Qualitative analysis of a one-dimensional laminar flame

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Abstract. In this report we discuss the combustion equations governing a one-dimensional, stationary and laminar flame. An important parameter for these equations is the Lewis number Le, which is the ratio of the coefficients for thermal conduction and mass diffusion. In the case $Le = 1$, referred to as the equidiffusive case, the combustion equations reduce to a single equation for the temperature. A qualitative analysis of the solution of the equations (mass flux, temperature, mass fractions and specific enthalpy) is presented both for the equidiffusive and the non-equidiffusive case.

Key words. Laminar flame, isobaric approximation, combustion equations, Lewis number, specific enthalpy, Shvab-Zeldovich variables.

AMS subject classifications. 80A32, 76V05, 34C11.

1 Introduction

The flow of a reacting gas mixture plays a central role in combustion theory. Laminar flames constitute a very important class of reacting flow problems, because they are often used in the numerical simulation of burners. In order to predict the behaviour of a burner, in terms of e.g. fuel consumption and NO_x-formation, one must be able to compute the flames in such a burner. The numerical computation of laminar flames in complex two- or three-dimensional burners is a difficult task and requires both advanced numerical techniques and powerful computers. In the last two decades, substantial progress in numerical flame simulation has been achieved and a lot of papers about this have been written; see e.g. [4, 10, 5].

However, numerical computation of a laminar flame usually doesn't give much insight in its structure. Therefore, we consider as a model problem a one-dimensional, laminar flame, which is accessible to analysis. The purpose of this paper is to analyze this flame using simple mathematical techniques, and in such a way gain insight in the structure of one-dimensional flames. Moreover, laminar flames in simple burner geometries can sometimes be considered as (nearly) one-dimensional, so even simulations of one-dimensional flames have been carried out [6].

The governing equations for laminar flames are derived from the conservation laws of reacting flow systems, and reduce to a set of ordinary differential equations for a one-dimensional and stationary flame. In laminar flame theory, the isobaric approximation is employed, i.e. the pressure is assumed to be almost constant, which is justified for low Mach number flow. As a consequence of the isobaric approximation, these equations can be split into the so-called combustion equations and the hydrodynamical equations. In a solution procedure, the mass flux, the mass fractions of the chemical species and the temperature are computed first from the combustion equations, and subsequently the hydrodynamical equations are solved for the density, velocity and pressure. In order to further simplify the model, we assume that only one irreversible chemical reaction takes place in the flame. This is not true, however, the global behaviour of a flame can often be modelled quite adequately by a single reaction.

An important parameter in the analysis is the Lewis number Le, which is the ratio of the thermal diffusion coefficient and the mass diffusion coefficient. In the equidiffusive case, i.e. $Le = 1$, all mass fractions can be expressed in the temperature and the set of equations reduces to one single equation for the temperature. For the case $Le \neq 1$ on the other hand, N equations have to be solved, with N the number of species in the flame.

The contents of the paper is the following. In the next section, the governing equations of a one-dimensional, stationary, laminar flame are presented. The underlying assumptions are stated explicitly. Boundary conditions for a stoichiometric flame are given in Section 3. In Section 4, the non-dimensional combustion equations are derived. A qualitative analysis of these equations for the case $Le = 1$ is given in Section 5. Finally, in Section 6 this analysis is generalized for the case $Le \neq 1$.

2 Governing equations

Consider a one-dimensional, stationary and laminar flame in a combustible mixture consisting of N different chemical species, denoted by $\mathcal{M}_i$ $(i = 1, \ldots, N)$. In the theory of laminar flames, it is customary to make the following assumptions [9]:

1. Fick's law of mass diffusion holds.
2. The gas mixture is inviscid.
3. External forces are negligible.
4. Fourier's law of heat conduction holds.
5. The heat flux as a consequence of concentration gradients (Dufour effect) and, conversely, mass diffusion as a consequence of a temperature gradient (Soret effect) are negligible.
6. Pressure-gradient diffusion is negligible.
7. Radiation is negligible.
8. The gas mixture is an ideal gas.

Under these assumptions, the equations for the above mentioned flame read [9, 8]:

$$(2.1) \quad \frac{\mathrm{d}}{\mathrm{d}x}(\rho u) = 0,$$

$$(2.2) \quad \frac{\mathrm{d}}{\mathrm{d}x}(\rho Y_i u) = \frac{\mathrm{d}}{\mathrm{d}x}(\rho D \frac{\mathrm{d}Y_i}{\mathrm{d}x}) + w_i, \ i = 1, \ldots, N,$$

$$(2.3) \quad \frac{\mathrm{d}}{\mathrm{d}x}(\rho u^2) = -\frac{\mathrm{d}p}{\mathrm{d}x},$$

$$(2.4) \quad \frac{\mathrm{d}}{\mathrm{d}x}(\rho h u) = \frac{\mathrm{d}}{\mathrm{d}x}(\lambda \frac{\mathrm{d}T}{\mathrm{d}x}) + \frac{\mathrm{d}}{\mathrm{d}x}(\rho D \sum_{j=1}^{N} h_j \frac{\mathrm{d}Y_j}{\mathrm{d}x}) + u \frac{\mathrm{d}p}{\mathrm{d}x},$$

$$(2.5) \quad p = \rho RT/\overline{W}, \ \overline{W}^{-1} = \sum_{j=1}^{N} Y_j/W_j.$$

The dependent variables in these equations are the mass density ρ of the mixture, the mass-weighted average velocity u of the mixture, the mass fractions Y_i of species $\mathcal{M}_i$, the hydrostatic pressure p, the specific enthalpy h of the mixture and the (absolute) temperature T. Physical/chemical quantities in (2.1)-(2.5) are successively, the binary diffusion coefficient D of all pairs of species, the reaction rates w_i of species $\mathcal{M}_i$, the thermal conductivity λ, the specific enthalpies h_i of species $\mathcal{M}_i$, the universal gas constant R and the molecular weights W_i of species $\mathcal{M}_i$. $\overline{W}$ in (2.5) is the average molecular weight of the mixture. Equations (2.1) and (2.2) describe, respectively, conservation of mass for the mixture as a whole and for each species individually. Momentum and energy conservation of the mixture are expressed by the equations (2.3) and (2.4), respectively. Finally, (2.5) is the equation of state of the mixture.

Obviously, the mass fractions Y_i and the reaction rates w_i satisfy

$$(2.6) \quad \sum_{j=1}^{N} Y_j = 1,$$

$$(2.7) \quad \sum_{j=1}^{N} w_j = 0.$$

This latter equation means that overall mass is neither created nor destroyed by chemical reactions. Because of (2.6) and (2.7) only N equations from (2.1) and (2.2) are linearly independent. Thus, the total system (2.1)-(2.5) consists of $N+3$ linearly independent equations. However, there are $N+4$ independent variables, namely the mass density ρ, the velocity u, $N-1$ mass fractions Y_i, the pressure p, the specific enthalpy h and the temperature T, and therefore one extra equation is needed. This equation is the thermodynamic identity

$$(2.8) \quad h = \sum_{j=1}^{N} Y_j h_j.$$

The specific enthalpies h_i in (2.8) are defined by the caloric equation of state

$$(2.9) \quad h_i = h_i^0 + \int_{T_0}^{T} c_{p,i}(\tau)\mathrm{d}\tau,$$

where h_i^0 is the specific heat of formation of species $\mathcal{M}_i$ at some reference temperature T_0 and $c_{p,i}$ is the specific heat at constant pressure of species $\mathcal{M}_i$. Equation (2.8) defines h as a function of Y_i $(i = 1, \cdots, N)$ and T through equation (2.9).

In order to specify the reaction rates w_i, we make the assumption:

9. Only one irreversible chemical reaction occurs in the mixture.

If we write this reaction as

$$(2.10) \quad \sum_{j=1}^{N} \nu_{r,j}\mathcal{M}_j \longrightarrow \sum_{j=1}^{N} \nu_{p,j}\mathcal{M}_j,$$

with $\nu_{r,i}$ and $\nu_{p,i}$ the stoichiometric coefficients of species $\mathcal{M}_i$, appearing as a reactant and as a product respectively, then, according to the law of mass action, w_i is given by

$$(2.11) \quad w_i = W_i(\nu_{p,i} - \nu_{r,i})k \prod_{j=1}^{N} \left(\frac{\rho Y_j}{W_j}\right)^{\nu_{r,j}}.$$

From (2.7) and (2.11) it follows immediately that

$$(2.12)\quad \sum_{j=1}^{N} \nu_{r,j} W_j = \sum_{j=1}^{N} \nu_{p,j} W_j.$$

The specific rate constant k in (2.11) is given by the Arrhenius' expression

$$(2.13)\quad k = A\mathrm{e}^{-E/RT},\ A = BT^{\alpha},$$

with A the frequency factor and E the activation energy for the reaction in (2.10).

Equation (2.1) implies that the mass flux $m = \rho u$ is a constant. Taking this into account, the conservation equations (2.1)-(2.4) reduce to

$$(2.14)\quad m = \rho u,$$

$$(2.15)\quad mY_i' = (\rho D Y_i')' + w_i,\ i = 1, \ldots, N-1,$$

$$(2.16)\quad mu' = -p',$$

$$(2.17)\quad mh' = (\lambda T')' + (\rho D \sum_{j=1}^{N} h_j Y_j')' + up'.$$

In these equations we used the prime symbol $'$ to denote differentiation, and we shall adhere to this notation in the following.

The energy equation (2.17) can be simplified by making the assumption:

10. All chemical species $\mathcal{M}_i$ have constant and equal specific heats at constant pressure.

Then, also the specific heat c_p of the mixture, defined by

$$(2.18)\quad c_p = \sum_{j=1}^{N} Y_j c_{p,j},$$

is equal to this constant. The specific enthalpies h and h_i, defined in (2.8) and (2.9), are in this case given by

$$(2.19)\quad h = \sum_{j=1}^{N} Y_j h_j^0 + c_p(T - T_0),$$

$$(2.20)\quad h_i = h_i^0 + c_p(T - T_0).$$

Substituting (2.19) and (2.20) into (2.17) and taking a linear combination with the equations (2.15) to eliminate the species diffusion term, gives the equation

$$(2.21)\quad mc_pT' = (\lambda T')' - \sum_{j=1}^{N} w_j h_j^0 + up'.$$

An important quantity is the specific heat of combustion Q, which is defined as [2]

$$(2.22)\quad \left(\sum_{j=1}^{N} \nu_{r,j} W_j\right) Q = \sum_{j=1}^{N} (\nu_{r,j} - \nu_{p,j}) W_j h_j^0,$$

thus Q is the heat per unit mass of reactants released by the reaction in (2.10). In combustion theory, the following usually holds:

11. The reaction in (2.10) is exothermic, i.e. $Q > 0$.

Substituting equation (2.11) for the reaction rates w_i into the reaction term $-\sum_{j=1}^{N} w_j h_j^0$, and using equation (2.22) for Q, it is easy to see that equation (2.21) can be rewritten as

$$(2.23)\quad mc_pT' = (\lambda T')' + \left(\sum_{j=1}^{N} \nu_{r,j} W_j\right) Q\omega + up'.$$

The variable ω in (2.23) is defined as

$$(2.24)\quad \omega = \frac{w_i}{W_i(\nu_{p,i} - \nu_{r,i})} = k \prod_{j=1}^{N} \left(\frac{\rho Y_j}{W_j}\right)^{\nu_{r,j}},$$

i.e. ω is the number of moles produced by the reaction in (2.10), per unit volume and per unit time, of any species for which $\nu_{p,i} - \nu_{r,i} = 1$. In the following, ω will be referred to as the reaction rate for the reaction in (2.10).

The equations to be solved are (2.14), (2.15) (for $N - 1$ different species), (2.16), (2.17) (or equivalently (2.23)) and (2.5). One of the difficulties associated with this set of equations is the presence of the mass fractions Y_i in the equation of state (2.5). In order to circumvent this problem, we assume:

12. $\overline{W}$ is constant, say $\overline{W} = W$.

The value of W is a characteristic value of $\overline{W}$ corresponding to a constant composition of the mixture. Assumption 12 only holds for the unimolecular reaction $\mathcal{R} \longrightarrow \mathcal{P}$, and is otherwise reasonable if the molecular weights W_i do not differ too much. This assumption is also quite good for combustion processes in air.

The frozen speed of sound a_f, i.e. the speed of sound at constant composition of the mixture, is given by [9]

$$(2.25)\quad a_f = \sqrt{\frac{\gamma p}{\rho}},$$

with $\gamma = c_p/c_v$ the specific heat ratio and $Ma = u/a_f$ is the corresponding Mach number. Now we make the following assumption:

13. The flow is highly subsonic, i.e. $| Ma | \ll 1$.

This assumption is the basis of a further simplification of the equations. From equation (2.16) we can easily derive the equation

$$(2.26)\quad \gamma Ma^2 \frac{u'}{u} + \frac{p'}{p} = 0,$$

from which we conclude that fractional changes in the pressure are very small for $| Ma | \ll 1$. Thus, we can write $p = p_0 + \delta p$ with p_0 a constant pressure and $| \delta p/p_0 | \ll 1$. In the isobaric approximation based hereon, the pressure is dealt with as follows. In (2.5) p is simply replaced by p_0, in (2.16) $p' = (\delta p)'$ is substituted and in (2.23) the pressure term up' is omitted altogether. This last approximation can be made plausible as follows. Taking into account the relation $R/W = c_p - c_v$, with c_v the specific heat at constant volume of the mixture, and using (2.5),(2.16) and (2.25), equation (2.23) can be simply rewritten as

$$(2.27)\quad mc_p\left(\left(1 + \frac{\gamma - 1}{2} Ma^2\right)T\right)' = (\lambda T')' + \left(\sum_{j=1}^{N} \nu_{r,j} W_j\right) Q\omega.$$

The term $mc_p\left(\frac{\gamma-1}{2}Ma^2T\right)'$ comes from the pressure term up' in (2.23) and can be neglected for highly subsonic flow. Consequently, also the term up' in (2.23) can then be omitted. For a further discussion, see e.g. [2, 3].

The final equations to be solved read:

$$(2.28)\quad m = \rho u,$$

$$(2.29)\quad mY_i' = (\rho D Y_i')' + (\nu_{p,i} - \nu_{r,i})W_i\omega, \; i = 1, \dots, N-1,$$

$$(2.30)\quad mu' = -(\delta p)',$$

$$(2.31)\quad mc_pT' = (\lambda T')' + \left(\sum_{j=1}^{N} \nu_{r,j}W_j\right) Q\omega,$$

$$(2.32)\quad p_0 = \rho RT/W,$$

with the reaction terms in (2.29) and (2.31) expressed in ω. The density ρ can be eliminated from (2.29) and (2.31) by virtue of (2.32) and hence these equations only contain the variables m,Y_i and T as unknowns. Equations (2.29) and (2.31) are often referred to as the combustion equations. Once we have computed the combustion variables m,Y_i and T from these equations, we successively compute ρ from (2.32), u from (2.28) and δp (and p) from (2.30). These latter equations are often called the hydrodynamical equations. In the remainder of this paper we only consider the combustion equations.

3 Boundary conditions

In this section we discuss boundary conditions for the combustion equations (2.29) and (2.31). The reaction rate ω in these equations can be written as a function of Y_i $(i = 1, \dots, N)$ and T:

$$(3.1)\quad \omega = k\left(\frac{p_0W}{RT}\right)^{\nu_r} \prod_{j=1}^{N}\left(\frac{Y_j}{W_j}\right)^{\nu_{r,j}}, \; \nu_r = \sum_{j=1}^{N} \nu_{r,j},$$

with the specific rate constant k defined in (2.13). For the specific heat of combustion Q we can write, cf. (2.22),

$$(3.2)\quad Q = -\sum_{j=1}^{N} r_j h_j^0,$$

with the quantities r_i defined by

$$(3.3)\quad r_i = (\nu_{p,i} - \nu_{r,i})W_i/(\sum_{j=1}^{N} \nu_{r,j}W_j).$$

It is obvious that

$$(3.4)\quad \sum_{j=1}^{N} r_j = 0,$$

according to (3.3) and (2.12).

Suppose, the combustion equations are defined on $I\!R$. We introduce the notation $f_\infty = \lim_{x\to\infty} f(x)$ and $f_{-\infty} = \lim_{x\to-\infty} f(x)$ for a generic variable f. For the sake of simplicity we assume that reactants and products are distinct, thus:

14. There are N_r reactants $\mathcal{M}_i$, $i = 1, \cdots, N_r$, and $N_p = N - N_r$ products $\mathcal{M}_i$, $i = N_r + 1, \cdots, N$.

Obviously, $\nu_{r,i} \neq 0$ and $\nu_{p,i} = 0$ hold for the reactants in (2.10), and $\nu_{r,i} = 0$ and $\nu_{p,i} \neq 0$ for the products. The following relations for the ratios r_i can be readily verified:

$$\sum_{j=1}^{N_r} r_j = -1, \tag{3.5}$$

$$\sum_{j=N_r+1}^{N} r_j = 1. \tag{3.6}$$

Furthermore, it is clear that $r_i < 0$ for the reactants and $r_i > 0$ for the products. To further simplify the discussion, we assume that for $x \to -\infty$ there are no products, i.e.

15. $Y_{i,-\infty} = 0$ for $i = N_r + 1, \cdots, N$.

The physical relevant solution of (2.29) and (2.31) is bounded for $x \to \pm\infty$ and consequently all derivatives should then vanish. Equations (2.29) and (2.31) imply that $\omega = 0$ should hold for $x \to \pm\infty$. However, $\omega_{-\infty} \neq 0$ but very small; typically $\omega_{-\infty} = \mathcal{O}(\mathrm{e}^{-10})$. This means that there is no bounded solution to (2.29) and (2.31). In physical terms, this means that the gas mixture, which is flowing in the positive x-direction, is forced to react all the way in from $x = -\infty$, so that by the time a finite x is reached, the combustion would be complete. This problem, which is a pure mathematical artefact, is called the cold-boundary difficulty [2, 9]. Therefore, the reaction rate ω is multiplied with the Heaviside function $H(T - T_{ign})$, i.e. the reaction rate is set equal to 0 for T below some ignition temperature $T_{ign} > T_{-\infty}$; see also Section 5. On the other hand, from the condition $\omega_\infty = 0$ we conclude that at least one of the reactants is depleted for $x \to \infty$. We even assume that all reactants are depleted:

16. $Y_{i,\infty} = 0$ for $i = 1, \cdots, N_r$.

Thus, the flame defined by the chemical reaction in (2.10) is stoichiometric because of the assumptions 14-16.

The boundary conditions for the mass fractions Y_i are completely determined by the stoichiometry of the flame. The mass fractions obviously satisfy

$$\sum_{j=1}^{N_r} Y_{j,-\infty} = 1, \tag{3.7}$$

$$\sum_{j=N_r+1}^{N} Y_{j,\infty} = 1. \tag{3.8}$$

Further, integration of the equations (2.29) and taking into account assumptions 15 and 16 gives, respectively,

$$mY_{i,-\infty} = \nu_{r,i} W_i \Omega, \quad i = 1, \ldots, N_r \tag{3.9}$$

for the reactants and

$$mY_{i,\infty} = \nu_{p,i} W_i \Omega, \quad i = N_r + 1, \ldots, N \tag{3.10}$$

for the products. In (3.9) and (3.10) $\Omega = \int_{-\infty}^{\infty} H(T - T_{ign})\omega \mathrm{d}x$, thus Ω is the total number of moles produced by the reaction in (2.10), per unit area and per unit time, of any product for which $\nu_{p,i} = 1$. The set of equations (3.7) and (3.9) constitute $N_r + 1$ linear independent equations for the unknowns $Y_{i,-\infty}$ $(i = 1, \cdots, N_r)$ and Ω. The solution of this system is

$$(3.11)\quad Y_{i,-\infty} = -r_i,\ i = 1, \ldots, N_r,$$

$$(3.12)\quad \Omega = m/(\sum_{j=1}^{N_r} \nu_{r,j} W_j).$$

Likewise, the product mass fractions $Y_{i,\infty}$ and Ω can be computed from the system (3.8) and (3.10):

$$(3.13)\quad Y_{i,\infty} = r_i,\ i = N_r + 1, \ldots, N,$$

$$(3.14)\quad \Omega = m/(\sum_{j=N_r+1}^{N} \nu_{p,j} W_j).$$

The expressions for Ω in (3.12) and (3.14) are equal by virtue of (2.12).

Finally, consider the boundary conditions for the temperature T. Integration of (2.31) over $I\!R$ gives

$$(3.15)\quad m c_p (T_\infty - T_{-\infty}) = \left(\sum_{j=1}^{N_r} \nu_{r,j} W_j\right) Q\Omega.$$

Summation of the equations (3.9), using (3.7), and substitution of the result into (3.15) then gives

$$(3.16)\quad T_\infty - T_{-\infty} = \frac{Q}{c_p}.$$

Since $Q > 0$, we see that $T_\infty > T_{-\infty}$.

4 Non-dimensional equations

In order to make the combustion equations (2.29) and (2.31) and the thermodynamic identity (2.19) dimensionless, we need representative values of the variables involved. Let $\tilde{f}$ denote this representative value of the variable f, then the associated dimensionless (scaled) variable f^* is defined by $f^* = f/\tilde{f}$. However, the mass fractions Y_i are not scaled since they are dimensionless already and instead of T^* we use the normalized dimensionless temperature $\vartheta = (T - T_{-\infty})/\tilde{T}$.

An important parameter in the non-dimensional equations is the Lewis number Le, which is defined by

$$(4.1)\quad Le = \frac{\lambda / c_p}{\rho D},$$

i.e. Le is the ratio of the diffusion coefficients λ / c_p in (2.31) and ρD in (2.29), respectively. To simplify the non-dimensionalization, we employ the final assumption:

17. Le and λ are constant.

Following [2], the non-dimensionalization is based on the following set of representative values:

$$(4.2) \quad \tilde{m},\, \tilde{x} = \frac{\lambda}{\tilde{m} c_p},\, \tilde{T} = T_{\infty} - T_{-\infty} = \frac{Q}{c_p},\, \tilde{\rho} = \frac{c_p p_0 W}{QR},\, \tilde{E},\, \tilde{h} = Q.$$

In (4.2), $\tilde{m}$ is a characteristic mass flux and $\tilde{x}$ is the diffusion length of equation (2.31) [9]. The choice of $\tilde{T}$ is suggested by (3.16) and $\tilde{\rho}$ is then computed from the ideal gas law (2.32). For $\tilde{E}$ several choices are possible and will be specified later.

The scaled combustion equations then read

$$(4.3) \quad m^* \frac{\mathrm{d}\vartheta}{\mathrm{d}x^*} = \frac{\mathrm{d}^2\vartheta}{\mathrm{d}x^{*2}} + s^*(\vartheta, Y_1, \cdots, Y_{N_r}),$$

$$(4.4) \quad m^* \frac{\mathrm{d}Y_i}{\mathrm{d}x^*} = \frac{1}{Le} \frac{\mathrm{d}^2 Y_i}{\mathrm{d}x^{*2}} + r_i s^*(\vartheta, Y_1, \cdots, Y_{N_r}).$$

In the following we will omit the asterisk $*$ and differentiation will again be denoted by a prime ($\prime$). The precise form of the chemical source term $s(\vartheta, Y_1, \cdots, Y_{N_r})$ depends on $\tilde{E}$. The obvious choice $\tilde{E} = R\tilde{T}$ would give

$$(4.5) \quad s(\vartheta, Y_1, \cdots, Y_{N_r}) = D_1(\vartheta)\, \mathrm{e}^{-E/(\vartheta+\beta)} \prod_{j=1}^{N_r} Y_j^{\nu_{r,j}},$$

with

$$(4.6) \quad D_1(\vartheta) = \frac{1}{\tilde{m}^2} \lambda B Q^{\alpha-\nu_r} c_p^{\nu_r-\alpha-1} \left(\frac{p_0}{R}\right)^{\nu_r} \left(\sum_{j=1}^{N_r} \nu_{r,j} W_j\right) \frac{W^{\nu_r}}{\prod_{j=1}^{N_r} W_j^{\nu_{r,j}}} (\vartheta + \beta)^{\alpha-\nu_r},$$

and with $\beta = T_{-\infty}/\tilde{T}$ the non-dimensional temperature of the unburnt gas. Another choice is $\tilde{E} = RT_{\infty}$, which is often used in activation energy asymptotics [2, 9]. In this case, $s(\vartheta, Y_1, \cdots, Y_{N_r})$ can be written as

$$(4.7) \quad s(\vartheta, Y_1, \cdots, Y_{N_r}) = D_2(\vartheta)\, \mathrm{e}^{-E(1-\vartheta)/(\vartheta+\beta)} \prod_{j=1}^{N_r} Y_j^{\nu_{r,j}},$$

with $D_2(\vartheta) = D_1(\vartheta)\mathrm{e}^{-E}$. Note that in the derivation of (4.7) a term e^{-E} is separated from the Arrhenius' factor. In the limit $E \to \infty$ it is then assumed that $D_2(\vartheta) = Const \neq 0$, so that $s(\vartheta, Y_1, \cdots, Y_{N_r}) \to 0$ except in the region where $\vartheta = 1 - O(1/E)$. The straightforward limit $E \to \infty$ would give $s(\vartheta, Y_1, \cdots, Y_{N_r}) \to 0$ everywhere and the chemical reaction would be completely eliminated from the formulation. For $E \to \infty$, only values of $D_2(\vartheta)$ for ϑ close to 1 are of importance, since for values of ϑ away from 1 the source term $s(\vartheta, Y_1, \cdots, Y_{N_r})$ is virtually 0 due to the exponential term. Therefore, $D_2(\vartheta)$ is often replaced by $D_2(1)$ and this number is referred to as the Damköhler number Da, although there are several Damköhler numbers [7]. An expression for the Damköhler number Da is

$$(4.8) \quad Da = D_2(1) = \frac{\lambda}{\tilde{m}^2 c_p} \left(\sum_{j=1}^{N_r} \nu_{r,j} W_j\right) \tilde{k} \prod_{j=1}^{N_r} \left(\frac{\rho_\infty}{W_j}\right)^{\nu_{r,j}},$$

with $\tilde{k} = BT_{\infty}^{\alpha}\mathrm{e}^{-E}$. Da can be interpreted as the ratio of a diffusion time to a reaction time [2].

The non-dimensional version of the thermodynamic identity (2.19) becomes

$$(4.9) \quad h = \frac{1}{Q} \sum_{j=1}^{N} Y_j h_j^0 + \vartheta - \vartheta_0,$$

with $\vartheta_0 = (T_0 - T_{-\infty})/\tilde{T}$ the normalized scaled reference temperature. Next, we will derive an alternative expression for h, in which it only depends on the reactant mass fractions Y_i $(i = 1, \cdots, N_r)$ and the normalized temperature ϑ. To that purpose, the product mass fractions Y_i $(i = N_r + 1, \cdots, N)$ have to be expressed in terms of the reactant mass fractions.

Consider equation (4.4) for a reactant $\mathcal{M}_{i_r}$ $(i_r \in \{1, \ldots, N_r\})$ and for a product $\mathcal{M}_{i_p}$ $(i_p \in \{N_r+1, \ldots, N\})$. In order to eliminate the chemical source terms, we take a suitable linear combination of both equations, and get the differential equation

$$(4.10) \quad m(r_{i_r} Y_{i_p} - r_{i_p} Y_{i_r})' = \frac{1}{Le}(r_{i_r} Y_{i_p} - r_{i_p} Y_{i_r})'',$$

which is subject to the boundary conditions

$$(4.11) \quad (r_{i_r} Y_{i_p} - r_{i_p} Y_{i_r})_{-\infty} = (r_{i_r} Y_{i_p} - r_{i_p} Y_{i_r})_{\infty} = r_{i_r} r_{i_p}.$$

The solution of the boundary value problem (4.10)-(4.11) is obviously

$$(4.12) \quad r_{i_r} Y_{i_p} - r_{i_p} Y_{i_r} = r_{i_r} r_{i_p},$$

and subsequently summation over all reactants gives

$$(4.13) \quad Y_{i_p} = r_{i_p}(1 - \sum_{j=1}^{N_r} Y_j), \; i_p = N_r + 1, \cdots, N.$$

Splitting the sum in (4.9) into a reactant part and a product part and substitution of (4.13) into this equation gives

$$(4.14) \quad h = \frac{1}{Q} \sum_{j=1}^{N_r} \left(h_j^0 - \sum_{l=N_r+1}^{N} r_l h_l^0 \right) Y_j + \frac{1}{Q} \sum_{j=N_r+1}^{N} r_j h_j^0 + \vartheta - \vartheta_0.$$

Using (3.2) and (3.5) the above equation can be rewritten as

$$(4.15) \quad h = \sum_{j=1}^{N_r} Y_j + \frac{1}{Q} \sum_{j=1}^{N_r} \sum_{l=1}^{N_r} (r_l Y_j - r_j Y_l) h_l^0 + \frac{1}{Q} \sum_{j=N_r+1}^{N} r_j h_j^0 + \vartheta - \vartheta_0.$$

Analogously to the derivation of (4.12) one can proof that $r_{i_1} Y_{i_2} - r_{i_2} Y_{i_1} = 0$ for any two reactants $\mathcal{M}_{i_1}$ and $\mathcal{M}_{i_2}$, and therefore the second sum in (4.15) cancels. The final expression for h is then

$$(4.16) \quad h = \sum_{j=1}^{N_r} Y_j + \frac{1}{Q} \sum_{j=N_r+1}^{N} r_j h_j^0 + \vartheta - \vartheta_0.$$

5 Qualitative analysis for the case $Le = 1$.

For $Le = 1$, the combustion equations reduce to

$$(5.1) \quad m\vartheta' = \vartheta'' + s(\vartheta, Y_1, \cdots, Y_{N_r}),$$

$$(5.2) \quad mY_i' = Y_i'' + r_i s(\vartheta, Y_1, \cdots, Y_{N_r}),$$

and these equations are subject to the boundary conditions

$$(5.3) \quad \vartheta_{-\infty} = 0, \; \vartheta_{\infty} = 1,$$

(5.4) $Y_{i,-\infty} = -r_i,\ Y_{i,\infty} = 0,\ i = 1, \cdots, N_r,$

(5.5) $Y_{i,-\infty} = 0,\ Y_{i,\infty} = r_i,\ i = N_r + 1, \cdots, N.$

For the chemical source term $s(\vartheta, Y_1, \cdots, Y_{N_r})$ we adopt the model (cf. (4.7))

(5.6) $$s(\vartheta, Y_1, \cdots, Y_{N_r}) = Da\, \mathrm{e}^{-E(1-\vartheta)/(\vartheta+\beta)} \prod_{j=1}^{N_r} Y_j^{\nu_{r,j}}.$$

The unknowns in the boundary value problem (5.1)-(5.5) are the mass flux m, the normalized temperature ϑ and the mass fractions Y_i.

We can eliminate the source term from all equations but one. To that purpose, we introduce the Shvab-Zeldovich variables Z_i, which are defined by [9]

(5.7) $Z_i = r_i\vartheta - Y_i,\ i = 1, \cdots, N.$

It is easy to see that the Shvab-Zeldovich variables satisfy

(5.8) $mZ_i' = Z_i'',\ i = 1, \cdots, N,$

(5.9) $Z_{i,-\infty} = Z_{i,\infty} = r_i,\ i = 1, \cdots, N_r,$

(5.10) $Z_{i,-\infty} = Z_{i,\infty} = 0,\ i = N_r + 1, \cdots, N.$

The solutions of (5.8)-(5.10) are evidently $Z_i = r_i$ for $i = 1, \cdots, N_r$ and $Z_i = 0$ for $i = N_r + 1, \cdots, N$. Consequently, $Y_i = -r_i(1 - \vartheta)$ for the reactants ($i = 1, \cdots, N_r$) and $Y_i = r_i\vartheta$ for the products ($i = N_r + 1, \cdots, N$). Substituting $Y_i = -r_i(1 - \vartheta)$ ($i = 1, \cdots, N_r$) into (5.6), it is clear that the equation for ϑ reads:

(5.11) $$m\vartheta' = \vartheta'' + \bar{s}(\vartheta),\ \bar{s}(\vartheta) = Da\, r(1 - \vartheta)^{\nu_r} \mathrm{e}^{-E(1-\vartheta)/(\vartheta+\beta)},\ r = \prod_{j=1}^{N_r} (-r_j)^{\nu_{r,j}}.$$

Once m and ϑ are computed from the boundary value problem (5.11) and (5.3) the mass fractions Y_i can easily be obtained.

For $x \to -\infty$ (cold boundary), ϑ' and ϑ'' should vanish in order to ensure that $\vartheta_{-\infty} = 0$. However, this is impossible since $\bar{s}(0) \neq 0$. Therefore, the boundary value problem (5.11) and (5.3) is improperly posed. A remedy to this cold-boundary difficulty is to introduce an ignition temperature ϑ_{ign} ($0 < \vartheta_{ign} < 1$), i.e. multiply the source term $\bar{s}(\vartheta)$ in (5.11) with the Heaviside function $H(\vartheta - \vartheta_{ign})$; see also Section 3. Further, note that ϑ is invariant under the translation $x \mapsto x + c$ for arbitrary c. Therefore, we impose the extra condition $\vartheta(0) = \vartheta_{ign}$. Thus, in the sequel of this section we will consider the following boundary value problem for ϑ:

(5.12) $m\vartheta' = \vartheta'' + H(\vartheta - \vartheta_{ign})\bar{s}(\vartheta),$

(5.13) $\vartheta_{-\infty} = 0,\ \vartheta(0) = \vartheta_{ign},\ \vartheta_{\infty} = 1.$

The existence and uniqueness of the solution of (5.12)-(5.13) is proven in [1].

The chemical source term in (5.12) is a production term for heat, as is stated in:

Lemma 5.1 *Let $\bar{s}(\vartheta)$ be defined in (5.11), then $\bar{s}(\vartheta) > 0$ for $\vartheta \neq 1$.*

Proof. The proof is trivial if ν_r is even. Therefore, suppose ν_r is odd and assume there exists an x_0 such that $\bar{s}(\vartheta(x_0)) < 0$, and consequently $\vartheta(x_0) > 1$. Because $\vartheta(0) < 1, \vartheta_\infty = 1$ and ϑ is at least twice continuously differentiable for $\vartheta > 1$, there exists an x_1 such that $\vartheta(x_1) > 1$, $\vartheta'(x_1) = 0$ and $\vartheta''(x_1) < 0$ (ϑ assumes a maximum at x_1). This is impossible because of (5.12). Now suppose $\bar{s}(\vartheta(x_0)) = 0$, or $\vartheta(x_0) = 1$, for some x_0. Similar to the previous case, the conditions $\vartheta'(x_0) > 0$ or $\vartheta'(x_0) < 0$ lead to a contradiction, so that $\vartheta'(x_0) = 0$ should hold. From (5.12) it follows that also $\vartheta''(x_0) = 0$. Repeatedly differentiation of (5.12) then gives $\vartheta^{(n)}(x_0) = 0$ for $n \geq 1$. This implies that $\vartheta(x) \equiv 1$, which is in contradiction with the boundary condition at $x = 0$. □

Some properties of m, ϑ and Y_i are formulated in the following theorems and corollaries.

Theorem 5.2 *Suppose the mass flux m satisfies (5.12), then $m > 0$.*

Proof. Since ϑ is bounded for $x \to \pm\infty$, $\vartheta'_{-\infty}$ and ϑ'_∞ should vanish. Integration of (5.12) over the whole real axis gives

$$m = \int_{-\infty}^{\infty} H(\vartheta(x) - \vartheta_{ign})\bar{s}(\vartheta(x))\mathrm{d}x,$$

and from Lemma 5.1 it is evident that $m > 0$. □

Theorem 5.3 *Suppose ϑ satisfies the boundary value problem (5.12)-(5.13), then*

$$\vartheta'(x) = \int_x^{\infty} \mathrm{e}^{m(x-y)} H(\vartheta(y) - \vartheta_{ign})\bar{s}(\vartheta(y))\mathrm{d}y. \tag{5.14}$$

Proof. Equation (5.12) can be rewritten as

$$(\vartheta'\mathrm{e}^{-mx})' = -\mathrm{e}^{-mx} H(\vartheta - \vartheta_{ign})\bar{s}(\vartheta).$$

Integration of this equation over (x, ∞) then gives (5.14) because $m > 0$. □

Corollary 5.4

(i) *$\vartheta(x) = \vartheta_{ign}\mathrm{e}^{mx}$ for $x \leq 0$.*

(ii) *ϑ is strictly increasing and $\vartheta_{ign} < \vartheta(x) < 1$ for $x > 0$.*

(iii) *$Y_i(x) = -r_i(1 - \vartheta_{ign}\mathrm{e}^{mx})$ $(i = 1, \cdots, N_r)$ and $Y_i(x) = r_i\vartheta_{ign}\mathrm{e}^{mx}$ $(i = N_r + 1, \cdots, N)$ for $x \leq 0$.*

(iv) *The reactant mass fractions are strictly decreasing and $0 < Y_i(x) < -r_i(1 - \vartheta_{ign})$ $(i = 1, \cdots, N_r)$ for $x > 0$. Likewise, the product mass fractions are strictly increasing and $r_i\vartheta_{ign} < Y_i(x) < r_i$ $(i = N_r + 1, \cdots, N)$ for $x > 0$.*

Because of this corollary, the boundary value problem (5.12)-(5.13) can be restricted to $x \geq 0$:

$$m\vartheta' = \vartheta'' + \bar{s}(\vartheta),\ x > 0, \tag{5.15}$$

$$\vartheta(0) = \vartheta_{ign},\ \vartheta'(0) = m\vartheta_{ign},\ \vartheta_\infty = 1. \tag{5.16}$$

The second boundary condition in (5.16) can be obtained by integrating (5.12) over $(-\infty, 0)$.

Theorem 5.5 *Suppose ϑ satisfies the boundary value problem (5.15)-(5.16), then $0 < \vartheta' < m$.*

Proof. The proof of $\vartheta' > 0$ is trivial. From (5.14) we can deduce the inequalities

$$\vartheta'(x) = \int_x^\infty \mathrm{e}^{m(x-y)}\bar{s}(\vartheta(y))\mathrm{d}y < \int_x^\infty \bar{s}(\vartheta(y))\mathrm{d}y \leq \int_0^\infty \bar{s}(\vartheta(x))\mathrm{d}x,$$

where we have used that $m > 0$ and $\bar{s}(\vartheta(y)) > 0$. Integration of (5.15) over $(0, \infty)$ gives

$$m = \int_0^\infty \bar{s}(\vartheta(x))\mathrm{d}x,$$

which completes the proof. □

Corollary 5.6 *$r_i m < Y_i'(x) < 0$ for the reactants $(i = 1, \cdots, N_r)$ and $0 < Y_i'(x) < r_i m$ for the products $(i = N_r + 1, \cdots, N)$.*

A priori estimates for m are given in:

Theorem 5.7 *Let*

$$\bar{m} = \left(2\int_{\vartheta_{ign}}^1 \bar{s}(\vartheta)\mathrm{d}\vartheta\right)^{\frac{1}{2}}$$

and m be the mass flux in (5.15)-(5.16),then

$$\text{(5.17)} \quad \bar{m} < m < \frac{1}{\vartheta_{ign}}\bar{m}.$$

Proof. Multiplying equation (5.15) with 1,ϑ or ϑ', and subsequently integrating the resulting equation over $(0, \infty)$ gives, respectively:

$$\text{(5.18)} \quad m = \int_0^\infty \bar{s}(\vartheta(x))\mathrm{d}x,$$

$$\text{(5.19)} \quad \frac{1}{2}m(1 + \vartheta_{ign}^2) = -\int_0^\infty \vartheta'(x)^2\mathrm{d}x + \int_0^\infty \bar{s}(\vartheta(x))\vartheta(x)\mathrm{d}x,$$

$$\text{(5.20)} \quad \frac{1}{2}m\vartheta_{ign}^2 = -\int_0^\infty \vartheta'(x)^2\mathrm{d}x + \frac{1}{m}\int_{\vartheta_{ign}}^1 \bar{s}(\vartheta)\mathrm{d}\vartheta.$$

The inequality $m < \bar{m}/\vartheta_{ign}$ follows immediately from (5.20). Subtracting (5.19) from (5.18) and adding the difference to (5.20) gives

$$\frac{1}{2}m = \frac{1}{m}\int_{\vartheta_{ign}}^1 \bar{s}(\vartheta)\mathrm{d}\vartheta + \int_0^\infty \bar{s}(\vartheta(x))(1 - \vartheta(x))\mathrm{d}x,$$

and because $\bar{s}(\vartheta) > 0$ and $\vartheta < 1$ the inequality $m > \bar{m}$ holds. □

We conclude this section with a theorem about the enthalpy.

Theorem 5.8 *The flow is isenthalpic, i.e. h is constant, and*

$$\text{(5.21)} \quad h = -\frac{1}{Q}\sum_{j=1}^{N_r} r_j h_j^0 - \vartheta_0.$$

Proof. Define $Z = \sum_{j=1}^{N_r} Y_j + \vartheta$. Summation of equation (5.1) and the equations (5.2) for all reactants $\mathcal{M}_i$, $(i = 1, \cdots, N_r)$, and using (3.5), gives the following boundary value problem for Z:

$$mZ' = Z'',$$

$$Z_{-\infty} = Z_\infty = 1.$$

The solution hereof is $Z = 1$, and combining this with (4.16) and (3.2) then gives (5.21). □

6 Qualitative analysis for the case $Le \neq 1$.

The complete boundary value problem for the general case $Le \neq 1$ reads:

$$(6.1)\quad m\vartheta' = \vartheta'' + H(\vartheta - \vartheta_{ign})\, s(\vartheta, Y_1, \cdots, Y_{N_r}),$$

$$(6.2)\quad mY_i' = \frac{1}{Le}Y_i'' + H(\vartheta - \vartheta_{ign})\, r_i s(\vartheta, Y_1, \cdots, Y_{N_r}),$$

$$(6.3)\quad \vartheta_{-\infty} = 0,\ \vartheta(0) = \vartheta_{ign},\ \vartheta_\infty = 1,$$

$$(6.4)\quad Y_{i,-\infty} = -r_i,\ Y_{i,\infty} = 0,\ i = 1, \cdots, N_r,$$

$$(6.5)\quad Y_{i,-\infty} = 0,\ Y_{i,\infty} = r_i,\ i = N_r + 1, \cdots, N,$$

with the chemical source term $s(\vartheta, Y_1, \cdots, Y_{N_r})$ defined in (5.6). Note that the ignition temperature ϑ_{ign} is introduced in (6.1) and (6.2) in order to circumvent the cold-boundary difficulty. The existence and uniqueness of the solution of a similar system of equations for laminar flames is established in [11]. Using the relation $r_{i_1}Y_{i_2} = r_{i_2}Y_{i_1}$, which holds for any two reactants $\mathcal{M}_{i_1}$ and $\mathcal{M}_{i_2}$, one can prove that $s(\vartheta, Y_1, \cdots, Y_{N_r}) \geq 0$. This proof is analogous to the proof of Lemma 5.1 and is therefore omitted.

The following two theorems are straightforward extensions of Theorem 5.2 and 5.3, and therefore their proofs are omitted.

Theorem 6.1 *Suppose the mass flux m satisfies (6.1) and (6.2), then $m > 0$.*

Theorem 6.2 *Suppose ϑ and Y_i ($i = 1, \cdots, N$) satisfy the boundary value problem (6.1)-(6.5), then*

$$(6.6)\quad \vartheta'(x) = \int_x^\infty e^{m(x-y)} H(\vartheta(y) - \vartheta_{ign})\, s(\vartheta(y), Y_1(y), \cdots, Y_{N_r}(y))\mathrm{d}y$$

and

$$(6.7)\quad Y_i'(x) = r_i Le \int_x^\infty e^{Le\, m(x-y)} H(\vartheta(y) - \vartheta_{ign})\, s(\vartheta(y), Y_1(y), \cdots, Y_{N_r}(y))\mathrm{d}y.$$

Corollary 6.3

(i) *$\vartheta(x) = \vartheta_{ign}e^{mx}$ for $x \leq 0$.*

(ii) *ϑ is strictly increasing and $\vartheta_{ign} < \vartheta(x) < 1$ for $x > 0$.*

(iii) *$Y_i(x) = -r_i + C_i e^{Le\, mx}$ ($i = 1, \cdots, N_r$) and $Y_i(x) = C_i e^{Le\, mx}$ ($i = N_r + 1, \cdots, N$) for $x \leq 0$. The integration constants satisfy $r_i \leq C_i \leq 0$ for $i = 1, \cdots, N_r$, $0 \leq C_i \leq r_i$ for $i = N_r + 1, \cdots, N$ and $\sum_{i=1}^N C_i = 0$.*

(iv) *The reactant mass fractions are strictly decreasing and $0 < Y_i(x) < -r_i + C_i$ ($i = 1, \cdots, N_r$) for $x > 0$. Likewise, the product mass fractions are strictly increasing and $C_i < Y_i(x) < r_i$ ($i = N_r + 1, \cdots, N$) for $x > 0$.*

When the solution of (6.1)-(6.5) is known for $x > 0$, then this solution is also known for $x \leq 0$ because of Corollary 6.3. Therefore, we restrict ourselves to the following boundary value problem, defined on $(0, \infty)$:

$$(6.8)\quad m\vartheta' = \vartheta'' + s(\vartheta, Y_1, \cdots, Y_{N_r}),\ x > 0,$$

$$mY_i' = \frac{1}{Le}Y_i'' + r_i s(\vartheta, Y_1, \cdots, Y_{N_r}),\ x > 0, \tag{6.9}$$

$$\vartheta(0) = \vartheta_{ign},\ \vartheta'(0) = m\vartheta_{ign},\ \vartheta_\infty = 1, \tag{6.10}$$

$$Y_i'(0) - Le\, m(Y_i(0) + r_i) = 0,\ Y_{i,\infty} = 0,\ i = 1, \cdots, N_r, \tag{6.11}$$

$$Y_i'(0) - Le\, mY_i(0) = 0,\ Y_{i,\infty} = r_i,\ i = N_r + 1, \cdots, N. \tag{6.12}$$

The boundary conditions for ϑ' and Y_i' at $x = 0$ are obtained by integrating (6.1) and (6.2), respectively, over $(-\infty, 0)$.

Theorem 6.4 *Suppose* ϑ *and* Y_i $(i = 1, \cdots, N)$ *satisfy the boundary value problem (6.8)-(6.12), then* $0 < \vartheta' < m$, $r_i Le\, m < Y_i' < 0$ $(i = 1, \cdots, N_r)$ *and* $0 < Y_i' < r_i Le\, m$ $(i = N_r + 1, \cdots, N)$.

Proof. We only proof the inequalities for the reactants ; the other inequalities can be proven analogously. It is trivial that $Y_i' < 0$ for $i = 1, \cdots, N_r$. From Theorem 6.2 we see that $Y_i'(x) = r_i Le \int_x^\infty \mathrm{e}^{Le\, m(x-y)} s(\vartheta(y), Y_1(y), \cdots, Y_{N_r}(y))\mathrm{d}y > r_i Le \int_0^\infty s(\vartheta(x), Y_1(x), \cdots, Y_{N_r}(x))\mathrm{d}x$, where we have used that $r_i < 0$ $(i = 1, \cdots, N_r)$, $m > 0$ and $s(\vartheta(x), Y_1(x), \cdots, Y_{N_r}(x)) \geq 0$. Lastly, integration of (6.8) over $(0, \infty)$ gives $m = \int_0^\infty s(\vartheta(x), Y_1(x), \cdots, Y_{N_r}(x))\mathrm{d}x$, which completes the proof. □

Consider the Shvab-Zeldovich variables Z_i defined in (5.7). Using these variables, we were able to proof the equalities $Y_i = -r_i(1 - \vartheta)$ $(i = 1, \cdots, N_r)$ and $Y_i = r_i\vartheta$ $(i = N_r + 1, \cdots, N)$ for the equidiffusive case $Le = 1$. In the general case $Le \neq 1$ these equalities do not hold anymore. Instead, lower and upper bounds for the mass fractions can be derived, based on bounds for the Shvab-Zeldovich variables. From (6.8) and (6.9) the following two equations for Z_i can be easily obtained:

$$mZ_i' = Z_i'' + (1 - \frac{1}{Le})Y_i'', \tag{6.13}$$

$$mZ_i' = \frac{1}{Le}Z_i'' + (1 - \frac{1}{Le})r_i\vartheta''. \tag{6.14}$$

The boundary conditions for Z_i are given in (5.9)-(5.10).

Bounds for Z_i are given in the following two lemmas.

Lemma 6.5 *For the Shvab-Zeldovich variables* Z_i $(i = 1, \cdots, N_r)$ *the following inequalities hold:*

$$\mid Z_i - r_i \mid \leq \mid 1 - \frac{1}{Le} \mid Y_i, \tag{6.15}$$

$$\mid Z_i - r_i \mid \leq \mid Le - 1 \mid r_i(\vartheta - 1). \tag{6.16}$$

Proof. To prove the first inequality, we integrate (6.13) over $(-\infty, x)$. Using the boundary conditions (5.9), this gives

$$m(Z_i - r_i) = Z_i' + (1 - \frac{1}{Le})Y_i'.$$

This equation can be rewritten as

$$((Z_i - r_i)\mathrm{e}^{-mx})' = -(1 - \frac{1}{Le})\mathrm{e}^{-mx}Y_i'.$$

Integration of this latter equation over (x, ∞) then yields

$$Z_i - r_i = (1 - \frac{1}{Le}) \int_x^{\infty} \mathrm{e}^{m(x-y)} Y_i'(y) \mathrm{d}y,$$

from which the above inequality can be easily derived, since $m > 0$.
Similarly we can deduce

$$Z_i - r_i = r_i(Le - 1) \int_x^{\infty} \mathrm{e}^{Le\, m(x-y)} \vartheta'(y) \mathrm{d}y$$

from equation (6.14) and the boundary conditions (5.9). From this equation the inequality (6.16) can easily be obtained. □

The following lemma holds for the Shvab-Zeldovich variables Z_i $(i = N_r + 1, \cdots, N)$ corresponding to the products. The proof is completely analogous to the proof of Lemma 6.5 and is therefore omitted.

Lemma 6.6 *For the Shvab-Zeldovich variables* Z_i $(i = N_r + 1, \cdots, N)$ *the following inequalities hold:*

$$(6.17) \quad | Z_i | \leq | 1 - \frac{1}{Le} | (r_i - Y_i),$$

$$(6.18) \quad | Z_i | \leq | Le - 1 | \, r_i(1 - \vartheta).$$

A straightforward combination of the inequalities in (6.15)-(6.18) gives the following bounds for the mass fractions Y_i.

Theorem 6.7 *The reactant and product mass fractions in (6.8)-(6.12) satisfy, respectively,*

$$(6.19) \quad f_l(Le) r_i(\vartheta - 1) \leq Y_i \leq f_u(Le) r_i(\vartheta - 1) \, (i = 1, \cdots, N_r)$$

and

$$(6.20) \quad f_l(Le) r_i(1 - \vartheta) \leq r_i - Y_i \leq f_u(Le) r_i(1 - \vartheta) \, (i = N_r + 1, \cdots, N),$$

with the functions f_l *and* f_u *defined by*

$$f_l(y) = \begin{cases} y, & 0 < y < 1 \\ \frac{y}{2y-1}, & y \geq 1 \end{cases}, \quad f_u(y) = \begin{cases} 2 - y, & 0 < y < 1 \\ y, & y \geq 1 \end{cases}.$$

Using the inequalities in Theorem 6.7, we can derive the following bounds for the mass flux m.

Theorem 6.8 *Let*

$$\bar{m} = \left(2Da\, r \int_{\vartheta_{ign}}^{1} \mathrm{e}^{-E(1-\vartheta)/(\vartheta+\beta)} (1 - \vartheta)^{\nu_r} \mathrm{d}\vartheta \right)^{\frac{1}{2}}, \quad r = \prod_{j=1}^{N_r} (-r_j)^{\nu_{r,j}},$$

and m *be the mass flux in (6.8)-(6.12), then*

$$(6.21) \quad f_l(Le)^{\nu_r/2} \bar{m} < m < \frac{1}{\vartheta_{ign}} f_u(Le)^{\nu_r/2} \bar{m}.$$

Proof. Analogous to the proof of Theorem 5.7, we can prove the inequalities

$$(6.22) \quad 2 \int_{\vartheta_{ign}}^{1} s(\vartheta, Y_1, \cdots, Y_{N_r}) \mathrm{d}\vartheta < m^2 < \frac{2}{\vartheta_{ign}} \int_{\vartheta_{ign}}^{1} s(\vartheta, Y_1, \cdots, Y_{N_r}) \mathrm{d}\vartheta.$$

Combining (6.22) with the inequalities of Theorem 6.7 then gives the bounds for m. □

Bounds for the enthalpy h are given in the following theorem.

Theorem 6.9 *Let* $\bar{h} = -\frac{1}{Q}\sum_{j=1}^{N_r} r_j h_j^0 - \vartheta_0$, *i.e.* $\bar{h}$ *is the specific enthalpy for* $Le = 1$, *then the following inequalities hold:*

$$(6.23)\quad \bar{h} - (\frac{1}{Le} - 1)\sum_{j=1}^{N_r} Y_j \leq h \leq \bar{h},$$

$$(6.24)\quad \bar{h} - (1 - Le)(1 - \vartheta) \leq h \leq \bar{h},$$

for $0 < Le < 1$, *and*

$$(6.25)\quad \bar{h} \leq h \leq \bar{h} + (1 - \frac{1}{Le})\sum_{j=1}^{N_r} Y_j,$$

$$(6.26)\quad \bar{h} \leq h \leq \bar{h} + (Le - 1)(1 - \vartheta),$$

for $Le > 1$.

Proof. From (6.1) and (6.2) we can deduce the following differential equation for h:

$$(6.27)\quad mh' = h'' + (\frac{1}{Le} - 1)\sum_{j=1}^{N_r} Y_j''.$$

Furthermore, h fulfils the boundary conditions

$$h_{-\infty} = h_{\infty} = \bar{h}.$$

First we integrate (6.27) over $(-\infty, x)$. This integrated version of (6.27) can be written as

$$((h - \bar{h})e^{-mx})' = (1 - \frac{1}{Le})\,e^{-mx}\sum_{j=1}^{N_r} Y_j'.$$

Integration of this latter equation over (x, ∞) then gives

$$h - \bar{h} = (\frac{1}{Le} - 1)\sum_{j=1}^{N_r}\int_x^{\infty} e^{m(x-y)} Y_j'(y)\mathrm{d}y,$$

from which (6.23) and (6.24) can easily be obtained since $m > 0$ and since the reactant mass fractions $Y_i\,(i = 1,\cdots,N_r)$ are strictly decreasing. An alternative differential equation for h, which can be derived from (6.1) and (6.2) is

$$mh' = \frac{1}{Le}h'' + (1 - \frac{1}{Le})\vartheta''.$$

The proof of (6.25) and (6.26) now proceeds in exactly the same way as the proof of (6.23) and (6.24). □

Appendix: Nomenclature

A	frequency factor $((\mathrm{mol}/\mathrm{m}^3)^{1-\nu_r}/\mathrm{s})$
a_f	frozen speed of sound (m/s)
B	constant in frequency factor $((\mathrm{mol}/\mathrm{m}^3)^{1-\nu_r}/(\mathrm{K}^\alpha \mathrm{s}))$
c_p	specific heat at constant pressure of gas mixture $(\mathrm{J}/(\mathrm{kg\,K}))$
$c_{p,i}$	specific heat at constant pressure for species $\mathcal{M}_i$ $(\mathrm{J}/(\mathrm{kg\,K}))$
c_v	specific heat at constant volume of gas mixture $(\mathrm{J}/(\mathrm{kg\,K}))$
D	binary diffusion coefficient for all pairs of species $(\mathrm{m}^2/\mathrm{s})$
Da	Damköhler number
E	activation energy (J/mol)
h	specific enthalpy of the gas mixture (J/kg)
h_i	specific enthalpy of species $\mathcal{M}_i$ (J/kg)
h_i^0	specific heat of formation of species $\mathcal{M}_i$ at a reference temperature T_0 (J/kg)
k	specific rate constant $((\mathrm{mol}/\mathrm{m}^3)^{1-\nu_r}/\mathrm{s})$
Le	Lewis number
m	mass flux $(\mathrm{kg}/(\mathrm{m}^2\mathrm{s}))$
Ma	Mach number
N	total number of chemical species present
p	hydrostatic pressure $(\mathrm{N}/\mathrm{m}^2)$
p_0	constant approximate pressure $(\mathrm{N}/\mathrm{m}^2)$
Q	specific heat of combustion (J/kg)
R	universal gas constant $(\mathrm{J}/(\mathrm{mol\,K}))$
r_i	mass of species $\mathcal{M}_i$ per unit mass of reactants, produced by the chemical reaction
T	(absolute) temperature of the gas mixture (K)
u	mass-weighted average velocity of the gas mixture (m/s)
$\overline{W}$	average molecular weight of the gas mixture (kg/mol)
w_i	reaction rate of species $\mathcal{M}_i$ $(\mathrm{kg}/(\mathrm{m}^3\mathrm{s}))$
W_i	molecular weight of species $\mathcal{M}_i$ (kg/mol)
Y_i	mass fraction of species $\mathcal{M}_i$
α	exponent determining the temperature dependence of the frequency factor
γ	specific heat ratio of the gas mixture
δp	perturbation of the constant pressure p_0 $(\mathrm{N}/\mathrm{m}^2)$
λ	thermal conductivity $(\mathrm{J}/(\mathrm{m\,s\,K}))$
$\nu_{r,i}$	stoichiometric coefficient for species $\mathcal{M}_i$ appearing as a reactant
$\nu_{p,i}$	stoichiometric coefficient for species $\mathcal{M}_i$ appearing as a product
ρ	mass density of the gas mixture $(\mathrm{kg}/\mathrm{m}^3)$
ω	reaction rate for a single reaction $(\mathrm{mol}/(\mathrm{m}^3\mathrm{s}))$

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