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Citation for published version (APA):

Document status and date:
Published: 01/01/1998

Publisher Version:
Publisher’s PDF, also known as Version of Record (includes final page, issue and volume numbers)

Please check the document version of this publication:
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RANA 98-13
July 1998

A Flamelet Description of Premixed Laminar Flames and
the Relation with Flame Stretch

by

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A Flamelet Description of Premixed Laminar Flames and the Relation with Flame Stretch

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ABSTRACT - A laminar flamelet description is derived for premixed laminar flames. The full set of 3D instationary combustion equations is decomposed in three parts: (1) a flow and mixing system without chemical reactions, described by the momentum, enthalpy and element conservation equations, (2) the G-equation for the flame motion and (3) a flamelet system describing the inner flame structure and the local mass burning rate. Local fields for the flame curvature and the flame stretch couple the flamelet system with the flow and flame motion. To derive an efficient model, the flamelet equations are analyzed in depth, using the Integral Analysis, first introduced by Chung and Law [4]. It appears that the flamelet response is governed by algebraic equations describing the influence of flame stretch on the local mass burning rate, the enthalpy variation and element composition. Known expressions for the mass burning rate, found by Joulin, Clavin and Williams are recovered in some special cases. Furthermore, the validity of the expressions has been shown for weak and strong stretch by comparing the results with numerical results of lean stretched premixed methane/air flames, computed with skeletal chemistry. Finally, the theory is illustrated for the tip of a 2D stationary Bunsen flame.

1 Introduction

The interest for flamelet models to simulate turbulent flames has increased significantly in the last decade. Flamelet models for turbulent diffusion flames have been derived by transforming the equations into mixture fraction, scalar dissipation-rate space using a local coordinate system adapted to the flame sheet [16, 17, 18]. For premixed flames [19], it is known that an additional equation (the kinematic G-equation, introduced by Williams [25]) has to be used to take the motion of the flame itself into account. In both systems, a number of assumptions and approximations has to be introduced to describe the coupling of the flamelet system with the turbulent flow field. However, it has not been pursued so far to derive a premixed flamelet model systematically from the full set of 3D instationary conservation equations. It is the purpose of this paper to derive and analyse a premixed flamelet description for laminar flames. It is anticipated that the method and results might also be of interest in future modelling studies of more-dimensional laminar and turbulent flames.
It will be shown that the set of 3D instationary equations can be decomposed in three parts: one part describing the fluid motion and mixing of enthalpy and elements, a second part for the flame motion through the G-equation and a third part consisting of a set of quasi-1D stationary flamelet equations governing the inner flame structure and local mass burning rate. These flamelet equations describe local transport perpendicular to suitably defined flame surfaces and they contain source terms proportional to the local flame stretch rate. Transport along the flame surfaces and instationary effects are incorporated in these flame stretch terms. The coupling between the 1D flamelet system and the flame motion (G-equation) is formed by scalar fields for the flame curvature and flame stretch.

It is well known that flame stretch, caused for instance by local velocity gradients near the flame front, may have an important influence on flames. This was first recognized by Karlovitz et al. [10] and Markstein [12]. Flames, experiencing flame stretch have been studied by a lot of researchers since, such as by Buckmaster, Matalon, Matkowsky, Chung and Law [1, 2, 13, 14, 4]. A rigorous mathematical analysis of stretched flames, based on matched asymptotic expansions, was given by Matalon and Matkowsky [13]. An Integral Analysis of flame stretch was presented by Chung and Law [4]. Flame sheet models with one-step chemistry and a single Lewis number are frequently used to study stretched flames. Stimulated by the ideas of Buckmaster [1], who first realized that variations in the preheating zone thickness are of importance and using the ideas of the Integral Analysis of Chung and Law [4], de Goey et al. [7, 8] recently applied the flame stretch formalism to flames with finite flame front thickness. It will be shown in this paper that the flame stretch field, there defined is precisely the local scalar field quantity that couples the flamelets with the flow and G-equation. This coupling, however, appears to be non-local, which means that a numerical implementation is far from easy and that the computational efficiency is expected not to be improved very much compared to a direct simulation. To derive efficient and accurate approximations for the flamelet response, the stretched and curved flamelet system is analysed analytically and numerically.

It is not clear at the moment whether presently existing flame stretch formalisms are able to describe the behaviour of flames governed by multiple-species transport and chemistry mechanisms, because these theories are based on a number of assumptions, such as an infinitely thin flame sheet, a single irreversible reaction and a single Lewis number. These assumptions are used in present flamelet models for turbulent flames. To make an extension to more general situations, an analysis will be proposed here which seems to be applicable to flames with multiple-species transport and chemistry. Analytical expressions are derived for the global flamelet behaviour (e.g. in terms of the mass burning rate), which seem to be valid even in case of stronger stretch. These expressions are verified to be accurate by comparing the results with numerical studies of the full flamelet system using the skeletal mechanism for methane/air combustion. This information is used to derive computationally more efficient and more accurate flamelet models for premixed flames.

The set of 3D instationary conservation equations, which governs laminar flames will be
presented in the next section. This set will be decomposed in parts in Section 3 and a set of quasi-1D flamelet equations for mass, species mass fractions, enthalpy and element mass fractions will arise. Using the Integral Analysis [4], the structure of the flamelet equations is analysed further in Sections 4, 5 and 6. The system is studied for the case of zero stretch in Section 4. It appears that the enthalpy and element mass fractions are conserved and an expression for the mass burning rate is derived. The analysis is extended to stretched flames in Section 5. There, it is shown that enthalpy and element mass fractions change through differential diffusion effects in the flame area. These changes in enthalpy and element mass fractions depend on the Karlovitz and Lewis numbers of all species. The subsequent consequences for the mass burning rate in the burnt gases are also studied. Apart from the known dependence of the mass burning rate on enthalpy changes, we find an additional sensitivity of the mass burning rate related to changes in the element mass fractions. Special cases of weak stretch, with constant \( \rho K \) or constant \( K \) in the flame area are studied in Section 6. Expressions derived by Joulin et al. [9] for constant \( \rho K \) and Clavin [5] for constant \( K \) are recovered for the case of a one-step irreversible reaction and a single Lewis number. The derived model system is compared with numerical results in Section 7. The quasi-1D flamelet equations are solved numerically using the skeletal mechanism for lean methane combustion. It appears that deviations of only a few percent arise with the analytical expressions. This shows the validity of the method to describe the mass burning rate of stretched flamelets with multiple-species transport and chemistry and it can be used to construct efficient and accurate flamelet models for premixed laminar and turbulent flames. Finally, the application of the theory to numerical results of a 2D stationary Bunsen flame tip is illustrated briefly in Section 8.

2 Problem Definition

Chemically reacting flows are governed by a set of conservation equations describing the flow, the chemical species mass fractions and the enthalpy. The governing equations for deflagration processes are the momentum and continuity equations

\[
\frac{\partial (\rho \mathbf{v})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathbf{v}) = -\nabla p + \nabla \cdot \mathbf{\tau},
\]

\[
\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0,
\]

\( \rho, p, \mathbf{v} \) and \( \mathbf{\tau} \) being the mass density, pressure, the flow velocity and the stress tensor, the conservation equations for the first \( N - 1 \) species mass fractions \( Y_i \)

\[
\frac{\partial (\rho Y_i)}{\partial t} + \nabla \cdot (\rho \mathbf{v} Y_i) - \frac{1}{Le_i} \nabla \cdot \left( \frac{\lambda}{c_p} \nabla Y_i \right) = \dot{\rho}_i, \quad (i = 1, \ldots, N - 1),
\]

and the balance equation for the specific enthalpy \( H \)

\[
\frac{\partial (\rho H)}{\partial t} + \nabla \cdot (\rho \mathbf{v} H) - \nabla \cdot \left( \frac{\lambda}{c_p} \nabla H \right) = \sum_{i=1}^{N} \left( \frac{1}{Le_i} - 1 \right) \nabla \cdot \left( \frac{\lambda}{c_p} H \nabla Y_i \right).
\]
Here, we introduced the thermal conductivity $\lambda$, the specific heat $c_p$, the chemical source terms $\dot{\rho}$, and the Lewis numbers $Le_i = \frac{\lambda}{\rho D_{im} c_p}$ (assumed to be constant), with $D_{im}$ the diffusion coefficients. Furthermore, the specific enthalpy $H = \sum_i H_i Y_i$ can be written as

$$H = H_T + \sum_{i=1}^{N} H_i^0 Y_i, \quad H_T = \int_{T_0}^{T} c_p(\xi) \, d\xi,$$

$H_T$, $H_i$, and $H_i^0$ being the thermal enthalpy, the total enthalpy of species $i$ and the enthalpy of formation of species $i$ at temperature $T_0$, respectively. As $N$ equations (3) together with the continuity equation (2) are overcomplete, only $N - 1$ species equations (3) are solved. The solution for the $N^{th}$ abundant species and its effective Lewis number (e.g. of nitrogen $N_2$) then follows from $\sum Y_i = 1$. Furthermore, we consider equal specific heats $c_{p,i} = c_p$, so that the $H_i^0$'s in the right-hand side term of Eq. (4) can be replaced by $H_i^0$'s. The system is closed with an expression for the stress tensor $\tau$ in terms of velocity gradients and the gas law

$$p = \rho RT/\sum_{i=1}^{N} \left( \frac{Y_i}{M_i} \right).$$

The analysis is restricted to low Mach-number flows and we neglect the effect of pressure variations in space and time on the combustion equations.

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. An element mass fraction $Z_j$ is defined by [16]

$$Z_j = \sum_{i=1}^{N} w_{ji} Y_i, \quad (j = 1, \cdots, N_e),$$

where the coefficients $w_{ji} = W_j \mu_{ji}/M_i$, denote the mass fraction of element $j$ in species $i$, $\mu_{ji}$ being 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. The conservation equations for $Z_j$ read

$$\frac{\partial(\rho Z_j)}{\partial t} + \nabla \cdot (\rho v Z_j) - \nabla \cdot (\frac{\lambda}{c_p} \nabla Z_j) = \sum_{i=1}^{N} w_{ji} (\frac{1}{Le_i} - 1) \nabla \cdot (\frac{\lambda}{c_p} \nabla Y_i), \quad (j = 1, \cdots, N_e),$$

stating that element mass fractions in a flame are only influenced by convection and diffusion and not by chemical reactions. These $N_e$ conservation equations are, of course, not independent of the set (3).

### 3 Flame Stretch and Flamelets

Numerical modelling of more-dimensional premixed flames is hampered by the inherent stiffness of the chemically reacting system, related with some extremely small chemical time scales and large local gradients in the thin flame front. Very small time steps and
grid cells are needed to solve the system. The modelling efficiency could be increased enormously, if it would be possible to decouple the chemical kinetic processes in the flame from the main flow and mixing processes. One way to accomplish such a decoupling is by using a flamelet model, in which the stiff set of equations in the form of 1D flamelet equations is solved separately from the flow and mixing processes. In this section, it is our purpose to deduce a flamelet description for premixed flames in a systematic way. The system of equations of the previous section is decomposed in three parts. The first part consists of the mass, momentum, enthalpy and element conservation equations and the gas law, which together describe the flow and mixing processes in the flame. Note that neither of these equations contains chemical source terms. These equations can therefore be solved with relatively large time steps and grid spacings, using standard numerical methods or CFD-packages. The second part (G-equation) describes the flame propagation and the third part the internal structure (1D flamelets) of the flame. These last two parts are derived by studying the mass, species and enthalpy equation in a flame-adapted coordinate system. This will be elaborated further in this section.

We define the premixed flame as the region in space, where a scalar variable \( \mathcal{G} \) has values between the unburnt (\( \mathcal{G}_u \)) and burnt (\( \mathcal{G}_b \)) values. For \( \mathcal{G} \) one may take for instance one of the species mass fractions, which obeys \( | \nabla \mathcal{G} | \neq 0 \) (e.g. \( \mathcal{G} = Y_{\text{CH}_4} \)). A 'flame surface' is defined as an iso-plane of \( \mathcal{G} \), i.e. a surface where \( \mathcal{G}(x,t) = \text{constant} \). The motion of such a surface is described by the kinematic equation [14]

\[
\frac{d \mathcal{G}}{dt} := \frac{\partial \mathcal{G}}{\partial t} + (v_f \cdot \nabla) \mathcal{G} = 0, \tag{9}
\]

stating that a point on a flame surface stays on this surface for all \( t \). Here, \( v_f \) is the local velocity of a flame surface. A local orthogonal coordinate system \( \eta = (\xi, \zeta, \eta) \) (see Figure 1) is defined in terms of these flame surfaces. The factors \( h_\xi = \left| \frac{\partial \xi}{\partial \eta} \right| \), \( h_\zeta = \left| \frac{\partial \zeta}{\partial \eta} \right| \) and \( h_\eta = \left| \frac{\partial \eta}{\partial \eta} \right| \) are scale factors, defining the arc-lengths in the \( \eta \)-coordinate system. Note that the unit normal vector \( e_\eta \) on a flame surface can be written as \( e_\eta = \text{sign}(\mathcal{G}_b - \mathcal{G}_u) \nabla \mathcal{G} / | \nabla \mathcal{G} | \), directed to the burnt gas mixture.

The tangential component \( v_{f,t} \) of the flame surface velocity is equal to the tangential component \( v_t \) of the fluid velocity and the difference \( \rho (v - v_f) \) is equal to the amount of mass, effectively consumed by the flame, so that we may write

\[
v - v_f = s_L e_\eta, \tag{10}\]

\( s_L \) being the local burning velocity. When Eq.(10) is substituted into Eq.(9) we find the well-known G-equation [25]:

\[
\frac{\partial \mathcal{G}}{\partial t} + (v \cdot \nabla) \mathcal{G} = s_L \left| \nabla \mathcal{G} \right|. \tag{11}\]

We now proceed with a reformulation of the continuity equation (2):

\[
\nabla \cdot (\rho (v - v_f)) = -\frac{\partial \rho}{\partial t} - \nabla \cdot (\rho v_f), \tag{12}\]

Figure 1
where the terms, describing transport perpendicular to the flame (in \( e_\eta \)-direction) are gathered in the left-hand side and all distortions from local 1D stationary flow shifted to the right-hand side. It is interesting to note that the right-hand side of (12) is exactly equal to \(-\rho K\), \( K \) being the local flame stretch rate, defined in [8]. In [8], the stretch rate \( K \) is defined as the relative rate of change of the mass

\[
M(t) = \int_{V(t)} \rho \, dV
\]

in a small part of the flame, enclosed by the volume \( V(t) \), moving with velocity \( \mathbf{v}_f \):

\[
K = \frac{1}{M} \frac{dM}{dt}.
\]

Applying the transport theorem to \( M(t) \) in Eq.(13) then leads to the following equation for the scalar field quantity \( K \):

\[
\rho \dot{K} = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}_f),
\]

which, apart from a minus sign, is equal to the right-hand side of (12). Using Eq.(10) this thus gives

\[
\nabla \cdot (\rho s_L e_\eta) = -\rho K
\]

for the continuity equation Eq.(12). Note that all distortions from local 1D flame behaviour are combined in the right-hand side term \(-\rho K\). Apart from the usual terms related with flame curvature and flow straining, this definition of \( K \) incorporates additional contributions, for instance due to flame thickness variations. A physical interpretation of the different contributions is presented in Ref.[8].

The conservation equation for the scalar variable \( \mathcal{G} \)

\[
\frac{\partial (\rho \mathcal{G})}{\partial t} + \nabla \cdot (\rho \mathbf{v} \mathcal{G}) - \frac{1}{Le_\mathcal{G}} \nabla \cdot \left( \frac{\lambda}{c_p} \nabla \mathcal{G} \right) - \dot{\rho} \mathcal{G} = 0,
\]

is now reformulated in the \( \eta \)-coordinate system. Using the G-equation (9) and Eqs. (15) and (10), the following quasi-1D form for \( \mathcal{G} \) is found rigorously:

\[
\nabla \cdot (\rho s_L \mathcal{G} e_\eta) - \frac{1}{Le_\mathcal{G}} \nabla \cdot \left( \frac{\lambda}{c_p} \frac{\partial \mathcal{G}}{\partial \eta} e_\eta \right) - \dot{\rho} \mathcal{G} = -\rho K \mathcal{G},
\]

with all transport terms along the flame surfaces gathered in the right-hand side term \(-\rho K \mathcal{G}\). We used here that the diffusive flux is already directed in the \( e_\eta \)-direction. It is important to note here that Eq.(18) is found from the full instationary conservation equation (17), using the stretch rate (15) and the G-equation (11). Alternatively, this means that the full conservation equation (17) for \( \mathcal{G} \) would be solved exactly, when a method would be available in which the G-equation and the flamelet equation (18) are solved in a combined way, using the coupling with the scalar stretch field \( K \) of Eq.(15).
The same procedure can be applied to the other scalar variables $Y_i$, $H$ and $Z_j$. This then leads to the following set of quasi-1D conservation equations:

\[
\nabla \cdot (\rho s_L e_n) = -\rho K,
\]

\[
\nabla \cdot (\rho s_L Y_i e_n) - \frac{1}{Le_i} \nabla \cdot \left( \frac{\lambda}{c_p} \frac{1}{h_q} \frac{\partial Y_i}{\partial \eta} e_n \right) - \dot{\rho}_i = -\rho K Y_i + Q_{Y_i}, \quad (i = 1, \cdots, N - 1),
\]

\[
\nabla \cdot (\rho s_L H e_n) - \nabla \cdot \left( \frac{\lambda}{c_p} \frac{1}{h_q} \frac{\partial H}{\partial \eta} e_n \right) = -\rho K H + Q_H,
\]

\[
\nabla \cdot (\rho s_L Z_j e_n) - \nabla \cdot \left( \frac{\lambda}{c_p} \frac{1}{h_q} \frac{\partial Z_j}{\partial \eta} e_n \right) = -\rho K Z_j + Q_{Z_j}, \quad (j = 1, \cdots, N_e),
\]

where the $Q_{Y_i}$, $Q_H$ and $Q_{Z_j}$ terms, which describe transport in the flame surfaces, arise because the local iso-surfaces of the variables $Y_i$, $H$ and $Z_j$ generally don't coincide with the iso-surfaces of $G$. However, it is expected that the contributions $Q_{Y_i}$, $Q_H$ and $Q_{Z_j}$ are small compared to the stretch terms in the right-hand side of Eq.(19) in most situations, although this might not be justified under extreme circumstances, such as near local flame quenching. In Ref.[7] the $Q_H$ term was computed numerically for the tip of a stationary 2D Bunsen flame and it appeared to be very small. Furthermore, it is obvious that $Q_G = 0$, $\sum_i Q_{Y_i} = 0$ and $Q_{Z_j} = \sum_j w_{ji} Q_{Y_i}$. This then implies that for a simple one-step reaction $R \rightarrow P$ where $G = Y_R$ all $Q$-terms vanish. Therefore, we assume in this paper that $Q_{Y_i} = Q_H = Q_{Z_j} = 0$. This approximation is related to the assumption that the length scales of the distortions along the flame surfaces are much larger than the flame thickness. In case of premixed turbulent flames this implies that the length scales of the turbulent structures would be so large that combustion takes place in the flamelet regime of the Borghi diagram.

Introducing the mass burning rate $m = \rho s_L$, the arc-length perpendicular to the flame surfaces $ds = h_q d\eta$ and the variable $\sigma = h_\xi h_\zeta = | \frac{\partial x}{\partial \xi} \times \frac{\partial x}{\partial \zeta} |$, which is a measure for the area on the flame surfaces through which transport takes place, the quasi-1D conservation equations in (19) can be expressed in the $\eta$-coordinate system. These equations, which we refer to as the 'flamelet' equations, then read:

\[
\frac{\partial}{\partial s}(\sigma m) = -\sigma \rho K,
\]

\[
\frac{\partial}{\partial s}(\sigma m Y_i) - \frac{1}{Le_i} \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} \frac{\partial Y_i}{\partial s}) - \sigma \dot{\rho}_i = -\sigma \rho K Y_i, \quad (i = 1, \cdots, N - 1),
\]

\[
\frac{\partial}{\partial s}(\sigma m H) - \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} \frac{\partial H}{\partial s}) = -\sigma \rho K H,
\]

\[
\sum_{i=1}^{N} \left( \frac{1}{Le_i} - 1 \right) \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} H^0 \frac{\partial Y_i}{\partial s}) = -\sigma \rho K H,
\]
A Flamelet Description of Premixed Laminar Flames ...

\[
\frac{\partial}{\partial s} (\sigma m Z_j) - \frac{\partial}{\partial s} (\sigma \frac{\lambda}{c_p} \frac{\partial Z_j}{\partial s}) - \sum_{i=1}^{N} w_{ji} \left( \frac{1}{L \epsilon_i} - 1 \right) \frac{\partial}{\partial s} (\sigma \frac{\lambda}{c_p} \frac{\partial Y_i}{\partial s}) = -\sigma \rho K Z_j, \quad (j = 1, \ldots, N_e). \tag{20}
\]

Note that the derivative \(\frac{1}{s} \frac{\partial \sigma}{\partial s}\) is equal to the curvature \(\frac{1}{R}\) of the flame surface. These flamelet equations describe the internal flame structure (in terms of \(G(s), Y_i(s), H(s), Z_j(s)\) or alternatively \(Y_i(G), H(G), Z_j(G)\)) and the eigenvalue for the mass burning rate \(m(s)\) or \(m(G)\) for a flamelet with a particular stretch field \(K(G)\) and curvature field \(\sigma(G)\). When Eqs. (20) are solved in combination with the G-equation for all G-surfaces, we in fact solve the full set of conservation equations of species, elements and enthalpy, assuming that diffusive transport along the G-surfaces is negligible (which is the case in the flamelet regime).

A possible numerical implementation of the above method is sketched schematically in Fig. 2. Such an implementation is not easy, has not been performed yet and is still under investigation in our group. The reason for this is that the flamelets are coupled with the flow and mixing processes in a non-local manner. The coupling is described by the scalar fields for \(K(G)\) and \(\sigma(G)\). These fields can be determined from the local structure of the flow and the G-surfaces. An explicit and easy to discretise expression for the \(K\) field, for example, follows when Eq. (15) is further elaborated [7]. Note, however, that the flame stretch and curvature functions \(K(G), \sigma(G)\) in the complete flamelet determine the structure and mass burning rate of the flamelet. Thus, as already observed by Buckmaster [1], there exists no local coupling of the flamelets with the flow: the behaviour of the flow and the G-surfaces in the complete preheating and reaction zones is of importance for the mass burning rate of the flamelet. This complicated coupling probably means that the computational efficiency has not been increased much, in spite of the fact that the stiff flamelet system has been decoupled from the flow.

To derive more efficient laminar flamelet models for premixed flames, we will analyse the flamelet system in more detail in the remainder of this paper. We will study the flamelet system Eq. (20) numerically in Section 7. First, however, we study the above system analytically in Sections 4, 5 and 6. More specifically, we will compute the mass burning rate \(m_e\) for both stretchless flames \((K = 0)\) and stretched flames \((K \neq 0)\), using the Integral Analysis [4]. This analysis might lead to more accurate approximations for both laminar and turbulent flamelet models.

4 Mass Burning Rate 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, enthalpy and element mass fractions of the set (20) from the unburnt to the burnt gas mixture gives:

\[
(\sigma m^0)_{b} = (\sigma m^0)_{u}, \tag{21}
\]

Figure 2
\[ (\sigma m^0 H^0)_{b} = (\sigma m^0 H)_u, \quad (22) \]
\[ (\sigma m^0 Z^0_j)_{b} = (\sigma m^0 Z_j)_u, \quad (j = 1, \cdots, N_e), \quad (23) \]

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 and the subscripts 'b' and 'u' denote the values of a variable in the burnt and unburnt gases, respectively. Eqs.(21), (22) and (23) simply indicate that the mass, enthalpy and element composition are constant in the flame area, i.e. \( H^0_b = H_u \) and \( Z^0_{j,b} = Z_{j,u} \), 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 \( m^0_b \) of the stretchless flame, which can be computed from the quasi-1D equation for \( G \):

\[ \mathcal{F}(s) - \frac{\partial}{\partial s} \mathcal{H}(s) = S(s), \quad (24) \]

where we introduced the functions \( \mathcal{F} \), \( \mathcal{H} \) and \( S \):

\[ \mathcal{F}(s) = \frac{\partial}{\partial s}(\sigma m G), \]
\[ \mathcal{H}(s) = \sigma \frac{1}{Lc_p c_p} \frac{\partial G}{\partial s}, \]
\[ S(s) = \sigma \beta c. \quad (25) \]

We multiply Eq.(24) with \( \mathcal{H}(s) \) and subsequently integrate the resulting equation over \( s \) from \( s_u \) to \( s_b \). The integral over the diffusion term \( \frac{1}{2} \frac{\partial^2 S}{\partial s^2} \) then drops out, as the diffusion fluxes are zero in the (un)burnt mixture and we find

\[ \int_{s_u}^{s_b} \mathcal{F}(s) \mathcal{H}(s) \, ds = \int_{s_u}^{s_b} \mathcal{H}(s) S(s) \, ds. \quad (26) \]

The integrals in this equation run over the complete flame region. The function \( \mathcal{H}(s) \) in the left-hand side of this equation can be approximated very well by the (integrated) solution of Eq.(24) in the preheating zone, where \( |S| \ll |\mathcal{F}| \):

\[ \mathcal{H}(s) = \int_{s_u}^{s} (\mathcal{F}(\psi) - S(\psi)) \, d\psi \approx \int_{s_u}^{s} \mathcal{F}(\psi) \, d\psi, \quad (27) \]

which, inserted into Eq.(26), leads to

\[ \int_{s_u}^{s_b} \mathcal{F}(s) \left( \int_{s_u}^{s} \mathcal{F}(\psi) \, d\psi \right) \, ds = \frac{1}{2} \left( \int_{s_u}^{s_b} \mathcal{F}(s) \, ds \right)^2 \approx \int_{s_u}^{s_b} \mathcal{H}(s) S(s) \, ds. \quad (28) \]

The validity of the approximation in Eq.(27) 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 \( \mathcal{F} \mathcal{H} \) in Eq.(26) is found in the preheating zone. It should be noted that Eq.(28) 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 [3, 24] to compute the mass burning rate.

The integrals in Eq.(28) can now be evaluated:

$$\int_{s_u}^{s_b} \mathcal{F}(s) \, ds = (\sigma m^0)_b (\mathcal{G}^0_b - \mathcal{G}_u),$$
$$\int_{s_u}^{s_b} \mathcal{H}(s) \mathcal{S}(s) \, ds = \int_{s_u}^{s_b} \sigma^2 \frac{1}{\mathcal{E}_c} \frac{\lambda}{c_p} \rho \, d\mathcal{G},$$

where we used Eq.(21). Substituted into Eq.(28), this gives the following approximation for the mass burning rate:

$$m^0_b(\mathcal{G}_u, H^0_b, Z_{1,b}^0, \ldots, Z_{N_e,b}^0) \approx \frac{1}{|\mathcal{G}^0_b - \mathcal{G}_u|} \sqrt{2 \int_{s_u}^{s_b} \left( \frac{\sigma}{\sigma_b} \right)^2 \frac{1}{\mathcal{E}_c} \frac{\lambda}{c_p} \rho \, d\mathcal{G}.}$$ (30)

It should be realized that Eq.(30) is not equal to the adiabatic mass burning rate $m^0_{b,1}$ of a flat flame, due to the factor $(\sigma/\sigma_b)^2$. For an infinitely thin reaction layer, though, this expression does reduce to the expression for the adiabatic mass burning rate of a planar flame, as the curvature terms then drop out.

Note that the expression Eq.(30) for $m^0_b$ depends on the initial state through $\mathcal{G}_u$ in the 'friction' factor $\frac{1}{|\mathcal{G}^0_b - \mathcal{G}_u|}$. Furthermore, we also explicitly emphasized that the mass burning rate $m^0_b$ also depends on the enthalpy $H^0_b$ and element composition $Z^0_{i,b}$ in the equilibrium state in Eq.(30). This follows from the observation that the factor $\frac{\lambda}{c_p} \rho$ in Eq.(30) is a function of all flame variables $Y_i \ (i = 1, \ldots, N)$ and $T$. However, the integral in Eq.(30) effectively runs only over the thin reaction layer, where $\rho \neq 0$ and where the system approaches the equilibrium state. From a time scale analysis of a number of combustion systems, it has become clear recently [23, 11, 6], that the reaction path in composition space is embedded in a low-dimensional manifold, which can be described by a small number of progress variables. Near the equilibrium point in composition space, all reaction paths are attracted to a one-dimensional subspace in most cases, independent of the initial composition. This means that for this case all flame variables can be written as function of $\mathcal{G}$ because $|\nabla \mathcal{G}| \neq 0$: $Y_i(\mathcal{G})$ and $T(\mathcal{G})$. Eq.(30) then indicates that the integral over $\mathcal{G}$ is independent of the initial composition in this case and depends only on 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. $H^0_b$ and $Z^0_{j,b}$ for $j = 1, \ldots, N_e$. 

A Flamelet Description of Premixed Laminar Flames ...
5 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 in (20) through the flame gives

\[(\sigma m)_b - (\sigma m)_u = - \int_{s_u}^{s_b} \sigma \rho K \, ds.\] (31)

In the same way, integration of the enthalpy equation and element mass fraction equations in (20) through the flamelet and using (31) results in

\[H_b - H_u = \frac{-1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma \rho K (H - H_u) \, ds\] (32)

and

\[Z_{j,b} - Z_{j,u} = \frac{-1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma \rho K (Z_j - Z_{j,u}) \, ds,\] (33)

respectively. When the definition equations (5) for \(H\) and \(H_u\) and (7) for \(Z_j\) and \(Z_{j,u}\) are inserted into the right-hand sides we find

\[H_b - H_u = - \frac{m_b^0}{m_b} \left( \sum_{i=1}^{N} H_i^0 \frac{K a_i}{L e_i} (Y_{i,b} - Y_{i,u}) + K a_T (H_{T,b} - H_{T,u}) \right),\] (34)

\[Z_{j,b} - Z_{j,u} = - \frac{m_b^0}{m_b} \left( \sum_{i=1}^{N} w_{ji} \frac{K a_i}{L e_i} (Y_{i,b} - Y_{i,u}) \right),\] (35)

where the Karlovitz numbers \(K a_i\) and \(K a_T\) are defined by:

\[K a_i = \frac{L e_i}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma \rho K \dot{Y}_i \, ds,\] (36)

\[K a_T = \frac{1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma \rho K \dot{H}_T \, ds.\] (37)

We also introduced normalised quantities

\[\dot{f} = \frac{f - f_u}{f_b - f_u}, \quad (f = Y_i, H_T).\] (38)

Using that \((H_{T,b} - H_{T,u}) = (H_b - H_u) - \Sigma_i H_i^0 (Y_{i,b} - Y_{i,u})\) and \(Z_{j,b} - Z_{j,u} = \Sigma_i w_{ji} (Y_{i,b} - Y_{i,u})\) in Eqs.(34) and(35) gives the exact equations

\[H_b - H_u = \frac{-m_b^0}{m_b + K a_T m_b^0} \sum_{i=1}^{N} H_i^0 \left( \frac{K a_i}{L e_i} - K a_T \right) (Y_{i,b} - Y_{i,u}),\] (39)
Equations (39) and (40) describe the influence of preferential diffusion and flame stretch, incorporated in the Karlovitz numbers, on the local enthalpy and element composition of the burnt mixture. It should be noted from the definition (36), (37) of the Karlovitz numbers that the influence of flame stretch \( \rho K \) in the preheating zone is effectively damped exponentially by the normalised variables \( \tilde{Y}_i \) and \( \tilde{H}_T \), which are equal to 1 in the burnt gases and go to zero for \( s \to s_u \). The enthalpy \( H_b \) and the element mass fractions \( Z_{j,b} \) in the burnt mixture determine the local stoichiometry and equilibrium composition of the burnt mixture. These quantities, following from Eqs.(39) and (40), have an important influence on the local mass burning rate \( m_b \), because \( m_b \) is determined to a large extent by the mixture composition and enthalpy in the reaction layer, close to the burnt mixture (see also Eq.(30)). 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 Eq.(24), where \( \mathcal{F}(s) \) is now given by

\[
\mathcal{F}(s) = \frac{\partial}{\partial s} (\sigma m \mathcal{G}) + \sigma \rho K \mathcal{G},
\]

while \( \mathcal{H} \) and \( \mathcal{S} \) are still given in (25). The computation of the mass burning rate is analogous to the computation presented in the previous section, with \( \mathcal{F} \) replaced by Eq.(41). For the integral over \( \mathcal{F} \) in (29) we now have

\[
\int_{s_u}^{s_b} \mathcal{F}(s) \, ds = \left( \sigma m \mathcal{G} \right)_b - \left( \sigma m \mathcal{G} \right)_u + \int_{s_u}^{s_b} \sigma \rho K \mathcal{G} \, ds
\]

\[
= \left( \sigma m \right)_b \left( \mathcal{G}_b - \mathcal{G}_u \right) + \int_{s_u}^{s_b} \sigma \rho K (\mathcal{G} - \mathcal{G}_u) \, ds,
\]

so that we find for the mass burning rate

\[
m_b(\mathcal{G}_u, H_b, Z_{1,b}, ..., Z_{N_e,b}) \approx \frac{1}{|\mathcal{G}_b - \mathcal{G}_u|} \left[ \frac{2 \int_{\mathcal{G}_u}^{\mathcal{G}_b} (\sigma_b)^2}{1 \frac{\lambda}{\ell_e} c_p} \int_{s_u}^{s_b} \sigma_b \rho \mathcal{G} \, ds \right]
\]

\[
- \frac{1}{\sigma_b} \int_{s_u}^{s_b} \sigma \rho K \tilde{\mathcal{G}} \, ds.
\]

The first term in the right-hand side is again a function of all combustion variables \( Y_i \) and \( T \). 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 low-dimensional manifold described by \( Y_i(\mathcal{G}) \) and \( T(\mathcal{G}) \). Comparison of this term with Eq.(30) for stretchless flames then indicates that this term can be related to the mass burning rate of a 'stretchless' flame \( m_b^0 \) with final enthalpy and composition given
by $H_b$ and $Z_{j,b}$ instead of $H_b^0$ and $Z_{j,b}^0$. Using Eq.(30) for $m_b^0$ and the definition of the Karlovitz number (36) for $K_{a_G}$ then gives for Eq.(43):

$$m_b(G_u, H_b, Z_{1,b}, \ldots, Z_{N_e,b}) \approx (1 - \frac{K_{a_G}}{L e_G}) m^0_b(G_u, H_b, Z_{1,b}, \ldots, Z_{N_e,b}).$$

(44)

For convenience we take here $G = H_T$ and choose a fixed initial temperature (so that $G_u = H_{T,u}$) of the stretchless flame, which then gives for (44):

$$m_b(H_{T,u}, H_b, Z_b) \approx (1 - K a_T) m^0_b(H_{T,u}, H_b, Z_b),$$

(45)

where the vector $Z$ denotes all the element mass fractions. Theoretically, it can be shown that other choices for $G$ or $G_u$ give the same final result for $m_b$. If we finally use (45) in Eqs.(39) and (40) we find the equations

$$\Delta H_b \approx -\sum_{i=1}^{N} H_i^0 (\frac{K a_i}{L e_i} - K a_T) (Y_{i,b} - Y_{i,u}),$$

$$\Delta Z_{j,b} \approx -\sum_{i=1}^{N} w_{ji} (\frac{K a_i}{L e_i} - K a_T) (Y_{i,b} - Y_{i,u}),$$

$$m_b(H_{T,u}, H_b, Z_b) \approx (1 - K a_T) m^0_b(H_{T,u}, H_b^0 + \Delta H_b, Z_b^0 + \Delta Z_b),$$

(46)

where $\Delta H_b = H_b - H_u = H_b - H_b^0$ and $\Delta Z_{j,b} = Z_{j,b} - Z_{j,u} = Z_{j,b}^0 - Z_{j,b}^0$. The set of Equations (46) for $H_b$, $Z_{j,b}$ and $m_b$ describe the enthalpy, element composition and mass burning rate of stretched and curved premixed flamelets and forms the basis of the subsequent analysis of the flamelet system. This set is also valid in case of strong stretch rates: Eqs.(39) and (40) follow rigorously from the flamelet equations and to derive Eq.(45) it only has been assumed that the reaction layer is thin. However, the system (46) is not closed because stretched flame solutions are needed in the Karlovitz numbers (36) and (37) to evaluate (46).

It is the aim of the analysis which follows to introduce smart approximations to close this set of equations in such a way that it may be used without solving the complete system (20) for each separate flamelet. There are many ways to do this. Two possible approaches will be presented here. The simplest method, which will be described in the next section, would be to restrict to weak stretch. A more accurate higher-order closure, which is also valid for stronger stretch is proposed in the Appendix.

### 6 Weak Stretch; Comparison with LAEA theory

The simplest way to close the system (46) is to evaluate $H_b$, $Z_{j,b}$ and $m_b$ from stretchless-flame information only. Instead of the Karlovitz numbers (36) and (37) we then use the 'stretchless' Karlovitz numbers

$$K a_i^0 = \frac{L e_i}{(\sigma m^0_b)^{1/2}} \int_{s_u}^{s_b} \sigma \rho^0 K \tilde{Y}_i^0 \, ds$$

(47)
and
\[ Ka_2^0 = \frac{1}{(\sigma m^0)_b} \int_{s_u}^{s_b} \sigma \rho^0 K \tilde{H}_2^0 \, ds \] (48)
in Eq.(46). With this last step we can now use Eq.(46) instead of solving the complete flamelet system (20) for each separate flamelet. This introduces a very large step in computational efficiency: when in a CFD calculation for a specific flamelet \( K(G) \) and \( \sigma(G) \) are determined (see Fig.2), the Karlovitz numbers \( Ka_2^0 \) and \( Ka_3^0 \) can be evaluated by integrating \( \rho K \sigma \) through the flamelet weighted with (stored) stretchless flamelet solutions \( f_0 \).

\( H_b, Z_{j,b} \) and \( m_b = m(G_b) \) can be evaluated subsequently for each flamelet from Eq.(46). The mass burning rate \( m(G) \) of each complete flamelet finally follows by integrating the continuity equation (see Eq.(68)).

To show the validity of the approach we will analyse (46) for weak stretch in the remainder of this section for some special cases. Well-known results from literature are recovered. For weak stretch it is possible to expand \( m_b^0(G, H_b, Z_b) \) around \( m_b^0(G, H^0_b, Z^0_b) \). We then find for \( m_b^0 \)
\[
\frac{m_b}{m_b^0} \approx 1 - Ka_2^0 + \Delta H_b \frac{\partial}{\partial H^0_b} (\ln m_b^0) + \sum_{j=1}^{N} \Delta Z_{j,b} \frac{\partial}{\partial Z^0_{j,b}} (\ln m_b^0) + \text{hot}, \tag{49}
\]
with \( \text{hot} \) containing higher-order terms in \( Ka_2^0, Ka_3^0 \).

Let us consider the physical significance of the different terms in Eq. (49). The term \( Ka_2^0 \) 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 the fact that the mass burning rate is proportional to \( \sqrt{\lambda} \). Note that the term \( 1 - Ka_2^0 \) does not vanish for unit Lewis numbers \( (Le_i = 1) \). The other terms in Eq.(49) are zero in that case. The \( \frac{\partial}{\partial H^0_b} (\ln m_b^0) \)-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 [4] for the case of a simple one-step reaction. The last term, proportional to \( \frac{\partial}{\partial Z_{j,b}} (\ln m_b^0) \), also arises from differential diffusion effects, which give rise to element composition and stoichiometry changes. This term has not been found in other studies because elements are conserved in one-step reaction mechanisms with a single Lewis number.

We now study the results for the special case of a flat flame \( (\sigma = \sigma_b) \) with constant \( \lambda \) and \( c_p \) in a stagnation flow with \( \rho K = \rho_b K_b \), so that \( \sigma \rho K = \text{Constant} \) in the flame region \( (s_u < s < s_b) \) (see e.g.[26]). For this special case, however, we find an identical expression for all Karlovitz numbers from Eq.(47) and (48):
\[
Ka_2^0 = \frac{\lambda \rho_b K_b}{c_p (m_b^0)^2}, \tag{50}
\]
where we substituted the approximate stretchless 1D solution for $\dot{Y}_i^0(s)$ and $\dot{H}_T^0(s)$:

$$\dot{Y}_i^0(s) = \exp\left(\frac{L_{e_i} (s - s_b)}{\delta^*}\right)$$ \quad and \quad $$\dot{H}_T^0(s) = \exp\left(\frac{(s - s_b)}{\delta^*}\right), \tag{51}$$

\[ \delta^* = \frac{1}{m_b^0 c_p} \]

being the flame thickness. Eqs.(46) and (49) now simplify considerably:

$$\Delta H_b \approx \mathcal{K} a^0 \left(\frac{1}{L_{e_{H}}} - 1\right) c_p(T_b^0 - T_u) + \mathcal{O}((\mathcal{K} a^0)^2),$$

$$\Delta Z_{j,b} \approx \mathcal{K} a^0 \left(\frac{1}{L_{e_{Z,j}}} - 1\right) Z_{j,u} + \mathcal{O}((\mathcal{K} a^0)^2),$$

$$\frac{m_b}{m_b^0} \approx 1 - \mathcal{K} a^0 \mathcal{M}_b + \mathcal{O}((\mathcal{K} a^0)^2), \tag{52}$$

where the Markstein number $\mathcal{M}_b$ has been introduced

$$\mathcal{M}_b = 1 - \left(\frac{1}{L_{e_{H}}} - 1\right) c_p(T_b^0 - T_u) \frac{\partial}{\partial H_b^0}(\ln m_b^0) - \sum_{j=1}^{N_e} \left(\frac{1}{L_{e_{Z,j}}} - 1\right) Z_{j,u} \frac{\partial}{\partial Z_{j,b}^0}(\ln m_b^0). \tag{53}$$

Furthermore, the effective Lewis numbers $L_{e_{H}}$ and $L_{e_{Z,j}}$ describing the enthalpy transport and element transport by the diffusive fluxes are given by

$$\frac{1}{L_{e_{H}}} - 1 = - \sum_{i=1}^{N_e} \left(\frac{1}{L_{e_i}} - 1\right) \frac{H_i^0 (Y_{i,b} - Y_{i,u})}{c_p(T_b^0 - T_u)},$$

$$\frac{1}{L_{e_{Z,j}}} - 1 = - \sum_{i=1}^{N_e} \left(\frac{1}{L_{e_i}} - 1\right) \frac{Y_{i,b} - Y_{i,u}}{Z_{j,u}}. \tag{54}$$

A conclusion, which might be drawn from the expressions 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 $\rho \mathcal{K} \sigma$ does not change in the flame zone. 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 Eq.(54)). 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 case of a one-step irreversible reaction $\mathcal{F} \rightarrow \mathcal{P}$ with a single Lewis number $L_{e_{\mathcal{F}}} = L_{e_{\mathcal{P}}} = L_e$ we find that $L_{e_{H}} = L_e$ and $L_{e_{Z,j}} = 0$. That the element Lewis numbers vanish means that elements are conserved. This is also clear from a physical point of view because the single element mass fraction $Z = Y_{\mathcal{F}} + Y_{\mathcal{P}}$ is constant in this case. Furthermore, using $m_b^0 \propto \exp(-E_a/2RT_b^0)$ yields for the derivative

$$c_p(T_b^0 - T_u) \frac{\partial}{\partial H_b^0}(\ln m_b^0) = (T_b^0 - T_u) \frac{\partial}{\partial T_b^0}(\ln m_b^0) = \frac{Ze^0}{2}, \tag{55}$$
where the Zeldovich number is given, as usual, by $Z_{e}^{0} = \frac{E_{a}(T_{u}^{0} - T_{b}^{0})}{\rho_{a}(T_{b}^{0})}$, $E_{a}$ being the activation energy. This finally leads to the Markstein number

$$\mathcal{M}_{b} = 1 + \frac{Le - 1}{Le} \frac{Z_{e}^{0}}{2}. \quad (56)$$

In 1979 Joulin and Clavin [9] studied the dynamic flame response with constant density, leading to a Markstein number for the unburnt and burnt gases equal to

$$\mathcal{M}_{b} = 1 + (Le - 1) \frac{Z_{e}^{0}}{2}. \quad (57)$$

They assumed that $(Le - 1) Z_{e}^{0} = O(1)$, so that deviations of the Lewis number from 1 are of order $\frac{1}{Le}$. To lowest-order in $Z_{e}^{0}$, Eqs.(56) and (57) are therefore equal.

In 1985 Clavin [5] extended the above approach to a constant stretch rate $K = K_{b}$, but with variable density in the flame zone

$$\rho^{0}(s) = \frac{\rho_{u}T_{u}}{T^{0}(s)} = \frac{\rho_{u}}{1 + \tau \exp\left(\frac{\Delta}{\delta^{*}}\right)}, \quad (58)$$

where the thermal expansion coefficient $\tau$ is defined by $\tau = T_{u}^{0} - T_{u} = \frac{\rho_{u} - \rho^{0}}{\rho^{0}}$. Now, substituting Eqs.(51) and (58) into Eqs.(47), (48) for $K a_{f}^{0}$ and $K a_{r}^{0}$ gives (taking $s_{b} = 0$ and $s_{u} \rightarrow -\infty$):

$$Ka_{f}^{0} = -\frac{\rho_{u}K_{b}}{m_{b}^{0}} \int_{-\infty}^{0} \frac{\exp\left(\frac{\Delta}{\delta^{*}}s^{*}\right)}{1 + \tau \exp\left(\frac{\Delta}{\delta^{*}}s^{*}\right)} \mathrm{d}s = Ka_{r}^{0} \left(\frac{\tau + 1}{\tau}\right) \ln(1 + \tau),$$

$$\frac{Ka_{r}^{0}}{Le} = -\frac{\rho_{u}K_{b}}{m_{b}^{0}} \int_{-\infty}^{0} \frac{\exp\left(\frac{Le}{\delta^{*}}s^{*}\right)}{1 + \tau \exp\left(\frac{Le}{\delta^{*}}s^{*}\right)} \mathrm{d}s = \frac{\rho_{u}K_{b}\delta^{*}}{m_{b}^{0}} \tau^{-Le} \int_{0}^{\tau} \frac{y^{Le-1}}{1 + y} \mathrm{d}y$$

$$= Ka_{r}^{0} - Ka_{f}^{0} (Le - 1) (1 + \tau) \int_{0}^{\tau} \frac{\ln(1 + y)}{y^{2}} \left(\frac{y}{\tau}\right)^{Le} \mathrm{d}y, \quad (59)$$

where the relation $\rho_{u} = \rho_{b}^{0}(1 + \tau)$ has been used. The final result for the Markstein number in the burnt gases follows from Eq.(49), in combination with $\Delta Z_{j} = 0$,

$$\Delta H_{b} = \left(\frac{Ka_{r}^{0}}{Le} - Ka_{f}^{0}\right)c_{p}(T_{b}^{0} - T_{u}) + \text{hot}, \quad (60)$$

Eq.(59) for the Karlovitz numbers and Eq.(55):

$$\mathcal{M}_{b} = \left(\frac{\tau + 1}{\tau}\right) \ln(1 + \tau) + \frac{Z_{e}^{0}}{2} (Le - 1) (1 + \tau) \int_{0}^{\tau} \frac{\ln(1 + y)}{y^{2}} \left(\frac{y}{\tau}\right)^{Le} \mathrm{d}y. \quad (61)$$

Clavin found the following result in 1985:

$$\mathcal{M}_{b} = \left(\frac{\tau + 1}{\tau}\right) \ln(1 + \tau) + \frac{Z_{e}^{0}}{2} (Le - 1) (1 + \tau) \int_{0}^{\tau} \frac{\ln(1 + y)}{y} \mathrm{d}y. \quad (62)$$
Clavin assumed in his analysis that \((Le - 1)\) is of order \(\frac{1}{Z^2}\). To lowest order in the Zeldovich number, Eq.(61) is therefore equal to the result of Clavin (1985) for \(M_b\), derived using LAEA.

7 Numerical Solution of the Flamelet System

The equivalence between the results presented in the previous section with well-known expressions from literature confirms the validity of the proposed description for weak stretch. However, as some approximations have been introduced, it is not clear how well the method predicts the response of more realistic complex-chemistry flames computed with numerical methods. It is the aim of this section to investigate this aspect. We will solve the flamelet system (20) numerically, using the skeletal reaction mechanism for methane/air combustion [20] and we will study how well the central flamelet response functions in Eq.(46) are reproduced. The comparison will be performed for flat \((\sigma = 1)\) stretched \((\rho K = \rho_b K_b\) or \(K = K_b\)) adiabatic methane/air flames with an equivalence ratio of \(\Phi = 0.8\). The analysis will be carried out for both weakly and strongly stretched flames. Non-unit Lewis numbers will be considered in the final part of this section; however, the simpler case of unit Lewis numbers is studied first.

As already mentioned in Section 6, the equations (39) and (40) for \(\Delta H_b\) and \(\Delta Z_{j,b}\) are exact in the sense that they are derived from first principles from (20). However, Eq.(45) for the mass burning rate has been found using the assumption that the reaction layer is very thin. This last equation thus forms the most critical part of the flamelet response model and it is not really necessary to compare Eqs.(39) and (40) with numerical data. We therefore, as a first step, take \(Le_i = 1\) in the numerical code, so that enthalpy and element mass fractions don't change, i.e. \(\Delta H_b = \Delta Z_{j,b} = 0\), focussing the comparison on the weakest part: Eq.(45) for \(m_b\). A conservative discretisation scheme of the enthalpy and element mass fraction equations, implemented in the numerical code [21], makes sure that enthalpy and elements are conserved exactly up to all orders. For this case Eq.(46) reduces to

\[
m_b(H_{T,u}, H_{T,b}^0, Z_{b}^0) \approx 1 - K a_{i,T} = 1 - \frac{1}{m_b^0} \int_{s_u}^{s_b} \rho K \bar{f}(s) ds = 1 - K a M_b, \tag{63}
\]

with \(K a = \frac{\delta_f \rho_b K_b}{m_b^0}\), independent of the chosen variable \(\bar{f}\). For the case \(\rho K = \rho_b K_b\), Eq.(63) indicates that the 'stretched' flame thickness \(\delta_f\) should be defined as

\[
\delta_f = \int_{s_u}^{s_b} \bar{f}(s) ds. \tag{64}
\]

Theoretically, the Markstein number \(M_b = 1\) for this situation. The Markstein number \(M_b(s_b) = -\left(\frac{m_b(s_b)}{m_b^0} - 1\right)/K a(s_b)\), computed numerically from the flamelet equations (20) is presented in Figure 3 for \(f = H_T, Y_{CH_4}\) as function of the boundary in the burnt gases \(s_b\), where the flame thickness \(\delta_f\) has been determined using (64). The scaled source terms \(S_T\)
of \( H_T \) and \( Y_{CH_4} \) are also included in Figure 3. The Markstein numbers found from \( f = H_T \) and \( f = Y_{CH_4} \) are equal to each other in the preheating zone because the solutions for \( H_T(s) \) and \( Y_{CH_4} \) are equal there for \( Le_i = 1 \). \( M_b \) still changes rapidly as function of \( s_b \) in the preheating zone and the first part of the reaction zone where the source terms are large. Furthermore, Fig.3 shows that the Markstein numbers both approach an asymptotic value for larger distances \( s_b \) in the burnt gases where the source terms are small. This behaviour is related to the fact that, although the Karlovitz number \( Ka \) increases linearly with \( s_b \) due to an increasing flame thickness \( \delta_f \propto s_b \) when \( \tilde{f} \approx 1 \) in the burnt flame zone, the mass burning rate compensates this rise like \( m_b(s_b) \propto -\rho_b K_b s_b \) (which follows from the continuity equation (16)). It thus may be concluded that the theory and the result for the Markstein number is independent of the choice of \( s_b \) and that we are completely free to choose the burnt flame boundary, as long as it is in the area where the source term is small enough.

Note that the asymptotic values for the Markstein numbers are equal to \( M_b = 1.09 \) when \( f = H_T \) and \( M_b = 0.98 \) when \( f = Y_{CH_4} \). This result is quite close to the expected analytical value \( M_b = 1 \). The result for methane is much better than the Markstein number computed from \( H_T \) because the source term of methane has a more limited range in space, while the source term of \( H_T \) has long tail due to the slow \( CO - CO_2 \) conversion in the burnt gases (see Fig.3). This has such an important effect on the accuracy of the flamelet response because the central assumption (27), introduced in Section 4 to derive the flamelet response model is that the reaction layer is thin. This assumption is a much better for methane which is consumed in a thin layer. This indicates that \( Y_{CH_4} \) is a better choice to serve as progress variable to evaluate the flame response functions.

The proposed description is also independent of the choice of the boundary \( S_u \) in the fresh mixture, because \( \tilde{f} = 0 \) in the area outside the preheating zone, where it does not influence the Karlovitz and Markstein numbers anymore. To show that the stretch rate in the preheating zone does have an influence on the flame response, for instance on the mass burning rate \( m_b \), a number of computations has been carried out with the numerical model, using a constant value for \( \rho K = \rho_b K_b \) not equal to zero in the area \([s_u, s_b] \) and equal to zero outside this region. \( s_b \) is chosen in the burnt gases where the sources are zero, but the position of \( s_u \) is varied in the preheating zone where \( \tilde{f} \neq 0 \). A fit through the obtained results shows that the mass burning rate \( m_b(s_u) \) behaves like \( \frac{m_b}{m_b^*} = 1 - \alpha \frac{\rho_b K_b \delta^*}{m_b^*} (1 - \exp(\frac{\delta_{su}}{\delta^*})) \) as a function of \( s_u \), with \( \alpha \approx 0.99 \), \( \beta \approx 1.05 \). \( \beta \) is not equal to 1 here, because of the temperature dependence of \( \lambda/c_p \). This observation confirms again the validity of the equation for the mass burning rate (63) and in particular the specific form of the Karlovitz numbers, being integrals of \( \rho K \sigma \) weighted with exponential functions \( \tilde{f} \).

In case of weak stretch and an infinite Zeldovich number when the solution of the flamelets is given by (51) and when \( \lambda \) and \( c_p \) are constant, it follows from Eq.(64) that the flame thickness reduces to \( \delta_f = \delta^* = \lambda/(m_b^2 c_p) \). With the numerically evaluated value for \( m_b \) at the position \( s_b \) where the source term reaches its full width half maximum in the burnt
gases, we then find \( g = 0.80 \) when the value for \( \lambda/c_p \) at 1200K is used for the flame thickness \( \delta^* \). The difference with the theoretical value is quite large in this case. Furthermore, it appears that the numerical value for \( M_b \) depends quite strongly on the position \( s_b \) where \( m_b \) is determined (see also Fig.3) and on the temperature, chosen to define the flame thickness \( \delta^* \), because \( \lambda/c_p \) is temperature dependent. This is a problem often encountered in the literature: which position should be chosen to define the flame and how should the flame thickness be defined? This problem is not encountered in the present approach.

The results for the normalised mass burning rate \( m_b/m_0 \) found from the numerical solution of (20) using \( \rho K = \rho_b K_b \) and \( Le_i = 1 \) are combined in Figure 4a as function of the stretchless Karlovitz number \( Ka^0 \) and in Figure 4b as function of the stretched Karlovitz number \( Ka \). The results in Fig.4a show that the deviation from the weak stretch limit (dashed line with Markstein number equal to 1) is not large for \( Ka^0 < 0.5 \), but the deviation is large for \( Ka^0 \) close to 1, where the flames are strongly stretched. Very interesting are the results of Figure 4b which show that \( M_b = 0.98 \) (using methane as progress variable) for the complete range of Karlovitz numbers \( 0 \leq Ka \leq 1 \). This result means that the theory, and specifically Eq.(63), is valid for strong stretch as well, up to the point where \( m_b \rightarrow 0 \) due to flame stretch. Note that this flame is not quenched at \( m_b = 0 \), but that the flow stagnates at \( s = s_b \) in the limit of \( Ka \rightarrow 1 \), so that the mass flow rate at position \( s \) in the flame zone is given by \( m(s) = \rho_b K_b (s_b - s) \). To obtain these results we have chosen the point \( s_b \) in the flue gases where the source term of methane has been decreased by a factor of 10 from its maximum value, but as we already saw, the conclusion is independent of the choice of \( s_b \). Note further that the temperature remains constant \( T_b = T_b^0 = 2012K \) for all Karlovitz numbers (because \( Le_i = 1 \)).

In Figure 5 the flame thickness \( \delta_f \) of Eq.(64) is displayed versus the Karlovitz number \( Ka \). Considering the definitions of \( Ka \) and \( Ka^0 \), it may be concluded that the flame thickness can also be expressed as \( \delta_f = \delta_f^0 \times Ka^0 \) when \( \rho K = \rho_b K_b \) is constant. The variation of the flame thickness \( \delta_f \) due to flame stretch thus also represents the deviation of the exact mass burning rate from the weak stretch limiting behaviour. For small \( Ka \), we approximately have \( \delta_f \approx \delta_f^0 (1 - 0.3 \times Ka^0 + ...) \), so that \( Ka \approx Ka^0 (1 - 0.3 \times Ka^0 + ...) \).

If \( K = K_b \) is constant instead of \( \rho K \), Eq.(63) indicates that the theoretical Markstein number should be equal to
\[
M_b = \int_{s^0}^{s_b} \frac{\rho}{\rho_b} \delta f ds / \int_{s^0}^{s_b} \delta f ds,
\]

instead of one. Note that this theoretical Markstein number is not independent of \( s_b \) now: it decreases asymptotically to 1 for increasing \( s_b \rightarrow \infty \). In Figure 6, we displayed this theoretical Markstein number as a function of \( s_b \), together with the Markstein numbers evaluated from the numerical solution of the flamelet system (20) using \( M_b = -(m_b - m_0^0)/(m_b - 1) / Ka \). As in Fig.3, the results found with \( f = H_T \) and \( f = Y_C H_4 \) are both equal to each other for small \( s_b \) in the preheating zone and they approach the theoretical curve in the burnt gases where the source term is zero. The result for methane is again much closer to
the theoretical curve (a few percent deviation) than the Markstein number of the thermal
enthalpy (ten percent deviation), because of the thinner reaction source term.

It should be noted that the Markstein number of Eq.(65) reduces to

$$\mathcal{M}_b = \left( \frac{\tau + 1}{\tau} \right) \ln(1 + \tau), \quad (66)$$

for weak stretch and infinite Zeldovitz number, when Eq.(51) describes the solution of
\( \dot{H}_T^0(s) \) and \( \dot{Y}_{CH_4}^0(s) \). This relation is also found by Clavin (1985) for \( Le = 1 \) (see Eq.(62)). Using this expression a value of \( \mathcal{M}_b = 2.24 \) is found for the Markstein number, using \( \tau = 5.75 \) (\( T_u = 298 \) K, \( T_b^0 = 2012 \) K for this \( \Phi = 0.8 \) flame). Note that this high value is only reached in Fig.6 by the theoretical curve in the preheating zone. From this comparison it may be concluded that the present approach gives a more accurate representation of the numerical behaviour. Only a small deviation of a few percent is found if methane is used as progress variable.

So far the enthalpy and element mass fractions were conserved due to the fact that the
Lewis numbers were all taken to be unity. We finally study the case of skeletal chemistry,
combined with realistic constant Lewis numbers for all species [20]. The numerically found
variation of the scaled element mass fractions \( \Delta Z_{i,b} \) for \( j = C, H \) and \( O \) and the enthalpy \( \Delta H_b \) due to preferential diffusion is presented in Figure 7a as a function of the Karlovitz
number \( Ka \) in case of constant \( \rho K = \rho_b K_b \). As the equations (40) and (39) for the
prediction of these variations are exact, we don't include the theoretical results. The most
important parts in the variation in enthalpy \( \Delta H_b \) are caused by diffusive fluxes of \( CO \) and
\( H \) radicals, but it appears that these contributions cancel each other almost completely in
\( \Delta H_b \). That these variations, which describe the effects of preferential diffusion, have a very
small effect on the mass burning rate of this methane flame is visible in Figure 7b, where
the numerical results for the stretched mass burning rate \( m_b(G_u, H_b, Z_b)/m_b(G_u, H_b, Z_b) \)
are compared with the theoretical prediction following from

$$m_b(G_{u, H_b, Z_b}) = m_b^0(G_u, H_b, Z_b) (1 - Ka) \quad (67)$$

as function of \( Ka \), taking methane as progress variable again. Note that the sole effect of preferential diffusion, described by \( m_b^0(G_u, H_b, Z_b) - m_b^0(G_u, H_b^0, Z_b^0) \), is very small for this flame. At first this might seem strange because theory predicts that changes in the
temperature are enhanced by the large Zeldovitz number (see also Eqs.(56) and (61)) in the
repons of the mass burning rate. However, it appears that the resulting increase of the
flame temperature \( \Delta T_b \) due to these variations in elements and enthalpy is very small,
at most 4 K for the highest Karlovitz number \( (Ka \approx 0.3) \) in this figure. This explains
the minimal effect of this deviation on the mass burning rate. This observation is also in
accordance with our expectations, because the Lewis number of methane \( Le_{CH_4} = 0.97 \),
which dominates the variation of flame temperature [22], is very close to 1.

It should be stressed that the result for \( m_b^0(G_u, H_b, Z_b) \) is evaluated from a stretchless
flame with 'conserved' values \( Z_b \) and \( H_b \) instead of \( Z_b^0 \) and \( H_b^0 \) for the elements and the
enthalpy. The corresponding initial state for this flame is found by varying the initial

Figure 6

Figure 7
composition of the flame. For the results of \(m_b\) and \(m^0_b\) (with x-symbols) in Figure 7b we have chosen to vary \(Y_{\text{CH}_4,u}, Y_{\text{O}_2,u}, Y_{\text{CO},u}, Y_{\text{H}_2,u}\) (and \(Y_{\text{N}_2,u}\)) to find the correct final element and enthalpy composition. To give an impression of the change in initial composition: for a Karlovitz number of \(\text{Ka} \approx 0.3\) about 10 (mol.) % of the initial fuel consists of \(\text{CO}\) and 15 % of \(\text{H}_2\). The theoretical result for the stretched mass burning rate \(m_b\) (line), evaluated from Eq.(67) is also included in Figure 7b. Note that the result is again close to the numerical behaviour. However, the correspondence is worse than for unit Lewis numbers. It might be guessed that this is related to the choice of initial composition, in which we have a freedom of choice. To check this thought, we performed another series of numerical computations, but now with varying initial values for \(Y_{\text{CH}_4,u}, Y_{\text{CO},u}, Y_{\text{CO}_2,u}, Y_{\text{O}_2,u}\) and \(Y_{\text{N}_2,u}\). The results for \(m^0_b(G_u, H_b, Z_b)\) are also included in Figure 7b (+-symbols). The difference between these two choices is small, but are large enough to justify the conclusion that the differences might be caused by the freedom of choice in the initial composition.

The results presented in this section have shown that the flamelet response is predicted by the algebraic model (46) to within a few percent for this methane/air flame. However, we only presented first numerical results and a more extensive validation is necessary on other flames and other fuels to give conclusive answers. Nevertheless, it can be concluded that the model forms a solid basis for further research into the development of accurate and efficient flamelet models with a sound physical basis.

8 Illustration: Tip of a 2D Stationary Bunsen Flame

So far, we only considered 1D stretched flames and we did not incorporate curved flames in the numerical analysis. In this section we will present a first confrontation of the theory with curved 2D Bunsen flames. In [7] the flame stretch formalism was applied to the numerical results of a 2D stationary, stoichiometric methane/air flammentip, computed using one-step chemistry. The stabilization of this flammentip was studied by computing the local stretch rate and the Karlovitz number. The local variations in the flame temperature due to flame stretch were studied and compared with direct numerical results. The reader is referred to this paper for details. Here we will use the same numerical data to confront a few of the new results of this paper with numerical results and with some new numerical results of the flammentip, computed with skeletal chemistry.

Let us study the local mass burning rate \(m_b\) on the central axis of the flammentip. The mass flow rate \(\rho v\) is presented in Figure 8 as a function of the distance \(y\) on the centre line, together with the stretch rate \(K = v/R - u_x\), the flow straining contribution \(u_x\), the curvature part \(v/R\) and the temperature \(T\) for a flame computed with one-step chemistry and with skeletal chemistry. In [7] 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. This is in accordance with results of the previous section. Using the numerical data in the flammentip, we find a value of \(\text{Ka} \approx -0.50\) using Eq.(36) with \(G = Y_{\text{CH}_4}\), for both flammentips. The term \(\text{Ka}\) in Eq.(67) then has the largest contribution to \(m_b/m^0_b\).
With \( m_b^0 = 0.35kg/(m^2 \text{ s}) \) a mass burning rate of \( m_b = 0.52kg/(m^2 \text{ s}) \) is found for this stoichiometric flame. This value is close to the values for \( (\rho_v)_b = 0.45kg/(m^2 \text{ s}) \) in the burnt gases of the one-step flame and \( (\rho_v)_b = 0.50kg/(m^2 \text{ s}) \) for the skeletal flame (see Figs. 8a,b).

These results indeed confirm the conclusion of Ref.[7]: although the curvature term has the largest contribution to \( \sigma p K \), it is the relatively small flow straining term \( u_x \), which causes a steady decrease of the mass flow rate of \( m_u = 1.2kg/(m^2 \text{ s}) \) in the unburnt gases to \( m_b = 0.50kg/(m^2 \text{ s}) \) in the burnt gases. Flow straining is responsible for the flame stabilization in this flame. 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.

9 Conclusions

The full set of combustion equations is decomposed in three parts: a flow part, the G-equation for the flame motion and a set of quasi-1D stationary flamelet equations for the inner flame structure and mass burning rate. The coupling is described by field quantities for the local flame curvature and stretch rate. The 1D flamelet equations are analysed to derive an efficient flamelet model for premixed flames. The burning velocity of stretched premixed flamelets with multi-component transport and chemistry is studied. Exact equations for the variations in combustion enthalpy and element mass fractions, induced by differential diffusion effects, are derived. Furthermore, approximate expressions are derived for the mass burning rate of stretched flames, in which the variations in the enthalpy and element mass fractions, giving rise to temperature and stoichiometry variations, play a role. The equations are also valid for strong stretch. Special cases of constant \( \rho K \) and constant \( K \) in the flamelets are also studied. For weak stretch and using additional simplifications for the transport and chemistry in the flame, these relations reduce to well-known expressions in established work of Joulin, Clavin and others. The expressions are also validated using a comparison with numerical results of flat skeletal chemistry flames, both in case of weak as in case of strong stretch. Deviations of only a few percent show the validity of the flamelet res pons model, which forms a solid basis for further research on the numerical implementation of laminar and turbulent premixed flamelet models. Some new aspects of the analysis are applied to a numerical study of the stabilization of a 2D Bunsen flametip as an illustration.

10 Acknowledgement

The support of Gastec n.v. and EnergieNed, the Netherlands, is grafully acknowledged.
References

Appendix: Higher-Order Flamelet Closure

Fields for the stretch rate $K(\mathcal{G})$ and curvature $R(\mathcal{G})$ are needed to close the set of equations (46). Furthermore, the curvature and stretch fields are needed to compute the stretched solution in terms of $\tilde{f}(\mathcal{G})$ ($f = Y_i, H_T$). It should be noted though, that the solution of (20) is especially sensitive to the stretch and curvature near the burnt flamelet boundary $\mathcal{G} = \mathcal{G}_b$ (see Eqs.(30), (36), (37)). We therefore propose the following approach:

(a) In Advance of Flame Calculations: Compute and Store Flamelets

Compute a series of solutions of (20) with constant values for $K(\mathcal{G}) = K_b$ and $R(\mathcal{G}) = R_b$ and store $m(\mathcal{G}), \tilde{f}(\mathcal{G})$ as function of enthalpy $H_b$, element composition $Z_{j,b}$, stretch $K_b$ and curvature $R_b$;

(b) During a CFD Calculation:

1. Determine $K(\mathcal{G})$ and $R(\mathcal{G})$ in each flamelet embedded in a 3D flame;
2. Determine the value $K_b = K(\mathcal{G}_b)$ and $R_b = R(\mathcal{G}_b)$ at the burnt flame boundary;
3. Use the stored solution $\tilde{f}(\mathcal{G})$ belonging to $K_b$ and $R_b$ in combination with $K(\mathcal{G})$ and $R(\mathcal{G})$ to determine $K_{a_1}$ and $K_{a_T}$ from Eqs.(36), (37);
4. Evaluate $H_b, Z_{j,b}$ and $m_b = m(\mathcal{G}_b)$ from (46);
5. Compute $m(\mathcal{G})$ in the rest of the flamelet from

$$m = \frac{\sigma_b}{\sigma} m_b + \frac{1}{\sigma} \int_s^{s_b} \sigma \rho K \, dt;$$

(68)

6. Use $m(\mathcal{G})$ and $\tilde{f}(\mathcal{G})$ in the next computational step for the flow-field and the kinematic G-equation (see Fig.2);
7. Repeat (1);

It is, as already indicated, possible to introduce various subtle changes to this approach.
Figure Captions

Figure 1: Generalized coordinate system $\eta = (\xi, \zeta, \eta)$ in a 3D instationary flame. The surfaces with constant $\mathcal{G}$ are the 'flame surfaces'.

Figure 2: Schematic picture of the flamelet model.

Figure 3: Markstein numbers for thermal enthalpy $H_T$ (dashed line) and methane $Y_{CH_4}$ ($\times$ symbols) as function of burnt gas boundary $s_b$, together with their arbitrarily scaled source terms $S_T$ ($\circ$ symbols) and $S_Y$ (drawn line). Lean ($\Phi = 0.8$) flat ($\sigma = 1$) skeletal chemistry flame with $Le_i = 1$ and small stretch rate with $\rho K = \rho_b K_b$ ($Ka_T \approx 0.01$).

Figure 4: Ratio of stretched and stretchless mass burning rate $m_b/m_b^0$ as function of stretchless Karlovitz number $Ka^0$ (a) and stretched Karlovitz number $Ka$ (b). Dashed line: weak-stretch limit. Lean ($\Phi = 0.8$) flat ($\sigma = 1$) skeletal chemistry flame with $Le_i = 1$ and small constant value of $\rho K = \rho_b K_b$ ($Ka_T \approx 0.01$).

Figure 5: 'Stretched' flame thickness $\delta = \int \dot{Y}_{CH_4}(s)ds$ as function of stretched Karlovitz number $Ka$. Lean ($\Phi = 0.8$) flat ($\sigma = 1$) skeletal chemistry flame with $Le_i = 1$ and small constant value of $\rho K = \rho_b K_b$ ($Ka_T \approx 0.01$).

Figure 6: Markstein numbers for thermal enthalpy $H_T$ (dashed line) and methane $Y_{CH_4}$ ($\times$ symbols) as function of burnt gas boundary $s_b$, together with their arbitrarily scaled source terms $S_T$ ($\circ$ symbols) and $S_Y$ ($\Delta$ symbols). The drawn line represents the theoretical Markstein number. Lean ($\Phi = 0.8$) flat ($\sigma = 1$) skeletal chemistry flame with $Le_i = 1$ and small constant stretch rate $K = K_b$ ($Ka_T \approx 0.01$).

Figure 7a: Variation in element mass fractions $\Delta Z_{j,b}$ ($j = C, H, O$) scaled with initial values $Z_{j,u}$ and variation in enthalpy $\Delta H_b$ scaled with $H_{T,b} - H_{T,u}$, as function of Karlovitz number $Ka$. Skeletal chemistry adiabatic methane/air flame ($\Phi = 0.8$); $\rho K = \rho_b K_b$.

Figure 7b: Scaled mass burning rate $m_b(G_u, H_b, Z_b)/m_b^0(G_u, H_b, Z_b)$ (line: theory according to Eq.(46); $\circ$-symbols: numerical results), sole effect of preferential diffusion $m_b^0(G_u, H_b, Z_b)/m_b^0(G_u, H_b^0, Z_b^0)$ ($\times$ symbols: $CO/H_2$ in initial mixture; $*$ symbols: $CO/CO_2$ in initial mixture). Skeletal chemistry adiabatic methane/air flame $\Phi = 0.8$; $\rho K = \rho_b K_b$.

Figure 8: Mass flow rate $\rho v$, stretch rate $K = v/R - u_x$, flame curvature $v/R$, flow straining $u_x$ and temperature $T$ through the flame tip; 2D methane/air Bunsen flame with $\Phi = 1.0$ and $v_{max} = 0.8 m/s$, one-step chemistry (a) and skeletal chemistry (b).
Fig. 1, de Goey et al. Combust. Flame
Flow and Mixing

* Navier-Stokes: \( \dot{v}, p \)
* Enthalpy: \( H \)
* Elements: \( Z_j \)

\[ \begin{align*}
\text{G-eqn: } G \\
\text{Stretch: } K \\
\text{Area: } \sigma
\end{align*} \]

Flamelets

* Mass fractions: \( Y_i \)
* Temperature: \( T \)
* Density: \( \rho \)
* Mass burning rate: \( m \)

Fig. 2 L.P.H. de Goey et al.
Fig. 3  L.P.H. de Goey et al.
Fig. 4a L.P.H. de Goey
Fig. 4b  L.P.H. de Goey et al.
Fig. 5 L.P.H. de Goey et al.
Fig. 6  L.P.H. de Goey et al.
Fig. 7a  L.P.H. de Goey et al.
Fig. 7b L.P.H. de Goey et al.
One-step chemistry

![Graph showing temperature (T), density (ρν), and shear stress (-v/R - K) as functions of vertical distance along the centerline (m).]

- Values of Kν, Eν, and Kν scaled with a factor T
- T, T, T

Skeletal chemistry

![Graph showing temperature (T), density (ρν), and shear stress (-v/R - K) as functions of vertical distance along the centerline (m).]

- u T, u T, u T
- u T, u T, u T

vertical distance along centerline [m]