) and \( S_L \)). The temperature in the attachment point \((R_0 - \delta_q, 0)\) can be determined from equation (4.13). The result \((T(R_0 - \delta_q) - Tu)/(T_b - Tu)\) is given in figure 4.11. The burning velocity in the attachment point \( S_L(R_0 - \delta_q, 0) \) is determined using the analytical relation between
4.2. Flame cooling by the burner wall

fig. 4.11: The temperature \( \frac{(T(R_0 - \delta_q) - T^w)/(T^b - T^w)}{T_{u}} \) (a) and the burning velocity \( \frac{S_L(R_0 - \delta_q, 0)/S_L}{S_L} \) (b) in the attachment point \( (R_0 - \delta_q, 0) \) for various values of \( R_0 \).

the burning velocity and the flame temperature for a flat burner-stabilised flame (Williams (1988), de Lange (1992))

\[
\ln \left( \frac{S_L(R_0 - \delta_q, 0)}{S_L} \right) = \frac{-T_a}{2T(R_0 - \delta_q, 0)} + \frac{T_a}{2T_b} + \frac{\alpha + \beta + 2}{2} \ln \left( \frac{T(R_0 - \delta_q, 0)}{T_b} \right). \tag{4.30}
\]

The burning velocity in the attachment point predicted by equation (4.30) is also given in figure 4.11 for three values of \( R_0 \). The estimated value for \( \delta_q \) is approximately 0.97 mm when the stabilisation criterion \( S_L(R_0 - \delta_q, 0)/S_L = 0.98 \) for slit burners \( (R_0 \rightarrow \infty) \) is taken. This estimate can also be made by using the same criterion for other values of \( R_0 \). The resulting values of \( \delta_q \) are 0.97 mm for \( R_0 \rightarrow \infty \) and 1.1 mm for \( R_0 = 1.6 \) mm. These values are significantly lower than the value of half the measured quenching distances obtained by Harris (1949): \( R_{q, car} = 1.2 \) and \( R_{q, cyl} = 1.6 \) mm, respectively. This is probably due to the assumptions in the analytical model, for example the assumption that the temperature at \( R_0 - \delta_q \) is approximately equal to the adiabatic flame temperature. The flame temperature near the quenching condition will become lower than the adiabatic temperature. To reduce the effect of the assumptions in the analytical model and the criterion \( S_L(R_0 - \delta_q, 0)/S_L = 0.98 \) we will study the ratio of the stand-off distances for cylindrical burners \( \delta_{q,cyl} \) and the slit burner \( \delta_{q,car} \). Variation of the value for the criterion \( S_L(R_0 - \delta_q, 0)/S_L \) between 0.97 and 0.99 did not significantly affect the ratio \( \delta_{q,cyl}/\delta_{q,car} \). Note that the resulting ratio \( \delta_{q,cyl}/\delta_{q,car} \) given in figure 4.12 only changes due to differences in conductive energy transport.
at different values of $R_0$ because the convective term in the energy equation (4.5) is independent of $R_0$.

### 4.2.7 The behaviour of $T$ and $Y_{fu}$ in the quenching layer

The profiles for $T$ and $Y_{fu}$ in the quenching layer for $y=0$ are given in figure 4.9. Note that the horizontal distance in figure 4.9 is normalised with the quenching distance $\delta_q$ so that effects due to differences in stand-off distance are not visible in figure 4.9. It is clearly visible in figure 4.9 that the temperature in the quenching layer decreases for when $R_0$ is smaller due to the enhanced cooling by these smaller burners. The decreasing temperature leads to higher fuel mass fractions in the quenching layer because of the conservation of $J_{fu}$ for $r<(R_0-\eta)$. The profiles of $T$ and $Y_{fu}$ for the cylindrical burners almost coincide with the profiles for the slit burner ($R_0 \to \infty$) for burner radii larger than approximately 3 mm, which is in agreement with the behaviour of $\delta_q$ discussed in the previous subsection.

The heat loss of the flame in the attachment point for $r=R_0-\delta_q$ and $y=0$ can be determined from

$$ Q_{\text{flame}} = \lambda \frac{\partial T}{\partial r} \bigg|_{r=R_0-\delta_q,y=0} = \frac{\lambda \Delta T}{(R_0-\delta_q) \ln \left(1 - \frac{\delta_q}{R_0}\right)}. \quad (4.31) $$

Evaluation of equation (4.31) in the attachment point $(R_0-\delta_q,0)$ results in values of $3.4 \cdot 10^5$, $2.2 \cdot 10^5$ and $2.1 \cdot 10^5 \text{ Jm}^{-2}\text{s}^{-1}$ for $R_0=1.5, 3.0$ and $R_0 \to \infty$, respectively. Note that the heat loss of the flame for $R_0=3.0$ mm differs 5% from the heat loss for $R_0 \to \infty$ which is comparable to the difference in the critical gradients for slit and cylindrical burners (see figure 4.7).

![Graph](attachment:F4q.png)

**fig. 4.12:** The ratio of the stand-off distances $(\delta_{q,cyl}/\delta_{q,car})$ as a function of $R_0$ predicted by the analytical model.
4.3 The dependence of the critical gradient on the burner size

We will now examine the dependence of the critical flash-back gradient on burner geometry and size by using the results obtained for $\delta_{q,cyl}/\delta_{q,car}$ in the previous section.

It is clearly visible in Figure 4.7 that $g_{f,lin}$ for the cylindrical burners shows a significantly larger variation with $R_0$ than the gradients for the slit burners. Also, the cylindrical values for $g_{f,lin}$ don’t seem to approach the slit burner values for large burners. This is probably due to the constant value for $\delta_{q,cyl}=1.6$ mm used in figure 4.7, while the analytical model predicts a decreasing stand-off distance $\delta_{q,cyl}$ with increasing $R_0$ (which is also expected from a physical point of view). This result will now be used to recalculate $g_{f,lin}$ for the cylindrical burners. The aim of this calculation is to investigate whether the larger variation of $g_{f,lin}$ for cylindrical burners and the observation that the gradients for large cylindrical and slit burners do not become equal are mainly caused by the assumption that $\delta_{q,cyl}$ is constant in figure 4.7. The absolute values of $\delta_{q,cyl} \approx 1.1$ mm for $R_0=1.6$ mm and $\delta_{q,car} \approx 0.97$ mm for $R_{d,cyl} = 1.6$ mm predicted by the analytical model, however, deviate about 19 to 31 % from the experimental values $R_{d,cyl}=1.6$ mm and $R_{d,car}=1.2$ mm. The stand-off distance of the flames computed numerically is probably much closer to the experimental values $R_{d,cyl}$ and $R_{d,car}$. This can be concluded from the good reproduction of $g_f$ by the numerical model. We, therefore, decided to use the experimental values $R_{d,cyl}$ and $R_{d,car}$ for $\delta_{q,cyl}$ and $\delta_{q,car}$ for $R_0=1.6$ mm. The decrease of $\delta_{q,cyl}/\delta_{q,car}$ is then used to calculate $\delta_{q,cyl}$ as a function of $R_0$. 

---

Fig. 4.13: The critical gradient based on a linear velocity profile (eq. (4.4)). For the slit burners we used $\delta_q=1.2$ (Harris (1949)); for the cylindrical burners we used $\delta_q=1.6$ mm (Harris (1949)) for $2R_0=3.2$ mm. For larger diameters $\delta_q$ is assumed to decrease according to $\delta_{q,cyl}/\delta_{q,car}$ given in figure 4.12.
Chapter 4. Flame stabilisation near flash-back

The stand-off distance \( \delta_{q,\text{car}} \) is assumed to be constant and equal to \( R_{d,\text{car}} = 1.2 \) mm. The result for \( g_{f,\text{lin}} \) is given in figure 4.13. The variation of \( g_{f,\text{lin}} \) with burner size for cylindrical burners in figure 4.13 is almost equal to the variation for the slit burners. This illustrates that \( g_{f,\text{lin}} \) becomes approximately equal for large slit and cylindrical burners if a decreasing value for \( \delta_{f,\text{cyl}} \) is used. Only near \( R_0 \approx 2 \) mm an increase is detected, which is caused by the steep decrease of \( g_{f,\text{cyl}} \) near the quenching diameter which, in turn, is caused by the large cooling rate near flame quenching (the flame quenches for \( R_{d,\text{cyl}} = 1.6 \) mm). Note that the critical gradient becomes zero for \( R_0 = R_{d,\text{cyl}} \) (also see Lewis (1943)). For slit burners the gradient becomes zero at \( R_{d,\text{car}} = 1.2 \) mm. The behaviour of the cylindrical \( g_{f,\text{lin}} \) as a function of \( R_0 \) is also physically more justified since it has the same behaviour as for slit burners for larger values of \( 2R_0 \).

4.4 Conclusions

The numerical model used to calculate the critical gradient only takes flame cooling into account; processes related to radicals and surface chemistry are not included. The agreement between the experimental and numerical results, therefore, shows that the flame stabilisation process is dominated by flame cooling by the burner wall, at least for the conditions studied in this chapter and for the burner materials (pyrex and brass) used in the experiments.

The differences between cylindrical and slit burners are only significant for small burners (smaller than 6 mm). This is supported by analytical and numerical results.

The results for \( g_{f,\text{lin}} \) shows that the curvature of the parabolic velocity profile is the main reason for the decrease of \( g_f \) for increasing burner size. An analysis has been presented to predict the effect of the burner wall curvature on the cooling rate by the burner. The analysis has been used to investigate the stand-off distance ratio of cylindrical and slit burners \( \delta_{q,\text{cyl}}/\delta_{q,\text{car}} \) as a function of \( R_0 \). The results show that the differences in stand-off distance between cylindrical and slit burners may induce an increase of about 10% of \( g_{f,\text{lin}} \) for a burner width/diameter of 4 mm. This is of the same order of magnitude as the observed differences between critical flash-back gradients based on a linear velocity profile of flames on slit and on cylindrical burners. This difference was not observable in the experimental results because it is of the same order of magnitude as the experimental errors.

Furthermore, the analysis shows that the effect of the burner wall curvature on the profiles of \( T \), \( Y_i \) and \( J_i \) is negligible for burners larger than about 6 mm. The study indicates that the observed differences in flash-back behaviour are dominated by differences in conductive heat transfer to the burner wall due to burner wall curvature.
Chapter 5

M- and V-shaped Flames

The stabilisation of M- and V-shaped flames on double slit burners is of interest because of the resemblance with the stabilisation of flames on perforated burners which are widely used in domestic heating equipment. The flames on perforated burners schematically look like flames confined between similar flames depicted in figure 3.1. The flames in the center area of these burners and their stabilisation is not affected by the surrounding atmosphere because the stabilisation point above the burner wall is surrounded by the combustible mixture flowing from the burner ports. The emissions of $NO_x$ and partially unburnt hydrocarbons from these burners increase at high mixture velocities, especially if the outer flames blow-off due to the cooling by and mixing with surrounding gases (also see chapter 1). The flames then only stabilise on the burner walls in the center of the burner.

On a double slit burner, which characterises the combustion phenomena of flames on perforated burners, M-shaped flames typically occur at low mixture velocities when the flame stabilises on the flameholder and on the outer burner walls of the double slit burner (see figure 5.1). At higher mixture velocities the mixing with and cooling by the surrounding atmosphere increases. This leads to lower burning velocities and eventually to blow-off at the outer burner walls. The flame then only stabilises at the flameholder and is referred to as a V-shaped or an inverted flame. An example of an M- and a V-shaped flame on the double slit burner is given in figure 5.3. The stabilisation point of a V-shaped flame is not surrounded by air, but by the combustible mixture flowing out of the burner. This implies that the stabilisation of V-shaped flames is not affected by the surrounding atmosphere, opposed to the stabilisation of Bunsen flames. This is the reason why the understanding of the stabilisation mechanisms of V-shaped flames is generally (Lewis and von Elbe (1961), Edmondson and Heap (1970), Kawamura et al. (1979,1982), Trevino et al. (1991) and Sung et al. (1992)) believed to be a necessary step towards the unravelling of the blow-off mechanisms of Bunsen-type flames.

Several phenomena are held responsible for the stabilisation of V-shaped flames, such as flow straining (Lewis and von Elbe (1961), Edmondson and Heap (1970)), the curvature of the flame front (Kawamura et al. (1979,1982) and heat loss to the stabilisation body or flameholder (Trevino et al. (1991)). Sung et al. (1992) demonstrated that V-shaped flames can be stabilised with no heat loss to the flameholder and presented an analysis of the stabilisation of a V-shaped flame which includes both strain and curvature. This analysis is, however, limited to weak strain rates
and a small curvature.

No attempt has been made so far to model V-shaped flames numerically. A numerical model can be a powerful means for investigating the mechanisms involved in the flame stabilisation process because the occurring mechanisms (e.g. curvature, flow straining and heat loss to the burner) can be studied in a systematic and detailed manner (see chapter 7). This study consists of the calculation of separate contributions to the stretch rate, involving flow straining and flame curvature in the tip of a two-dimensional Bunsen flame and in a V-shaped flame.

![Diagram of rectangular double slit burner](image)

**fig. 5.1:** The rectangular double slit burner used for the experiments (dimensions in [mm]). The figure denotes a cross-section perpendicular to the flameholder plate and the rectangular slits.

In this chapter, experimental results and numerical results of lean M- and V-shaped methane/air flames are presented. The aim of this study is to validate the results obtained with the numerical model by comparing the data for M- and V-shaped flames with experimental results (Laser
5.1. The experimental set-up

Doppler velocity measurements and flame shapes). Also, the numerically predicted critical gradients at the transition from the M- to the V-shaped flame and at blow-off of the V-shaped flame are compared with experimental results. The stabilisation mechanism of V-shaped flames is further investigated in chapter 7, after the treatment of the flame stretch theory in chapter 6.

![Diagram of the computational domain](image)

fig. 5.2: The computational domain.

A short description of the experimental set-up is given in the following section. Modelling results of an M- and a V-shaped flame with an equivalence ratio $\phi=0.7$ will be discussed and compared with experimental results in section 5.2. The experimental results consist of Laser Doppler velocity measurements near and within the flames and flame shapes. The modelling of the transition from M- to V-shaped flame and blow-off of the V-shaped flames is discussed in section 5.3. The chapter ends with conclusions in section 5.4.

5.1 The experimental set-up

The experiments to validate the model are performed on a rectangular slit burner (see figure 5.1). The slit is divided in two equal parallel slits of $1.75 \times 55$ mm separated by a flat plate (the flameholder) with a thickness of $2t=0.5$ mm. The velocity profiles at the burner exit are fully developed. The shape of the profiles is parabolic in the plane perpendicular to the slits and top-hat like along the slits, so that a 2D numerical study is sufficient (Mallens and de Goey (1995)). The velocity profiles at the outflow of the burner measured using Laser Doppler Velocimetry deviate no more than a few percent from the theoretical profiles for a fully developed flow. Both the flame shapes and the measured velocity profiles are symmetrical within a few percent.
Chapter 5. M- and V-shaped Flames

fig. 5.3: Direct photographs of an M-shaped flame (top, mean burner exit velocity 0.53 m/s) and a V-shaped flame (bottom, mean burner exit velocity 0.73 m/s) for $\phi = 0.7$.

The flow rate at which the transition from M- to V-shaped flame or blow-off of the V-shaped flame occurs is determined by gradually increasing the flow rate until transition or blow-off occurs. The theoretical profile is then used to determine the gradient $\partial v/\partial x|_{wall}$ at the burner wall. The accuracy of the gradients determined in this way mainly depends on the accuracy of the mass flow controllers and is equal to about 10 to 15%.

5.2 Results for M-shaped and V-shaped flames for $\phi=0.7$

In this section we will present modelling results for two flames: an M-shaped flame with a mean inlet velocity ($V$) of 0.53 m/s and a V-shaped flame with $V=0.73$ m/s. The computational domain is given in figure 5.2. The domain dimensions (in mm) are: $b = 2.0$, $B = 9.0$, $L_x = 30.0$ and $L_y = 40.0$. The height of the burner wall and the flameholder in $y$ direction is equal to 1.0 mm and $t=0.25$ mm in figure 5.2.

In the remainder of this section numerical results will be presented and compared with experimental results for the M-shaped flame and the V-shaped flame. Photographs of the M- and
5.2. Results for M-shaped and V-shaped flames for $\phi=0.7$

fig. 5.4: Numerical results of an M-shaped flame at a mean burner exit velocity of 0.53 m/s and $\phi=0.7$. Top: contours of the stream function $\varphi$ from $\varphi=-0.003$ kg m$^{-1}$s$^{-1}$ to $\varphi=0.0$ kg m$^{-1}$s$^{-1}$ with steps equal to 0.00025 kg m$^{-1}$s$^{-1}$. Bottom: contours of temperature are shown from 400 K to 1600 K with steps equal to 200 K.

V-shaped flame considered in this section are given in figure 5.3.

5.2.1 The M-shaped flame

The numerical results for the chosen M-shaped flame, consisting of contour plots of the temperature and the stream function, are given in figure 5.4. The results clearly show the typical shape of the flame. The maximum temperature is equal to 1793 K. This is close to the adiabatic flame temperature ($T_{\text{ad}}=1815$ K) due to the large stand-off distance of the flame. Note that the burnt gases above the flame are cooled significantly by the cold surrounding gases and are accelerated by buoyancy forces. The model also predicts a recirculation area above the flameholder. The numerical solution will be validated in more detail below.

The experimental flame shape (defined as the upstream boundary of the luminous zone) and the shape of the numerical flame (defined as the locus of the maximum $\rho_fu$) is given in figure 5.5. The reproduction of the flame shape by the model is quite well above the thin flameholder and
burner exit ($x \leq 0.002$ m), apart from small differences in stand-off distance and a slightly larger curvature of the experimental flame. The discrepancy becomes somewhat larger above the outer burner wall. The stand-off distance (defined as the vertical distance between the top of the burner and the locus of the maximum $\dot{\rho}_{fu}$) at the flameholder ($x = 0.0$) and the outer burner rim is quite large. The stand-off distance is equal to about 1.4 and 1.9 mm at the flameholder and burner rim, respectively. The experimental stand-off distance is equal to 1.0 and 1.7 mm. It should be noted that discrepancies in flame position up to approximately 0.4 mm may occur due to differences in flame front definition.

The profiles of the vertical velocity component $v$ at four heights $y$ are given in figure 5.6. The velocity profiles at the burner outflow ($y=1.0$ mm) produced by the model and the outflow profiles of the experimental burner (see figure 5.6) differ only a few percent. The velocity profiles in the flame region change rapidly with increasing $y$ and are, therefore, extremely sensitive to small differences in flame position or stand-off distance, i.e. the flow field near and within the flame is, in the cases studied here, mainly determined by the vertical position relative to the flame. Therefore, we corrected the numerical $y$ values for the difference in the stand-off distance between the numerical and the experimental flame ($=0.5$ mm). The $y$ values given in figure 5.6 are the experimental values. The profiles at $y=1.95$ mm in figure 5.6, however, still show a different behaviour for $x < 1$ mm due to slightly different flame positions or flame shapes at the symmetry axis. Above the flame base, the experimental values of $v$ are up to 25% higher.
5.2. Results for M-shaped and V-shaped flames for \( \phi = 0.7 \)

![Graph comparing experimental and numerical values of velocity profiles in a M-shaped flame](image)

**fig. 5.6:** Measured (left) and computed (right) velocity profiles in the M-shaped flame of the velocity component \( v \) at various heights \( y \). The numerical \( y \) values have been corrected for the different stand-off distance of the numerical flame.

The numerical values deviate from the experimental values. The difference might be related to several items: the grid inside the flame base, the boundary conditions at the symmetry axis, the reproduction of the flow rate in the surrounding atmosphere, the reproduction of the flame temperature and burning velocity by the one-step chemical model and the shape of the flame base. The discretisation of the boundary conditions at the symmetry axis is such that both mass- and energy conservation is satisfied at the symmetry axis (also see chapter 3). Additional numerical calculations with finer grids and a different calculation of the mixture viscosity (which affects the velocities in the surrounding atmosphere) did not change the reproduction of the vertical velocity profile significantly. The adiabatic flame temperature and the adiabatic one-dimensional burning velocity reproduced by the one-step chemical model at \( \phi = 0.7 \) deviate only a few percent from measurements performed by van Maaren (1994). All the items mentioned above don't seem to explain the observed differences. It should be noted that the poor reproduction of the vertical velocity above the flameholder can also be related to flame shape differences such as a different curvature of the flame base around \( x=0 \). Small differences in the radius of curvature \( (R) \) of the flame front at \( x=0 \) have a large effect on the vertical velocity, especially because the radius of curvature is very small at \( x=0 \). The decrease of the stream tube area which, together with the temperature increase, causes the velocity increase, is very sensitive for small changes in \( R \) because of its approximate proportionality.
to $1/R$ with $R = O(10^{-3})$. The difference in flame curvature is probably caused by the lacking of highly diffusive radicals in the model. The highly curved flame may lead to high diffusive transport of these intermediates towards the unburnt mixture (out of the central stream tube) which, in turn, modifies the burning velocity and the flame shape. These effects are not incorporated in the one-step model. Calculations with more detailed chemical schemes would certainly shed more light on the reasons behind the poor reproduction of the vertical velocity profile. We, however, have not been able to obtain a converged solution with skeletal chemistry up to now because these calculations are very time consuming (also see Somers (1995)).

\[ \text{fig. 5.7: Numerical results of a V-shaped flame at a mean burner exit velocity of 0.73 m/s and } \phi=0.7. \text{ Contours of the stream function } \varphi \text{ (top) are shown from } \varphi=-0.003 \text{ kgm}^{-1}\text{s}^{-1} \text{ to } \varphi=0.0 \text{ kgm}^{-1}\text{s}^{-1} \text{ with steps equal to } 0.00025 \text{ kgm}^{-1}\text{s}^{-1}. \text{ Below contours of temperature are shown from } 400 \text{ } K \text{ to } 1600 \text{ } K \text{ with steps equal to } 200 \text{ } K. \]

It can be concluded from the above that the numerical model describes the global flame properties (flame shape, stand-off distance) of the M-shaped flame ($\phi = 0.7$) reasonably accurate. The absolute values of $v$ predicted by the model are, however, considerably lower (up to 25 %) than the measured values.
5.2 Results for M-shaped and V-shaped flames for \( \phi = 0.7 \)

5.2.2 The V-shaped flame

![Graph showing experimental and numerical flame positions](image)

Fig. 5.8: The experimental V-shaped flame (defined as the upstream boundary of the luminous flame; markers) and the locus of the maximum fuel source term \( \dot{\rho}_f u \) (line) in the modelled equivalent of the experimental flame.

Figure 5.7 shows the numerical results for the V-shaped flame \( (\phi = 0.7; V = 0.73 \text{ m/s}) \). The maximum temperature of the V-shaped flame \( (1800.0 \text{ K}) \) is almost equal to that of the M-shaped flame. The model also predicts a recirculation area above the flameholder for this flame. The results given in figure 5.7 will be discussed and verified below by comparing the flame shape, stand-off distance and \( v \) profiles of the numerical flame with experimental results.

The shape of the numerical V-shaped flame and its experimental equivalent is given in figure 5.8. The difference between the stand-off distance (at \( x = 0.0 \)) of the numerical flame \( (2.1 \text{ mm}) \) and the experimental flame \( (1.3 \text{ mm}) \) has increased to \( 0.8 \text{ mm} \). This difference in flame attachment point has a direct influence on the flame position at other locations. The difference between the position of the numerical and the experimental flame seems significant despite possible differences caused by different flame front definitions. Another difference between the numerical and the experimental flame is that the experimental flame wing \( (x \geq 2 \text{ mm}) \) is less curved than the numerical flame wing.

Profiles of the vertical velocity \( v \) as a function of \( x \) are given in figure 5.9. As in the case of the M-shaped flame, the \( y \) coordinates (except \( y = 1.0 \text{ mm} \)) have been corrected for the difference in stand-off distance between the experimental and the numerical flame. The profiles at the burner outflow \( (y = 1.0 \text{ mm}) \) are well reproduced by the model. The shape of the profiles at higher \( y \) values is also reproduced reasonably well. The absolute values of \( v \), however, differ up to as much as 35 %. The values for the vertical velocities \( v \) produced by the model are smaller than the experimental
values. This was also the case for the M-shaped flame described in the previous section. In this case the discrepancies are probably also caused by flame shape differences, especially a different flame curvature at $x=0$. The profile at $y=1.95$ mm in figure 5.9 shows that the vertical velocity $v$ for $x < 0.6$ mm is lower for the numerical flame. This implies that the lateral velocities in the positive $x$ direction are higher for the numerical flame, i.e. the numerical flame wing stabilises with a smaller angle with the $x$-axis and is less curved around the central axis. As explained in the previous sub-section, a slightly lower curvature of the flame around $x=0$ gives rise to lower velocities $v$ above the flame.

The above has shown that the model describes the global flame shape and the global behaviour of the velocity field of the V-shaped flame reasonably well. The stand-off distance and the vertical velocity, however, differ significantly. The reasons for this probably lie in the absence of highly diffusive radicals in the one-step model.
5.3 The transition from M- to V-shaped flame and blow-off of the V-shaped flame

The velocity gradient at the burner wall at which the modelled M-shaped flame changes to a V-shaped flame and the velocity gradient at which the modelled V-shaped flame blows-off will be compared with experimental results in this section.

The critical transition ($g_t$) and blow-off ($g_b$) velocity gradient at the burner wall is computed as follows:

$$g_{t,b} = \frac{6V_{t,b}}{(b - t)}, \tag{5.1}$$

where $V_{t,b}$ denotes the mean velocity at the burner exit at the transition and blow-off condition, respectively. The dimensions $b$ and $t$ are defined in figure 5.2. The gradient $g_{t,b}$ is determined by increasing the inlet velocity of a converged numerical solution by steps of 5 % of the inlet velocity. After each velocity adjustment the calculation process is resumed until the solution is converged again. Note that the step size of 5 % introduces an uncertainty in the numerical critical gradients of 5 %. Smaller steps would increase the calculation time too much and it is expected that assumptions in the model as well as experimental irregularities give errors of the same order of magnitude.
Chapter 5. M- and V-shaped Flames

The transition from M- to V-shaped flame generally does not happen suddenly at a certain mixture velocity. Instead, the transition starts with the detachment of the M-shaped flame at the outer burner wall (say, at a velocity $V_{t,1}$) and ends with a clearly V-shaped flame (at a velocity $V_{t,2} > V_{t,1}$). The critical transition gradients reported in figure 5.10 are calculated with $V_t = (V_{t,1} + V_{t,2})/2$. The uncertainty $(V_{t,2} - V_{t,1})/V_t$ is equal to about 6% for the experimental and numerical transition gradients. The critical transition gradients predicted by the numerical model are in good agreement with the experimental values (see figure 5.10). The good prediction of the transition gradients for $\phi = 0.7$ by the model indicates that the effect of the surrounding atmosphere on the behaviour of the temperature and the species (fuel and oxygen) is described well by the model, at least for the cases studied here.

Blow-off of the inverted flame is only well reproduced by the model at $\phi = 0.7$. At $\phi = 0.8$, numerical blow-off is found at a lower velocity than experimental blow-off. We haven't been able to determine a numerical blow-off gradient for $\phi = 0.9$. The calculation of $g_b$ at $\phi = 0.8$ and 0.9 is very difficult because, for these equivalence ratios, the numerical flames tend to stabilise due to cooling in the wake behind the flameholder. From a physical point of view, the stabilisation very close to the flameholder is possible in the numerical model because of the low velocities (smaller than the adiabatic burning velocity) downstream of the flameholder and because of the unlimited cooling capacity of the numerical flameholder (which is kept at 300 K in the computations). However, experimentally, this stabilisation point is not observed. Generally, there are two possible causes which might explain the difficulties to model blow-off for $\phi = 0.8$ and 0.9: the poor reproduction of the stand-off distance and small errors in the reproduction of the flame shape in the attachment point which, in turn, may be caused by the one-step chemical model or by the flow field modelling in the surrounding atmosphere. A short discussion of these causes is presented below.

The stabilisation and blow-off of V-shaped flames is determined by the local balance between the vertical mixture velocity and the local burning velocity. The poor reproduction of blow-off of the V-shaped flame at $\phi = 0.8$ and 0.9 is, therefore, related to the poor reproduction of the vertical mixture velocity and/or the burning velocity. Previous investigations (Mallens (1995,1996)) have shown that the vertical mixture velocity is extremely sensitive to the value of the stand-off distance and the flame curvature at the flame base. The stand-off distance (defined as the vertical distance between the flameholder and the lower boundary of the luminous zone) of the experimental V-shaped flames increases from about 1.5 mm for $\phi = 0.7$ to 2.5 mm for $\phi = 0.9$. The numerical V-shaped flames tend to stabilise on top of the flameholder (inside the wake very close to the flameholder) for $\phi = 0.8$ and $\phi = 0.9$ and do not blow-off. When the numerical flame is quenched locally above the flameholder and the computation is resumed a 'new' solution is found with a stand-off distance significantly larger than the experimental values. Also, small differences with the experimental flame shape occur.

The flameholder is situated outside the preheat zone (about 0.8 mm thick) for the experimental and numerical V-shaped flames which, in turn, means that the heat loss of the flame to the flameholder is negligible. This implies that the V-shaped flame stabilises at a position where the vertical velocity balances the adiabatic local burning velocity (determined by the mixture composition, flame curvature and - stretch). Deviations of about 10% of the unstretched adiabatic burning velocity are possible due to errors in the chemical parameters. Furthermore, as already mentioned before, the absence of highly diffusive radical species in the one-step chemistry model...
can lead to a different curvature of the flame base (Mallens, 1996). Small differences in flame curvature have a large effect on the local burning velocity, especially because the radius of curvature is very small.

5.4 Conclusions

One-step chemistry results of lean M- and V-shaped flames have been presented and validated. The model describes the flame shape reasonably well. The velocity field above the burner is, however, only predicted qualitatively, i.e. the velocity values produced by the model differ considerably from the experimental values. This is probably caused by (relatively small) flame shape differences which can be caused by the absence of highly diffusive intermediate species in the one-step chemistry model.

In the last section of this chapter predicted transition and blow-off gradients of M- and V-shaped flames are presented for $\phi=0.7$, 0.8 and 0.9. A comparison with experimental results shows that the transition gradient is well reproduced by the model for all three equivalence ratios considered. The blow-off gradient is, however, only reproduced for $\phi=0.7$. The difficult reproduction of blow-off of the V-shaped flames at $\phi = 0.8$ and 0.9 is caused by the strong sensitivity of the critical blow-off gradient to small changes in stand-off distance and flame shape. This makes a good prediction of the stand-off distance and the flame shape vital for a good prediction for the blow-off gradient.
Chapter 5. M- and V-shaped Flames
Chapter 6

Flame Stretch in 2D Stationary Premixed Flames

It is well known that deviations from pure one-dimensional flow and transport in premixed flames, such as flame curvature and non-uniform flow along the flame, might lead to local variations in flame temperature and mass burning rate (also see chapter 1). These stretch effects were first studied by Karlovitz (1953) to describe flame extinction. Subsequently, Lewis and von Elbe (1961) used flame stretch to study flame stabilisation. Markstein (1964) investigated the influence of stretch on flame front instability. Since these early publications, significant progress has been made in the understanding of flame stretch and in particular the structure and propagation of stretched flames has been studied in numerous papers.

The definition of the flame stretch $K_A$, given by Karlovitz (1953), reads

$$K_A = \frac{1}{A} \frac{dA}{dt}, \quad (6.1)$$

i.e. $K_A$ is the fractional area change of a small area $A$ in the flame surface, which moves along the flame with a tangential velocity equal to the local tangential fluid velocity. This definition of flame stretch only holds at the flame surface. Practical expressions for $K_A$, based on kinematic considerations, are given by Buckmaster (1979) and Matalon (1983).

In the analysis of stretched flames, relations between flame temperature and burning velocity on one hand and flame stretch on the other hand are derived. A rigorous mathematical analysis of stretched flames, based on matched asymptotic expansions, is given by Matalon and Matkowsky (1982). Buckmaster (1982) derived a relation between the burning velocity and stretch for two examples of stretched flames. An integral analysis of flame stretch is presented by Chung and Law (1988).

The significance of stretch for premixed flames is controversial. Buckmaster (1979) gives a critical assessment of flame stretch. He claims that flame behaviour does not solely depend on flame stretch, because of the following reasons. First, heat transfer in a flame cannot only depend on the local value of flame stretch defined at the flame surface, but it must also depend on the stretch in the preheat zone. Second, also variations in the preheat zone thickness are of importance for the heat transfer rate. Finally, the burning velocity does not only depend on flame stretch.
but also on the Lewis number $Le$ of the flame. This last observation is confirmed by Law (1988), who asserts that flame stretch can only influence flame response in combination with preferential diffusion effects.

As the existing theory is not directly applicable to numerical flame studies, we approach the problem in an alternative way. We define our flame stretch in the flame region between the burnt and unburnt gases, comprising the reaction zone and the preheat and reactant diffusion zones. In this flame region, we can identify iso-lines of a suitably chosen variable $Y$. The new flame stretch is then defined in terms of the mass flux along these lines. It will turn out that flame thickness variations are included in our stretch definition. The method is restricted to stationary 2D flames for the time being.

We believe that our definition of flame stretch has a sound physical basis, because it is based on the mass conservation equation and no restricting assumptions are made. In contrast, the existing theory of flame stretch is based on assumptions such as the existence of a single reaction with one Lewis number or the applicability of perturbation theory. The classical theory is therefore of limited value for numerical combustion studies with complex transport and complex chemistry models. Numerical flame studies are our primary interest and it is our aim to apply the extended theory to study the importance of flame stretch on the mechanisms of flame stabilisation. We like to emphasise, that it is not our purpose to give a final assessment of flame stretch, but instead present a new approach which can be used in the analysis of numerically computed flames. As an example, we compare our results with the results of the integral analysis by Chung and Law (1988). In the chapter 7 we will use the theory to study the stabilisation of numerically computed V-shaped flames.

The contents of this chapter is the following. In section 6.1, the new flame stretch definition is introduced, starting from the mass conservation equation. Our definition of flame stretch contains the strain rate of the tangential velocity along the flame surface, as in other studies. Moreover, additional terms due to density variations along the flame surface and flame thickness variations are also incorporated in our definition. The influence of the stretch field on the behaviour of some scalar variables is studied in section 6.2. The burning velocity of stretched flames is studied in section 6.3. In particular, we have applied the new stretch definition to the enthalpy equation in order to investigate the relation between the local flame temperature and the stretch field. As an illustration, in section 6.4 we have computed the different contributions to the flame stretch rate for the flame tip of a two-dimensional Bunsen flame. Finally, some conclusions are formulated in section 6.5.

### 6.1 The New Flame Stretch Definition

Consider a 2D stationary flame 'front' in a premixed gas mixture, defined in terms of a given scalar field $Y$, which might be the temperature or the mass fraction of any species in the flame for the time being. We assume that flame front 'contours' correspond with iso-contours of $Y$ (see figure 6.1) and that the unburned and burned boundaries of the flame front are given by the contours $Y = Y_u$ and $Y = Y_b$, respectively. An orthogonal coordinate system $(\xi, \eta)$ is introduced, with axes
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fig. 6.1: Generalised coordinates \((\xi, \eta)\) in a 2D stationary flame. The arrows indicate the stream lines. The contours with constant \(\eta\) are perpendicular to the contours with constant \(\xi\). The small hatched area is a diffusive cell with magnitude \(h_\xi d\xi h_\eta d\eta\).

locally adapted to the contours of \(\mathcal{Y}\), i.e. the unit vector normal to the contours is given by

\[
e^{-\eta} = \frac{\nabla \mathcal{Y}}{||\nabla \mathcal{Y}||} = \frac{1}{\mathcal{Y}_L} \begin{pmatrix} \mathcal{Y}_x \\ \mathcal{Y}_y \end{pmatrix},
\]

where \(\mathcal{Y}_x = \frac{\partial \mathcal{Y}}{\partial x}, \mathcal{Y}_y = \frac{\partial \mathcal{Y}}{\partial y}\) and \(\mathcal{Y}_L = \sqrt{\mathcal{Y}_x^2 + \mathcal{Y}_y^2}\) and the unit vector along the contours is defined as

\[
e^x = \frac{1}{\mathcal{Y}_L} \begin{pmatrix} \mathcal{Y}_y \\ -\mathcal{Y}_x \end{pmatrix}.
\]

Note that the \(e^x\)-unit vector can also be defined in the opposite direction. Here, we choose \(\mathcal{Y}_y > 0\). It is interesting to realise that diffusive transport of the scalar quantity \(\mathcal{Y}\) is always directed in \(e^x\)-direction, i.e. perpendicular to the local iso-contours of \(\mathcal{Y}\). However, the local velocity vector \(\vec{v}\) is generally not in \(e^\eta\)-direction. This means that variations in the convective transport in \(e^x\)-direction might introduce local distortions in the behaviour of \(\mathcal{Y}\) through the flame, compared to the behaviour in cases where the convective and diffusive transport directions are parallel (such as in perfectly flat, cylindrical or spherical flames). Following this reasoning, we define the generalised
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The stretch rate in terms of the convective transport contributions in $\xi$-direction. To compute these convective transport terms in $\xi$-direction, the conservation equation of mass will be analysed.

Consider the continuity equation $\nabla \cdot (\rho v) = 0$ in the $(\xi, \eta)$-coordinate system of figure 6.1.

$$\frac{1}{h_\xi h_\eta} \left( \frac{\partial}{\partial \xi} (\rho v_\xi h_\eta) + \frac{\partial}{\partial \eta} (\rho v_\eta h_\xi) \right) = 0,$$

(6.4)

where the velocity vector is written as $\vec{v} = v_\xi \vec{e}_\xi + v_\eta \vec{e}_\eta$. Furthermore, $h_\xi$ and $h_\eta$ are the scale factors of the $(\xi, \eta)$-coordinate system, defined by $h_\xi = |\frac{\partial}{\partial \xi}|$ and $h_\eta = |\frac{\partial}{\partial \eta}|$. The scalar stretch field $K(\xi, \eta)$ is now defined as the term in equation (6.4) which gives rise to transport in $\xi$-direction divided by $\rho$, i.e.

$$K = \frac{1}{\rho h_\xi h_\eta} \frac{\partial}{\partial \xi} (\rho v_\xi h_\eta),$$

(6.5)

defined in the zone for $\eta$ between $\eta_a$ and $\eta_b$, where $\mathcal{Y}$ equals $\mathcal{Y}_a$ and $\mathcal{Y}_b$, respectively. Equation (6.5) for $K$ can be further elaborated to

$$K = \frac{1}{\rho h_\xi} \frac{\partial}{\partial \xi} (\rho v_\xi) + v_\xi \nabla \cdot \vec{e}_\xi.$$

(6.6)

Let $\alpha$ denote the angle between $\vec{e}_\xi$ and the positive x-axis, then it is easy to see that

$$\nabla \cdot \vec{e}_\xi = \frac{d\alpha}{ds_\xi} = C_\xi,$$

(6.7)

with $s_\xi$ the arc length along the contour $\xi = Const$ and $C_\xi$ the curvature of this contour. The radius of curvature $R_\xi$ of the contour $\xi = Const$ is defined by

$$R_\xi = |R_\xi|$$

with $R_\xi = \frac{1}{C_\xi}$. (6.8)

Using (6.7) and (6.8), equation (6.6) can be rewritten as

$$K = \frac{1}{\rho h_\xi} \frac{\partial}{\partial \xi} (\rho v_\xi) + \frac{v_\xi}{R_\xi}.$$

(6.9)

This equation for the flame stretch field is an extension of the expression

$$K_a = \frac{1}{h_\xi} \frac{\partial v_\xi}{\partial \xi},$$

(6.10)

which can be derived from the conventional definition of stretch in equation (6.1); see e.g. Buckmaster (1979) and Matalon (1983). The first term in equation (6.9) arises in case of a non-uniform mass flux along a flame 'contour' $\eta = Const$. It should be noted that density variations along a flame 'contour' are neglected in the analysis of other authors. The first term in equation (6.9) then reduces to $K_a$. However, in real flames the contours $\eta = Const$ generally don't coincide with isotherms, because stretch may induce local differences in flame temperature. The second
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A flame with flat $\eta$ iso-contours and thickness variations in a homogeneous flow field; a: a convective cell (with areas $A_1$ and $A_2$) and a diffusive cell (with areas $A_2$ and $A_3$); b: enlargement of the area variation.

That the variation in flame thickness indeed gives a contribution to the stretch rate as presented in equation (6.9) can be shown by considering figure 6.2. In this figure we analyse the special case of a uniform flow through a hypothetical flame with flat $\eta = \text{Const}$-contours and circular $\xi = \text{Const}$-contours, so that we find a zero stretch rate $K_\eta = \frac{1}{h_\xi} \frac{\partial h_\xi}{\partial \xi} = 0$ when formula (6.10) is used. We now estimate the fractional area change $K_A = \frac{1}{A} \frac{dA}{dt}$ of a piece of a flame contour $A$ with constant $\eta$, caused by differences in convective and diffusive transport in the flame. In figure 6.2 it is observed that the flame thickness is not constant, so that $R_\xi$ (the radius of curvature of the $\xi$-contours) is finite. In figure 6.2a we define two transport cells. The convective cell has an initial area $A_1$, a final area $A_2$ and walls along the local stream tube. The diffusive transport cell has initial area $A_3$, final area $A_2$ and walls along the contours with constant $\xi$. Diffusive transport takes place along the contours with constant $\xi$, so that there is no area change in the diffusive transport cell, thus $A_2 - A_3 = 0$. We may therefore consider the area change of the convective transport cell in figure 6.2 only. As can be seen in the enlargement in figure 6.2b, for small angles $\epsilon$ we may write $\epsilon = \frac{dh}{A} = \frac{h_\eta}{h_\xi} \frac{dn_\eta}{\epsilon_\xi}$. Furthermore, it is observed that $\frac{dh}{dA} = \frac{\nu_\eta}{\nu_\xi}$. Using these relations
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gives

\[
\frac{1}{A} \frac{dA}{dt} = \frac{v_\eta}{h_\eta d\eta} \frac{dA}{A} = \frac{v_\xi}{h_\xi d\eta} \frac{dh}{A} = \frac{v_\xi}{R_\xi}.
\]

(6.11)

This shows that the last term in equation (6.9) is indeed related with stretch effects due to flame thickness variations.

![Diagram](image)

**fig. 6.3:** Visualisation of the area variation in a flame. The convective and diffusive cells are hatched; the thicker lines indicate the initial and final area’s of the cells.

In figure 6.3 we present the general case with non-uniform flow, flame curvature and flame thickness variation. In this figure we introduce the convective transport cell ABFE and the diffusive transport cell CDFE. We will show that the stretch rate \( K(\xi, \eta) \) defined in equation (6.9) can be interpreted as the total fractional area change of a part AB of an arbitrary flame contour with constant \( \eta \), due to convection in ABFE and diffusion in CDFE. Note that we speak of the area of AB, while in the present 2D case we mean the length of AB. First consider the convective cell ABFE. The line segments AE and BF are stream lines and AB and EF are flame contours a distance \( h_\eta d\eta = v_\eta dt \) apart. Due to conservation of mass in ABFE it is clear that \( (\rho v_\eta A)(\eta + d\eta) = (\rho v_\eta A)(\eta) \), from which we can conclude that

\[
A(\eta + d\eta) = \frac{(\rho v_\eta)(\eta)}{(\rho v_\eta)(\eta + d\eta)} A(\eta) = \left(1 - d\eta \frac{\partial}{\partial \eta} \frac{\rho v_\eta}{\rho v_\eta} + O(d\eta^2)\right) A(\eta).
\]

(6.12)
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Substitution of \( d\eta = v_\eta dt/\eta \) into (6.12) and letting \( dt \to 0 \) gives the following expression for the fractional area change of AB due to convection in ABFE:

\[
\left( \frac{1}{A} \frac{dA}{dt} \right)_c = -\frac{1}{\rho \eta \partial \eta} (\rho v_\eta).
\] (6.13)

In the diffusive cell CDFE, the parametrisations of the line segments CD and EF are related by \( \vec{r}(\xi, \eta) = \vec{r}(\xi, \eta + d\eta) - v_\eta(\xi, \eta + d\eta) dt \vec{e}_\eta \). Thus, substitution of \( \vec{d} = -v_\eta(\xi, \eta + d\eta) dt \vec{e}_\eta \) into equation (A.6) of Appendix A gives the following relation between the areas \( A(\eta) \) of CD and \( A(\eta + d\eta) \) of EF:

\[
A(\eta) = \left( 1 - \frac{v_\eta dt}{h_\xi h_\eta} + \mathcal{O}(dt^2) \right) A(\eta + d\eta).
\] (6.14)

The fractional area change due to diffusion in CDFE can be easily derived from equation (6.14) whenever \( dt \to 0 \)

\[
\left( \frac{1}{A} \frac{dA}{dt} \right)_d = -\frac{v_\eta}{h_\xi h_\eta} \frac{\partial h_\xi}{\partial \eta}.
\] (6.15)

Adding the two fractional area changes of equations. (6.13) and (6.15) then gives for the total fractional area change:

\[
\frac{1}{A} \frac{dA}{dt} = \frac{1}{\rho h_\xi h_\eta} \frac{\partial}{\partial \eta} (\rho v_\eta h_\xi) = \frac{1}{\rho h_\xi h_\eta} \frac{\partial}{\partial \xi} (\rho v_\xi h_\eta) = K(\xi, \eta).
\] (6.16)

This analysis shows that our definition of stretch indeed includes those terms which give rise to flame area variations for convective and diffusive transport. Equation (6.9) defines a scalar stretch field not only on an infinitesimal (i.e. infinitely thin) flame sheet but in the whole region for \( \mathcal{Y}(x, y) \) between \( \mathcal{Y}_u \) and \( \mathcal{Y}_b \), and the separate terms can be computed from the numerical solution of the flow field \( \vec{v} \) and the scalar fields \( \rho \) and \( \mathcal{Y} \). Explicit expressions for the different terms of \( K(\xi, \eta) \) are derived in terms of \( \vec{v}, \rho \) and \( \mathcal{Y} \) in a 2D Cartesian coordinate system in Appendix B.

A question not yet answered is which scalar field in the flame should be used to define the flame front. It is important to realise that the results for \( K \) depend on the choice of \( \mathcal{Y} \). In most cases there is no unique choice. The only mathematical restriction is that, in order to be able to introduce a well-defined \( (\xi, \eta) \)-coordinate system, \( \mathcal{Y} \) has to be a monotonous field without local extremes. This eliminates the possibility to use the mass fraction of intermediate species in the flame for \( \mathcal{Y} \). Also, it seems to be unwise to use the temperature for \( \mathcal{Y} \), because local temperature variations along the flame contours induced by stretch effects may be of interest. Any other choice, i.e. the mass fraction of one of the main species is possible. In our case it seems obvious to use the mass fraction of fuel for \( \mathcal{Y} \). The position of the flame contours then depends on the amount of fuel already consumed in the combustion process.

### 6.2 Flame Stretch and the Conservation Equations

It is well known that stretch has important effects on the local behaviour of flames through local variations in scalar quantities, such as the (flame) temperature. In this section it will be shown...
that the terms in equation (6.9) which arise from a non-uniform flow and from flame thickness variations are precisely those contributions which induce such variations in the behaviour of \( Y \) and in the other scalar fields of the flame. As an example, the effect of stretch on the flame temperature will be studied and it will be shown that the theory gives identical results as the analysis of Chung et al., when a number of assumptions and approximations are introduced. For that purpose, we will study the conservation equation of the scalar quantity \( Y \) in the coordinate system of figure 6.1.

Again, we start from the mass conservation equation (6.4). The total amount of mass which enters or leaves the diffusive cell (hatched area in figure 6.1) at the boundaries \( \eta = \eta_u \) or \( \eta = \eta_b \) can be obtained by integration of equation (6.9) over this cell

\[
\int_{\xi_1}^{\xi_2} \int_{\eta_u}^{\eta_b} \frac{1}{h_\xi h_\eta} \left[ \frac{\partial}{\partial \xi} (\rho v_\xi h_\eta) + \frac{\partial}{\partial \eta} (\rho v_\eta h_\xi) \right] | J | \, d\eta \, d\xi = 0,
\]

(6.17)

where \( | J | = h_\xi h_\eta \) denotes the Jacobian of the transformation \((x, y) \to (\xi, \eta)\). Substitution of equation (6.5) into equation (6.17) gives

\[
\int_{\xi_1}^{\xi_2} [(\rho v_\eta h_\xi)_b - (\rho v_\eta h_\xi)_u] d\xi = -\int_{\xi_1}^{\xi_2} \int_{\eta_u}^{\eta_b} \rho K(\xi, \eta) h_\xi h_\eta d\eta,
\]

which holds for arbitrary \( \xi_1 \) and \( \xi_2 \) and therefore

\[
(\rho v_\eta h_\xi)_b - (\rho v_\eta h_\xi)_u = -\int_{\eta_u}^{\eta_b} \rho K(\xi, \eta) h_\xi h_\eta d\eta.
\]

(6.18)

(6.19)

The coefficients \( h_{\xi, u} \) and \( h_{\xi, b} \) are measures for the area of the unburned and burned boundaries of the diffusive cell through which the scalar variable \( Y \) diffuses. Differences in \( h_{\xi, u} \) and \( h_{\xi, b} \) are accounted for by the curvature term

\[
\frac{\rho v_\eta}{h_\xi h_\eta} \frac{\partial h_\xi}{\partial \eta} = \rho v_\eta \nabla \cdot \vec{e}_\eta = \frac{\rho v_\eta}{R_\eta}
\]

(6.20)

with \( R_\eta \) being the radius of curvature of the \( \eta = \text{Const}\)-contours (see equation (6.4)). Note that the mass fluxes at the unburned and burned cell boundaries are equal, i.e. \((\rho v_\eta h_\xi)_u = (\rho v_\eta h_\xi)_b\), when the local stretch rate is zero.

Now consider the conservation equation for the scalar quantity \( Y \)

\[
\nabla \cdot (\rho \vec{v} Y) - \nabla \cdot (\rho D_Y \nabla Y) = S_Y,
\]

(6.21)

with \( D_Y \) and \( S_Y \) the diffusion coefficient and the (chemical) source term, generally depending on the other field variables in the flame. In the coordinate system of figure 6.1 we find

\[
\frac{1}{h_\xi h_\eta} \frac{\partial}{\partial \eta} (\rho v_\eta h_\xi Y) - \frac{1}{h_\xi h_\eta} \frac{\partial}{\partial \eta} (\rho D_Y h_\xi \frac{\partial Y}{\partial \eta}) - S_Y = -\frac{1}{h_\xi h_\eta} \frac{\partial}{\partial \xi} (\rho v_\xi h_\eta Y) = -\rho K Y,
\]

(6.22)
where we used that the diffusive transport is directed in $\bar{e}_1$-direction, so that $\partial N/\partial \bar{e}_1 = 0$. The left-hand side of equation (6.22) is a quasi '1D' conservation equation in $\bar{e}_1$-direction. All distortions from 1D behaviour, being the transport contributions in $\bar{e}_\xi$-direction, are gathered in the right-hand side of equation (6.22). Integrating this equation over the diffusive cell of figure 6.1, analogous to equation (6.17), then gives

$$\int h_{\xi b} m_0 \Delta Y^0 - \int S_{\xi} h_{\eta} h_{\eta} d\eta = 0,$$

(6.25)

To arrive at equation (6.23), we used that the diffusive fluxes vanish in the unburned and burned mixture. The mass burning rate $\rho S_L$ for stationary flames is now defined as

$$\rho(\bar{v} \cdot \bar{e}_1) = \rho S_L \bar{e}_1 = m \bar{e}_1.$$

(6.24)

Let us now consider the variation $\Delta Y = Y_b - Y_u$ of $Y$ through the flame and compare this variation with $\Delta Y^0 = Y^0_b - Y^0_u$ in case of stretch-less flames. The undistorted value $\Delta Y^0$ follows from equation (6.23)

$$h_{\xi b} m_0 \Delta Y^0 - \int S_{\xi} h_{\eta} h_{\eta} d\eta = 0,$$

(6.25)

where we used that $(\rho v_{\eta} h_{\xi})_b = (\rho v_{\eta} h_{\xi})_u$ is equal to $h_{\xi b}$ times the adiabatic mass burning rate $m^0_b$ for $K = 0$. Furthermore, $S^0_{\eta}$ denotes the undistorted chemical source term. In case $K \neq 0$ we find from equation (6.23)

$$\Delta Y = \frac{m_b}{m^0_b} \Delta Y^0 + \Delta S + \frac{1}{h_{\xi b} m^0_b} \int \rho K(\xi, \eta) [Y_u - Y(\eta)] h_{\xi} h_{\eta} d\eta.$$

(6.26)

In equation (6.26) we used the mass balance (6.19) and equation (6.25). Furthermore, we introduced

$$\Delta S = \frac{1}{h_{\xi b} m^0_b} \int (S_{\xi} - S^0_{\xi}) h_{\xi} h_{\eta} d\eta.$$

(6.27)

Equation (6.26) indicates that a non-uniform flow and flame thickness variations may change the local value of $\Delta Y$ in the flame, through the terms in $K(\xi, \eta)$ we considered in the previous section.

We will now derive equation (6.26) in terms of the enthalpy $H$, being the mass weighted average of the species enthalpies $H_i$

$$H = \sum_{i=1}^{N} H_i Y_i, \quad H_i = H^0_i + \int_{\tau_0}^{T} c_{p,i}(\tau) d\tau,$$

(6.28)

in order to compute the local variations in the flame temperature. We start from the stationary enthalpy conservation equation

$$\nabla \cdot (\rho \bar{v} H) = -\nabla \cdot \bar{q},$$

(6.29)
with
\[ q = -\lambda \nabla T + \sum_{i=1}^{N} \rho Y_i H_i V_i, \]

where \( V_i \) being the diffusion velocity of species \( i \). After introducing the constant Lewis numbers \( Le_i = \frac{\lambda}{\rho D_{im} c_p} \), \( D_{im} \) being the diffusion coefficient of species \( i \) in the mixture, the equation can be written as (Peters, 1992)

\[ \nabla \cdot (\rho \bar{v} H) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla H \right) = \sum_{i=1}^{N} (1 - Le_i) \nabla \cdot (\rho D_{im} H_i \nabla Y_i). \]

When equation (6.5) is used, equation (6.31) evolves to

\[ \nabla \cdot (\rho v H \bar{c}_{\eta}) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla H | \bar{c}_{\eta} \right) - \sum_{i=1}^{N} (1 - Le_i) \nabla \cdot (\rho D_{im} H_i | \nabla Y_i | \bar{c}_{\eta}) = -p KH - Q_H. \]

The left-hand side is again a '1D' conservation equation in \( \bar{c}_{\eta} \)-direction. Distortions from local 1D behaviour are gathered in the right-hand side. Most convective enthalpy fluxes are now combined in the \( pKH \) term. The convective flux \( \frac{\partial H}{\partial \xi} \frac{C_{p}^2}{\partial t} \) and the diffusive enthalpy fluxes along the flame contours, due to terms arising from the factors \( \frac{\partial Y_i}{\partial \xi} \frac{C_{p}^2}{\partial t} \) and \( \frac{\partial \tau}{\partial \xi} \frac{C_{p}^2}{\partial t} \) in equation (6.31) are combined in the term \( Q_H \). It must be realised that \( \frac{\partial Y_i}{\partial \xi} \frac{\partial \tau}{\partial t} \neq 0 \) in general, as the iso-contours of the scalar quantities are not parallel. Local variations in e.g. the temperature along flame contours would not be possible otherwise.

We now continue with integrating equation (6.32) through the flame from \( \eta = \eta_u \) to \( \eta = \eta_b \)

\[ (\rho v \eta h_{\xi} H)_{b} - (\rho v \eta h_{\xi} H)_{u} = - \int_{\eta_u}^{\eta_b} (pKH + Q_H) h_{\xi} h_{\eta} d\eta, \]

where we used that \( | \nabla H | = | \nabla Y_i | = 0 \) in the (un)burnt mixture. Substituting equation (6.19) finally gives

\[ H_b - H_u = \frac{1}{(\rho S_{h} h_{\xi})_{u}} \int_{\eta_u}^{\eta_b} (pK(H_u - H) - Q_H) h_{\xi} h_{\eta} d\eta. \]

equation (6.34) is our final equation, which can be used in numerical computations to study the effects of flame stretch on local variations in the flame temperature. In the remainder of this section, we will derive an approximation of equation (6.34).

When it is assumed that the composition of the mixture at the 'unburned' flame boundary \( \eta = \eta_u \) is equal to the composition of the related stretchless flame with which the behaviour is compared, we have \( H_u = H_u^0 = H_b^0 \), so that

\[ H_b - H_u = H_b - H_b^0 \approx c_p(T_b - T_b^0). \]
Note that $c_p$ is taken to be constant. The last step in equation (6.35) follows because local enthalpy variations mainly introduce temperature differences; changes in the mixture composition have a smaller contribution, especially in lean mixtures. In equation (6.35), $T_b - T_b^0$ is the local deviation from the undistorted adiabatic temperature $T_b^0$.

In the weak flame-stretch limit, we may assume that the dimensionless stretch rate $K = \frac{\lambda}{h_{\eta}} \frac{\partial \eta}{\partial t}$ is small enough so that terms of order $K^2$ and higher are negligible in equation (6.34). The contribution of the parallel diffusive fluxes of, for instance, the temperature $\frac{\lambda h_{\xi} \partial T}{c_p h_{\eta} \partial \xi}$ compared to the parallel convective flux $\rho v_{\xi} c_p T$, are small for weakly stretched flames, as $\frac{\partial T}{\partial \xi} \to 0$ when $K \to 0$. That $\frac{\partial T}{\partial \xi}$ is indeed small follows also from the numerical illustration in the next section, where it is shown that the density variations along the flame (directly coupled with the tangential temperature variations) are very small. From the above it is reasonable to assume that terms like $\frac{\partial}{\partial \xi} (\lambda h_{\xi} \frac{\partial T}{c_p h_{\eta} \partial \xi})$ are small compared to $\frac{\partial}{\partial \xi} (\rho v_{\xi} h_{\eta} c_p T) \approx \rho K c_p T h_{\xi} h_{\eta}$. This indicates that $| Q_H |$ is negligible compared to $| \rho K H |$. Numerical data of the flame tip, discussed extensively in the next section, have shown that the $Q_H$ term gives a contribution which is two to three orders of magnitude smaller than the $\rho K H$ term. We therefore neglect the $Q_H$ term in the following.

For weak stretch rates, we may restrict ourselves to the lowest-order $K^0$ contribution to calculate $H_u - H$ in the right-hand side of equation (6.34). This means that, when integrating equation (6.32) over $\eta$ from $\eta$ to $\eta_b$, we may neglect the term $\rho K H + Q_H$. This gives

$$
(\rho v_{\eta} h_{\xi} H)_u - (\rho v_{\eta} h_{\xi} H) + \frac{\lambda h_{\xi}}{c_p h_{\eta}} \frac{\partial H}{\partial \eta} = - \sum_{i=1}^{N} H_{i0} (1 - L e_i) \rho D_{im} \frac{h_{\xi}}{h_{\eta}} \frac{\partial Y_i}{\partial \eta} + O(\tilde{K}).
$$

In the right hand side of this expression, $H_i$ has been replaced by the dominant part $H_i^0$. The contribution arising from $\int c_p dT$ can be neglected in hydrocarbon flames (Smooke, 1991). From mass conservation we know that

$$
(\rho v_{\eta} h_{\xi})_u = \rho v_{\eta} h_{\xi} + O(\tilde{K}),
$$

so that

$$
(H_u - H) = - \delta_f \frac{\partial H}{h_{\eta}} - \frac{1}{\delta_f} \sum_{i=1}^{N} H_{i0} (1 - L e_i) \frac{1}{h_{\eta}} \frac{\partial Y_i}{\partial \eta} + O(\tilde{K}),
$$

where $\delta_f = \frac{\rho v_{\eta} c_p}{\rho v_{\xi}}$ is constant up to $O(\tilde{K})$. To continue, we search expressions for $\frac{1}{h_{\eta}} \frac{\partial H}{\partial \eta}$ and $\frac{1}{h_{\eta}} \frac{\partial Y_i}{\partial \eta}$ of order $K^0$. It is assumed that the reaction zone is thin and that the behaviour of these terms is determined predominantly by the solution in the preheating zone. Integration of the conservation equations of $Y_i$ and $H$ through the flame then results in

$$
\frac{1}{h_{\eta}} \frac{\partial Y_i}{\partial \eta} = L e_i \frac{(Y_i - Y_{i,u})}{\delta_f}
$$

and

$$
\frac{1}{h_{\eta}} \frac{\partial H}{\partial \eta} = \frac{(H_b - H_u)}{\delta_f} \exp \left[ \frac{1}{\delta_f} \int_{\eta_b}^{\eta} h_{\eta} d\tilde{\eta} \right].
$$
equations, (6.35), (6.38), (6.39) and (6.40) are now substituted into equation (6.34). The term arising from $\frac{\partial H}{\partial \eta}$ is proportional to $H_b - H_u$ and is therefore of $O(K^2)$ in equation (6.34) and is neglected. We thus finally have

$$T_b - T^0_b \approx \frac{1}{c_p} (H_b - H_u) = - \sum_{i=1}^{N} \frac{H^0_u}{Le_i} \left( \frac{1}{Le_i} - 1 \right) (Y_{i,b} - Y_{i,u}) \frac{K a_i + O(K^2)}{1},$$

(6.41)

where the Karlovitz numbers $K a_i$ are given by

$$K a_i = \frac{Le_i}{(\rho S L h_\xi)_b} \frac{\eta_b}{\eta_u} \int \rho K(\xi, \eta) \left[ \frac{Y_i - Y_{i,u}}{Y_{i,b} - Y_{i,u}} \right] h_\xi h_\eta d\eta.$$  

(6.42)

This expression indicates that the local stretch rate $\rho K$ has to be weighted with a factor $(Y_i - Y_{i,u})/(Y_{i,b} - Y_{i,u})$ which behaves exponentially in numerical studies, so that the contribution of $\rho K$ in the cold part of the preheating zone is damped and the predominant contribution to $K a_i$ is found near the reaction zone. This demonstrates that flame stretch throughout the whole preheat zone influences the flame temperature, in agreement with remarks made by Buckmaster (1979).

In most analytical studies so far, a one-step reaction is used. To show that we arrive at the same result as Chung, we finally consider only one chemical species (e.g. fuel) with one Lewis number. Further, assuming that $H^0_u(Y_{fu,u} - Y_{fu,b})/(c_p T^0_b) = 1$ (as Chung also does), finally gives

$$\frac{T_b}{T^0_b} = 1 + K a \left( \frac{1}{Le} - 1 \right) + O(Ka^2)$$

(6.43)

for equation (6.41). Note that equation (6.43) can also be found from equation (6.41) in case of multi-species combustion, when $\rho K h_\xi = (\rho K h_\xi)_b$ is constant in the range $\eta_u < \eta < \eta_b$, so that the integral equation (6.42) reduces to the usual definition for the Karlovitz number $K a_i = Ka(Le = 1) = \frac{K \delta \xi}{S L_b}$. The effective Lewis number $Le$, taking into account the combined effect of all species which have an impact on diffusive energy transport in the flame, is then found by equating equations (6.41) and (6.43)

$$\left( \frac{1}{Le} - 1 \right) = \sum_{i=1}^{N} \left( \frac{1}{Le_i} - 1 \right) (Y_{i,u} - Y_{i,b}) \frac{H^0_i}{c_p T^0_b}.$$

(6.44)

The result (6.43) is equal to the result of Chung. The analysis shows that equation (6.26) gives identical results as the analysis of others, when the appropriate assumptions are used.

### 6.3 The burning velocity

In this section expressions will be derived from the conservation equations for the mass burning rate of stretched flames. The conservation equations used for this analysis are those for mass, the mass fractions $Y_i$, the enthalpy $H$ and the element mass fractions $Z_j$ which are defined by (Peters, 1992)

$$Z_j = W_j \sum_{i=1}^{N} \mu_{ji} Y_i / M_i, \quad (j = 1, \ldots, N_e),$$

(6.45)
6.3. The burning velocity

where the $\mu_{ij}$ coefficients denote the element composition (i.e. the number of atoms of type $j$ in species $i$) and where $M_i$ and $W_j$ are the molar masses of species $i$ and element $j$, respectively. $N_e$ is the number of elements in the flame. It is instructive to analyse the specific element mass fractions in stretched flames, because flame stretch in combination with preferential diffusion might influence the local stoichiometry of the flame.

Before we turn to the derivation of expressions for the mass burning rate $\rho S_L$ the conservation equations have to be expressed in terms of $\rho S_L$ and $K$ (instead of $\rho \vec{v}$). The introduction of $K$ into the conservation equation is treated in the previous section. With the definition (6.24) of $m$ the conservation equations become 1D equations like (6.22)

$$
\frac{1}{h_\eta} \frac{\partial}{\partial \eta} (h_\xi \cdot m) = -h_\xi \rho K,
$$

$$
\frac{1}{h_\eta} \frac{\partial}{\partial \eta} (h_\xi \cdot m \cdot Y_i) - \frac{1}{h_\eta} \frac{\partial}{\partial \eta} \left( h_\xi \rho D_{im} \frac{1}{h_\eta} \frac{\partial Y_i}{\partial \eta} \right) - h_\xi \dot{Y}_i = -h_\xi \rho K Y_i, \quad (i = 1, \ldots, N),
$$

$$
\frac{1}{h_\eta} \frac{\partial}{\partial \eta} (h_\xi \cdot m \cdot H) - \frac{1}{h_\eta} \frac{\partial}{\partial \eta} \left( h_\xi \frac{\lambda}{c_p} \frac{1}{h_\eta} \frac{\partial H}{\partial \eta} \right) - \sum_{i=1}^N \left( \frac{1}{L_{ei}} - 1 \right) \frac{1}{h_\eta} \frac{\partial}{\partial \eta} \left( h_\xi \frac{\lambda}{c_p} H_i \frac{1}{h_\eta} \frac{\partial Y_i}{\partial \eta} \right) = -h_\xi \rho KH, \quad (6.46)
$$

$$
\frac{1}{h_\eta} \frac{\partial}{\partial \eta} (h_\xi \cdot m \cdot Z_j) - \frac{1}{h_\eta} \frac{\partial}{\partial \eta} \left( h_\xi \frac{\lambda}{c_p} \frac{1}{h_\eta} \frac{\partial Z_j}{\partial \eta} \right) - \sum_{i=1}^N w_{ji} \left( \frac{1}{L_{ei}} - 1 \right) \frac{1}{h_\eta} \frac{\partial}{\partial \eta} \left( h_\xi \frac{\lambda}{c_p} \frac{1}{h_\eta} \frac{\partial Y_i}{\partial \eta} \right) = -h_\xi \rho KZ_j, \quad (j = 1, \ldots, N_e).
$$

Note that the diffusive flux along the flame contours (the $Q_i$ terms) is neglected and that the derivative of $h_\xi$ is related to the curvature of the flame. In the following subsections we study the above system analytically for arbitrary $h_\xi$ and $K$ as function of $\eta$. More specifically, we will compute the mass burning rate $m$ for both stretchless flames ($K = 0$) and stretched flames ($K \neq 0$). These equations are also a suitable model in numerical flame simulations, when the stretch rate $K$ and the area function $h_\xi$ are given.

6.3.1 The burning velocity of stretchless flames

Let us first study the case of stretchless flames, i.e. $K = 0$. Note that flames may still be curved when $K = 0$. Integration of the conservation equations for mass and enthalpy from the unburnt to the burnt gas mixture gives

$$
(h_\xi m^0)_b = (h_\xi m^0)_u, \quad (6.47)
$$

$$
(h_\xi m^0 H^0)_b = (h_\xi m^0 H)_u, \quad (6.48)
$$

$$
(h_\xi m^0 Z^0_j)_b = (h_\xi m^0 Z_j)_u, \quad (j = 1, \ldots, N_e), \quad (6.49)
$$

where it has been used that the diffusive fluxes all vanish in the unburnt and burnt gases. The superscript '0' refers to the stretchless solution. equations (6.47), (6.48) and (6.49) simply indicate
that the mass, enthalpy and element composition are constant in the flame area, i.e. $H_0 = H_u$ and $Z_{j,b}^0 = Z_{j,u}$, as expected. This means that the stoichiometry of the mixture near the reaction zone is also unchanged.

Let us now turn to the mass burning rate $m_b^0$ of the stretchless flame, which can be computed from the quasi-1D equation for $Y$

$$F(\eta) - \frac{\partial}{\partial \eta} \mathcal{G}(\eta) = \mathcal{S}(\eta),$$  \hspace{1cm} (6.50)

where we introduced the functions $F$, $G$ and $S$

$$F(\eta) = \frac{\partial}{\partial \eta} (h_\xi m Y),$$

$$G(\eta) = h_\xi \rho D Y \frac{1}{h_\eta} \frac{\partial Y}{\partial \eta},$$

$$S(\eta) = h_\eta h_\xi \rho Y.$$ \hspace{1cm} (6.51)

We multiply equation (6.50) with $G(\eta)$ and subsequently integrate the resulting equation over $\eta$ from $\eta_u$ to $\eta_b$. The integral over the diffusion term $\frac{1}{2} \frac{\partial^2}{\partial \eta^2}$ then drops out, as the diffusion fluxes are zero in the (un)burnt mixture and we find

$$\int_{\eta_u}^{\eta_b} F(\eta) G(\eta) \, d\eta = \int_{\eta_u}^{\eta_b} G(\eta) \, S(\eta) \, d\eta. $$ \hspace{1cm} (6.52)

The integrals in this equation run over the complete flame area. The function $G(\eta)$ in the left-hand side of this equation can be approximated very well by the (integrated) solution of equation (6.50) in the preheating zone, where $S \ll F$

$$G(\eta) = \int_{\eta_u}^{\eta} (F(\psi) - S(\psi)) \, d\psi \approx \int_{\eta_u}^{\eta} F(\psi) \, d\psi,$$ \hspace{1cm} (6.53)

which leads to

$$\int_{\eta_u}^{\eta_b} F(\eta) \left( \int_{\eta_u}^{\eta} F(\psi) \, d\psi \right) \, d\eta = \frac{1}{2} \left( \int_{\eta_u}^{\eta_b} F(\eta) \, d\eta \right)^2 \approx \int_{\eta_u}^{\eta_b} G(\eta) \, S(\eta) \, d\eta. $$ \hspace{1cm} (6.54)

The validity of the approximation in equation (6.53) is related to the fact that the reaction layer is much thinner than the preheating zone, so that the major contribution to the integral over $FG$ in equation (6.52) is found in the preheating zone. It should be noted that equation (6.54) is exact when the reaction sheet thickness goes to zero (e.g. for infinite activation energy). This approach is equivalent to the Large Activation Energy Asymptotics treatment (Bush (1970), Williams (1975)) to compute the mass burning rate.
The integrals in equation (6.54) can now be evaluated

\[
\int_{\eta_u}^{\eta_b} F(\eta) \, d\eta = (h_\xi m_b^0) (Y_b^0 - Y_u),
\]

\[
\int_{\eta_u}^{\eta_b} G(\eta) S(\eta) \, d\eta = \int_{\eta_u}^{Y_b^0} h_\xi^2 \rho D_Y \dot{\rho}_Y \, dY,
\]

where we used equation (6.47). Substituted into equation (6.54), this gives the following expression for the mass burning rate

\[
m_b^0(H_b^0, Z_{1,b}^0, \ldots, Z_{N_e-1,b}^0) \approx \frac{1}{|Y_b^0 - Y_u|} \sqrt{2 \int_{\eta_u}^{Y_b^0} \left( \frac{h_\xi}{h_\xi^b} \right)^2 \rho D_Y \dot{\rho}_Y \, dY}.
\]

(6.56)

It should be realised that equation (6.56) is not equal to the adiabatic mass burning rate \(m_{b,1}\) of a flat flame, due to the \(h_\xi\)-terms. For an infinitesimal reaction layer, though, this known expression does reduce to the expression for the adiabatic mass burning rate of a planar flame, as the curvature factor \((h_\xi/h_\xi^b)^2\) then drops out. Note that we explicitly emphasised the dependence of the mass burning rate \(m_b^0\) on the enthalpy and element composition in the equilibrium state (or the burnt state) in equation (6.56), while the integral is expressed as a function of a scalar variable \(Y\). Strictly, the factor \(\rho D_Y \dot{\rho}_Y\) in equation (6.56) is a function of all flame variables \(Y_i\) \((i = 1, \ldots, N)\) and \(T\). However, the integral in equation (6.56) effectively runs only over the thin reaction layer, where \(\dot{\rho}_Y \neq 0\) and where the system approaches the equilibrium state. From a time scale analysis (see e.g. Eggels (1995)) it has become clear recently that the reaction path near the equilibrium or the burnt state is one-dimensional, i.e. it can be described by one so-called progress variable (in this case \(Y\)). The observation that the integral effectively runs over the reaction zone, which is close to the equilibrium state, also implies that the integral over \(Y\) and \(m_b^0\) are mainly determined by the equilibrium state. The local equilibrium state is described completely by the pressure (assumed to be constant), total enthalpy and element composition in the reaction layer, i.e. \(H_b^0\) and \(Z_{j,b}^0\) for \(j = 1, \ldots, N_e - 1\); \(Z_{N_e}\) follows from \(\sum_j Z_j = 1\).

### 6.3.2 Mass Burning Rate of Stretched Flames

In this section we consider stretched flames. As in the previous section, we first study the conservation equations for mass, enthalpy and element mass fractions. Integration of the mass conservation equation and the enthalpy conservation equation in (6.47) through the flame leads to equations (6.19), (6.34) and (6.41) with \(m = \rho S_L = \rho v_\eta\). Equation (6.41) describes the influence of preferential diffusion and flame stretch, incorporated in the Karlovitz numbers, on the local enthalpy of the burnt mixture. It should be noted from the definition (6.42) of the Karlovitz numbers that the influence of flame stretch \(\rho K\) in the preheating zone is effectively damped exponentially by the factor \(\frac{Y_i - Y_{i,m}}{Y_{i,b} - Y_{i,m}}\), which is equal to 1 in the burnt gases and tends to zero for \(\eta \rightarrow \eta_u\).
To determine the local element mass fractions in the burnt mixture of stretched flames, the same procedure can be followed as for the enthalpy. Integrating the equations for \( Z_j \) in the set (6.47) through the flame gives

\[
Z_{j,b} - Z_{j,u} = \frac{-1}{(h_{\xi} \rho K \eta)} \int h_{\xi} \rho K (Z_j - Z_{j,u}) \, d\eta.
\]  

When the definition equation (6.45) for \( Z_j \) and \( Z_{j,u} \) is inserted into the right-hand side we find, using equation (6.42)

\[
Z_{j,b} - Z_{j,u} = - \sum_{i=1}^{N} w_{ji} \frac{1}{Le_i} (Y_{i,b} - Y_{i,u}) K a_i.
\]

This equation describes the effect of preferential diffusion and flame stretch on the local element mass fractions in the burnt mixture. The enthalpy \( H_b \) and the element mass fractions \( Z_{j,b} \) in the burnt mixture, determine the local stoichiometry and equilibrium composition in the burnt mixture. These quantities, following from equations (6.41) and (6.58), have an important influence on the local mass burning rate \( m_b \), because it is determined to a large extent by the mixture composition and enthalpy in the reaction layer, close to the burnt mixture. The precise description of this influence will be studied hereafter.

Let us now turn to the evaluation of the mass burning rate for stretched flames. The mass burning rate is again determined from the quasi-1D \( \mathcal{Y} \)-equation (6.50), where \( \mathcal{F}(\eta) \) is now given by

\[
\mathcal{F}(\eta) = \frac{\partial}{\partial \eta}(h_{\xi} \rho K \mathcal{Y}) + h_{\xi} \rho K \mathcal{Y},
\]

while \( \mathcal{G} \) and \( \mathcal{S} \) are still given in (6.51). The computation of the mass burning rate is analogous to the computation presented in the previous section, with \( \mathcal{F} \) replaced by equation (6.59). For the integral over \( \mathcal{F} \) in (6.55) we now have

\[
\int_{\eta_u}^{\eta_b} \mathcal{F}(\eta) \, d\eta = (h_{\xi} \rho K \mathcal{Y})_b - (h_{\xi} \rho K \mathcal{Y})_u + \int_{\eta_u}^{\eta_b} h_{\xi} \rho K \mathcal{Y} h_{\eta} \, d\eta
\]

so that we find for the mass burning rate

\[
m_b(H_b, Z_{1,b}, \ldots, Z_{N_c-1,b}) \approx \frac{1}{\sqrt{\mathcal{Y}_b - \mathcal{Y}_u}} \left[ \int_{\mathcal{Y}_u}^{\mathcal{Y}_b} \left( \frac{h_{\xi} \rho K \mathcal{Y}}{h_{\xi} \rho} \right)^2 \rho D\mathcal{Y} \, d\mathcal{Y} \right]^{-1/2} \int_{\eta_u}^{\eta_b} h_{\xi} \rho K \left( \frac{\mathcal{Y} - \mathcal{Y}_u}{\mathcal{Y}_b - \mathcal{Y}_u} \right) h_{\eta} \, d\eta.
\]
The first term in the right-hand side is again a function of all variables $Y_i$ and $T$. However, as before, the integral effectively runs over the thin reaction layer, where the source term is non-zero and where the composition approaches the equilibrium point, following the 1D reaction path described by $Y_i(Y)$ and $T(Y)$. Comparison of this term with equation (6.56) for stretchless flames then indicates that this term is equal to the mass burning rate of a 'stretchless' flame $m_b^0(H_b, Z_{1,b}, ..., Z_{N_e-1,b})$ with enthalpy and composition given by $H_b$ and $Z_{j,b}$ instead of $H_b^0$, $Z_{j,b}^0$. Using the definition of the Karlovitz numbers (6.42) then gives for equation (6.61)

$$m_b(H_b, Z_{1,b}, ..., Z_{N_e-1,b}) \approx m_b^0(H_b, Z_{1,b}, ..., Z_{N_e-1,b}) - m_b \frac{K_{aY}}{L_{eY}}. \quad (6.62)$$

Comparing the mass burning rate $m_b = m_b(H_b, Z_{1,b}, ..., Z_{N_e-1,b})$ to the mass burning rate $m_b^0 = m_b^0(H_b^0, Z_{1,b}^0, ..., Z_{N_e-1,b}^0)$ for the stretchless counterpart and taking into account that $H_b = H_u$ and $Z_{j,b}^0 = Z_{j,u}(j = 1, \cdots, N_e)$, this last equation can be written as

$$\frac{m_b}{m_b^0} = 1 - \frac{K_{aY}}{L_{eY}} + (H_b - H_u) \frac{\partial}{\partial H_b^0} (\ln m_b^0)$$

$$+ \sum_{j=1}^{N_e-1} (Z_{j,b} - Z_{j,u}) \frac{\partial}{\partial Z_{j,b}^0} (\ln m_b^0) + \text{hot}, \quad (6.63)$$

with hot containing higher-order terms in $K_{aY}$. The differences $H_b - H_u$ and $Z_{j,b} - Z_{j,u}$ in (6.63) follow from equation (6.41) and (6.58), respectively.

Let us consider the physical significance of the different terms in equation (6.63). The term $K_{aY}/L_{eY}$ is related to the fact that effective upstream transport of heat and mass from the reaction zone to the preheating zone is modified by flame stretch. The rate of upstream transport has an important influence on the propagation velocity of a premixed flame. This can, for instance, be understood from equation (C.13), where it is observed that the mass burning rate is proportional to $\sqrt{\lambda L_e}$. Note that this term does not vanish for unit Lewis numbers ($L_e = 1$). The other terms are zero in that case. The $\frac{\partial}{\partial Z_{j,b}^0} (\ln m_b^0)$-term in the right-hand side is related to the effect of preferential diffusion on the local enthalpy, leading to a change in the mass burning rate on its turn. Both terms appear in the analysis of Chung and Law (1988) for the case of a simple one-step reaction. The last term, proportional to $\frac{\partial}{\partial Z_{j,b}^0} (\ln m_b^0)$, also arises from differential diffusion effects, which give rise to element composition and stoichiometry changes (at constant enthalpy). This term is not found in other studies. It is probably smaller than the second term, because the burning velocity is quite sensitive to variations in the temperature for large $E_a$ in most situations. However, burning velocity changes, due to local stoichiometry fluctuations may be important in some cases, for instance near the flammability limits.

We finally turn to the mass burning rate $m_u$ in the upstream part of the flame, which is frequently considered in the literature. Combining equation (6.19) and its stretchless counterpart equation (6.47) gives

$$\frac{m_u}{m_u^0} = \frac{m_b}{m_b^0} \left( 1 + \frac{1}{(h_{\xi} m_b)^{\eta_p}} \int_{h_{\xi} \rho K h_{\eta} d\eta} \right). \quad (6.64)$$
For \( \frac{m_b}{m_u} \) we may substitute equation (6.63). It is important to realise, that the integral over \( \rho K \) here is not proportional to the Karlovitz number, as is assumed in some studies. The factor \( \rho K \) in the definition (6.42) of the Karlovitz number is damped exponentially in the preheating zone. However, in equation (6.64), \( \rho K \) is not damped in the preheating zone, which might result in a value, significantly larger than the \( K_a \). Equations (6.63) and (6.64) describe the mass burning rate in the burnt and unburnt mixture, compared to the mass burning rate for the stretchless case. Finally, the mass burning rate \( m_u^0 \) follows from the equation

\[
 m_u^0 = m_b^0 \frac{h_{\xi b}}{h_{\xi u}} = m_b^0 \left( 1 - \frac{1}{h_{\xi b}} \int_{\xi_u}^{\xi_b} \frac{\partial h_{\xi}}{\partial \eta} \, d\eta \right)^{-1}
\]  

(6.65)

where the second term between large brackets describes the effect of flame curvature. Note that \( m_b^0 \) and \( m_u^0 \) are not equal to the mass burning rate of a flat adiabatic flame \( m_{b,1} \), due to the curvature factors in the integrals over the flame. However, the expression for \( m_u^0 \) is approximately equal to the adiabatic mass burning rate of a flat flame, because the integral in equation (6.56) has the largest contribution in the reaction layer, where the factor \( h_{\xi} \) is close to \( h_{\xi b} \). For the case of an infinitesimal reaction layer, \( m_u^0 \) in equation (6.56) is equal to the adiabatic mass burning rate. Expressions for the mass burning rate for constant \( \rho K \) and for lean flames with one-step chemistry are derived in appendix C. These expressions are used to investigate the effect of the Lewis number on the mass burning rate of lean V-shaped flames in chapter 7.

### 6.4 Illustration: Flame Stretch in the Tip of a Bunsen Flame

As an illustration we will compare the typical order of magnitude of the different contributions to the stretch rate \( K \) in this section. The contributions are determined for the tip of a stationary premixed Bunsen flame on a multiple-slit burner. This study gives an indication of the importance of the corresponding terms on the flame behaviour and flame stabilisation of the tip. The burner slits have a width of 4.0\( \text{mm} \) and a burner wall thickness of 0.4\( \text{mm} \). A stoichiometric methane/air mixture enters the computational domain with a parabolic velocity profile and a maximum velocity of 0.8\( \text{m/s} \). The stoichiometric methane/air flame on this burner is computed using the model described in chapter 2. The mass fraction of fuel \( Y_{fu} \) is used as the scalar quantity \( Y \) to define the stretch rate. For \( K \) we may write

\[
 K(\xi, \eta) = K_a + K_b + K_c,
\]  

(6.66)

where \( K_a \) is the usual stretch rate (given by equation (6.10)). Furthermore, \( K_b \) and \( K_c \) are given by

\[
 K_b = \frac{v_{\xi}}{\rho h_{\xi}} \frac{\partial \rho}{\partial \xi}
\]  

(6.67)

and

\[
 K_c = \frac{v_{\xi}}{R_{\xi}}
\]  

(6.68)
fig. 6.4: The different stretch field contributions in the flame tip on a 2D multiple-slit burner. Lines: $\eta$-contours (fuel mass fraction $Y_{fu}$) and contours of the stream function $\phi$; a: $K_a$, b: $K_b$, c: $K_c$ and d: $K$.

arising from density variations along the iso-contours and flame thickness variations. False-colour plots of $K_a$, $K_b$, $K_c$ and $K$ in the flame tip are presented in figures 6.4a, 6.4b, 6.4c and 6.4d, respectively. A number of iso-contours of $Y_{fu}$ ($\eta = constant$) and the stream function is also presented in the figure 6.4. Note that the maximum values for $|K_a|$, $|K_b|$, $|K_c|$ and $|K|$ are about 17000, 700, 4000 and 17000, respectively. This means that $K_b$ is negligible in the flame tip. However, the contribution of $K_c$ to $K$ is significant.

The behaviour of $K$ on the central symmetry axis ($\xi = 0$) is shown in figure 6.5. Note that $K = K_a$ because $K_b = K_c = 0$ on this axis for symmetry reasons. From equation (B.4) it is seen that $K' = K_a = u_x - v\dot{Y}_{xx}$ for $\xi = 0$ (see appendix B). Furthermore, for the flame front curvature
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we can deduce that \( \frac{1}{R_\eta} = \bar{Y}_{xx} \) for \( \xi = 0 \), so that \( K \) can also be written as

\[
K = K_a = u_x - \frac{v}{R_\eta},
\]
for the central axis. The different contributions \( u_x \) and \( v\bar{Y}_{xx} \) to \( K \) are also presented in figure 6.5. It is clearly seen that, although the flow divergence term \( u_x \) is not negligible, the curvature term has the most significant contribution, which is also concluded by other authors, such as Law (1992) and Poinset (1992). It should, however, be noted that \( R_\eta \) shows large variations through the flame. This indicates that the simple formula \( K = -v/R_f \) is valuable to approximate the stretch rate in a flame tip, when the correct value for the flame tip radius \( R_f \) is used.

The stretch rate \( K \) near the upstream boundary of the flame tip, where the tip radius \( R_\eta \) becomes smaller than the grid spacing is not shown in figures 6.4 and 6.5. The gradients are small there and the curvature terms are not reliable in this region. It should be noted that this is not a problem, because the exponential function in equation (6.42) for the Karlovitz number \( K_{\alpha} \) damp the contribution of the upstream part of \( \rho K \). To show this, both \( \rho K \) and the integrand \( \rho K \frac{Y_{i,b} - Y_{i,a}}{Y_{i,b} - Y_{i,a}} \) of equation (6.42) for \( K_{\alpha,CH_4} \) are presented in figure 6.6. Note that this figure indicates that the exponential damping of the preheating part of the stretch rate is essential. For the Karlovitz number, we find \( K_{\alpha}(Le_i = 1) = -0.51 \) in the tip with equation (6.42). The computed value for \( K_{\alpha} \) appears to be not very sensitive to variations of the Lewis number \( Le_i \) from 1. The contribution of the curvature part \( v\bar{Y}_{xx} \) is again dominant.

To quantify the importance of flame stretch on the flame temperature and the tip stabilization in our case, we computed the effective Lewis number \( Le \) from equation (6.44) for the case of the one-step chemical model presented in chapter 2. For stoichiometric methane/air flames a Lewis
number \( Le = 0.92 \) is found. Combining this with \( Ka(Le) = -0.47 \) leads to \( \frac{T_b}{T^0_b} \approx 0.96 \) with equation (6.43). For skeletal chemistry we find \( Le = 0.98 \) for \( \phi = 1 \), which indicates an even smaller variation in the flame temperature when a more complex chemical model is used. A direct analysis of the local flame temperature data in the numerically computed tip shows that \( T_b - T^0_b \approx -80K \), so that \( \frac{T_b}{T^0_b} \approx 0.96 \). This result is in good agreement with the value found with equation (6.43) and this analysis shows that temperature variations due to flame stretch are small.

Let us study the local mass burning rate \( m_b \) and \( m_u \) on the central axis of the flame tip. In figure 6.7 the mass flow rate \( \rho v \) as a function of the distance \( y \) on the center line is presented, together with the temperature \( T \). In the above we already saw that the effects of preferential diffusion on the burning velocity are smaller than 10\%, because the effective Lewis numbers are close to 1. For the Karlovitz number we find a value of \( Ka_{CH_4} \approx -0.47 \) using equation (6.42). The term \( \frac{K_a}{Le} \) in equation (6.63) which is equal to -0.51 then has the largest contribution to \( m_b/m^0_b \). With \( m^0_b = 0.35 \frac{kg}{(m^2 s)} \) a mass burning rate of \( m_b = 0.53 \frac{kg}{(m^2 s)} \) is found for this stoichiometric flame. This value should be close to the value for \( \rho v \) in the burnt gases \((\rho v)_b = 0.55 \frac{kg}{(m^2 s)}\); see figure 6.7).

For the mass burning rate in the unburnt gases we use equation (6.64). The term with the integral between brackets in this equation is quite large, so that the effect of this term on the unburnt mass burning rate, given by \( \frac{m_u}{m^0_u} \approx 0.2 \), is very large in the unburnt gases. The small value for \( \frac{m_b}{m^0_b} \) implies that the flame area at the unburnt side due to pure curvature is much smaller than the flame area based on curvature and flow divergence. The contribution of the curvature term between large brackets in equation (6.65) is also quite large, so that \( m^0_u \approx 17m^0_b \). When the
results for $m_u/m_u^0$ and $m_v/m_v^0$ are combined, the largest parts of these terms cancel and we find $m_u \approx 1.2\text{kg/(m}^2\text{s})$. This is also quite close to the result for $\rho v$ in the unburnt gases (see figure 6.7). That the terms in the integrals are quite large is related to the fact that these terms in equation (6.64) and (6.65) are not damped by an exponential factor in the unburnt gases, as in the case of the stretch rate in the Karlovitz numbers. Both these terms are large because of the large flame curvature contribution in the preheating zone, also present in the stretch rate $\rho K$. The cancellation of these curvature contributions can also be understood when equations (6.64) and (6.65) are observed more closely. If $h_\xi\rho K = -\frac{1}{h_o} \frac{\partial(h_\xi\rho v)}{\partial \eta}$ is substituted into equation (6.64) and combined with equation (6.65) we find the obvious result

$$m_u = m_b - \int_{\eta_b}^{\eta_a} \frac{\partial}{\partial \eta} (\rho v) d\eta.$$

(6.70)
Only the flow straining term \( \frac{\partial (\rho v)}{\partial y} = \rho \frac{\partial u}{\partial y} \) remains. Although the curvature term has the largest contribution to \( \rho K \), it is the relatively small flow straining term, which causes a steady decrease of the mass flow rate of \( m_u = 1.2kg/(m^2 \text{ sec}) \) in the unburnt gases to \( m_b = 0.55kg/(m^2 \text{ sec}) \) in the burnt gases. Flow straining is responsible for the flame stabilisation in this case. Note that this analysis also teaches us that the mass burning rate in the burnt gases is the only physically relevant quantity: \( m_b \) indicates the amount of mass that is actually converted into products in the flame. The mass burning rate \( m_u \) has no real physical meaning: the mass flow rate in the unburnt gases may be changed significantly by flow straining before it is actually consumed.

Another proof of the importance of flow straining can be found in figure 6.8. In this figure the contributions to \( K \) in the flame tip on the symmetry axis are plotted together with the vertical mass flux \( \rho v \) and the normalised temperature for four different velocities. The maximum temperature \( T_{\text{max}} \) is equal to about 2220 K for all cases. The mass flux \( m_b \) in the burnt gases is equal to about 0.5 kg/m\(^2\)s for all inlet velocities despite an increase of \( K \) and \( v/R_\eta \) with a factor 2 in the preheat zone and the increase by almost a factor 2 of the maximum mass flux just in front of the flame tip. The necessary decrease of the mass flux \( \rho v \) is achieved by the flow straining contribution \( u_z \) to \( K \) because the decrease is proportional to \( \partial \rho v / \partial y = \rho u_z \). Another important observation in figure 6.8 is that the largest part of the decrease of \( \rho v \) is accomplished in the preheat zone.

Furthermore, the observation that \( m_b \) and \( m_u \) are (obviously) equal to the mass flux \( \rho v \) and independent of \( V_{\text{max}} \) implies that the stabilisation criterion \( m = \rho v \) has to be satisfied throughout the flame front for stable flame propagation.

### 6.5 Conclusions

The flame stretch concept has been extended to the case of 2D stationary flames with a finite flame front thickness. Additional terms due to density variations along the flame and flame thickness variations appear. The generalised formalism is applied to study the local variations in scalar quantities, such as the enthalpy, flame temperature and mass burning rate. From this, it appears to be possible to derive generalised equations for these variations, starting from the conservation equations. Furthermore, these generalised equations reduce to known expressions, when a number of approximations is introduced.

Finally, the order of magnitude of the separate terms is computed for the tip of a Bunsen flame as an illustration. The contribution to the stretch rate arising from density variations along the flame contours appears to be negligible in this case, while the term caused by flame thickness variations has a non-negligible contribution. It is shown that the Karlovitz number is not large and that the effective Lewis number is close to one, so that flame stretch has a small effect on the local temperature and mass burning rate for the particular flame studied. The stabilisation of the tip seems to be dominated by hydrodynamic effects, in particular by the flow straining term \( u_z \), which induces a steady decrease of the mass flow rate through the tip. The decrease of the mass flux is mainly achieved upstream of and inside the preheat zone.

It is concluded that the proposed method is a valuable tool to quantify the contribution of different effects on the local flame behaviour in numerical studies, such as the stabilisation of
flames on burners. The theory will be applied to the study of the stabilisation of inverted flames in the following chapter.
Chapter 7

The stabilisation of V-shaped flames

In this chapter we will investigate the stabilisation mechanism of V-shaped flames. A schematic drawing of a V-shaped or an inverted flame is given in figure 7.1. The stabilisation of V-shaped flames is an important subject of research because of several reasons (also see chapter 5). The stabilisation of V-shaped flames resembles the stabilisation of flames on multiple slit or porous plate burners which are widely used in domestic heating equipment. Also, the stabilisation of V-shaped flames is not affected by the surrounding atmosphere. This implies that the stabilisation of V-shaped flames can only be affected by heat loss to the flameholder, flow straining, stretch and Lewis number effects (also see the previous chapter).

The stabilisation of V-shaped flames has already been investigated by many authors. The most important investigations by Lewis and von Elbe (1961), Edmondson and Heap (1970), Kawamura et al. (1979, 1982), Trevino et al. (1991) and Sung et al. (1992) will be discussed briefly in section 7.1. Still, the exact stabilisation mechanism and the relative importance of, e.g., heat loss to the flameholder and Lewis number effects remains obscure. This is mainly due to the experimental and intuitive nature of previous investigations which makes a systematical investigation of the various phenomena difficult.

The stabilisation of lean V-shaped flames ($\phi = 0.7$) is investigated in section 7.2. There, the various contributions to the stretch rate $K$ (such as flow straining, curvature and the Lewis number) are calculated in the base of lean V-shaped flames ($\phi = 0.7$) stabilised at various mixture velocities. The stabilisation mechanism is then analysed by looking at the behaviour of these contributions to $K$ and the behaviour of the mass burning rate in the unburnt and the burnt mixture as a function of the mixture velocity. The analysis also leads to a better insight in the relative importance of the various quantities that affect the stabilisation process. Finally, in section 7.3, conclusions will be drawn from the results presented in this chapter.

7.1 Literature overview

In this section we will discuss several stabilisation concepts found in the literature. First, in subsection 7.1.1, the stabilisation theory based on a critical Karlovitz number (given by Lewis and von Elbe (1961) and Edmondson and Heap (1970)) will be discussed. The area-increase concept
(based upon pure flame curvature) by Kawamura et al. (1979, 1982) is presented subsequently. A description with the general stretch theory by Sung et al. (1992) will also be presented. Finally, the influence of heat loss to the flameholder is discussed.

\[ \text{fig. 7.1: A scheme of a V-shaped flame stabilised above a flameholder. Note the small recirculation zone just above the flameholder.} \]

### 7.1.1 The Karlovitz number

This stabilisation concept, developed by Lewis and von Elbe, is based on the flame stretch theory by Karlovitz (see chapter 1). Karlovitz has shown analytically that the burning velocity can deviate from its adiabatic value by velocity gradients in the unburnt mixture and that this deviation can be expressed in terms of the stretch rate \( K \). The Karlovitz number at blow-off is then defined by Lewis and von Elbe as

\[
K_{ab} = \frac{\delta}{S_{L,ad}} g_b, 
\]

(7.1)
7.1. Literature overview

with $g_b$ the velocity gradient $\partial v/\partial x$ at the flameholder at blow-off while $\delta$ follows from

$$\delta = \frac{\lambda}{c_p \rho_u S_{L,ad}}. \tag{7.2}$$

Lewis and von Elbe assume that the inverted flame blows off because the (increasing) positive stretch in the flame base leads to a large heat loss to the unburnt mixture, a subsequent decrease of the mass burning rate and, eventually, to local extinction and blow-off at a critical value of the Karlovitz number $K_{ab}$, approximately equal to one. The heat loss is attributed to the conduction of heat out of the central stream tubes at the flame base. Lewis and von Elbe, however, curiously neglect the effect of reactant diffusion towards the flame front. This diffusion process increases the amount of energy near the flame front because it is directed into the central stream tubes (also see Buckmaster (1979)). Since the investigation by Lewis and von Elbe several authors (e.g. Law (1988)) have shown that positive stretch only leads to a lower flame temperature when the Lewis number is larger than one (i.e. the diffusivity of heat is larger than the diffusivity of the deficient reactant; also see chapter 6).

Lewis and von Elbe implicitly assume a direct correlation between the velocity gradient at the burner wall and the gradient near the stabilisation point above the flameholder, independent of the flameholder thickness. Hertzberg (1990) shows that this is only valid for an infinitely thin flameholder. Hertzberg also shows that the gradient at the stabilisation point becomes increasingly lower than the gradient at the burner wall for a larger flameholder thickness which leads to an increase of $K_{ab}$ at blow-off for an increasing flameholder thickness. This implies that the theory by Lewis and von Elbe doesn’t have a sound physical basis for the description of the stabilisation of V-shaped flames.

The comments given above also apply to the investigation by Edmondson and Heap (1970) because they apply the same theory developed by Lewis and von Elbe. Although the stabilisation concept based on the Karlovitz number gives a reasonable description for the stabilisation process for thin flameholders it does not give much insight in the stabilisation process of inverted flames (and premixed flames in general) because of the omission of the Lewis number effect, the negligence of the flame curvature in the flame base and the poor correlation between the velocity gradient at the burner wall and the flow field above the burner (also see Melvin and Moss (1973)).

7.1.2 The area-increase concept

The stabilisation of inverted flames according to the area increase concept is described by Kawamura et al (1979,1982). The area-increase concept is based on the assumption that the flame stabilises because the local burning velocity and mixture velocity become equal above the flameholder. Kawamura assumes that the effect of flow straining ($\equiv \partial p_u/\partial x$) at the symmetry axis on the burning velocity is negligible compared to the effect of flame curvature on the burning velocity. The area change through the flame front (the area-increase factor) which describes the relative area increase from the ignition zone to the beginning of the preheat zone

$$A = \frac{\delta}{R}, \tag{7.3}$$
with $R$ the radius of curvature and $\delta$ the flame thickness. Kawamura assumes that the burning velocity decreases with increasing $A$ due to the divergent nature of the heat flow from the reaction zone towards the preheat zone. The diffusion of reactants to the reaction zone (which is convergent) is not taken into account by Kawamura. Measurements of $A$ (with $R$ determined from photographs) and $K_{a_b}$, related to $g_b$ according to (7.1), for various inlet velocities and flameholder thicknesses show that the area-increase factor $A$ at blow-off ($A_{b}$; determined by extrapolation) varies less with the flameholder thickness than $K_{a_b}$. This observation indicates that the area-increase concept gives a physically more correct description of the stabilisation of V-shaped flames than the description with the Karlovitz number. Kawamura also derives a stabilisation criterion which states that the conditions $S_L = v$ and $\partial S_L / \partial y > \partial v / \partial y$ have to be satisfied in the attachment point of a stable flame.

Despite the fact that $A_b$ varies less with the flameholder thickness than $K_{a_b}$, it remains uncertain if the flow divergence is unimportant in the stabilisation process. Especially the extrapolation of $A$ to the blow-off condition is a weak point in the area-increase concept. Experimental results given by Kawamura of the mass flux perpendicular to and along the flame front near the flame base do not show a zero flow divergence. Further note that the area-increase concept states that the burning velocity in the flame base can only become lower than $S_{L,ad}$, regardless of the Lewis number. This is in contradiction with experimental and theoretical results of other references (see e.g. Buckmaster (1979), Law (1988) and the previous chapter). The area-increase concept, therefore, doesn't provide a good basis for the physical understanding of the stabilisation process.

Finally note that the stabilisation criterion $\partial S_L / \partial y > \partial v / \partial y$ can only be applied to flames with a finite thickness if $\partial S_L / \partial y$ and/or $\partial v / \partial y$ in the flame front change if the mixture velocity is changed. If $\partial S_L / \partial y$ and $\partial v / \partial y$ in the flame front would be independent of the mixture velocity, the criterion would be satisfied for every disturbance in the mixture velocity. This matter will be discussed further in subsection 7.2.4.

### 7.1.3 A description with the stretch theory

Sung and Law present an analytical analysis which includes the effects of the stretch rate $K$ (which includes flow divergence and curvature) and the Lewis number on the stabilisation of inverted flames. In this analysis, the flow field is approximated by a uniform isothermal flow with a local potential sink above the flameholder. The flow field is fixed, which means that the flow field in the flame front changes if the position of the flame changes. An important difference between this and a physically realistic flow field is that the recirculation area above the flameholder is not present. A comparison with experimental results shows that the analytical model predicts the effect of $K$ on the stand-off distance qualitatively. This is probably due to the poor reproduction of the flow field by the model.

The results presented by Sung and Law indicate that both the flow divergence and the curvature contributions to the total stretch rate $K$ are important. Also, the results indicate that a physically correct reproduction of the flow field is important when investigating (inverted) flame stabilisation. All together, the results obtained by Sung and Law show that a complete flame stretch description together with a physically correct combustion and flow field model is important for investigating the stabilisation of inverted flames and premixed flames in general.
7.1.4 Heat loss to the flameholder

It is claimed by Trevino et al. (1991) that heat transfer between the flame and the flameholder is necessary for the stabilisation of a V-shaped flame. This conclusion is based on the observation that the flameholder of the burner they used had to be heated to stabilise the flame. Measurements of the temperature of the top of the flameholder by Kawamura et al. also show that the flame is cooled by the flameholder plate up to mixture velocities close to the blow-off limit. Sung et al., however, demonstrated that a V-shaped flame can stabilise at various velocities without heat loss to the flameholder. This is confirmed by the numerical and experimental results presented in chapter 5, which can be concluded from the observation that the stand-off distance is much larger than the thickness of the preheat zone (less than 1 mm).

The observations made by Trevino et al. seem to contradict the observations in chapter 5 and the observations of Sung and Law. One should, however, realise that the importance of heat transfer for the stabilisation of V-shaped flames largely depends on the specific burner geometry and on the shape of the velocity profile near the burner exit. A velocity profile with a relatively small gradient at the flameholder would lead to a smaller stand-off distance and, possibly, more heat transfer between the flame and the flameholder than a velocity profile with a large gradient at the flameholder. The results presented in chapter 5 and those presented by Sung and Law merely show that V-shaped flames can stabilise without significant heat transfer between the flame and the flameholder.

7.2 The stabilisation of lean V-shaped flames at various velocities

In this section a detailed investigation of the stabilisation of lean V-shaped flames (\( \phi = 0.7 \)) computed numerically at various inlet velocities is presented. The computational domain used for the computations is given in figure 5.2. The aim of the investigation is to study the importance of the different contributions to flame stretch such as flow divergence, flame curvature and Lewis number effects. The effect of the stretch rate and the Lewis number on the mass burning rate in the unburnt and the burnt mixture will also be investigated at various inlet velocities.

In the following subsection, \( \rho u \) and the various contributions to the stretch rate on the symmetry axis at \( x = 0 \) (figure 7.2) are evaluated for \( V_{\text{max}} \) ranging from 0.8 to 1.2 m/s. The effect of the stretch rate and the Lewis number on the mass burning rate (calculated from the equations derived in chapter 6 and appendix C) is investigated afterwards. The section ends with a comparison with the work described in the literature.

7.2.1 The contributions to the stretch rate

As shown in chapter 6, the stretch rate contains contributions due to flow straining, flame curvature, density variations along the flame front and flame thickness variations. The contributions due to density variations along the flame front and due to flame thickness variations (\( K_b \) and \( K_c \), given by equations (6.67) and (6.68)) are zero on the symmetry axis. As shown in section 6.4, the
Chapter 7. The stabilisation of V-shaped flames

Fig. 7.2: Strain $u_z$, curvature $v/R_\eta$, total stretch rate $K = K_a$, temperature $T$ and vertical mass flux $\rho v$ on the symmetry axis of inverted flames at four inlet velocities $V_{\max}$.

The flame blows off for $V_{\max} > 1.2$ m/s. It is apparent from figure 7.2 that the behaviour of the different quantities $K$, $u_z$ and $v/R_\eta$ does not change much when $V_{\max}$ is increased. The most important effect of an increasing $V_{\max}$ is an increase of the curvature part of $K$. Together with the almost negligible change in $u_z$ this also leads to an increase in the total stretch rate $K$. The increasing curvature can be explained straightforwardly by the upward movement of the flame wings at higher mixture velocities. This inevitably leads to larger curvatures in the flame base. The increasing stretch rate is, therefore, caused by the increasing curvature in the flame base. Some

\[ K = K_a = u_z - \frac{v}{R_\eta}, \quad (7.4) \]

with $1/R_\eta$ equal to $\tilde{Y}_{zz}$. In figure 7.2 the contributions $u_z$, $v/R$ and the total stretch rate are plotted as a function of the vertical distance $y$ for values of $V_{\max}$ ranging from 0.9 to 1.2 m/s. The flame blows off for $V_{\max} > 1.2$ m/s. It is apparent from figure 7.2 that the behaviour of the different quantities $K$, $u_z$ and $v/R_\eta$ does not change much when $V_{\max}$ is increased. The most important effect of an increasing $V_{\max}$ is an increase of the curvature part of $K$. Together with the almost negligible change in $u_z$ this also leads to an increase in the total stretch rate $K$. The increasing curvature can be explained straightforwardly by the upward movement of the flame wings at higher mixture velocities. This inevitably leads to larger curvatures in the flame base. The increasing stretch rate is, therefore, caused by the increasing curvature in the flame base. Some
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Key values have been listed below in Table 7.1 to clarify the effect of \( V_{\text{max}} \) on the various quantities.

**Table 7.1:** The minimum values of \( u_x \), the maximum values of \( \frac{v}{R_\eta} \), and \( K \), and the stand-off distance \( \delta_y \) (defined as the vertical distance between the top of the flameholder and the maximum \( \rho_f u \) at \( x=0 \)) for various values of \( V_{\text{max}} \).

<table>
<thead>
<tr>
<th>( V_{\text{max}} ) [m/s]</th>
<th>( \frac{v}{R_\eta} ) [max] [s(^{-1})]</th>
<th>( u_x ) [max] [s(^{-1})]</th>
<th>( K_{\text{max}} ) [s(^{-1})]</th>
<th>( \delta_y ) [mm]</th>
</tr>
</thead>
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<tr>
<td>0.8</td>
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<td>-287</td>
<td>826</td>
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</tr>
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<td>-310</td>
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</tr>
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<td>1160</td>
<td>3.5</td>
</tr>
<tr>
<td>1.2</td>
<td>1475</td>
<td>-305</td>
<td>1170</td>
<td>4.1</td>
</tr>
</tbody>
</table>

![Graph showing temperature and vertical mass flux](image)

**Fig. 7.3:** Temperature \( T \) (line) and vertical mass flux \( \rho v \) (markers) on the symmetry axis of a V-shaped flame at \( V_{\text{max}} = 1.3 \) m/s. Note that this flame is not stabilised anymore.

Note that \( u_x \) is equal to \( \frac{(1/\rho)\partial \rho u/\partial x}{(1/\rho)\partial \rho v/\partial y} \) on the symmetry axis because \( \partial \rho/\partial x \) is zero there. The most important effect of \( V_{\text{max}} \) on the profiles of \( u_x \) is the translation of the profile to higher \( y \)-values, which is caused by the increasing stand-off distance. The observation that \( u_x \) and the profiles of \( \rho v \) hardly change with increasing \( K \) implies that the stream tube contraction...
is about the same for all inlet velocities. Also, the mass flux \( \rho v \) in the burnt gases becomes equal to about 0.21 kg/m²s - approximately equal to \( m_b \) - for all values of \( V_{max} \) despite an increase of about 40 % in \( K \). The mass flux in front of the flame \( \approx m_u \) (at, e.g., 400 K) is equal to about 0.06 kg/m²s for all inlet velocities. This indicates that the effect of \( K \) on the amount of mass consumed in the flame is negligible. Apparently the mass flux consumed by the flame is limited to a physical maximum (in this case approximately 0.21 kg/m²s) and this value is accomplished by stream tube contraction by the non-zero flow convergence, described by \( u_x \). This indicates that \( u_x \) controls the stabilisation of the flame. The mass flux \( \rho u \) and the temperature \( T \) on the symmetry axis slightly above the blow-off limit (\( V_{max} = 1.3 \) m/s) is given in figure 7.3 as an illustration. It should be stressed that this is not a converged solution anymore. A clear difference with the results of figure 7.2 is that \( \rho_u v_u \) is significantly larger, thus leading to a larger value of \( \rho_b v_b \approx 0.225 > m_b \), kgm⁻²s⁻¹. This indicates that the amount of mass \( \rho_u v_u \) has increased too much for the flame to stabilise.

The effect of a V-shaped flame on the flow field is illustrated in figure 7.4. Figure 7.4 shows that the length of the recirculation area above the flameholder increases from 0.5 mm to 1.0 mm for \( V_{max} = 1.2 \) m/s if a flame is present. An increase of this order was observed for all V-shaped flames. This increase of the length of the recirculation area can be explained from the decrease of \( \rho v \) when a flame is present. This decrease, in turn, is caused by the flow resistance of the flame base and the flame wings which push the flow outwards. Note that the flame affects the behaviour of \( \rho v \) up to approximately 2 mm upstream of the upstream boundary of the preheating zone of the flame base, due to the flow resistance of the flame base and the flame wings.
7.2. The stabilisation of lean V-shaped flames at various velocities

The effect of the stretch rate on the flame temperature and the mass burning rate for inverted flames will be studied in more detail in the following subsections. We will also investigate the role of the various contributions to $K$ further to find more evidence for the importance of $u_x$ for the stabilisation of V-shaped flames.

7.2.2 The effect of stretch on the flame temperature

The effect of stretch on the flame temperature is analysed with equations (6.34) for $H_b - H_u$ and (6.35) which relates $H_b - H_u$ to the flame temperature. Calculation of $H_b - H_u$ from equation (6.34) resulted in values of about $3.3 \times 10^4$ J kg$^{-1}$. This results in values of about 1.03 for $T_b/T_b^0$, with $T_b^0 = 1814$ K. The temperature ratio $T_b/T_b^0$ obtained directly from the numerical flame data is about 1.02. The flame temperatures predicted by the combustion model are, therefore, somewhat lower (approximately 18 K) but still in reasonable agreement with equations (6.34) and (6.35). The calculations of $T_b$ have shown that the Lewis number effect at this equivalence ratio (0.7) gives rise to small deviations of $T_b$ from its adiabatic value and that the Lewis number effect is not large for the flames considered here.

7.2.3 The mass burning rate in the unburnt and the burnt mixture

In this subsection the relations for the mass burning rate will be used to analyse the stabilisation of V-shaped flames. More specifically, the investigation should lead to insight in the relative importance of curvature, flow straining and Lewis number effects for the mass burning rate of V-shaped flames.

The Karlovitz number used for the calculations is given by equation (6.42). Note that the Karlovitz number contains an integral of the stretch rate $K$ which implies that $Ka$ is a direct measure for the stretch rate $K$. The mass burning rate in the burnt mixture for $K=0$ ($m_b^0$) and $m_b = m_b^0 - Ka$ (with $K \neq 0$) for $Le=1$ are then calculated from equations (6.56) and (6.61). The contribution due to non-unit Lewis numbers is calculated from the last terms of equation (C.19) in appendix C. The mass burning rate in the unburnt mixture $m_u$ is calculated subsequently from equations (6.64) and (6.65). The amount of stream tube contraction in the flame is investigated by calculating the integral in equation (6.70). The quantities mentioned above are plotted as a function of $V_{max}$ in figure 7.5.

In figure 7.5 it is shown that the mass burning rate for a stretchless flame ($m_b^0$) increases with $V_{max}$ due to the increasing curvature of the flame front, which leads to an increase of the factor $(h_b/h_b^0)^2$ in equation (6.56). The mass burning rate $m_b^0$ can be interpreted as the mass flux that can be converted into products by the flame if $K$ would be zero. The stretch rate $K$ is, however, quite large in the flames considered here. In fact, the stretch rate $K$ increases due to the increasing curvature although the flow straining part of $K$ ($u_x$) remains approximately constant in the flame. The positive Karlovitz number $Ka$ leads to a decrease of the mass burning rate $m_b^0$ in the burnt mixture to the value of $m_b$. The mass burning rate $m_b$ with $Le=1$ is also shown in figure 7.5 to show that the magnitude of the Lewis number effect on $m_b$ is rather small. It is clear from figure 7.5 that the Karlovitz number increases to a value of about 0.8 near the blow-off limit. In spite of the variation of $m_b^0$ and $Ka$ the mass burning rate $m_b$ is constant, which confirms the observation
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fig. 7.5: The mass burning rate \([\text{kgm}^{-2}\text{s}^{-1}]\) in the burnt mixture without the stretch contribution \((m_b^0)\), with stretch contribution \((m_s; Le_t = 1)\) and with Lewis number effects \((m_b)\) and in the unburnt mixture \((m_u)\).

The Karlovitz number \(K_a(Le_{eff})\) according to (6.42).

The integral in equation (6.70) is an important quantity because it denotes the difference between \(m_b\) and \(m_u\). A large difference between \(m_b\) and \(m_u\) indicates that the flame can sustain a large amount of stream tube contraction (i.e. a large \(u_z\)) and a large flame curvature in the flame base. The magnitude of the integral is denoted by the drawn line in figure 7.5. Apparently the flame base adjusts itself to a higher mixture velocity and to a higher curvature in such a way that the amount of flow straining \(u_z\) and \(m_b\) do not change. Note that \(m_u = \rho_u u_u\) before the flame also do not change significantly for the flames in figure 7.2. This implies that the flow from the burner ports is partly pushed outwards upstream of the flame base in such a way that the flow rate in front of the flame reaches a certain constant value \(m_u \approx 0.15 \text{ kgm}^{-2}\text{s}^{-1}\).

The flow is pushed outwards by the flow resistance over the flame base which affects \(\rho u\) up to a distance \(L \approx 2 \text{ mm}\) upstream of the flame base for the higher values of \(V_{max}\). The part of the
7.2. The stabilisation of lean V-shaped flames at various velocities

flow which is pushed outwards increases with $V_{\text{max}}$. The flame accomplishes this by the increase of $\delta_f$, which gives the flow more time to flow outwards. This situation becomes unstable (i.e. the flame blows off) when $y_u - L$, with $y_u$ the $y$ coordinate of the upstream boundary of the preheat zone, becomes larger than the length of the recirculation zone for the cold flow because this leads to an increasing positive value of $\rho v$ at $y_u - L$ and to a value $\rho_u v_u > m_u$ and eventually to a value $\rho_b v_b > m_b$.

7.2.4 Discussion

In this subsection the results of the investigation presented in the previous subsections will be compared with the results of the investigations of other authors, introduced in section 7.1.

The results for the flame temperature $T_b$ show that $T_b$ in the flame base increases about 3 % above the adiabatic temperature $T_b^0$ due to flame stretch. This is in accordance with investigations of the flame temperature of stretched flames by e.g. Law (1988) and Buckmaster (1979). The increase of the flame temperature shows that blow-off of lean methane/air inverted flames can't be induced by flame quencing, as was stated by Lewis and von Elbe (1943). The above also shows that the assumption made by Kawamura that flame stretch can only lead to lower flame temperatures ($n/T_b < 1$) is not justified.

The results presented in the previous subsections have also shown that flow straining (the $u_x$ contribution to $K$), which is neglected by Kawamura, is essential for the stabilisation of V-shaped flames. The observation that the profiles of $\rho v$, $m_u$ and $m_b$ are almost independent of $V_{\text{max}}$ shows that $\partial v/\partial y \approx (\rho_u v_u - \rho_b v_b)/(y_b - y_u)$ is equal to $\partial S_L/\partial y \approx (m_u - m_b)/(y_b - y_u)$ for all values of $V_{\text{max}}$ ($y_u$ and $y_b$ denote the $y$-value at the unburnt and burnt boundary of the flame, respectively). This, in turn, shows that the stabilisation criterion $\partial S_L/\partial y > \partial v/\partial y$ derived by Kawamura can't be applied directly to flames with a finite thickness because the results for $m_u$, $m_b$ and $\rho v$ in figures 7.2 and 7.5 show that $\rho v = m$ throughout the flame front for a stable flame. This condition, which is an extension for flames with a finite thickness of the known condition $S_L = u_g$ mentioned in chapter 1, is more or less trivial because a violation of the condition $\rho v = m$ on an arbitrary flame contour $\mathcal{Y}$ implies that the contour of $\mathcal{Y}$ is would be moving. The above doesn't mean that the stabilisation criterion of Kawamura is physically incorrect or invalid. The criterion is still valid if the stand-off distance $\delta_y$ instead of the vertical coordinate $y$ is used for the vertical distance.

The flow field used by Sung and Law is not affected by the flame. This implies that the effect of the flame on the flow field is not taken into account and that the flow field near and inside the flame front changes if the flame position changes. Figure 7.4 shows the large effect of the flame on $\rho v$ at the symmetry axis, which implies that it is not justified to assume a flow field which is not affected by the flame when an analysis of flame stabilisation is made. The results presented in figure 7.2 show that the flow field near and inside the flame base is independent of the flame position.
7.3 Conclusions

This investigation has shown that the stabilisation mechanism of the V-shaped flames considered in this chapter, stabilised without heat transfer towards the flameholder, is determined by flow straining inside and upstream of the flame base. The mass burning rate \( m_b \) appears to be independent of the stretch rate \( K \). This shows that the flame adjusts itself to the flow field in such a way that the mass flux \( \rho v \) before and inside the flame front eventually becomes equal to \( m_b \). This value of \( m_b \) is, apparently, only determined by the mixture composition and the flame temperature. The flame affects the profile of \( \rho v \) up to a distance \( L \approx 2 \text{mm} \) upstream of the flame at the higher values of \( V_{\text{max}} \). The flame blows off when the mass flux \( \rho v \) at \( y = y_u - L \) becomes positive (i.e. when \( y_u - L \) lies above the recirculation area of the cold flow).

The effect of the Lewis number on the flame temperature appears to be small for the cases studied here. It should, however, be noted that the magnitude of the Lewis number effect predicted by the numerical model can be affected by the use of a one-step chemical model. The use of a more complex chemical model which includes highly diffusive radicals can give different results for the magnitude of the Lewis number effect. This also applies to the effect of the Lewis number on the mass burning rate. The observation that the magnitude of the Lewis number effect does not change significantly is, however, an indication that the Lewis number effect doesn't play a decisive role in the stabilisation of methane/air flames.
Appendix A

Area change of flame front contours

Consider two flame front contours $C_1 : \mathcal{Y}(x,y) = \eta_1$ and $C_2 : \mathcal{Y}(x,y) = \eta_2$ ($\eta_1 < \eta_2$) with parametrisations $\mathbf{r} = \mathbf{r}(\xi, \eta_1)$ and $\mathbf{r} = \mathbf{r}(\xi, \eta_2)$, respectively. Let $A(\eta_1)$ and $A(\eta_2)$ denote the areas (lengths) of infinitesimal segments on $C_1$ and $C_2$, respectively, then

$$A(\eta_1) = \left| \frac{\partial \mathbf{r}}{\partial \xi}(\xi, \eta_1) \right| d\xi, \quad A(\eta_2) = \left| \frac{\partial \mathbf{r}}{\partial \xi}(\xi, \eta_2) \right| d\xi. \quad (A.1)$$

In this appendix we study the relation between $A(\eta_1)$ and $A(\eta_2)$. Suppose $\mathbf{r}(\xi, \eta_2) = \mathbf{r}(\xi, \eta_1) + \mathbf{a}(\xi)$, with $\mathbf{a}(\xi)$ an arbitrary displacement vector. Substitution of this relation into the second equation of (A.1) gives

$$A(\eta_2) = \left( \left| \frac{\partial \mathbf{r}}{\partial \xi}(\xi, \eta_1) \right|^2 + 2 \left( \frac{\partial \mathbf{r}}{\partial \xi}(\xi, \eta_1), \frac{d\mathbf{a}}{d\xi}(\xi) \right) + \left| \frac{d\mathbf{a}}{d\xi} \right|^2 \right)^{1/2} d\xi. \quad (A.2)$$

Introducing the unit vectors $\mathbf{e}_\xi = \frac{1}{h_\xi} \frac{\partial \mathbf{r}}{\partial \xi}$ and $\mathbf{e}_\eta = \frac{1}{h_\eta} \frac{\partial \mathbf{r}}{\partial \eta}$ with $h_\xi = \left| \frac{\partial \mathbf{r}}{\partial \xi} \right|$ and $h_\eta = \left| \frac{\partial \mathbf{r}}{\partial \eta} \right|$ the corresponding scale factors, equation (A.2) can also be written as

$$A(\eta_2) = \left( 1 + \frac{2}{h_\xi} (\mathbf{e}_\xi, \frac{d\mathbf{a}}{d\xi}) + \frac{1}{h_\xi^2} \left| \frac{d\mathbf{a}}{d\xi} \right|^2 \right)^{1/2} A(\eta_1), \quad (A.3)$$

where $\mathbf{e}_\xi$ and $h_\xi$ have to be evaluated at $\eta = \eta_1$. Anticipating that $|d(\xi)|$ and $\left| \frac{d\mathbf{a}}{d\xi}(\xi) \right|$ are small, we only elaborate the inner product $(\mathbf{e}_\xi, \frac{d\mathbf{a}}{d\xi})$. Let $\mathbf{a} = a_\xi \mathbf{e}_\xi + a_\eta \mathbf{e}_\eta$ in the $(\xi, \eta)$-coordinate system, then it is easy to verify that (note that $\mathbf{e}_\eta \cdot \mathbf{e}_\xi = 0$)

$$(\mathbf{e}_\xi, \frac{d\mathbf{a}}{d\xi}) = \frac{da_\xi}{d\xi} + a_\eta (\mathbf{e}_\xi, \frac{d\mathbf{e}_\eta}{d\xi}). \quad (A.4)$$

Furthermore, from the identity $h_\xi \frac{\partial h_\eta}{\partial \eta} = \frac{1}{2} \frac{\partial}{\partial \eta} \left( \frac{\partial \mathbf{r}}{\partial \xi} \cdot \frac{\partial \mathbf{r}}{\partial \xi} \right)$, one can easily derive the following expression for the last term in (A.4):

$$(\mathbf{e}_\xi, \frac{d\mathbf{e}_\eta}{d\xi}) = \frac{1}{h_\eta} \frac{\partial h_\xi}{\partial \eta}. \quad (A.5)$$
Combining (A.3), (A.4) and (A.5) then finally results in

$$A(\eta_2) = \left(1 + \frac{2}{h_\xi} \left( \frac{da_{\xi}}{d\xi} + a_\eta \frac{\partial h_\xi}{\partial \eta} \right) + \frac{1}{h_\xi^2} \left| \frac{d\bar{a}}{d\xi} \right|^2 \right)^{1/2} A(\eta_1). \quad \text{(A.6)}$$

This latter expression will be used in section 6.1 to derive the formula for the stretch rate $K(\xi, \eta)$. 
Appendix B

Evaluation of stretch rate contributions in flame computations

Explicit expressions for the different contributions to the generalised stretch rate $K$ and for the conventional stretch rate $K_a$ will be presented in this appendix. For $K$ we may write

$$K = K_a + K_b + K_c,$$

where $K_a$, $K_b$ and $K_c$ are given by equations (6.10) and (6.67-6.68).

To be able to compare the different contributions to $K$ in case of a flame, computed numerically in the Cartesian $(x,y)$-coordinate system, we express the different terms of equation (B.1) in the $\tilde{v}$ and $\tilde{\mathcal{V}}$ variables computed in this coordinate system. We already saw that the local unit vectors $\tilde{e}_n$ and $\tilde{e}_\xi$ are given by equations (6.2) and (6.3). For the flow vector $\tilde{v}$ we have $\tilde{v} = u \tilde{e}_x + v \tilde{e}_y = v_\xi \tilde{e}_\xi + v_\eta \tilde{e}_\eta$, so that:

$$v_\xi = \tilde{e}_\xi \cdot \tilde{v} = \tilde{y}_y u - \tilde{y}_x v,$$

$$v_\eta = \tilde{e}_\eta \cdot \tilde{v} = \tilde{y}_x u + \tilde{y}_y v,$$

where $\tilde{y}_x = \mathcal{Y}_x / \mathcal{Y}_L$ and $\tilde{y}_y = \mathcal{Y}_y / \mathcal{Y}_L$. For the vector $\tilde{\mathcal{V}}$ we may write $\tilde{\mathcal{V}} = \tilde{e}_x \frac{\partial}{\partial x} + \tilde{e}_y \frac{\partial}{\partial y} = \frac{1}{h_\xi} \frac{\partial}{\partial \xi} + \frac{1}{h_\eta} \frac{\partial}{\partial \eta}$, leading to:

$$\frac{1}{h_\xi} \frac{\partial}{\partial \xi} \cdot \tilde{\mathcal{V}} = \tilde{y}_y \frac{\partial}{\partial x} - \tilde{y}_x \frac{\partial}{\partial y},$$

$$\frac{1}{h_\eta} \frac{\partial}{\partial \eta} \cdot \tilde{\mathcal{V}} = \tilde{y}_x \frac{\partial}{\partial x} + \tilde{y}_y \frac{\partial}{\partial y}.$$ (B.3)

With the use of these relations we find for $K_a$:

$$K_a = \frac{1}{h_\xi} \frac{\partial v_\xi}{\partial \xi} = [\tilde{y}_y \frac{\partial (\tilde{y}_y u - \tilde{y}_x v)}{\partial x} - \tilde{y}_x \frac{\partial (\tilde{y}_y u - \tilde{y}_x v)}{\partial y}]$$

$$= [\tilde{y}_x u + \tilde{y}_y v] [-\tilde{y}_y^2 \tilde{y}_{xx} + 2 \tilde{y}_x \tilde{y}_y \tilde{y}_{xy} - \tilde{y}_x^2 \tilde{y}_{yy}]$$

$$+ [u_x \tilde{y}_y^2 - v_x \tilde{y}_x \tilde{y}_y - u_y \tilde{y}_x \tilde{y}_y + v_y \tilde{y}_y^2].$$ (B.4)
where e.g. $\tilde{Y}_{xx} = Y_{xx}/Y_L$. For $K_b$ we obtain:

$$K_b = \frac{v_\xi \partial \rho}{\rho h_\xi} \frac{\partial x}{\partial \xi} = \left[ \tilde{Y}_u - \tilde{Y}_z v \right] \left[ \tilde{Y}_y \frac{\partial \rho}{\partial x} - \tilde{Y}_x \frac{\partial \rho}{\partial y} \right]$$  \hspace{1cm} (B.5)

and for $K_c$:

$$K_c = \frac{v_\xi \epsilon_\eta}{h_\eta} \frac{\partial \xi}{\partial \eta} = \left[ \tilde{Y}_u - \tilde{Y}_z v \right] \left[ \tilde{Y}_x \frac{\partial \xi}{\partial \eta} - \tilde{Y}_y \frac{\partial \xi}{\partial \eta} \right]$$

$$= \left[ \tilde{Y}_u - \tilde{Y}_z v \right] \left[ \tilde{Y}_x \frac{\partial \xi}{\partial \eta} - \tilde{Y}_y \frac{\partial \xi}{\partial \eta} \right] + (\tilde{Y}_{xx}^2 - \tilde{Y}_{yy}^2) \frac{\partial \xi}{\partial \eta}. \hspace{1cm} (B.6)$$

These expressions can be evaluated in the computational orthogonal $(x,y)$ coordinate system. It should be stressed, however, that it is preferable to evaluate the derivatives in $x$ and $y$ direction, identically as they are calculated in the flame computation. We use a conservative finite volume method in combination with an exponential fitting scheme to evaluate the fluxes in the numerical flame computations. Therefore, we also apply the exponential fitting scheme to determine the derivatives.
Appendix C

The mass burning rate for constant $\rho K$ and for lean flames

C1: Mass Burning Rate of Flames with Constant Stretch Rate

In this section we elaborate the results presented in section 6.3 for the special case that $\sigma \rho K = (\sigma \rho K)_b = \text{Const.}$ in the flame region ($\eta_u < \eta < \eta_b$). An example of such a flame is a flat flame $(\sigma = \sigma_b)$ in a stagnation flow with $\rho K = (\rho K)_b$, which is frequently studied in literature; see e.g. Zeldovich (1985). This approximation, however, is certainly not valid for premixed flames in general. For this special case, though, we find an identical expression for all Karlovitz numbers from equation (6.42):

$$K_a \approx \left( \frac{\lambda \rho K}{c_p m^2} \right)_b,$$

where we substituted the approximate stretchless 1D solution for $Y_i(\eta)$:

$$\frac{Y_i - Y_{i,u}}{Y_{i,b} - Y_{i,u}} = \exp \left( \frac{m}{\rho D_m} \int_{\eta_u}^{\eta_b} h_\eta(\psi)d\psi \right)$$

in the preheating zone. The expressions in the previous section now simplify considerably. equation (6.41) reduces to

$$H_b - H_u = K_a \left( \frac{1}{Le_H} - 1 \right) c_p(T_b - T_u) + O(Ka^2),$$

where the effective Lewis number $Le_H$, describing the enthalpy transport by the diffusive fluxes, follows from

$$\frac{1}{Le_H} - 1 = - \sum_{i=1}^{N} \left( \frac{1}{Le_i} - 1 \right) \frac{H_i^0 (Y_{i,b} - Y_{i,u})}{c_p(T_b - T_u)}.$$  

Note that $1/Le_H - 1$ is a weighted average of the factors $1/Le_i - 1$, because

$$- \sum_{i=1}^{N} H_i^0 (Y_{i,b} - Y_{i,u}) = c_p(T_b - T_u).$$

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for constant $c_p$.

Analogous to the enthalpy equation, equation (6.58) may be written as

$$Z_{j,b} - Z_{j,u} = K_a \left( \frac{1}{Le_{Z_j}} - 1 \right) Z_{j,u}. \quad (C.6)$$

Here, the effective Lewis numbers $Le_{Z_j}$, describing the diffusive transport of the elements, are defined by

$$\frac{1}{Le_{Z_j}} - 1 = -\sum_{i=1}^{N} \frac{1}{Le_i} w_{ji} \frac{Y_{i,b} - Y_{i,u}}{Z_{j,u}}. \quad (C.7)$$

Finally, for the equation of the mass burning rate equation (6.63) we find

$$\frac{m_b}{m_b^0} \approx 1 - \frac{K_a}{Le_y} + K_a \left( \frac{1}{Le_H} - 1 \right) c_p(T_b - T_u) \frac{\partial}{\partial H_b^0} (\ln m_b^0) + O(Ka^2). \quad (C.8)$$

An important conclusion, which might be drawn from the analysis presented here, is that there is in general no unique Karlovitz number. Each species has its own Karlovitz number, because the effective transport by diffusion in the flame is different for each species. However, the Karlovitz numbers are all equal, when the stretch rate does not change in the flame zone. Only for this special case or when the stretch rate does not vary too much in the flame zone, the analysis leads to a unique Karlovitz number and to comparable results as found in the literature. Furthermore, the choice of Lewis numbers is critical in real multi-component combustible mixtures. The Lewis numbers considered should be related to the effective diffusive transport of enthalpy, when variations in the enthalpy are considered and to the effective transport of elements, when variations in composition are of interest (see equations (C.4) and (C.7)). Furthermore, effects of the local flame temperature on the mass burning rate are not automatically governed by the same Lewis numbers as the Lewis numbers which predict variations in the enthalpy. In the next section, equation (C.8) is used to compute the burning rate in case of a one-step irreversible reaction describing lean methane/air combustion. It is shown that results of the literature for the mass burning rate (see e.g. Chung (1988)) are recovered, with additional terms related with stoichiometry changes in the flame.

C2: Mass Burning Rate for Lean Methane/Air Flames

In this section, we discuss the special case of combustion of lean methane/air mixtures, described by a single-step irreversible reaction. We will first calculate the stretchless mass burning rate of a flat flame and subsequently study the influence of flame stretch.

For the case of a stretchless flat flame, equation (6.56) reduces to

$$m_{b,1}^0 = m_{u,1} \approx \frac{1}{\sqrt{2} \int_{Y_u}^{Y_b^0} \rho D_y \rho_y \, dY}, \quad (C.9)$$
since $\sigma = \sigma_b = \text{const.}$, equation (C.9) is equivalent to expressions for the adiabatic mass burning rate, derived by other authors. Williams (1975) has given an overview of the results in literature on this matter. Usually, the mass burning rate is computed from the equation for the temperature. The equation for the temperature can be readily derived from the set (6.47). Assuming constant specific heat $c_p$ and neglecting all diffusion terms, this equation reads

$$\frac{1}{h} \frac{\partial}{\partial \eta} (\sigma m T) - \frac{1}{h} \frac{\partial}{\partial \eta} (\sigma \lambda \frac{1}{h} \frac{\partial T}{\partial \eta}) - \frac{\sigma}{c_p} \dot{\rho}_T = -\sigma \rho K T,$$

where $\dot{\rho}_T = -\sum_i H_i^0 \dot{n}_i$. Following the procedure in section 6.3, a similar expression for $m_{b,1}^0$ can be derived

$$m_{b,1}^0 = m_{u,1} \approx \frac{1}{c_p(T_b^0 - T_u)} \sqrt{\int_{T_u}^{T_b^0} \lambda \dot{\rho}_T \, dT}.$$  

(C.11)

Let us now we compute the adiabatic mass burning rate from equation (C.11), for lean methane/air flames. The source term for equation (C.10) is given by (also see chapter 2):

$$\dot{\rho}_T = \Delta H A \rho^{a+\beta} Y_{CH_4}^a Y_{O_2}^b \exp(-E_a/RT).$$

(C.12)

In case of lean combustion we find the following expression for the adiabatic mass burning rate (de Lange (1992)):

$$m_{b,1}^0 = m_{u,1} \approx \left(2 A \Gamma(\alpha + 1) \frac{\lambda}{c_p} L e_{CH_4}^a \rho_b^{a+\beta}(Y_{O_2,b}^b)^{\beta} \right)^{1/2} \left(\frac{c_p T_b^0}{\Delta H} \right)^{(a+1/2)} \left(\frac{T_b^0}{T_b^0 - T_u} \right)^{(a+1/2)} \exp(-E_a/2RT_b^0).$$

(C.13)

In the derivation of equation (C.13), we used the approximate relation $Y_{CH_4} \approx L e_{CH_4} c_p (T_b^0 - T)/\Delta H$ between $Y_{CH_4}$ and $T$ near the reaction layer.

For stretched flames with constant $\sigma \rho K$ we have derived equation (C.8) for the mass burning rate. This expression requires the computation of the partial derivatives of $m_b^0$ with respect to $H_b^0$ and $Z_{j,b}^0$. However, in equation (C.13) the mass burning rate is expressed in terms of $T_b^0$ and $Y_{b}^0$. The partial derivatives in equation (C.8) can only be computed if there exists a one-to-one relation between the set of variables $(H_b, Z_{j,b})$ on the one hand and $(T_b, Y_{b})$ on the other hand. The equilibrium relations have to be used to define this relation. However, in case of a one-step irreversible reaction with 5 species $CH_4$, $O_2$, $H_2O$, $CO_2$ and $N_2$ and 4 elements $C$, $O$, $H$ and $N$, there is a unique relationship between the set of variables $(H_b, Z_{C,b}, Z_{O,b}, Z_{H,b}, Z_{N,b})$ and $(T_b, Y_{O_2,b}, Y_{CO_2,b}, Y_{H_2O,b}, Y_{N_2,b})$, simply because $Y_{CH_4,b} = 0$ at the equilibrium state. This is a very good approximation for lean methane/air flames, since the other species appear in extremely small quantities.

For the equilibrium state of methane/air flames the following relations hold:

$$H_b = c_p(T_b - T_{ref}) + H_{O_2}^0 Y_{O_2,b} + H_{CO_2}^0 Y_{CO_2,b} + H_{H_2O}^0 Y_{H_2O,b},$$
$$Z_{C,b} = w_{C,O_2} Y_{CO_2,b},$$
$$Z_{O,b} = w_{O,O_2} Y_{O_2,b} + w_{O,CO_2} Y_{CO_2,b} + w_{O,H_2O} Y_{H_2O,b},$$
$$Z_{H,b} = w_{H,H_2O} Y_{H_2O,b}.$$  

(C.14)
which can be easily inverted. Subsequently, the partial derivatives of the set \((T, Y_{O_2}, Y_{CO_2}, Y_{H_2O})\) with respect to the variables \(H, Z_C, Z_O\) and \(Z_H\) can be computed:

\[
\frac{\partial T}{\partial H} = \frac{1}{c_p} \frac{\partial T}{\partial Z_C} = \frac{1}{c_p W_C} (M_{O_2}H_{O_2}^0 - M_{CO_2}H_{CO_2}^0),
\]

\[
\frac{\partial T}{\partial Z_O} = -\frac{1}{c_p W_O} \frac{1}{2} M_{O_2}H_{O_2}^0, \quad \frac{\partial T}{\partial Z_H} = \frac{1}{c_p W_H} \left(\frac{1}{4} M_{O_2}H_{O_2}^0 - \frac{1}{2} M_{H_2O}H_{H_2O}^0\right),
\]

\[
\frac{\partial Y_{O_2}}{\partial H} = 0, \quad \frac{\partial Y_{O_2}}{\partial Z_C} = -M_{O_2}, \quad \frac{\partial Y_{O_2}}{\partial Z_O} = M_{O_2}, \quad \frac{\partial Y_{O_2}}{\partial Z_H} = -\frac{M_{O_2}}{4W_H},
\]

\[
\frac{\partial Y_{CO_2}}{\partial H} = 0, \quad \frac{\partial Y_{CO_2}}{\partial Z_C} = M_{CO_2}, \quad \frac{\partial Y_{CO_2}}{\partial Z_O} = 0, \quad \frac{\partial Y_{CO_2}}{\partial Z_H} = 0,
\]

\[
\frac{\partial Y_{H_2O}}{\partial H} = 0, \quad \frac{\partial Y_{H_2O}}{\partial Z_C} = 0, \quad \frac{\partial Y_{H_2O}}{\partial Z_O} = 0, \quad \frac{\partial Y_{H_2O}}{\partial Z_H} = \frac{M_{H_2O}}{2W_H}.
\]

The partial derivatives in equation (C.8) can now be computed using the chain rule. We have for example

\[
\frac{\partial (\ln m_b^0)}{\partial H_b^0} = \frac{\partial (\ln m_b^0)}{\partial T_b^0} \frac{\partial T_b^0}{\partial H_b^0} + \frac{\partial (\ln m_b^0)}{\partial Y_{O_2,b}^0} \frac{\partial Y_{O_2,b}^0}{\partial H_b^0} + \frac{\partial (\ln m_b^0)}{\partial Y_{CO_2,b}^0} \frac{\partial Y_{CO_2,b}^0}{\partial H_b^0} + \frac{\partial (\ln m_b^0)}{\partial Y_{H_2O,b}^0} \frac{\partial Y_{H_2O,b}^0}{\partial H_b^0}. \tag{C.16}
\]

Similar expressions can be derived for the other derivatives. Application of the differentiation rules in (C.15) and (C.16) to equation (C.8) gives the following expression for the mass burning rate:

\[
\frac{m_b}{m_b^0} \approx 1 - \frac{\kappa a}{L_{ECH_4}} + \kappa a \left(\frac{1}{L_{ECH_4}} - 1\right) \left(T_b - T_u\right) \frac{\partial}{\partial T_b} (\ln m_b^0),
\]

\[
- \kappa a \left(\frac{1}{L_{ECH_4}} - \frac{1}{L_{O_2}}\right) (Y_{O_2,b}^0 - Y_{O_2,b}^0) \frac{\partial}{\partial Y_{O_2,b}^0} (\ln m_b^0)
\]

\[
+ \kappa a \left(\frac{1}{L_{ECH_4}} - \frac{1}{L_{CO_2}}\right) Y_{CO_2,b}^0 \frac{\partial}{\partial Y_{CO_2,b}^0} (\ln m_b^0)
\]

\[
+ \kappa a \left(\frac{1}{L_{ECH_4}} - \frac{1}{L_{H_2O,b}}\right) Y_{H_2O,b}^0 \frac{\partial}{\partial Y_{H_2O,b}^0} (\ln m_b^0) + O(\kappa a^2). \tag{C.17}
\]

It should be stressed that this equation is also valid for more-step chemistry models, as long as the mass fractions of \(\text{CH}_4\) and the extra species are negligible in the burnt gas mixture compared to the mass fractions of \(\text{O}_2, \text{CO}_2\) and \(\text{H}_2\text{O}\).

Note that in equation (C.13) the mass burning rate \(m_b^0\) is a function of \(T_b^0\) and \(Y_{O_2,b}^0\) only, when \(\rho_b\) and \(\Delta H\) are assumed to be constant. Using equation (C.13) for the adiabatic mass burning rate of a flat stretchless flame with one-step chemistry, we then find for the relevant partial derivatives:

\[
\frac{\partial}{\partial T_b^0} (\ln m_b^0) = \frac{1}{T_b - T_u} \left(\alpha - (\alpha + 1) \frac{T_u}{T_b} + \frac{E_a(T_b - T_u)}{2RT_b^2}\right),
\]

\[
\frac{\partial}{\partial Y_{O_2,b}^0} (\ln m_b^0) = \frac{\beta}{2Y_{O_2,b}^0}. \tag{C.18}
\]
Substituted into equation (C.17) this gives us the final result for the lean methane-air flames:

$$\frac{m_b}{m_b^0} \approx 1 - \frac{K_a}{Le_{CH_4}} + K_a(\frac{1}{Le_{CH_4}} - 1) \left( \alpha - (\alpha + 1) \frac{T_u}{T_b} + \frac{E_a(T_b - T_u)}{2RT_b^2} \right)$$

$$- K_a(\frac{1}{Le_{CH_4}} - \frac{1}{Le_{O_2}}) \frac{\beta}{2} \frac{(Y_{O_2,b} - Y_{O_2,a})}{Y_{O_2,b}} + O(Ka^2).$$  \hspace{1cm} (C.19)

This expression for $m_b$, determined by a one-step irreversible reaction, is comparable to the result found by others in the literature, such as Chung (1988). However, equation (C.19) shows that different Lewis numbers appear when multi-component transport is taken into account. Furthermore, extra terms, related to local stoichiometry changes by differential diffusion effects, play a role when more than one species is considered. The effective Lewis number $\frac{1}{Le_{CH_4}} - \frac{1}{Le_{O_2}}$ of this mechanism is related to the difference in diffusivity of the reactant species. Moreover, it is interesting to note that the effective Lewis number $Le^{-1}$, being a sum of species diffusivities weighted by the species enthalpies, describes variations in the local enthalpy of the mixture through equation (C.3). However, the effect of temperature variations on the mass burning rate $m_b$ is only related to the Lewis number of the deficient reactant $Le_{CH_4}$ in this case (see equation (C.19)). This last observation is also clear from a physical point of view, because the temperature variation by preferential diffusion is obviously independent of the Lewis number of $O_2$ in a bulk of air and of the product species $CO_2$ and $H_2O$ in an irreversible reaction, in which the products play no more role in the propagation speed of the flame when the reaction is finished. From this point of view it also follows that other species Lewis numbers should play a role in case of reversible reactions. This is described by the original equation (C.8) and may be calculated when the equilibrium relations of the mixture are taken into account.
Appendix C. The mass burning rate for constant $\rho K$ and for lean flames
Samenvatting

Laminaire vlamstabilisatie is de laatste decennia een belangrijk onderwerp van onderzoek geworden. Dit komt vooral door de introductie van branders met een geforceerde luchttoevoer. Met de introductie van deze branders werd het mogelijk om met volledig voorgemengde, brandstofarme mengsels te werken. Deze voorgemengde vlammen hebben echter het nadeel dat ze gevoeliger zijn voor stabilisatieproblemen zoals inslag en afblazen.

Het doel van het onderzoek dat beschreven wordt in dit proefschrift is het kunnen beschrijven en verklaren van de invloed van de omgeving (menging, koeling), stretch en kromming in/van het vlamfront en koeling (door de branderwand en de omgeving) op laminaire voorgemengde vlammen en op de stabilisatie van deze vlammen. Een groot deel van het onderzoek is uitgevoerd met een twee-dimensionaal numeriek vlammodel. Dit model maakt gebruik van een stroomfunctie-vorticiteitsformulering en één-staps chemie. Experimentele validatie van het model laat zien dat het model de vlamvorm en het stromingsveld in en dichtbij de vlam tot op 10 % nauwkeurig beschrijft.

Een groot deel van het onderzoek richt zich op verschillen in vlamvorm, energietransport en inslaggedrag tussen vlammen op kleine (tot 9 mm) spleetbranders en cilindrische branders. Voor beide geometriëën worden vlammen bekeken die ingeklemd zijn tussen gelijke vlammen en vlammen die branden in een open omgeving. De resultaten laten zien dat de vlamvormen en de massaflux stroomopwaarts van de vlamtip duidelijk beïnvloed wordt door de brander geometrie en door de omgeving. Deze verschillen worden vooral veroorzaakt door de extra massaflux in radiële richting bij de cilindrische vlammen en de beperking van de massaflux loodrecht op de symmetrieas bij vlammen die ingeklemd zijn tussen gelijke vlammen.

Het onderzoek naar het inslaggedrag van vlammen op ronde - en spleetbranders laat zien dat de kritische gradiënten die voorspeld worden door het numerieke model niet meer dan 8 % afwijken van experimentele waarden. De verschillen tussen kleine spleetbranders en cilindrische branders zijn niet groter dan 10 %. Een analyse van de invloed van branderwandkromming op de vlamkoeling bevestigt deze verschillen. Een analytisch model voor de daling van de kritische gradiënt met toenemende branderbreedte laat zien dat deze daling vooral veroorzaakt wordt door de kromming van het parabolische snelheidsprofiel bij de wand.

De stabilisatie bij hoge snelheden wordt onderzocht aan de hand van vlammen op 2-spletenbranders. Er worden numerieke resultaten gepresenteerd van M- en V-vormige vlammen. De numerieke resultaten worden vergeleken met experimentele resultaten, die bestaan uit vlamvormen, Laser doppler snelheidsmetingen en omslag- en afblaasgradiënten. De vlamvorm en de omslaggradiënten worden voor arme vlammen redelijk goed voorspeld door het model. De verticale
snelheden boven de vlam die voorspeld worden door het model zijn echter tot 35 % lager dan de experimentele waarden. De afblaasgradiënten worden alleen goed voorspeld voor $\phi = 0.7$. De afwijkingen worden waarschijnlijk veroorzaakt door relatief kleine vlamkrommingsverschillen in de vlamvoet tussen het numerieke en de experimentele vlam. Kleine vlamkrommingsverschillen kunnen aanleiding geven tot grote verschillen in de verticale snelheid omdat de kromtestraal van het vlamfront in de vlamvoet zeer klein is. De vlamkrommingsverschillen worden hoogstwaarschijnlijk veroorzaakt door het ontbreken van hoog-diffusieve radicalen in the één-staps model.

Voor de beschrijving van de stabilisatie bij hoge mengselsnelheden wordt een nieuwe stretch-definietie geïntroduceerd die, vergeleken met de definitie uit de literatuur, ook bijdragen bevat ten gevolge van dichtheidsvariaties en vlamdikteverschillen. Er worden ook relaties afgeleid voor de vlamsnelheid en vlamtemperatuur van gestretchte vlammen die nagenoeg geen aannames over bijvoorbeeld de grootte van de stretch of de vlamdikte bevatten. De stabilisatie van de tip van een Bunsenvlam en de voet van een V-vlam wordt onderzocht door de verschillende bijdragen aan de stretch, de vlamsnelheid en vlamtemperatuur te berekenen. Uit deze analyse blijkt dat de krommingsbijdrage aan de stretch factor veel groter is dan de bijdrage ten gevolge van stromingsdivergentie. Uit een onderzoek van het gedrag van de stretchbijdragen en de vlamsnelheid bij verschillende inlaatsnelheden blijkt echter dat de stromingsdivergentie zorgt voor de stabilisatie van de vlamtip en de voet van de V-vlam. De stromingsdivergentie leidt tot een vlamsnelheid, gedefinieerd in het verbrande mengsel, die nagenoeg onafhankelijk is van de snelheid voor de vlam.
Summary

Laminar flame stabilisation in small-scale combustion equipment has become an important issue of research in the past decades. This is mainly due to the introduction of burners with a forced air supply which made it possible to use fully premixed flames with a lean fuel/air mixture. Fully premixed flames are, however, more sensitive to stabilisation problems. This can lead to, for instance, blow-off or flash-back.

The aim of the investigation described in this thesis is to formulate a description and explanation of the effects of various phenomena on steady laminar premixed flames and their stabilisation. A two-dimensional numerical flame model is used for large parts of the research to facilitate a detailed and systematic investigation of the various phenomena. The two-dimensional model uses a vorticity-stream function formulation for the flow field in combination with a one-step chemical model. Experimental validation of the model shows that the model is capable of describing the flame shape and the flow field near and inside the flame cone with an accuracy of about 10%.

The influence of a surrounding atmosphere and burner curvature on the flame shape, flow field and mass transport in 2D laminar premixed Bunsen flames is investigated in chapter 3. It is found that flames on cylindrical burners confined between similar flames have a smaller flame length and flame tip curvature than flames on slit burners with comparable dimensions. These effects are caused by the larger available expansion space (in radial direction) for the cylindrical flames. Furthermore, it is shown that the flames in a surrounding atmosphere are less curved than flames confined between other flames; the curvature of the tip is also smaller. These effects are explained by the fact that the confined flames push the mass flow and the flame front towards the central axis. This in turn results in differences in flame length.

The investigation of flash-back of flames on cylindrical and slit burners shows that the critical gradients predicted by the numerical model deviate about 8% from experimental values. The differences between the cylindrical and slit burner gradients is equal to about 10% for smaller burners (≈ 4 mm). An analysis of the effect of burner wall curvature on flame cooling confirms these differences. An analytical model for the decrease of the critical gradient with increasing burner size shows that this decrease is mainly caused by the curvature of the parabolic velocity profile near the burner wall.

Flame stabilisation at high mixture velocities is investigated for flames on two-slit burners (M- and V-shaped flames). Numerical modelling results of M- and V-shaped methane/air flames with an equivalence ratio of 0.7 are presented and compared with experimental results in chapter 5. The experimental results used to validate the model consist of flame shapes, stand-off distances, velocity profiles measured with Laser Doppler Velocimetry and critical transition and blow-off
Summary

Gradients. The flame shape and the stand-off distance of the M-shaped flame are reproduced well by the model. The values of the vertical velocity are, however, up to 25% lower than the experimental values. The lower vertical velocities computed with the model are due to relatively small differences between the computed and the experimental flame shape. The shape of the V-shaped flame is also reproduced reasonably well by the model. The stand-off distance predicted by the model differs 0.8 mm from the experimental value. The vertical velocities predicted by the model are, as for the M-shaped flame, lower (up to 35%) than the experimental values. This is also caused by flame shape differences. The small differences between the computed and experimental flame shapes is probably related with the absence of highly diffusive radicals in the one-step model. The model is also used to compute the critical transition (from M- to V-shaped flame) and blow-off (of the V-shaped flame) gradients for equivalence ratios 0.7, 0.8, and 0.9. The values for the critical gradients at $\phi=0.7$ predicted by the model differ no more than 10% from the experimental values obtained with our burner. The transition from M- to V-shaped flames is also well reproduced at $\phi=0.8$ and 0.9. Blow-off of the V-shaped flame is, however, only well predicted at an equivalence ratio of 0.7. At the higher equivalence ratios, blow-off is much harder to model. This is probably caused by the numerical model having problems with the reproduction of the stand-off distance and the vertical velocity profile.

A new stretch definition is introduced for the description of flame stabilisation at high mixture velocities. Compared to the usual definition, additional contributions to the stretch rate due to changes in the flame thickness and due to density variations along the flame arise. Extended expressions are derived that describe the effect of stretch on variations in scalar quantities, such as the enthalpy. These expressions are used to determine local variations in the flame temperature and it is shown that known results are recovered when a number of approximations are introduced. Also, expressions for the mass burning rate in the unburnt and the burnt mixture are derived. The different contributions to the total stretch rate and the effects thereof on the flame stabilization are numerically computed for the flame tip of a two-dimensional Bunsen flame. This analysis shows that the contribution to the total stretch rate due to curvature is much larger than the contribution due to flow divergence.

The stabilisation of the tip of a Bunsen flame and the base of a V-shaped flame is investigated by calculating the different contributions to stretch rate, the burning velocity in the burnt and unburnt mixture and the flame temperature, all this for various inlet velocities. The investigation shows that the flow divergence contribution to the stretch rate is responsible for the stabilisation of the flame tip and the flame base. Also, the flow field near and inside the flame front appears to be nearly independent of the inlet velocity.
Bibliography


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Curriculum Vitae

1969 Geboren te Tilburg

1981-1987 Maurick College te Vught
VWO-B

1987-1992 Technische Universiteit Eindhoven
Faculteit Werktuigbouwkunde
Fabrieks- en Apparatenbouw voor de procesindustrie


Hobbies: Onderwatersport, Fotografie
Stellingen

behorende bij het proefschrift

Stabilisation of Laminar Premixed Methane/Air Flames

van

Roel Mallens
1. Nagenoeg alle verschillen tussen de stabilisatie van vlammen op cilindrische branders en die op spleetbranders kunnen verklaard worden uit de verschillende mate van expansie van de verbrandingsgassen. *Hoofdstuk 3, dit proefschrift.*

2. De kromming van de branderwand veroorzaakt een verschil van ten hoogste 10% tussen de inslaggradiënt voor spleetbranders met een breedte van 4 mm en cilindrische branders met een even grote diameter. *Hoofdstuk 4, dit proefschrift.*

3. In twee-dimensionale stationaire vlammen wordt de stretch rate niet alleen bepaald door snelheidsgradiënten, maar ook door dichtheidsgradiënten en vlamdikteveranderingen. *Hoofdstuk 6, dit proefschrift.*

4. Het effect van preferentiële diffusie en de stretch rate op de vlamtemperatuur en de verbrandingssnelheid is minder dan 5% voor de in dit proefschrift beschreven vlammen. *Hoofdstuk 6 en 7, dit proefschrift.*

5. Vanuit fysisch oogpunt verdient het de voorkeur om de verbrandingsniet alleen bepaald door fysische groot- heden aan de verbrande zijde van de vlam. *Hoofdstuk 6 en 7, dit proefschrift.*


7. De in stabilisatiemodiellen veel gemaakte aanname dat de vlam geen effect heeft op het stromingsveld is niet gerechtvaardigd. *Hoofdstuk 7, dit proefschrift.*

9. Evolutie leidt niet tot beschaving. Darwins 'Survival of the fittest' kan dan ook gedeeltelijk geïnterpreteerd worden als 'Survival of the uncivilised'.

10. De enige plek waar succes eerder komt dan werk, is het woordenboek. *Vidal Sassoon*

11. Iemand die eerlijk is, hoeft niets te onthouden.

12. Het enerzijds opdelen van grote steden in deelraden om de burger dichter bij de politiek te brengen en anderzijds het samenvoegen van gemeenten tot grotere gemeenten is in direkte tegenspraak met elkaar.

13. Door de opstelling van de stadsbesturen van sommige brabantse steden is de gemeentelijke herindeling van een op zichzelf nuttige ope- ratie verworden tot een ordinair spelletje 'landje pik'.