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Mass burning rate of premixed stretched flames: integral analysis versus large activation energy asymptotics

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Abstract. New expressions for the mass burning rate are derived from a recently introduced flamelet model using Integral Analysis and results are compared with well-known expressions, based on Large Activation Energy Asymptotics. There is no restriction on Lewis numbers and the expressions reduce to the same results as found earlier with asymptotic techniques if Lewis numbers are close to 1. From our analysis it appears that the burnt edge of a stretched flamelet is most appropriate to determine the mass burning rate. The consequences for experimental and numerical studies are investigated.

Keywords: premixed stretched flames, flat stagnation flame, flamelet model, integral analysis, large activation energy asymptotics, mass burning rate, Karlovitz integral, Markstein number.

1 Introduction

It is well known that flame stretch plays an important role in the dynamics, stability and structure of premixed flames. Stretch effects were first studied by Karlovitz et al. [14], Lewis and von Elbe [15] and Markstein [16] to investigate flame extinction, flame stabilization and flame front instability. Since these early publications, significant progress has been made in the understanding of flame stretch and in particular the structure, propagation and dynamics of stretched flames has been studied in numerous papers using Large Activation Energy Asymptotics (LAEA); see e.g., Buckmaster [5], Matalon [17] and Matalon and Matkowsky [18]. Clavin [7] and Clavin and Williams [8] rigorously derived expressions for the mass burning rate using LAEA for flames described by simple chemistry and Lewis numbers close to 1. This theory has been used, for instance, in laminar flamelet models for turbulent premixed flames, see e.g., Peters [21]. Chung and Law [6] used another approach, the Integral Analysis (IA), to study stretched flames. Identical phenomena are predicted with their theory, although the resulting expressions are different. The LAEA and IA theories have never been compared in a thorough way so far.

Using the IA in a rigorous way, de Goey et al. [10, 12, 11] and ten Thijs Boonkkamp et al. [23, 24] studied the mass burning rate of stretched flames with multiple-species transport and chemistry. They introduced a mass-based stretch field for a spatially resolved flame and derived expressions for the mass burning rate, containing integrals of the stretch field, describing the flame response. There is no restriction on the Lewis numbers. In the present paper we will use this approach to show that LAEA results, first found by Joulin and Clavin [13], are recovered with the IA method to lowest-order in the Zeldovich number for flat, weakly strained flames when density variations are neglected and for Lewis numbers close to 1. Furthermore, the same results as derived by Clavin and Williams [7, 8] are found to lowest order in the Zeldovich number when density variations due to the gas expansion are included, again for Lewis numbers close to 1. Finally, from a (theoretical and numerical) investigation of the spatially resolved stretched flame, it is shown that the mass burning rate in the burnt mixture (and the

corresponding Markstein number) is more accurate to describe the actual behaviour of the stretched mass burning rate in premixed flames. This is very important for the quantitative interpretation of experimental and numerical data of stretched flames. If not the burnt flame edge but another position is chosen to derive the mass burning rate, correction terms have to be used, which are also derived in this paper.

The paper is organized as follows. In Section 2, we summarize the flamelet model of de Goeij and ten Thije Boonkkamp. General expressions for the mass-burning rate m_b in the burnt gases of stretched flames are presented in Section 3. These expressions have been applied with success in the last few years to analyse and describe strong stretch effects in turbulent flames in case of unit Lewis numbers [19] and in weakly stretched flames governed by multiple-species chemistry and transport with non-unit Lewis numbers [22]. In Section 4, we study the mass burning rate m_b for the case of flat weakly strained premixed flames without gas expansion, described by a one-step irreversible reaction. Variations in the density caused by gas expansion are studied in the subsequent section. The mass burning rate m_u in the unburnt gases is studied in Section 6. Different results are found for the Markstein numbers in the burnt (\mathcal{M}_b) and unburnt (\mathcal{M}_u) gases. In Section 7 our analysis shows that the Markstein numbers for the burnt gases previously found by Joulin and Clavin [13] and Clavin [8] are reproduced for Lewis numbers close to 1. For the unburnt gases, the Markstein number of Clavin and Williams [7] is also found if Lewis numbers are close to 1. A clear physical picture of how m_u and m_b are to be interpreted inside the flame structure is also presented in Section 7.

2 Flamelet model for premixed stretched flames

In this section we summarize the flamelet model for premixed, stretched flames, as introduced in our papers [10, 12, 23].

We define a flame as the region in space where a suitable progress variable \mathcal{Y} assumes values between the unburnt (\mathcal{Y}_u) and burnt (\mathcal{Y}_b) values, in other words, it consists of the preheat zone and the reaction layer. For \mathcal{Y} we may take, e.g., one of the species mass fractions Y_i or the temperature T , provided $\nabla\mathcal{Y} \neq \mathbf{0}$ everywhere in the flame. In this paper we choose $\mathcal{Y} = T$. We introduce flame surfaces as isotherms, i.e., surfaces where $T(\mathbf{x}, t) = \text{Const}$, and define a curvilinear coordinate system $\boldsymbol{\xi} = (\xi^1, \xi^2, \xi^3)$ by the relations

$$T(x_1, x_2, x_3, t) = T(\xi^1), \quad \frac{\partial \mathbf{x}}{\partial \xi^1} \cdot \frac{\partial \mathbf{x}}{\partial \xi^\alpha} = 0 \quad (\alpha = 2, 3) \quad \text{for} \quad T_u \leq T \leq T_b, \quad (2.1)$$

i.e., the coordinate surfaces $\xi^1 = \text{Const}$ coincide with flame surfaces and the ξ^1 -coordinate lines are orthogonal to the ξ^α -coordinate lines ($\alpha = 2, 3$). Note that the ξ^1 -coordinate is not uniquely defined by the relations in (2.1), since these also hold for $f(\xi^1)$ with f a sufficiently smooth and monotone function. In each flame surface, (ξ^2, ξ^3) is a curvilinear coordinate system, not necessarily orthogonal, and will not be further specified. For time-dependent flames, the flame surfaces will move in the spatial domain with velocity $\mathbf{v}_f = \mathbf{v} + s_L \mathbf{n}$, where \mathbf{v} is the local flow velocity, s_L the local laminar burning velocity and \mathbf{n} the unit normal directed towards the unburnt gas mixture, resulting in a time dependent coordinate system $\boldsymbol{\xi} = \boldsymbol{\xi}(\mathbf{x}, t)$. Moreover, we introduce the variable τ as the time corresponding to the curvilinear coordinate system. Obviously, $\tau = t$.

In the flamelet model that follows, we use the mass based definition of the stretch rate K [11], that is an extension of the usual definition [26] and applicable to flames of finite thickness. It is defined as

$$K := \frac{1}{M} \frac{dM}{dt} \quad \text{with} \quad M(t) := \int_{\Omega(t)} \rho dV, \quad (2.2)$$

where $d/dt := \partial/\partial t + \mathbf{v}_f \cdot \nabla$ is the time derivative when following the flame surfaces and where ρ is the density of the gas mixture, i.e., K is the fractional rate of change of the mass $M(t)$ contained in a

small volume $\Omega(t)$ in the flame, moving with velocity \mathbf{v}_f . Applying the transport theorem [2] to (2.2), we obtain the following expression for K :

$$\rho K = \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}_f). \quad (2.3)$$

Formulated in $(\boldsymbol{\xi}, \tau)$ -variables, the expression for K reads

$$K = \frac{1}{\sqrt{g}} \frac{\partial}{\partial \tau} (\sqrt{g}) + \frac{1}{\rho} \frac{\partial \rho}{\partial \tau}, \quad (2.4)$$

where \sqrt{g} is the Jacobian of the coordinate transformation $\mathbf{x} \mapsto \boldsymbol{\xi}$, given by

$$\sqrt{g} = h_1 \sigma, \quad h_1 := \left| \frac{\partial \mathbf{x}}{\partial \xi^1} \right|, \quad \sigma := \left| \frac{\partial \mathbf{x}}{\partial \xi^2} \times \frac{\partial \mathbf{x}}{\partial \xi^3} \right|. \quad (2.5)$$

Clearly, $dV := \sqrt{g} d\xi^1 d\xi^2 d\xi^3$ is the volume element in the $\boldsymbol{\xi}$ -coordinate system, $dS := \sigma d\xi^2 d\xi^3$ is the area element on a flame surface $\xi^1 = \text{Const}$ and $ds := h_1 d\xi^1$ is the arc-length element along a ξ^1 -coordinate line. Apart from the usual terms related to flame curvature and flow straining, relation (2.4) for K incorporates additional terms, e.g., due to flame thickness variations. Note that K is a scalar field, defined in the entire flame zone, whereas in other theories the stretch rate is restricted to a single flame surface.

The set of governing equations for premixed flames can be classified in the following three groups, i.e., first, the flamelet equations for the *combustion variables* Y_i, T and the mass burning rate $m := \rho s_L$, describing transport and chemistry in the flame, second, the momentum equations coupled with the flamelet equations for the specific enthalpy h and element mass fractions Z_j , describing flow and mixing without chemical reactions, and third, a kinematic equation describing the motion of the flame. We have derived the first system of equations by rewriting the corresponding conservation equations in terms of the curvilinear coordinate system $\boldsymbol{\xi}$ and inserting expression (2.3) for the stretch rate; for more details see e.g. [12, 25]. This way we obtain the following set of quasi-one-dimensional flamelet equations

$$\frac{\partial}{\partial s} (\sigma m) = -\sigma \rho K, \quad (2.6a)$$

$$\frac{\partial}{\partial s} (\sigma m Y_i) - \frac{1}{Le_i} \frac{\partial}{\partial s} \left(\sigma \frac{\lambda}{c_p} \frac{\partial Y_i}{\partial s} \right) = \sigma (\omega_i - \rho K Y_i), \quad (i = 1, \dots, N_s), \quad (2.6b)$$

$$\frac{\partial}{\partial s} (\sigma m T) - \frac{1}{c_p} \frac{\partial}{\partial s} \left(\sigma \lambda \frac{\partial T}{\partial s} \right) = \sigma (\omega_T - \rho K T), \quad \omega_T := \frac{-1}{c_p} \sum_{i=1}^{N_s} h_i \omega_i. \quad (2.6c)$$

Other variables/parameters in (2.6) are the number of different species N_s , the species reactions rates ω_i , the temperature source term ω_T , the thermal conductivity λ , the specific heat (at constant pressure) c_p and the Lewis numbers Le_i (assumed to be constant). In the derivation of (2.6) we have assumed that conduction and diffusion fluxes along the flame surfaces are negligible compared to the stretch terms, proportional to K , which is justified in the so-called flamelet combustion regime where chemistry is fast compared to the flow time scales. We further assumed that all specific heats are equal and constant, i.e., $c_{p,i} = c_p$. The set has to be closed with an equation of state, which for constant ambient pressure p_{amb} , describing low Mach number deflagrations, may be written as

$$\frac{\rho R T}{M} = p_{\text{amb}}, \quad \frac{1}{M} = \sum_{i=1}^{N_s} \frac{Y_i}{M_i}, \quad (2.7)$$

with R the universal gas constant, M the average molar mass of the mixture and M_i the species molar masses.

Since the mass burning rate depends on the enthalpy and element composition in the reaction layer [12], we have to take into account the flamelet equations for the specific enthalpy h and the mass fractions Z_j of the N_e elements involved. Recall, that these variables are defined by

$$h = \sum_{i=1}^{N_s} h_i Y_i, \quad h_i = h_{i,\text{ref}} + \int_{T_{\text{ref}}}^T c_{p,i}(T') dT', \quad Z_j := \sum_{i=1}^{N_s} w_{j,i} Y_i, \quad (j = 1, \dots, N_e), \quad (2.8)$$

where h_i , $h_{i,\text{ref}}$ and $c_{p,i}$ are the specific enthalpy, the specific enthalpy of formation at reference temperature T_{ref} and the specific heat (at constant pressure), respectively, of species i . Moreover, the coefficients $w_{j,i}$ are defined by $w_{j,i} := W_j \mu_{j,i} / M_i$, with W_j the molar mass of element j and $\mu_{j,i}$ the number of atoms of element j in species i . Analogous to the derivation of (2.6) we find

$$\frac{\partial}{\partial s}(\sigma m h) - \frac{\partial}{\partial s} \left(\sigma \frac{\lambda}{c_p} \frac{\partial h}{\partial s} \right) - \sum_{i=1}^{N_s} \left(\frac{1}{Le_i} - 1 \right) \frac{\partial}{\partial s} \left(\sigma \frac{\lambda}{c_p} h_i \frac{\partial Y_i}{\partial s} \right) = -\sigma \rho K h, \quad (2.9a)$$

$$\frac{\partial}{\partial s}(\sigma m Z_j) - \frac{\partial}{\partial s} \left(\sigma \frac{\lambda}{c_p} \frac{\partial Z_j}{\partial s} \right) - \sum_{i=1}^{N_s} \left(\frac{1}{Le_i} - 1 \right) w_{j,i} \frac{\partial}{\partial s} \left(\sigma \frac{\lambda}{c_p} \frac{\partial Y_i}{\partial s} \right) = -\sigma \rho K Z_j, \quad (j = 1, \dots, N_e). \quad (2.9b)$$

Note that the flamelet equations (2.9) do not contain a chemical source term, and for that reason we refer to h and Z_j as the *conserved variables*. Moreover, the set of equations (2.9b) is of course *not* independent of (2.6b).

3 Mass burning rate: the general case

We derive a general expression for the mass burning rate m_b at the burnt side of the flame. This mass burning rate depends on the conserved variables $\psi := (h, Z_j)$ in the burnt mixture, which we therefore determine first from the corresponding flamelet equations.

Suppose, $\sigma = \sigma(s)$ and $K = K(s)$ are given along an s -coordinate line. Integrating the flamelet equations (2.9) across the flame, we obtain

$$\Delta h := h_b - h_u = \frac{-1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) (h(s) - h_u) ds, \quad (3.1a)$$

$$\Delta Z_j := Z_{j,b} - Z_{j,u} = \frac{-1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) (Z_j(s) - Z_{j,u}) ds, \quad (j = 1, \dots, N_e), \quad (3.1b)$$

where we have assumed that all diffusive/conductive fluxes vanish at the unburnt (at $s = s_u$) and the burnt (at $s = s_b$) sides of the flame. The subscripts b and u denote the value of the corresponding variable in the burnt and unburnt gas, respectively. For the special case of a stretchless flame, i.e., $K = 0$, we obtain $\Delta h^0 = 0$ and $\Delta Z_j^0 = 0$ ($j = 1, \dots, N_e$), where the superscript 0 indicates that the variable is considered to be the solution of the corresponding stretchless flamelet equation. Using the expressions for h and Z_j in (2.8), we can derive the following formulae for Δh and ΔZ_j :

$$(1 + K a_{T,b}) \Delta h = - \sum_{i=1}^{N_s} \left(\frac{K a_{i,b}}{Le_i} - K a_{T,b} \right) h_{i,\text{ref}} (Y_{i,b} - Y_{i,u}), \quad (3.2a)$$

$$(1 + K a_{T,b}) \Delta Z_j = - \sum_{i=1}^{N_s} \left(\frac{K a_{i,b}}{Le_i} - K a_{T,b} \right) w_{j,i} (Y_{i,b} - Y_{i,u}), \quad (j = 1, \dots, N_e), \quad (3.2b)$$

where the Karlovitz integrals $Ka_{T,b}$ and $Ka_{i,b}$ are defined by, respectively,

$$Ka_{T,b} := \frac{1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) \tilde{T}(s) ds, \quad (3.3a)$$

$$Ka_{i,b} := \frac{Le_i}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) \tilde{Y}_i(s) ds, \quad (i = 1, \dots, N_s). \quad (3.3b)$$

In (3.3) we introduced the normalized variables $\tilde{T}(s)$ and $\tilde{Y}_i(s)$, defined by

$$\tilde{f}(s) := \frac{f(s) - f_u}{f_b - f_u}, \quad (f = Y_i, T). \quad (3.4)$$

Clearly, $0 = \tilde{f}_u \leq \tilde{f}(s) \leq \tilde{f}_b = 1$ for $s_u \leq s \leq s_b$. Thus, $Ka_{T,b}$ is the weighted fbw rate $\sigma(s)\rho(s)K(s)\tilde{T}(s)$ along the flame surfaces, integrated across the flame and scaled with the normal mass fbw rate $(\sigma m)_b$; a similar interpretation holds for $Ka_{i,b}$.

An expression for the mass burning rate m_b of a premixed flame can be derived in a similar manner. Integrating the flamelet equation (2.6c) for the temperature across the flame, we obtain the relation [12]

$$(1 + Ka_{T,b})m_b(\psi_b) = m_b^0(\psi_b), \quad (3.5)$$

where we have explicitly denoted the dependence of m_b and m_b^0 on the vector ψ_b . Note that the variable $m_b^0(\psi_b)$ in the right hand side of (3.5) is the mass burning rate of a stretchless flame, however, to be evaluated as a function of the state vector ψ_b of a stretched flame. In the derivation of (3.5) it has been assumed, first, that the reaction zone is infinitely thin and, second, that the conductive flux vanishes at the burnt and unburnt sides of the flame. There are no other assumptions introduced and the relations (3.2), (3.3) and (3.5) together describe the effect of flame stretch and preferential diffusion on the mass burning rate of premixed flames. There is in principle no restriction on the stretch rate, curvature or reaction mechanism. It has been shown in a number of recent publications that this model accurately describes these influences for strongly stretched turbulent flames, modelled using DNS including reduced chemistry in the form of the flamelet-generated manifold technique and unit Lewis numbers [19, 4]. Furthermore, it was recently observed that the model also successfully predicts stretch related phenomena in weakly stretched methane and propane flames, modelled using complex chemistry in combination with non-unit Lewis numbers [22].

In the following we restrict ourselves to weak stretch because existing theories based on LAEA are restricted to weak stretch. Then, taking into account that $m_b^0 = m_b^0(\psi_b^0)$, $h_b = h_b^0 + \Delta h$ and $Z_{j,b} = Z_{j,b}^0 + \Delta Z_j$ ($j = 1, \dots, N_e$), we can expand $m_b^0(\psi_b)$ in a Taylor series, to obtain

$$\frac{m_b - m_b^0}{m_b^0} = -Ka_{T,b} + \Delta h \frac{\partial}{\partial h_b} (\ln m_b^0) + \sum_{j=1}^{N_e} \Delta Z_j \frac{\partial}{\partial Z_{j,b}} (\ln m_b^0) + \text{h.o.t.} \quad (3.6)$$

Expression (3.6) is only applicable to weakly stretched flames, i.e., K is small enough to neglect second (and higher) order terms in the Karlovitz integrals; see (3.2) and (3.3). Otherwise, we can use both expressions (3.5) and (3.6) for arbitrary flames with multiple-species chemistry and transport. Thus, we do not have to impose any restrictions on the Lewis numbers, unlike in asymptotic theories, where $|Le_i - 1|$ are assumed to be small (of the order of the reciprocal Zeldovich number).

Summarizing, the derivation of an expression for the mass burning rate requires the following steps. First, we have to solve the flamelet equations (2.6) for the normalized combustion variables $\tilde{Y}_i(s)$ and $\tilde{T}(s)$, either analytically or numerically. In the following sections, we will use analytical expressions for $\tilde{Y}_i^0(s)$ and $\tilde{T}^0(s)$, assuming constant coefficients. Second, we have to compute the Karlovitz integrals

in (3.3). With regard to the density in these integrals, we distinguish two case, i.e., constant density and variable density. Third, we determine from (3.2) the differences Δh and ΔZ_j due to differential diffusion and flame stretch. Finally, assuming that K is small enough to neglect higher order terms, we have to evaluate expression (3.6).

4 Mass burning rate: the constant density approximation

We will elaborate the formulae (3.2), (3.3) and (3.6) for the special case of a lean stagnation flame in a constant density fbw, thus we ignore expansion of the gas mixture due to combustion. So, consider a model flame determined by a one-step irreversible reaction $\mathcal{F} \rightarrow \mathcal{P}$, with one rate determining lean species \mathcal{F} . The main assumptions are:

- I The flame is flat, i.e., $\sigma(s) = 1$.
- II Both species have the same Lewis number, i.e., $Le_{\mathcal{F}} = Le_{\mathcal{P}} = Le$.
- III The thermal conductivity λ and the specific heat c_p are constant.
- IV The flame is weakly stretched.
- V The density is constant, i.e., $\rho(s) = \text{Const} = \rho_b^0$.
- VI The reaction zone is infinitely thin and located at $s = s_b = 0$ and the preheat zone extends to infinity, i.e., $s_u \rightarrow -\infty$.

As a consequence of assumption IV, we can neglect the higher order terms in (3.6) and replace the combustion variables in (3.2) and (3.3) by their stretchless counterparts. Moreover, we can prove that in the preheat zone $K(s)$ is nearly constant and equal to the applied strain rate a ; see the Appendix. Therefore, we take $K(s) = a$ in the preheat zone.

First, we solve the stretchless flamelet equations (2.6) for the combustion variables $\tilde{T}^0(s)$, $\tilde{Y}_{\mathcal{F}}^0(s)$ and $\tilde{Y}_{\mathcal{P}}^0(s)$. Note that $m^0(s) = \text{Const} = m_u^0 = m_b^0 = m^0$. Since the reaction zone is considered infinitely thin, we can replace the thermal/chemical source terms by delta functions, i.e., $\omega_T = Q\delta(s)$, where the coefficient Q should be chosen such that $T(s)$ remains bounded for $s \rightarrow \infty$, and likewise for ω_i . This way, we obtain in the preheat zone $s < 0$ the solution

$$\tilde{T}^0(s) = e^{\eta(s)}, \quad \tilde{Y}_{\mathcal{F}}^0(s) = \tilde{Y}_{\mathcal{P}}^0(s) = e^{Le\eta(s)}, \quad \eta(s) := \frac{s}{\delta_f}, \quad \delta_f := \frac{\lambda}{m^0 c_p}, \quad (4.1)$$

where $\eta(s)$ is the scaled coordinate in the preheat zone and δ_f is the thermal thickness of the stretchless flame. On the other hand, in the burnt gas mixture, we have $\tilde{T}^0(s) = \tilde{Y}_{\mathcal{F}}^0(s) = \tilde{Y}_{\mathcal{P}}^0(s) = 1$, with $s > 0$ the usual Cartesian coordinate; see Figure 1.

Substituting the stretchless solution (4.1) in (3.3), we obtain the following expressions for the Karlovitz integrals

$$Ka_{T,b} = Ka_{\mathcal{F},b} = Ka_{\mathcal{P},b} = Ka_b, \quad Ka_b := \frac{a\delta_f\rho_b^0}{m^0}, \quad (4.2)$$

where Ka_b is the usual Karlovitz number at the burnt side of the flame.

Next, we have to compute the differences Δh and ΔZ_j . Since the one-step reaction $\mathcal{F} \rightarrow \mathcal{P}$ involves only one element, its mass fraction Z has to be constant, i.e., $Z(s) = \text{Const}$, and consequently all ΔZ_j -terms in (3.6) cancel. Taking into account that \mathcal{F} and \mathcal{P} have the same Lewis number and Karlovitz integral, we can write the Δh -term as

$$\begin{aligned} \Delta h &= (h_{\mathcal{F},\text{ref}}Y_{\mathcal{F},u}^0 - h_{\mathcal{P},\text{ref}}Y_{\mathcal{P},b}^0) \left(\frac{1}{Le} - 1 \right) Ka_b + \mathcal{O}(Ka_b^2) \\ &= c_p(T_b^0 - T_u^0) \left(\frac{1}{Le} - 1 \right) Ka_b + \mathcal{O}(Ka_b^2). \end{aligned} \quad (4.3)$$

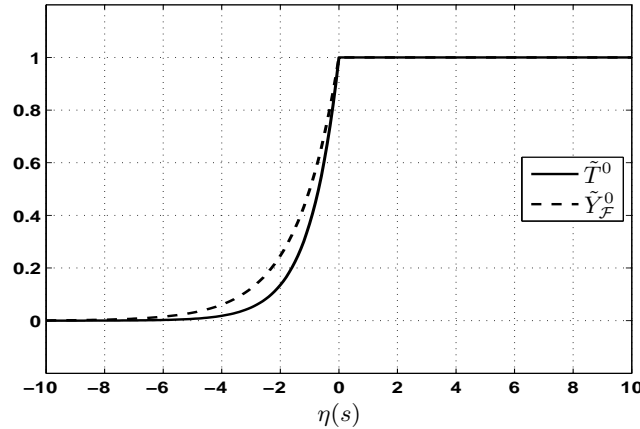


Figure 1: The normalized variables $\tilde{T}^0(s)$ and $\tilde{Y}_{\mathcal{F}}^0(s)$, for $Le = 0.7$, as a function of the dimensionless coordinate $\eta(s)$.

The second equality in (4.3) follows readily from the definition of h in (2.8) and the relation $\Delta h^0 = 0$. For the mass burning rate m^0 we adopt the same model as used by Barenblatt et al. [3], i.e.,

$$m^0 = m^0(T_b) = Ae^{-T_a/(2T_b)}, \quad (4.4)$$

where $T_a := E_a/R$ is the activation temperature and E_a the activation energy. Combining (3.6), (4.2)-(4.4) and applying the chain rule

$$\frac{\partial}{\partial h_b}(\ln m^0) = \frac{1}{c_p} \frac{\partial}{\partial T_b}(\ln m^0),$$

we get the following relation

$$\begin{aligned} \frac{m_b - m^0}{m^0} &= -Ka_b + c_p(T_b^0 - T_u^0) \left(\frac{1}{Le} - 1 \right) Ka_b \frac{T_a}{2(T_b^0)^2} \frac{1}{c_p} + \mathcal{O}(Ka_b^2) \\ &= - \left(1 + \frac{Ze}{2} \left(1 - \frac{1}{Le} \right) \right) Ka_b + \mathcal{O}(Ka_b^2), \end{aligned} \quad (4.5)$$

where $Ze := T_a(T_b^0 - T_u^0)/((T_b^0)^2)$ is the Zeldovich number [27]. Finally, we can rewrite relation (4.5) in the equivalent form

$$\frac{m_b - m^0}{m^0} = -\mathcal{M}_b Ka_b + \mathcal{O}(Ka_b^2), \quad (4.6)$$

where \mathcal{M}_b is the Markstein number given by

$$\mathcal{M}_b = 1 + \frac{Ze}{2} \left(1 - \frac{1}{Le} \right). \quad (4.7)$$

The Markstein number is a measure for the relative change in the mass burning rate m_b due to flame stretch. The second term in \mathcal{M}_b accounts for preferential diffusion when $Le \neq 1$.

5 Mass burning rate: variable density

In a similar way as in Section 4, we derive an expression for the mass burning rate m_b , however, this time for variable density, thus accounting for gas expansion due to combustion. All assumptions remain valid, except assumption V. Instead, we determine the density from the equation of state (2.7). Consequently, we have the following expression for the density in the preheat zone

$$\rho^0(s) = \frac{\rho_b^0 T_b^0}{T^0(s)} = \rho_b^0 \frac{\theta + 1}{1 + \theta \tilde{T}^0(s)}, \quad \theta := \frac{T_b^0 - T_u^0}{T_u^0} = \frac{\rho_u^0 - \rho_b^0}{\rho_b^0}; \quad (5.1)$$

see Figure 2. In the derivation of (5.1) we have used that $\rho^0(s)T^0(s) = \text{Const} = \rho_b^0 T_b^0$, which is a consequence of the equation of state (2.7) and the assumption that $M = \text{Const}$. The parameter θ is the thermal expansion coefficient. Obviously, in the burnt gas mixture $\rho(s) = \rho_b^0$. Thus we can interpret the preheat zone as a layer of variable density connecting the incompressible unburnt and burnt gas mixtures. The expressions in (4.1) for the combustion variables in the preheat zone still hold.

Substituting the formulae for $\rho^0(s)$ and $\tilde{T}^0(s)$ in (3.3a), we obtain the following expression for the Karlovitz integral $Ka_{T,b}$,

$$Ka_{T,b} = Ka_b(\theta + 1) \frac{\ln(\theta + 1)}{\theta}. \quad (5.2)$$

Likewise, substituting the expressions for $\rho^0(s)$, $\tilde{T}^0(s)$ and $\tilde{Y}_{\mathcal{F}}^0(s)$ in (3.3b), we obtain for $Ka_{\mathcal{F},b}$ the expression,

$$\frac{Ka_{\mathcal{F},b}}{Le} = Ka_b(\theta + 1) \int_0^1 \frac{\nu^{Le-1}}{1 + \theta\nu} d\nu. \quad (5.3)$$

The integral in (5.3) can be expressed in terms of hypergeometric functions; see e.g. [1]. Note, that in the limit for $\theta \rightarrow 0$ the expressions for $Ka_{T,b}$ and $Ka_{\mathcal{F},b}$ reduce to the ones in (4.2).

Next, we have to compute the enthalpy difference Δh . Analogous to the derivation in the previous section, we find

$$\Delta h = c_p(T_b^0 - T_u^0) \left(\frac{Ka_{\mathcal{F},b}}{Le} - Ka_{T,b} \right) + \mathcal{O}(Ka_b^2), \quad (5.4)$$

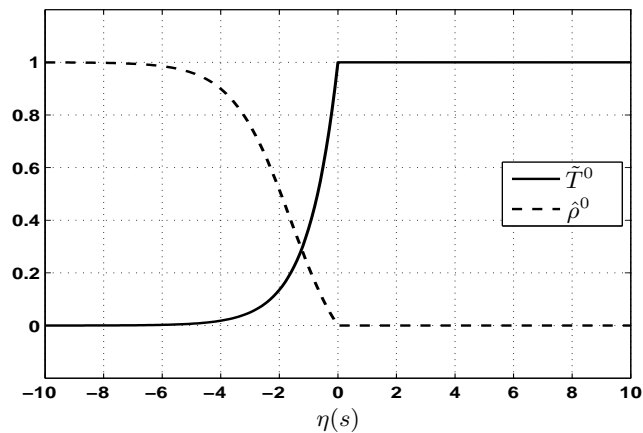


Figure 2: The normalized variables $\tilde{T}^0(s)$ and $\hat{\rho}^0(s) := 1 - \tilde{\rho}^0(s)$, for $\theta = 5$, as a function of the dimensionless coordinate $\eta(s)$.

with $Ka_{T,b}$ and $Ka_{\mathcal{F},b}$ given in (5.2) and (5.3), respectively. Using relation (4.4) for the mass burning rate m^0 , we get the following generalisation of (4.5),

$$\frac{m_b - m^0}{m^0} = -Ka_{T,b} + \frac{Ze}{2} \left(\frac{Ka_{\mathcal{F},b}}{Le} - Ka_{T,b} \right) + \mathcal{O}(Ka_b^2). \quad (5.5)$$

Applying integration by parts to the integral in (5.3) and subsequently substituting the resulting expression for $Ka_{\mathcal{F},b}/Le - Ka_{T,b}$ in (5.5), we obtain the familiar relation (4.6), with the Markstein number \mathcal{M}_b given by

$$\mathcal{M}_b = (\theta + 1) \frac{\ln(\theta + 1)}{\theta} + \frac{Ze}{2} (Le - 1) \frac{\theta + 1}{\theta} \int_0^1 \nu^{Le-2} \ln(1 + \theta\nu) d\nu. \quad (5.6)$$

The first term in \mathcal{M}_b describes the effect of gas expansion on the mass burning rate m_b and the second term the effect of preferential diffusion. Note that for $\theta \rightarrow 0$ expression (5.6) reduces to (4.7).

6 The mass burning rate in the unburnt mixture

In the previous sections we derived expressions for the mass burning rate m_b at the burnt side of the flame, i.e., at the reaction layer. Alternatively, in this section we derive a model for the mass burning rate m_u in the unburnt gas mixture, equivalent to the model for m_b presented in Section 3. First, we give alternative expressions for Δh and ΔZ_j . Analogous to the derivation of (3.2), we find

$$(1 + Ka_{T,u}) \Delta h = - \sum_{i=1}^{N_s} \left(\frac{Ka_{i,u}}{Le_i} - Ka_{T,u} \right) h_{i,\text{ref}} (Y_{i,b} - Y_{i,u}), \quad (6.1a)$$

$$(1 + Ka_{T,u}) \Delta Z_j = - \sum_{i=1}^{N_s} \left(\frac{Ka_{i,u}}{Le_i} - Ka_{T,u} \right) w_{j,i} (Y_{i,b} - Y_{i,u}), \quad (j = 1, \dots, N_e), \quad (6.1b)$$

where the Karlovitz integrals $Ka_{T,u}$ and $Ka_{i,u}$ are defined by, respectively,

$$Ka_{T,u} := \frac{-1}{(\sigma m)_u} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) (1 - \tilde{T}(s)) ds, \quad (6.2a)$$

$$Ka_{i,u} := \frac{-Le_i}{(\sigma m)_u} \int_{s_u}^{s_b} \sigma(s) \rho(s) K(s) (1 - \tilde{Y}_i(s)) ds, \quad (i = 1, \dots, N_s), \quad (6.2b)$$

i.e., the Karlovitz integral $Ka_{T,u}$ is the weighted fbw rate $\sigma(s)\rho(s)K(s)(1 - \tilde{T}(s))$, integrated across the flame and scaled with the normal mass fbw rate $(\sigma m)_u$ and likewise for $Ka_{i,u}$. From their definitions and the flamelet equation (2.6a), we can derive the following relations between the Karlovitz integrals $Ka_{T,b}$, $Ka_{\mathcal{F},b}$ for the burnt side of the flame, and $Ka_{T,u}$, $Ka_{\mathcal{F},u}$ for the unburnt side, i.e.,

$$(\sigma m)_b (Ka_{T,b} + 1) = (\sigma m)_u (Ka_{T,u} + 1), \quad (6.3a)$$

$$(\sigma m)_b (Ka_{\mathcal{F},b} + Le_i) = (\sigma m)_u (Ka_{\mathcal{F},u} + Le_i). \quad (6.3b)$$

Next, equivalent to relation (3.5), we have the following relation for m_u ,

$$(1 + Ka_{T,u}) m_u(\psi_b) = m_u^0(\psi_b), \quad (6.4)$$

where we again assume that m_u^0 depends on the conserved variables ψ_b in the *burnt* gas mixture. For weakly stretched flames, we can expand $m_u^0(\psi_b)$ in a Taylor series, to find

$$\frac{m_u - m_u^0}{m_u^0} = -Ka_{T,u} + \Delta h \frac{\partial}{\partial h_b} (\ln m_u^0) + \sum_{j=1}^{N_e} \Delta Z_j \frac{\partial}{\partial Z_{j,b}} (\ln m_u^0) + \text{h.o.t.} \quad (6.5)$$

Summarizing, the model for m_u consists of either relation (6.4) or (6.5), coupled with (6.1) and (6.2) to determine the differences Δh and ΔZ_j .

In the following, we restrict ourselves to the variable density case of the stagnation flame of the previous sections, and use the stretchless variables in (4.1) to derive expressions for the Karlovitz integrals and the difference Δh . Straightforward substitution of (4.1) and (5.1) in (6.2) would lead to divergent Karlovitz integrals for $s_u \rightarrow -\infty$. The reason for this divergence is that $(1 - \tilde{T}(s))K(s) \neq 0$ in the entire flame and does not tend to 0 for $s \rightarrow -\infty$. Consequently, the mass burning rate m_u becomes unbounded for $s_u \rightarrow -\infty$, in agreement with the flamelet equation (2.6a). To remedy this problem, we cut off the integration interval at some finite reference value s_{ref} . Then, substituting $\nu = \exp(s/\delta_f)$ and applying the method of partial fractions, we obtain

$$Ka_{T,u} \sim Ka_u \left(\eta_{\text{ref}} + (\theta + 1) \frac{\ln(\theta + 1)}{\theta} \right), \quad \eta_{\text{ref}} := \frac{s_{\text{ref}}}{\delta_f}, \quad Ka_u := \frac{a\delta_f \rho_u^0}{m^0}, \quad (6.6a)$$

$$\frac{Ka_{\mathcal{F},u}}{Le} \sim Ka_u \left(\eta_{\text{ref}} + \ln(\theta + 1) + \int_0^1 \frac{\nu^{Le-1}}{1 + \theta\nu} d\nu \right), \quad (6.6b)$$

where Ka_u is the Karlovitz number in the unburnt gas mixture. Note that $Ka_u = (\theta + 1)Ka_b$. Next, we have to derive an expression for Δh from (6.1a). Applying the same assumptions as before, we find

$$\Delta h = c_p(T_b^0 - T_u^0) \left(\frac{Ka_{\mathcal{F},u}}{Le} - Ka_{T,u} \right) + \mathcal{O}(Ka_u^2). \quad (6.7)$$

Note from relations (6.6), that the Karlovitz integrals diverge, whereas Δh remains bounded for $\eta_{\text{ref}} \rightarrow -\infty$. Substituting (6.7) in relation (6.5), we find for the relative change in m_u the following expression

$$\frac{m_u - m^0}{m^0} = -Ka_{T,u} + \frac{Ze}{2} \left(\frac{Ka_{\mathcal{F},u}}{Le} - Ka_{T,u} \right) + \mathcal{O}(Ka_u^2). \quad (6.8)$$

Finally, substituting the expressions for the Karlovitz integrals in (6.6) and applying integration by parts to the integral involved, we can rewrite relation (6.8) in the form

$$\frac{m_u - m^0}{m^0} = -\mathcal{M}_u(\eta_{\text{ref}})Ka_u + \mathcal{O}(Ka_u^2), \quad (6.9)$$

where the Markstein number at the unburnt side of the flame is given by

$$\begin{aligned} \mathcal{M}_u(\eta_{\text{ref}}) &= \eta_{\text{ref}} + (\theta + 1) \frac{\ln(\theta + 1)}{\theta} + \frac{Ze}{2}(Le - 1) \frac{1}{\theta} \int_0^1 \nu^{Le-2} \ln(1 + \theta\nu) d\nu \\ &= \eta_{\text{ref}} + \frac{1}{\theta + 1} \mathcal{M}_b + \ln(\theta + 1). \end{aligned} \quad (6.10)$$

Thus, expressions (4.6) and (5.6) for m_b and \mathcal{M}_b can be used to determine the influence of flame stretch on the mass burning rate in the burnt gases at the reaction layer $\eta(s) = 0$. On the other hand, expressions (6.9) and (6.10) for m_u and \mathcal{M}_u describe what happens in the unburnt gases, but as there is no natural

position in the unburnt gases, the reference position $\eta = \eta_{\text{ref}}$ indicates the point where m_u is considered. Thus, compared to expression (5.6) for \mathcal{M}_b , this expression contains the additional term η_{ref} , that accounts for the finite thickness of the preheat zone. Note that the above relation implies that there is a difference between m_u and m_b given by

$$\frac{m_u - m_b}{m^0} = (-\eta_{\text{ref}} - \ln(\theta + 1))Ka_u, \quad (6.11)$$

which is not equal to zero even if they are evaluated at the same position, i.e., if we choose $\eta_{\text{ref}} = 0$. The term proportional to $\ln(\theta + 1)$ is related to the gas expansion in the preheat zone. In the limit of no expansion, i.e., $\theta \rightarrow 0$, relation (6.10) reduces to

$$\mathcal{M}_u(\eta_{\text{ref}}) = 1 + \eta_{\text{ref}} + \frac{Ze}{2} \left(1 - \frac{1}{Le}\right) = \mathcal{M}_b + \eta_{\text{ref}}, \quad (6.12)$$

which gives identical Markstein numbers and mass burning rates at $\eta_{\text{ref}} = 0$.

7 A review on the mass burning rate

In this final section we review the relations for the mass burning rate derived in the previous sections. In particular, we compare it to results obtained with LAEA from literature and show the consistency of our model. Finally, we will discuss the implications for numerical and experimental studies.

In order to compare our results with literature, we first have to relate our stretch rate K with the classical stretch rate κ , which is used in flame sheet models, where flames are considered a single surface separating the burnt and unburnt gases. It is defined as the fractional rate of change of the area element on the flame sheet, when it is moving with velocity v_f . For a properly defined coordinate system $\xi = \xi(x, t)$ for which the scale factor $h_1 = \text{Const}$, we have

$$K = \kappa + \frac{1}{\rho} \frac{\partial \rho}{\partial \tau}, \quad \kappa := \frac{1}{\sigma} \frac{\partial \sigma}{\partial \tau}, \quad (7.1)$$

with σ defined in (2.5). Since by definition $\partial T / \partial \tau = 0$ and $\rho T = \text{Const}$ by virtue of the equation of state (2.7), we also have $\partial \rho / \partial \tau = 0$, and consequently $K = \kappa$. We like to emphasize that this equality only holds at the flame sheet, since κ is not defined elsewhere. Next, we will reformulate our results in terms of the burning velocity s_L . Assuming weak stretch, so that we can replace ρ_b by ρ_b^0 , we obtain at the burnt side of the flame

$$\frac{s_{L,b} - s_{L,b}^0}{s_{L,b}^0} = -\mathcal{M}_b Ka_b + \mathcal{O}(Ka_b^2), \quad Ka_b := \frac{\kappa \delta_f}{s_{L,b}^0}, \quad (7.2)$$

with the Markstein number \mathcal{M}_b defined in (4.7) for the constant density approximation, and in (5.6) for variable density. Relation (7.2) was previously derived by Joulin and Clavin [13] for the constant density case and by Clavin [7] for the variable density case. However, their Markstein numbers differ slightly from ours. In particular, according to Joulin and Clavin [13]

$$\mathcal{M}_b = 1 + \frac{Ze}{2}(Le - 1), \quad (7.3a)$$

whereas Clavin obtained the result [7]

$$\mathcal{M}_b = (\theta + 1) \frac{\ln(\theta + 1)}{\theta} + \frac{Ze}{2}(Le - 1) \frac{\theta + 1}{\theta} \int_0^1 \nu^{-1} \ln(1 + \theta \nu) d\nu. \quad (7.3b)$$

In their derivations, they considered the flame as a surface separating the (incompressible) burnt and unburnt gas mixtures. They first integrated the conservation equations across the reaction zone, to give boundary conditions and jump conditions for the flow in the (un)burnt gas mixtures, which they subsequently solved using asymptotic expansions. However, in their derivations they had to assume that $|Le - 1| = \mathcal{O}(1/Ze)$, so that (7.3a) and (7.3b) are to lowest order in $1/Ze$ equal to (4.7) and (5.6), respectively. Our expressions do not suffer from this assumption and are valid for general Lewis numbers.

Alternatively, at the unburnt side of the flame we have

$$\frac{s_{L,u} - s_{L,u}^0}{s_{L,u}^0} = -\mathcal{M}_u(\eta_{\text{ref}})Ka_u + \mathcal{O}(Ka_u^2), \quad Ka_u := \frac{\kappa\delta_f}{s_{L,u}^0}, \quad (7.4)$$

with the Markstein number $\mathcal{M}_u(\eta_{\text{ref}})$ given in (6.10). A very similar result was obtained by Clavin and Williams [7]; they found (7.4), with Markstein number \mathcal{M}_u given by

$$\mathcal{M}_u = (\theta + 1) \frac{\ln(\theta + 1)}{\theta} + \frac{Ze}{2}(Le - 1) \frac{1}{\theta} \int_0^1 \nu^{-1} \ln(1 + \theta\nu) d\nu. \quad (7.5)$$

Apart from the small difference in the preferential diffusion term, again due to the fact that Clavin and Williams had to assume $|Le - 1| = \mathcal{O}(1/Ze)$, the term η_{ref} is also missing. This is a consequence of their model, where the entire flame is considered a surface, i.e., they implicitly take $\eta_{\text{ref}} = 0$.

This shows indeed that the LAEA theory uses the position $s = 0$ (at the reaction layer) to identify the unburnt mass burning rate m_u as well as the burnt mass burning rate m_b . This is a direct consequence of the LAEA theory which assumes that the complete flame structure is viewed as an interface (at $s = 0$) separating unburnt and burnt gases, in contrast with the Integral Analysis where the flame zone has a finite thickness. What the LAEA theory implicitly comes down to is that the asymptotic behaviour of $m(s)$ in the (un)burnt gases is evaluated and that it is extrapolated linearly to the position $s = 0$ to identify the reported results for m_b and m_u . Or, alternatively, the limit of an infinitely thin flame is taken, i.e., $\delta_f \rightarrow 0$ (reaction layer including preheat zone). This procedure gives different results for m_b and m_u (or \mathcal{M}_b and \mathcal{M}_u), although they are evaluated at the same point.

To understand this difference more clearly, let us now study the variation of $m(s)$ in the flame. We will consider two cases: as reference we will consider the theoretical model considered in this paper where the preheat zone thickness is infinite, while the reaction layer is infinitely thin (see Figure 3) and compare this with a numerical simulation where both the reaction layer and the preheat zone have a finite thickness (see Figure 4). We can determine the mass burning rate $m(s)$ from the first flamelet equation in (2.6), that describes conservation of mass. Thus, integrating equation (2.6a) from $s = s_b = 0$, where the infinitely thin reaction layer is situated, to a location $s \neq 0$ in either the preheat zone or the burnt gas mixture, we obtain

$$m(s) - m_b = -a \int_0^s \rho^0(s') ds', \quad (7.6)$$

where we have replaced ρ by its stretchless counterpart ρ^0 . Note that we have taken $K(s) = a$, which is justified for the complete preheat zone and the burnt gas mixture in the vicinity of the reaction layer; see Appendix. In the burnt gas mixture, for $s > 0$, we may take $\rho^0(s) = \rho_b^0$, to find the mass burning rate linearly decreasing with $\eta(s)$, i.e.,

$$\frac{m(s) - m_b}{m^0} = -Ka_b\eta(s), \quad (7.7)$$

which has been plotted in Figure 3. This linear decrease of $m(s)$ in the burnt gases can also be seen in Figure 4, that presents numerical results for a weakly strained lean methane-air flame (equivalence ratio

$\varphi = 0.7$, strain rate $a = 10 \text{ s}^{-1}$) computed from the full set of conservation equations using GRI-mech 3.0. Let us next investigate $m(s)$ in the preheat zone, i.e., for $-\infty < s \leq 0$. Substituting expression (5.1) for $\rho^0(s)$ in (7.6), we obtain the following relation

$$\frac{m(s) - m_b}{m^0} = K a_b (\theta + 1) \left(-\eta(s) + \ln \left(\frac{\theta e^{\eta(s)} + 1}{\theta + 1} \right) \right). \quad (7.8)$$

This relation is also plotted in Figure 3 and is similar to the numerical results in Figure 4. Theoretical and numerical results are almost identical in the complete flame except in the neighbourhood of the reaction layer, as expected. If we now take the limit $s \rightarrow -\infty$, we recover relation (6.11), as found from the Integral Analysis presented in the previous section:

$$\frac{m(s) - m_b}{m^0} \sim K a_u (-\eta(s) - \ln(\theta + 1)). \quad (7.9)$$

This means that the mass burning rate $m(s)$ is also linearly varying with $\eta(s)$ in the preheat zone, sufficiently far away from the reaction layer. However, substituting $\eta(s) = 0$ in the left hand side of (7.9), we obtain for the mass burning rate the extrapolated value $m^*(0) := m_b - \ln(\theta + 1) K a_u m^0 \neq m_b$, due to expansion of the gas mixture. If we next replace the mass burning rate m_u by $m(s_{\text{ref}})$, and if we take $|s_{\text{ref}}|$ large enough, we have

$$\begin{aligned} \frac{m_u}{m^0} &\sim \frac{m_b}{m^0} + (-\eta_{\text{ref}} - \ln(\theta + 1)) K a_u \\ &= 1 - \mathcal{M}_b K a_b + (-\eta_{\text{ref}} - \ln(\theta + 1)) K a_u + \mathcal{O}(K a_b^2) \\ &= 1 - \mathcal{M}_u(\eta_{\text{ref}}) K a_u + \mathcal{O}(K a_u^2), \end{aligned} \quad (7.10)$$

implying also that the relations (4.6) and (6.9) with the Markstein numbers \mathcal{M}_b and $\mathcal{M}_u(\eta_{\text{ref}})$ defined in (5.6) and (6.10), respectively, are consistent with the model presented in the previous sections. Finally, if we let the flame shrink to a surface, i.e., $\eta_{\text{ref}} \rightarrow 0$, we recover from (7.9) relation (6.11):

$$\frac{m_u - m_b}{m^0} = -\ln(\theta + 1) K a_u. \quad (7.11)$$

This way, we can define two alternative mass burning rates, one at the reaction zone at $s = 0$ and one extrapolated from the unburnt gas mixture, and the difference between these is given by (7.11), and only when $\theta = 0$ these are equal. Alternatively, we can derive (7.11) from the relations (4.6) and (6.9).

Figure 3 clearly shows that the mass burning rate m_b in the burnt gases gives a more accurate representation of the mass burning rate of stretched flames, because the extrapolated value $m^*(0)$ deviates considerably from $m(0)$. One should realize, though, that the reaction layer is in reality not infinitely thin. In case of a finite reaction layer thickness, the value for m_b describes the asymptotic behaviour of $m(s)$ in the burnt gases, extrapolated to the heart of the reaction layer at $s = 0$, e.g., the position of the maximum heat release. In that case, m_b is not exactly on the $m(s)$ curve either because $m(s)$ is not completely linear then for $s > 0$. However, m_b is much closer to $m(0)$ than $m^*(0)$, because the reaction layer is much thinner than the preheat zone. In other words, the 'error' in the Markstein number \mathcal{M}_b is of the order of $\delta_r/\delta_f = 1/Ze$, where δ_r is the reaction layer thickness, while it is of the order of 1 in the Markstein number of the unburnt gas \mathcal{M}_u .

A very important question is what can be learnt from this. First of all, it should be noted that in general, the burning velocity s_L at the *unburnt* flame boundary is used as reference value. For instance, in experiments on spherically expanding flames one often uses Schlieren photography to determine the unburnt boundary or another position in the flame to derive s_L or the Markstein number. The above analysis shows that m_b is more appropriate than m_u to predict the mass burning rate in the flame structure.

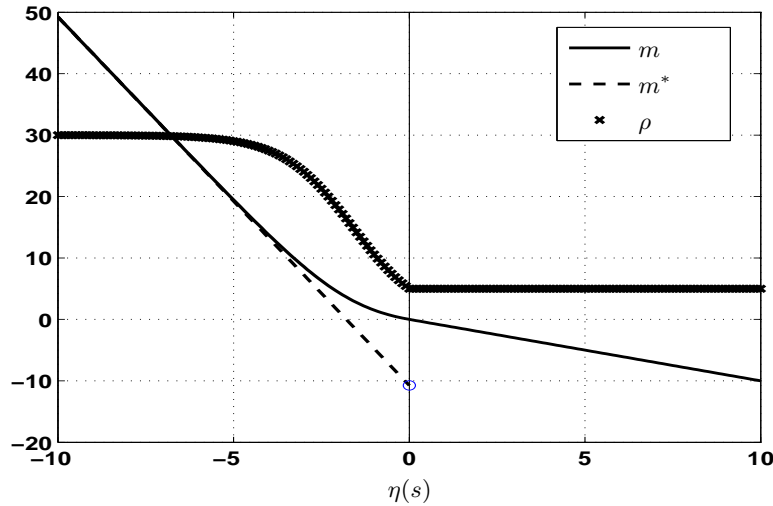


Figure 3: The (scaled) mass burning rate $m(s)$ and density $\rho(s)$ of a flame with infinitely thin reaction layer at $\eta(s) = 0$ subject to a constant stretch rate $K(s) = a$.

We therefore suggest to use the burnt flame boundary instead of the unburnt boundary as a reference to determine the mass burning rate in experiments. If another position is preferred for some reason, one should bear in mind that the use of (6.9) and (6.10) could lead to inaccuracies. However, accurate predictions of the mass burning rate $m(s)$ at other positions in the flame structure are possible if we take m_b as reference value and apply the correction suggested by (7.9).

8 Conclusions

A recently introduced theory using Integral Analysis to describe the influence of flame stretch on the mass burning rate of premixed flames has been elaborated for general flames and for flat weakly strained flames governed by simple chemistry. New expressions are derived for the Markstein numbers in the burnt and unburnt mixture for general Lewis numbers, and it has been shown that these expressions become identical to previous results found by Joulin et al. [13] and Clavin et al. [7, 8] in the limit of small values for $|Le - 1| = \mathcal{O}(1/Ze)$. A clear physical picture of how $m^*(0)$ and m_b are to be interpreted inside the flame structure is presented, i.e., $m^*(0)$ is the asymptotic behavior of $m(s)$ in the unburnt mixture and m_b is the asymptotic behavior of $m(s)$ in the burnt mixture, both extrapolated linearly to the reaction layer at $s = 0$. From this analysis it appears that the mass burning rate m_b in the burnt gases seems to be more accurate than $m^*(0)$ to identify the mass burning rate of stretched flames. Furthermore, an additional correction is derived to describe the mass burning rate in experimental and numerical studies, in which another position is preferred to identify the burning velocity.

A The stretch rate of a plane stagnation flame

In this appendix we derive expressions for the stretch rate $K(s)$ of a plane stagnation flame and show that it is nearly constant in the entire preheat zone and in the burnt gas mixture close to the reaction layer, provided the flame is only weakly stretched. Therefore, we restrict ourselves to weakly stretched flames, i.e., the Karlovitz number $Ka_b \ll 1$. In this appendix we frequently refer to the parameters δ_f , Ka_b and

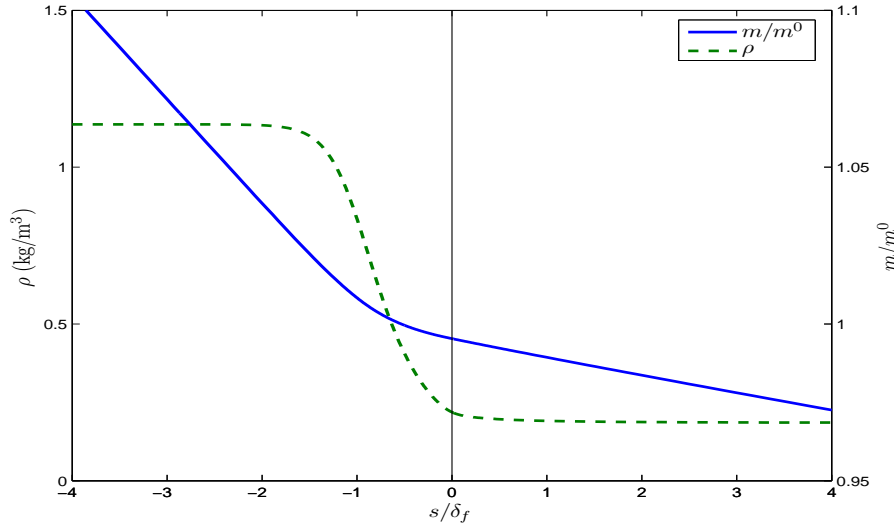


Figure 4: The mass burning rate $m(s)$ and the density $\rho(s)$ of a methane/air flame computed numerically from the flamelet equations (2.6) using GRI-mech 3.0. Parameter values are: $\varphi = 0.7$, $a = 10 \text{ s}^{-1}$, $\delta_f = 6.22 \times 10^{-2} \text{ cm}$, $m^0 = 2.13 \times 10^{-2} \text{ gr}/(\text{cm}^2\text{s})$.

θ , which are defined in (4.1), (4.2) and (5.1), respectively.

From the momentum equations, describing the two-dimensional stagnation flow in the flame, we can derive the following differential equation for K [9, 20]:

$$m \frac{dK}{ds} - \frac{d}{ds} \left(\mu \frac{dK}{ds} \right) = \rho_u a^2 - \rho K^2, \quad (\text{A.1})$$

where μ is the dynamic viscosity of the gas mixture and a the applied strain rate at the unburnt side of the flame. This equation has to be coupled with flamelet equation (2.6a), with $\sigma(s) = 1$, in order to determine $K(s)$ and $m(s)$. We derive approximate solutions of these equations, separately for the preheat zone and for the burnt gas mixture. Let ℓ be the stand-off distance, i.e., the stagnation plane is located at $s = \ell$, and assume that $\ell \gg \delta_f$. Applying an appropriate scaling to (A.1) and (2.6a), with length scales δ_f for the preheat zone and ℓ for the burnt gas mixture, respectively, we conclude that in the preheat zone the convective and viscous terms are of comparable size whereas the stretch terms in both equations are negligible. On the other hand, in the burnt gas mixture, the viscous term is negligible but the stretch terms have to be included. Finally, taking μ constant, replacing $m(s)$ in the preheat zone by m^0 , ρ_u by ρ_u^0 and $\rho(s)$ in the burnt gas by ρ_b^0 , we obtain the following set of equations

$$m^0 \frac{dK}{ds} - \mu \frac{d^2 K}{ds^2} = 0, \quad -\infty < s < 0, \quad (\text{A.2a})$$

$$m \frac{dK}{ds} = \rho_u^0 a^2 - \rho_b^0 K^2, \quad \frac{dm}{ds} = -\rho_b^0 K, \quad 0 < s < \ell, \quad (\text{A.2b})$$

which we have to solve subject to the following boundary conditions

$$K(-\infty) = a, \quad \frac{dK}{ds}(\ell) = 0, \quad m(\ell) = 0. \quad (\text{A.2c})$$

Moreover, we require continuity of $K(s)$, $\frac{dK}{ds}(s)$ and $m(s)$ at $s = 0$.

The solution of equation (A.2a), subject to the first boundary condition in (A.2c), reads

$$K(s) = a \left(1 + A e^{\eta(s)/Pr} \right), \quad \eta(s) := \frac{s}{\delta_f}, \quad -\infty < s < 0, \quad (\text{A.3})$$

where A is a coefficient to be determined later and $Pr := \mu c_p / \lambda$ is the Prandtl number of the gas mixture. The solution of (A.2b) is more involved. Combining both equations, we obtain the following differential equation for the mass burning rate m :

$$m \frac{d^2 m}{ds^2} - \left(\frac{dm}{ds} \right)^2 + \rho_u^0 \rho_b^0 a^2 = 0. \quad (\text{A.4})$$

The solution of (A.4), subject to the third boundary condition in (A.2c), can be written in the form $m(s) = -B \sin q\eta(s - \ell)$ with $B, q > 0$, provided $Bq/\delta_f = a\sqrt{\rho_u^0 \rho_b^0}$. Substituting this expression in the second equation in (A.2b), we obtain

$$K(s) = a\sqrt{\theta + 1} \cos q\eta(s - \ell), \quad 0 < s < \ell. \quad (\text{A.5})$$

The solution in (A.3) and (A.5) contains three unknown constants, viz. A, q and ℓ , that we determine from continuity of $K(s)$, $\frac{dK}{ds}(s)$ and $m(s)$ at $s = 0$. This gives the following set of nonlinear equations

$$1 + A = \sqrt{\theta + 1} \cos q\eta(\ell), \quad \eta(\ell) = \frac{\ell}{\delta_f}, \quad (\text{A.6a})$$

$$A = Prq\sqrt{\theta + 1} \sin q\eta(\ell), \quad (\text{A.6b})$$

$$m^0 q = a\delta_f \rho_b^0 \sqrt{\theta + 1} \sin q\eta(\ell). \quad (\text{A.6c})$$

Using the Taylor series $\sqrt{1+x} = 1 + \frac{1}{2}x - \frac{1}{8}x^2 + \mathcal{O}(x^3)$ for $x \rightarrow 0$, we can show that the solution of (A.6), to first order accuracy, is given by

$$A = \theta Pr K a_b + \mathcal{O}(K a_b^2), \quad (\text{A.7a})$$

$$q = \sqrt{\theta} K a_b + \mathcal{O}(K a_b^2), \quad (\text{A.7b})$$

$$\tan\left(\frac{q\ell}{\delta_f}\right) = \sqrt{\theta} + \mathcal{O}(K a_b^2). \quad (\text{A.7c})$$

Combining the solutions in (A.3) and (A.5), we have

$$K^*(s) := \frac{K(s) - a}{a} = \begin{cases} A e^{\eta(s)/Pr}, & -\infty < s < 0, \\ \sqrt{\theta + 1} \cos q(\eta(s) - \ell) - 1, & 0 < s < \ell, \end{cases} \quad (\text{A.8})$$

with the parameters A, q and ℓ given in (A.7); see Figure 5. Clearly, the relative deviation of $K(s)$ from a is at most 2×10^{-2} in the preheat zone. Note that also in the burnt gas mixture, close to the reaction layer, $K^*(s)$ is still small. For example, $K^*(s) < 0.1402$ for $0 \leq \eta(s) \leq 5$. Finally, note that $\ell \gg \delta_f$ indeed, as we assumed in the derivation of (A.2).

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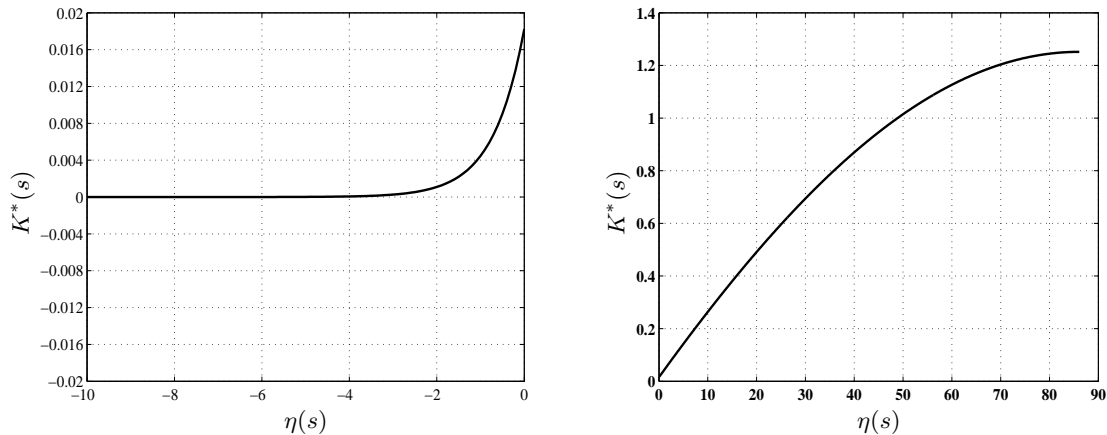


Figure 5: $K^*(s)$ of a flame with infinitely thin reaction layer at $\eta(s) = 0$, in the preheat zone (left) and in the burnt gas mixture (right). Parameter values are: $a = 10 \text{ s}^{-1}$, $Pr = 0.71$, $\theta = 4$, $\delta_f = 6.22 \times 10^{-2} \text{ cm}$ and $Ka_b = 6.4 \times 10^{-3}$.

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