

# A comparison of the integral analysis and large activation energy asymptotics for studying flame stretch

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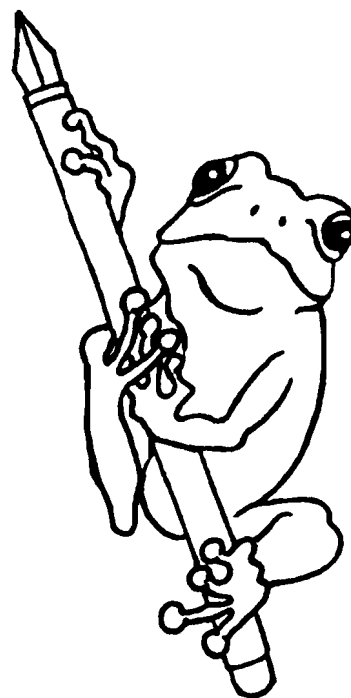
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# A Comparison of the Integral Analysis and Large Activation Energy Asymptotics for Studying Flame Stretch

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**ABSTRACT** - Expressions for the mass burning rate derived recently with the Integral Analysis are compared with well-known expressions by Joulin, Clavin and Williams, based on Large Activation Energy Asymptotics. Equivalent results are found for the asymptotic behaviour of the mass burning rate in the burnt and unburnt gases for the special case in which the flame is subject to a flow with a constant value of the flame stretch rate  $K$  in the flame zone. This applies to the case where gas expansion is neglected as well as when it is taken into account properly. It is shown that the Integral Analysis does not only predict identical Markstein numbers in the asymptotic regions of the flame as the asymptotic methods do, but also describes the mass burning rate in the complete internal flame structure.

*Key Words: Flame stretch, Large Activation Energy Asymptotics, Integral Analysis*

## 1 Introduction

Flame stretch is an important quantity in the understanding of flame phenomena such as extinction and the local structure of turbulent flames. Stretch effects were first studied by Karlovitz et al. (1953) and Lewis and von Elbe (1961) to study flame extinction and flame stabilization. Markstein (1964) investigated the influence of stretch on flame front instability. Since these early publications, significant progress has been made in the understanding of flame stretch and in particular the structure, propagation and dynamics of stretched flames has been studied in numerous papers using Large Activation Energy Asymptotics (LAEA), see e.g. Buckmaster (1979), Matalon and Matkowsky (1982) and Matalon (1983). Clavin and Williams (1982) and Clavin (1985), for instance, rigorously

derived expressions for the mass burning rate, taking into account density variations in the flame. This theory has been used for instance in laminar flamelet models for turbulent premixed flames, see e.g. Peters (1992). Chung and Law (1988) used another approach, the Integral Analysis (IA), to study stretched flames. Identical phenomena are predicted with their theory, although the resulting expressions are different and have lead, so far, to different results. An analysis of differences between the LAEA and IA theories has never been performed so far.

In some recent papers, de Goeij et al. (1996), (1997a), (1997b) and ten Thijs Boonkcamp et al. (1997a), (1997b) used the IA method to study the mass burning rate of stretched flames with multiple-species transport and chemistry. A mass-based flame stretch field has been introduced and expressions containing integrals of the stretch field through the flamelet are derived describing the flame response. The mass burning rate of lean methane/air flames has been computed for the case in which the flame is stabilised in a flow with a constant value for the density weighted stretch rate  $\rho^0 K$ . In the present paper we will use this approach to show that the LAEA results of Joulin and Clavin (1979) are recovered with the IA method to lowest-order in the Zeldovich number for constant  $K$  and when density variations are neglected. Furthermore, the same results as Clavin and Williams (1982,1985) are found to lowest order in the Zeldovich number when density variations due to the gas expansion are included, i.e. when the stretch rate  $K$  is taken to be constant instead of  $\rho^0 K$ .

The paper is organized as follows. In Section 2, we summarize the approach of de Goeij and ten Thijs Boonkcamp. Expressions are presented for the mass-burning rate  $m_b$  in the burnt gases of stretched flames. In Section 3, we study the mass burning rate  $m_b$  for the special case of a constant stretch rate  $K$  and constant density  $\rho^0$  in the flame, described by a one-step irreversible reaction. The analysis shows that the Markstein number  $\mathcal{M}_b$  found by Joulin and Clavin (1979) is recovered in this case. Variations in the density  $\rho^0$  caused by gas expansion are studied in the subsequent section. Different results are found for the Markstein number in the burnt ( $\mathcal{M}_b$ ) and unburnt ( $\mathcal{M}_u$ ) gases. For the burnt gases, the result  $\mathcal{M}_b$  of Clavin (1985) is reproduced. The mass burning rate in the unburnt gases  $m_u$  is analysed subsequently in Section 5 and the Markstein number  $\mathcal{M}_u$  of Clavin and Williams (1982) is found in the limit of an infinitely thin flame thickness. The behaviour of the local mass burning rate in the internal flame structure, predicted with the IA method, is studied in the final section. It is shown that the IA method describes the structure of the mass burning rate  $m(s)$  in the complete domain of the flame  $s_u < s < s_b$ , between the unburnt ( $s_u$ ) and burnt ( $s_b$ ) flame boundaries. The results show the equivalence of the LAEA and IA theories and that the LAEA asymptotic results are recovered from the IA results for infinitely thin flames.

## 2 Mass Burning Rate of Stretched Flames

A premixed flame is defined as the region in space, where a scalar variable  $\mathcal{Y}$  assumes values between the unburnt ( $\mathcal{Y}_u$ ) and burnt ( $\mathcal{Y}_b$ ) values. For  $\mathcal{Y}$  we may use for instance

one of the species mole numbers, which obeys  $|\nabla\mathcal{Y}| \neq 0$ . In this paper, however, we choose  $\mathcal{Y} = T$ . A 'flame surface' is defined as an iso-plane of  $\mathcal{Y}$ , i.e. a surface where  $\mathcal{Y}(\mathbf{x}, t) = \text{constant}$ . A local orthogonal coordinate system  $\boldsymbol{\eta} = (\xi, \zeta, \eta)$  (see Figure 1) is defined in terms of these flame surfaces. The coordinates  $\xi, \zeta$  constitute an orthogonal system in each flame surface and  $\eta$  is the coordinate perpendicular to the flame surfaces. The factors  $h_\xi = |\frac{\partial\mathbf{x}}{\partial\xi}|$ ,  $h_\zeta = |\frac{\partial\mathbf{x}}{\partial\zeta}|$  and  $h_\eta = |\frac{\partial\mathbf{x}}{\partial\eta}|$  are scale factors, defining the arc-lengths in the  $\boldsymbol{\eta}$ -coordinate system.

In this coordinate system, a set of quasi-1D stationary flamelet equations for the mass burning rate  $m = \rho s_L$ , the  $N_s$  species mole numbers  $\phi_i$  and the temperature  $T$  can be derived from the set of 3D combustion equations (de Goey, 1996, ten Thije Boonkkamp, 1997a,b):

$$\begin{aligned} \frac{\partial}{\partial s}(\sigma m) &= -\sigma \rho K, \\ \frac{\partial}{\partial s}(\sigma m \phi_i) - \frac{\partial}{\partial s}(\sigma \rho D_{im} \frac{\partial \phi_i}{\partial s}) - \sigma \omega_i &= -\sigma \rho K \phi_i, \quad (i = 1, \dots, N_s), \\ \frac{\partial}{\partial s}(\sigma m T) - \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} \frac{\partial T}{\partial s}) - \sigma \omega_T &= -\sigma \rho K T, \end{aligned} \quad (1)$$

where the coordinate  $s$  is the arc length through the flame, defined by  $ds = h_\eta d\eta$ , and  $\sigma = |\frac{\partial\mathbf{x}}{\partial\xi} \times \frac{\partial\mathbf{x}}{\partial\zeta}| = h_\xi h_\zeta$  is a measure of the local flame surface area. In (1),  $\omega_i$  is the chemical source term of species  $i$  and  $\omega_T$  is the source term of the temperature. Furthermore,  $\lambda$ ,  $c_p$  and  $D_{im}$  denote the thermal conductivity, specific heat and diffusion coefficient of species  $i$  in the mixture, respectively. The set is closed with an equation of state, which, for constant pressure  $p_u$  (describing low Mach number deflagarations) may be written as:

$$\rho R T \sum_{i=1}^{N_s} \phi_i = p_u. \quad (2)$$

To derive Eq.(1), it has been assumed that terms associated with diffusion fluxes along the flame iso-planes are negligible compared to the stretch terms, proportional to  $K$  (ten Thije Boonkkamp, 1997a). Although the set (1) describes the internal flame structure properly, it will be interesting to study the equations for the 'conserved scalars' without chemical source terms, i.e. the specific enthalpy  $H = \sum_i H_i M_i \phi_i$  and the  $N_e$  element mole numbers  $\psi_j = \sum_i \mu_{ji} \phi_i$ :

$$\begin{aligned} \frac{\partial}{\partial s}(\sigma m H) - \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} \frac{\partial H}{\partial s}) - \\ \sum_{i=1}^{N_s} M_i \left( \frac{1}{Le_i} - 1 \right) \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} H_i \frac{\partial \phi_i}{\partial s}) &= -\sigma \rho K H, \\ \frac{\partial}{\partial s}(\sigma m \psi_j) - \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} \frac{\partial \psi_j}{\partial s}) - \\ \sum_{i=1}^{N_s} \mu_{ji} \left( \frac{1}{Le_i} - 1 \right) \frac{\partial}{\partial s}(\sigma \frac{\lambda}{c_p} \frac{\partial \phi_i}{\partial s}) &= -\sigma \rho K \psi_j, \quad (j = 1, \dots, N_e), \end{aligned} \quad (3)$$

where  $Le_i = \frac{\lambda}{\rho D_{im} c_p}$  is the Lewis number of species  $i$ ,  $M_i$  the molar mass of species  $i$  and  $\mu_{ji}$  the stoichiometry factor, indicating the number of atoms of type  $j$  in a molecule of type  $i$ . In the remainder it will be assumed that the specific heats of all species are equal and constant ( $c_{p,i} = c_p$ ), so that the specific enthalpy of species  $i$  is given by  $H_i = H_i^* + c_p(T - T^*)$ ,  $H_i^*$  being the enthalpy of formation of species  $i$  at reference temperature  $T^*$ . Then, the  $H_i$ 's in equation (3) may be replaced by  $H_i^*$ 's, as the thermal contributions to  $H_i$  then drop out.

The definition of the stretch rate  $K$ , introduced above, is an extension of the usual definition (Williams, 1975) for flames with a finite thickness and was introduced in de Goey (1997a) for 2D stationary flames and in de Goey (1997b) for 3D instationary flames. It is defined as the relative rate of change of the mass  $M(t) = \int_{V(t)} \rho \, dV(t)$  in a small volume  $V(t)$  in the flame, which moves with velocity  $\mathbf{v}_f$  of the flame surfaces:

$$K = \frac{1}{M} \frac{dM}{dt}. \quad (4)$$

Note that the flamelet equations in Eq.(1-3) describe transport in the flame perpendicular to the flame surfaces.

Expressions for the change in flame enthalpy  $H_b - H_u$  and the element mole numbers  $\psi_{j,b} - \psi_{j,u}$ , caused by flame stretch, can be derived by integrating the corresponding equations in (3) through the flamelet from the boundary  $s_u$  in the unburnt gases to the boundary  $s_b$  in the burnt gases. In the weak stretch limit the results are given by (de Goey 1996, ten Thijs Boonkamp, 1997a,b):

$$H_b - H_u = \frac{-1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma \rho K (H - H_u) ds = - \sum_{i=1}^{N_s} M_i H_i^* \left( \frac{Ka_i}{Le_i} - Ka_T \right) (\phi_{i,b}^0 - \phi_{i,u}) + hot, \quad (5)$$

and

$$\psi_{j,b} - \psi_{j,u} = \frac{-1}{(\sigma m)_b} \int_{s_u}^{s_b} \sigma \rho K (\psi_j - \psi_{j,u}) ds = - \sum_{i=1}^{N_s} \mu_{ji} \left( \frac{Ka_i}{Le_i} - Ka_T \right) (\phi_{i,b}^0 - \phi_{i,u}) + hot, \quad (6)$$

where the Karlovitz numbers  $Ka_i$  and  $Ka_T$  are defined by:

$$Ka_i = \frac{Le_i}{(\sigma m^0)_b} \int_{s_u}^{s_b} \sigma \rho^0 K \tilde{\phi}_i^0 ds, \\ Ka_T = \frac{1}{(\sigma m^0)_b} \int_{s_u}^{s_b} \sigma \rho^0 K \tilde{T}^0 ds, \quad (7)$$

with  $\tilde{\phi}_i^0$  and  $\tilde{T}^0$  the normalized mole fraction and temperature, respectively, defined by

$$\tilde{\phi}_i^0 = \frac{\phi_i^0 - \phi_{i,u}}{\phi_{i,b}^0 - \phi_{i,u}}, \quad \tilde{T}^0 = \frac{T^0 - T_u}{T_b^0 - T_u}. \quad (8)$$

The terms *hot* in Eqs.(5,6) indicate higher-order Karlovitz number terms and the superscript <sup>0</sup> denotes quantities, undisturbed by flame stretch.

The mass burning rate  $m_b$  of stretched flames can be derived using a similar IA procedure. The analysis leads to the following expression for the mass burning rate in the weak stretch limit (de Goeij 1996,1997a, ten Thijs Boonkamp 1997b):

$$\begin{aligned} \frac{m_b}{m_b^0} &= 1 - Ka_T + (H_b - H_u) \frac{\partial}{\partial H_b^0} (\ln m_b^0) \\ &+ \sum_{j=1}^{N_e} (\psi_{j,b} - \psi_{j,u}) \frac{\partial}{\partial \psi_{j,b}^0} (\ln m_b^0) + hot. \end{aligned} \quad (9)$$

Eqs.(5-9) are quite generally applicable to flames with multiple-species transport and chemistry models, with  $K(s)$  being an arbitrary function in the flame area, as long as it remains small enough to neglect second-order Karlovitz terms. Note that it is not necessary to introduce restrictions with respect to the magnitude of the Lewis numbers as in the asymptotic theories, where it is been assumed that  $Le - 1$  is small (of order of the reciprocal Zeldovich number).

### 3 Comparison with the LAEA theory

The results of this IA approach will now be compared with the results of the LAEA method of Joulin, Clavin and others. The analysis will be restricted to flat flames ( $\sigma(s) = 1$ ), so that  $m_b^0 = m^0$ . Consider a one-step irreversible reaction  $\mathcal{F} \rightarrow \mathcal{P}$ , with one rate-determining lean species  $\mathcal{F}$  and a single constant Lewis number  $Le_{\mathcal{F}} = Le_{\mathcal{P}} = Le$ . The coefficient  $\lambda/c_p$  is also treated as a constant. Note that the single element mole number  $\psi = \phi_{\mathcal{F}} + \phi_{\mathcal{P}} = \phi_{\mathcal{F},u}$  is constant as  $\mathcal{F}$  and  $\mathcal{P}$  have identical Lewis numbers, so that the last term with the summation in Eq.(9) vanishes. The term with the factor containing  $H_b - H_u$  in Eq.(9) can be simplified by evaluating Eq.(5) to yield:

$$H_b - H_u = (M_{\mathcal{F}} H_{\mathcal{F}}^* \phi_{\mathcal{F},u} - M_{\mathcal{P}} H_{\mathcal{P}}^* \phi_{\mathcal{P},b}^0) \left( \frac{Ka_{\mathcal{F}}}{Le} - Ka_T \right) + hot. \quad (10)$$

In the derivation of 10) we have used that both species have the same Lewis number, so that  $\check{\phi}_{\mathcal{F}}^0(s) = \check{\phi}_{\mathcal{P}}^0(s)$  and consequently  $Ka_{\mathcal{F}} = Ka_{\mathcal{P}}$ . Furthermore, using the chain rule

$$\frac{\partial}{\partial H_b^0} (\ln m_b^0) = \frac{1}{c_p} \frac{\partial}{\partial T_b^0} (\ln m_b^0) \quad (11)$$

for this one-step irreversible reaction together with the relation  $M_{\mathcal{F}} H_{\mathcal{F}}^* \phi_{\mathcal{F},u} - M_{\mathcal{P}} H_{\mathcal{P}}^* \phi_{\mathcal{P},b}^0 = c_p(T_b^0 - T_u)$  for enthalpy conservation, we can derive from Eq.(9):

$$\frac{m_b}{m_b^0} = 1 - Ka_T + \left( \frac{Ka_{\mathcal{F}}}{Le} - Ka_T \right) \frac{Ze^0}{2} + hot. \quad (12)$$

The dominant behaviour of  $m_b^0$  with respect to the flame temperature  $T_b^0$ , given by  $m_b^0 \propto \exp(-E_a/2RT_b^0)$  has been used here and the Zeldovich number is given, as usual,



by  $Ze^0 = \frac{E_a(T_b^0 - T_u)}{R(T_b^0)^2}$ ,  $E_a$  being the activation energy.

In this section, the special case of a constant  $\rho^0 K = (\rho^0 K)_b$  will be treated. For an infinitely thin reaction layer (in the limit of infinite activation energy) we may solve the stretchless 1D equations for the fuel mole number  $\tilde{\phi}_{\mathcal{F}}^0(s)$  and the temperature  $\tilde{T}^0(s)$  from Eq.(1) in the preheat zone, fixing  $s_b = 0$  to the reaction layer without loss of generality and assuming that  $s_u \rightarrow -\infty$ :

$$\begin{aligned}\tilde{\phi}_{\mathcal{F}}^0(s) &= \exp(Le s/\delta_f), \\ \tilde{T}^0(s) &= \exp(s/\delta_f),\end{aligned}\tag{13}$$

where we introduced the flame thickness  $\delta_f = \lambda/(m^0 c_p)$ . Using this solution for  $\tilde{T}^0(s)$  and  $\tilde{\phi}_{\mathcal{F}}^0(s)$ , the expressions for the Karlovitz numbers in Eq.(7) may be evaluated to give  $\mathcal{K}a_b = \left(\frac{\rho^0 K}{m^0}\right)_b \delta_f$  for  $\mathcal{K}a_{\mathcal{F}}$  and  $\mathcal{K}a_T$ . Then, Eq.(12) can be rewritten as:

$$\frac{m_b}{m_b^0} = 1 - \mathcal{K}a_b \mathcal{M}_b + \mathcal{O}(\mathcal{K}a_b^2),\tag{14}$$

with  $\mathcal{M}_b$  the Markstein number, given by:

$$\mathcal{M}_b = 1 + \frac{Le - 1}{Le} \frac{Ze^0}{2}.\tag{15}$$

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

$$\mathcal{M}_b = 1 + (Le - 1) \frac{Ze^0}{2}.\tag{16}$$

They assumed that  $(Le - 1) Ze^0 = \mathcal{O}(1)$ , so that deviations of the Lewis number from 1 are of order  $\frac{1}{Ze^0}$ . To lowest-order in  $Ze^0$ , Eqs.(15) and (16) are therefore equal.

## 4 Comparison with LAEA: Variable Density

In this section we will repeat the above analysis, but now for the case that  $K = K_b = K_u$  is constant, while the density  $\rho^0$  in the expressions (7) for the Karlovitz numbers varies as in a non-stretched deflagration wave with negligible pressure variation:

$$\rho^0(s) = \frac{\rho_u T_u}{T^0(s)} = \frac{\rho_u}{1 + \tau \exp\left(\frac{s}{\delta_f}\right)},\tag{17}$$

where we introduced the thermal expansion coefficient  $\tau = \frac{T_b^0 - T_u}{T_u} = \frac{\rho_u - \rho_b^0}{\rho_b^0}$ . Now, substituting Eqs.(13) and (17) into Eq.(7) for  $\mathcal{K}a_T$  gives:

$$\mathcal{K}a_T = \frac{\rho_u K_b}{m_b^0} \int_{-\infty}^0 \frac{\exp\left(\frac{s}{\delta_f}\right)}{1 + \tau \exp\left(\frac{s}{\delta_f}\right)} ds = \frac{\rho_u K_b \delta_f}{m_b^0 \tau} \int_0^{\tau} \frac{1}{1 + y} dy = \mathcal{K}a_b \left(\frac{\tau + 1}{\tau}\right) \ln(1 + \tau),\tag{18}$$

where the relation  $\rho_u = \rho_b^0(1 + \tau)$  has been used in the last step.

The expression for  $Ka_{\mathcal{F}}$  can be derived in the same way. Eq.(13) for  $\tilde{\phi}_{\mathcal{F}}^0$  and Eq.(17) for  $\rho^0(s)$  is substituted into Eq.(7) for  $\frac{Ka_{\mathcal{F}}}{Le}$ , which gives

$$\frac{Ka_{\mathcal{F}}}{Le} = \frac{\rho_u K_b}{m_b^0} \int_{-\infty}^0 \frac{\exp\left(\frac{Le s}{\delta_f}\right)}{1 + \tau \exp\left(\frac{s}{\delta_f}\right)} ds = \frac{\rho_u K_b \delta_f}{m_b^0} \tau^{-Le} \int_0^{\tau} \frac{y^{Le-1}}{1+y} dy. \quad (19)$$

This last integral  $\mathcal{I} = \int_0^{\tau} \frac{y^{Le-1}}{1+y} dy$  can be rewritten as follows, using partial integration:

$$\mathcal{I} = \int_0^{\tau} \frac{y^{Le-1}}{1+y} dy = \tau^{Le-1} \ln(1+\tau) - (Le-1) \int_0^{\tau} y^{Le-2} \ln(1+y) dy. \quad (20)$$

Note that  $\mathcal{I}$  is convergent for all  $Le > 0$ . We thus find

$$\frac{Ka_{\mathcal{F}}}{Le} = Ka_T - \mathcal{K}a_b (Le-1) (1+\tau) \int_0^{\tau} \frac{\ln(1+y)}{y^2} \left(\frac{y}{\tau}\right)^{Le} dy. \quad (21)$$

Combining Eqs.(18) and (21) for the Karlovitz numbers with Eq.(12) then gives for the Markstein number in the burnt gases:

$$\mathcal{M}_b = \left(\frac{\tau+1}{\tau}\right) \ln(1+\tau) + \frac{Ze^0}{2} (Le-1) (1+\tau) \int_0^{\tau} \frac{\ln(1+x)}{x^2} \left(\frac{x}{\tau}\right)^{Le} dx. \quad (22)$$

Clavin found the following result in 1985:

$$\mathcal{M}_b = \left(\frac{\tau+1}{\tau}\right) \ln(1+\tau) + \frac{Ze^0}{2} (Le-1) \frac{(1+\tau)}{\tau} \int_0^{\tau} \frac{\ln(1+x)}{x} dx. \quad (23)$$

Clavin assumed in his analysis that  $(Le-1)$  is of order  $\frac{1}{Ze^0}$ . To lowest order in the Zeldovich number, Eq.(22) is therefore equal to the result of Clavin (1985) for  $\mathcal{M}_b$ , derived using LAEA.

## 5 The mass burning rate in the unburnt mixture

For the mass burning rate  $m_u$  in the unburnt mixture, an equation equivalent to Eq.(9) can be derived. This can be done by following the same procedure as for  $m_b$ , which has been described in ten Thije Boonkamp (1997a,b). This procedure then yields

$$\begin{aligned} \frac{m_u}{m_u^0} &= 1 - Ka_T^* + (H_b - H_u) \frac{\partial}{\partial H_b^0} (\ln m_u^0) \\ &+ \sum_{j=1}^{N_e} (\psi_{j,b} - \psi_{j,u}) \frac{\partial}{\partial \psi_{j,b}^0} (\ln m_u^0) + hot. \end{aligned} \quad (24)$$

$Ka_T^*$  is given by

$$Ka_T^* = \frac{-1}{(\sigma m^0)_u} \int_{s_u}^{s_b} \sigma \rho^0 K \hat{T}^0 ds = \frac{1}{(\sigma m^0)_u} \int_{s_u}^{s_b} \sigma \rho^0 K (\tilde{T}^0 - 1) ds, \quad (25)$$

with  $\tilde{T}^0 = \frac{T^0 - T_b^0}{T_u - T_b^0}$  the normalized temperature with respect to the burnt mixture instead of the unburnt mixture, as used in Eq.(7). The results of the IA approach will be compared again with those of the LAEA theory, so we assume that  $\sigma(s) = 1$  and  $K(s) = K_u = K_b$  is constant. The preferential diffusion terms in Eq.(24), which are proportional to  $Ze^0$  as in the previous section, have the same contribution to  $m_u/m_u^0$  as to  $m_b/m_b^0$ . Instead of Eq.(12) we thus have

$$\frac{m_u}{m_u^0} = 1 - Ka_T^* + \left( \frac{Ka_{\mathcal{F}}}{Le} - Ka_T \right) \frac{Ze^0}{2} + \text{hot}. \quad (26)$$

Note that Karlovitz numbers in the preferential diffusion term might be normalised with respect to the burnt mixture as well, because  $Ka_{\mathcal{F}}/Le - Ka_T = Ka_{\mathcal{F}}^*/Le - Ka_T^*$ . Using  $\rho^0(s)$  from Eq.(17) and  $\tilde{T}^0(s)$  from Eq.(13) we obtain for  $Ka_T^*$ :

$$Ka_T^* = \frac{\rho_u K_u}{m_u^0} \int_{-\infty}^0 \frac{\exp\left(\frac{s}{\delta_f}\right) - 1}{\tau \exp\left(\frac{s}{\delta_f}\right) + 1} ds = \mathcal{K}a_u \int_0^1 \frac{y - 1}{\tau y^2 + y} dy, \quad (27)$$

where the Karlovitz number  $\mathcal{K}a_u = \left(\frac{\rho K}{m\sigma}\right)_u \delta_f = (1 + \tau) \mathcal{K}a_b$  in the unburnt mixture is introduced. Note that this integral diverges logarithmically as  $y = \exp(s/\delta_f) \rightarrow 0$ . This divergence originates from the fact that  $m_u$  is defined at the unburnt boundary of the flame, i.e. for  $s_u \rightarrow -\infty$ . However,  $K$  is constant everywhere in the flame area  $-\infty < s < \infty$ , so the local mass burning rate  $m(s)$  keeps on changing for decreasing  $s \rightarrow -\infty$  (this follows from the continuity equation in (1)). The origin of the problem associated with this divergence is that there is no specific position in the preheat zone, except at  $s_u \rightarrow -\infty$ , to define the unburnt boundary of the flame. To tackle this problem, let us first separate the term responsible for the logarithmic divergence of  $Ka_T^*$ . The consequences hereof will be studied furtheron. We thus write for the integrand in Eq.(27):

$$\frac{y - 1}{\tau y^2 + y} = \frac{1 + \tau}{\tau y + 1} - \frac{1}{y}, \quad (28)$$

where the integral of the first term converges and the one of the second term leads to the logarithmic divergence. For a positive value of  $y_u$ , (or a finite value of  $s_u = \delta_f \ln y$ ), we thus find for Eq.(27), when Eq.(28) is used:

$$Ka_T^*(s_u) = \mathcal{K}a_u \left( \frac{1 + \tau}{\tau} \ln(1 + \tau) + \frac{s_u}{\delta_f} \right), \quad (29)$$

where  $s_u$  now denotes the position in the unburnt mixture where the unburnt flame boundary is chosen. It is now possible to evaluate the Markstein number  $\mathcal{M}_u$  in the unburnt gases from Eq.(26) and the relation

$$\frac{m_u(s_u)}{m_u^0} = 1 - \mathcal{K}a_u(s_u) \mathcal{M}_u(s_u) + \mathcal{O}(\mathcal{K}a_u^2). \quad (30)$$

Using Eqs.(29) and (21) in Eq.(26) then gives :

$$\mathcal{M}_u(s_u) = \frac{s_u}{\delta_f} + \frac{\tau + 1}{\tau} \ln(1 + \tau) + \frac{Ze^0}{2} (Le - 1) \int_0^\tau \frac{\ln(1 + x)}{x^2} \left(\frac{x}{\tau}\right)^{Le} dx. \quad (31)$$

This equation is equivalent to the equation of Clavin and Williams (1982) up to order  $Ze^0$ , when  $Le = 1 + \mathcal{O}(1/Ze^0)$  is substituted into the integral and when the equation is evaluated at  $s_u = 0$ .

## 6 Discussion

Some of the results, presented in the previous section are studied in more detail to identify their origin and consequences. First of all, it should be noted that the constant stretch rate  $K = K_u = K_b$ , applied in the last three sections in combination with  $\sigma(s) = 1$ , means, according to the mass conservation equation in Eq.(1), that the 'local' mass burning rate  $m(s)$  behaves like

$$m(s) - m(0) = -K \int_0^s \rho(s) ds. \quad (32)$$

A typical example of the behaviour of  $\rho^0(s)K$  (continuous line) and  $m(s)$  (dashed line) is presented in Figure 2 for a flat stagnation flame as a function of  $s/\delta_f$ . When the reaction layer is infinitely thin and located at  $s = 0$ , we may substitute  $\rho(s) = \rho_b$  in the burnt gases ( $s > 0$ ), so that Eq.(32) gives for  $s > 0$ :

$$m(s) - m(0) = -K \rho_b s = -m^0 \mathcal{K} a_b \frac{s}{\delta_f}. \quad (33)$$

It should be noted that this result for  $m(s)$  in the burnt gases, in fact, also follows from Eq.(12). Evaluating  $m(s_b)$  with Eq.(12) at position  $s_b$  and subtracting the result  $m(0)$  of Eq.(12) at  $s = 0$  gives

$$m(s_b) - m(0) = -m^0 (K a_T(s_b) - K a_T(0)) = -K \rho_b \int_0^{s_b} ds = -m^0 \mathcal{K} a_b \frac{s_b}{\delta_f}, \quad (34)$$

where we used that  $H^0(s) - H_b^0$  is constant for  $s > 0$  so that the contributions induced by preferential diffusion cancel when Eq.(12) is used to evaluate Eq.(34). Furthermore, it has been used that  $\tilde{T}^0(s) = 1$  for  $s > 0$  in the equation for  $K a_T$ . The equivalence of Eqs.(33) and (34) shows that Eqs.(9) and (12) correctly take into account the dependence of the result for  $m_b$  on the position  $s_b$  in the burnt gases where the burnt flame boundary is defined. Furthermore, from the equivalence of Eq.(22) for  $\mathcal{M}_b$  and the result found by Clavin, it becomes clear that Clavin defines the burnt flame boundary to be at  $s_b = 0$  where the reaction layer is positioned (see Fig.2).

Let us now study  $m(s)$  in the region  $s < 0$ . For  $s < 0$  a similar reasoning can be applied. However, the correct dependence of  $\rho(s)$  has to be used in Eq.(32) and this equation

cannot be simplified as easy now. However, outside the preheating zone, for  $s \rightarrow -\infty$ , we again find a linear asymptotic behaviour of  $m(s)$ :

$$m(s) - m^*(0) = -K \rho_u s = -m_u^0 \mathcal{K} a_u \frac{s}{\delta_f}, \quad (35)$$

where  $m^*(0)$  denotes the extrapolated value of the linear asymptotic behaviour of  $m(s)$  to  $s = 0$ . As in the burnt gases, Eq.(26) for  $m(s_u)$  describes the same asymptotic behaviour in the unburnt gases as Eq.(35). Furthermore, it is interesting to note that the linear dependence of  $\mathcal{M}_u$  on  $s_u$ , described by the term  $\frac{s_u}{\delta_f}$  in Eq.(31) has exactly the same origin as the linear dependence of Eq.(35). This explains the origin of the divergence, observed in the previous section once more. Clavin's result is equal to Eq.(31) for  $s_u = 0$ . This means that Clavin et al. in their theory use the position  $s = 0$  of the reaction layer to identify the unburnt mass burning rate  $m_u$  as well as the burnt mass burning rate  $m_b$ . What they in fact implicitly do is computing the asymptotic behaviour of  $m(s)$  in the (un)burnt gases and extrapolate linearly to the position  $s = 0$  to identify the reported results for  $m_b$  and  $m_u$  (see Fig.2). Or, alternatively, they take the limit of an infinitely thin flame  $\delta_f \rightarrow 0$  (reaction layer including preheating zone).

Fig.2 shows, in our opinion, 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  $m_u$  might be quite far away from the  $m(s)$  curve. It should be realized, though, that the reaction layer, is, in practice, also not infinitely thin. The value for  $m_b$  then describes again the asymptotic value of  $m(s)$  in the burnt gases, extrapolated to the heart of the reaction layer. In this case,  $m_b$  is not on the  $m(s)$  curve of Fig. 2 either. However, as the reaction layer is much thinner than the preheating zone, it is expected that  $m_b$  is always closer to the  $m(s)$ -curve than  $m_u$ .

## 7 Conclusions

The mass burning rate of stretched flames described by a single irreversible reaction has been studied. It has been shown that the results of the Integral Analysis, first introduced by Chung et al.(1988) and elaborated further by de Goey and ten Thije Boonkkamp (1996,1997), leads to the same results for the Markstein numbers as the theory of Joulin and Clavin (1979) and Clavin et al. (1982,1985) in case of a constant stretch rate  $K$  through the flame to lowest order in the Zeldovich number. This is true for a constant density in the flame as well as for a density  $\rho^0(s)$  varying according to the gas law. This analysis shows that the expressions (9) and (24) for the mass burning rate of stretched flames describe the mass burning rate in the full flame area  $-\infty < s < \infty$  and the asymptotic values are equal to the asymptotic values for the mass burning rate, found by the LAEA theory. The mass burning rate  $m_b$  in the burnt gases, seems to be more appropriate to identify the mass burning rate in stretched flames. It remains to be seen whether the assumption that the stretch field  $K(s)$  can be described by a constant value  $K_b$  through the flame is accurate enough to describe the behaviour of real laminar and turbulent flamelets. In principle it is possible to study the effect of variations in the stretch rate  $K(s)$  as a function of  $s$  using the Integral Analysis, presented here.

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## Figure Captions

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

Figure 2: Density  $\rho^0(s)$  from Eq.(17) (continuous line) and the mass burning rate  $m(s)$  according to the continuity equation of Eq.(1) (dashed line) as a function of the scaled distance  $s/\delta_f$  from the reaction layer in the flame for a constant stretch rate  $K$ . Extrapolations  $m_b$  and  $m_u$  of the asymptotic behaviour of  $m(s)$  for  $s/\delta_f > 0$  and  $s/\delta_f \ll -1$  to the reaction layer at  $s = 0$  are also indicated.

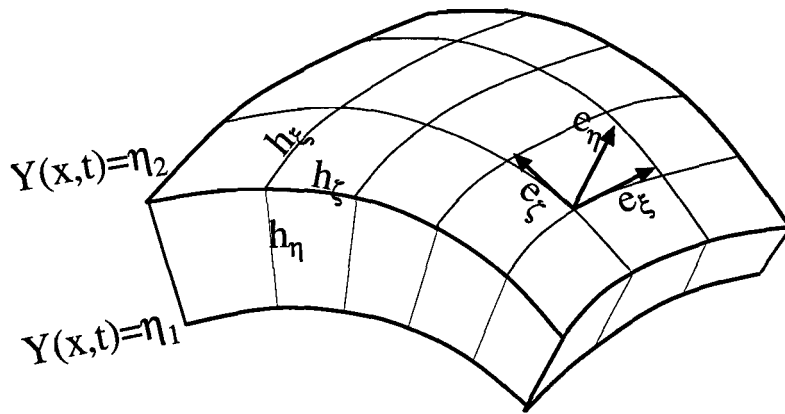


Fig.1 L.P.H. de Goey



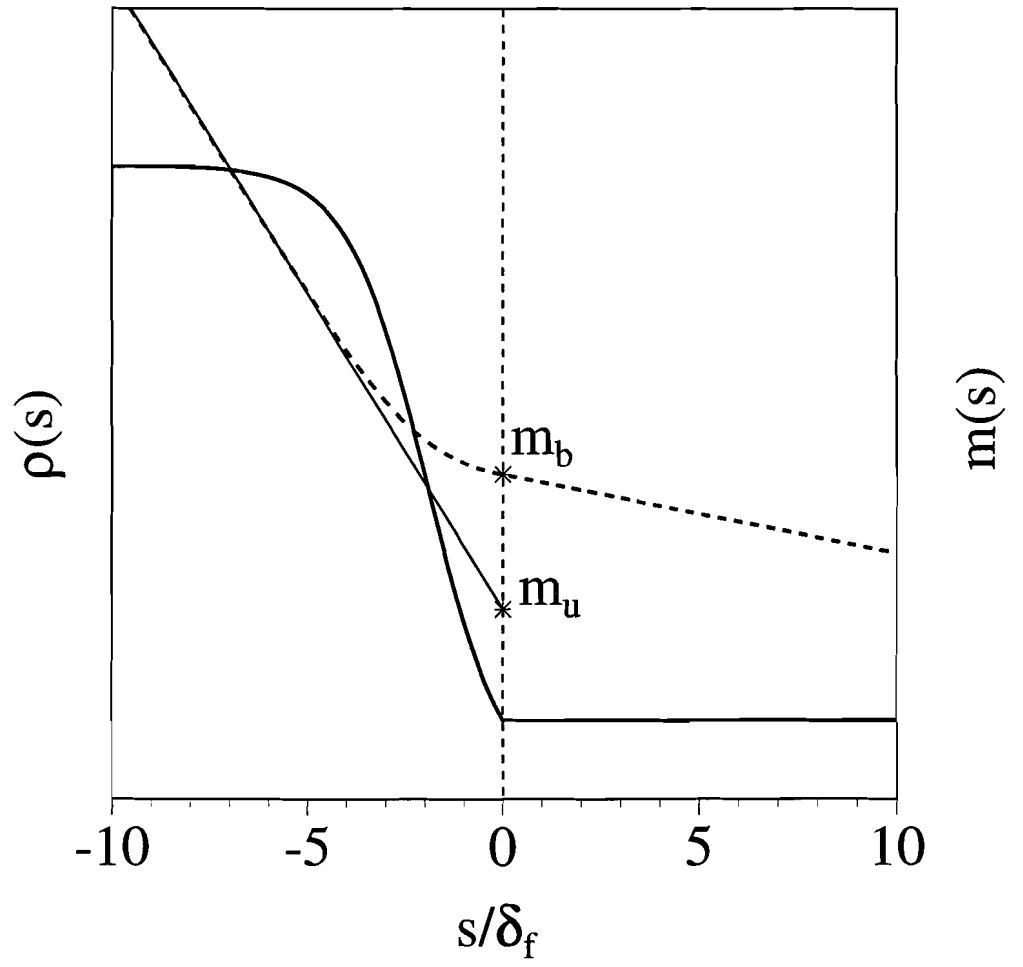


Fig.2 L.P.H. de Goey

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