Laminar Flame Propagation in a Premixed Particle Cloud: Effect of Vaporization Rate

C. Vázquez-Espí

Department of Applied Mathematics, E. T. S. de Ingeniería Aeronáutica y del Espacio, Universidad Politécnica de Madrid (UPM), Madrid, Spain

ABSTRACT

The propagation of a flame in a mixture of air and small solid fuel particles is analyzed. It is assumed that solid particles suffer a vaporization, after which the resulting gaseous fuel mixes with air and a premixed combustion occurs. The combustion reaction is modeled by a global reaction of Arrhenius type with large activation energy and the analysis is carried out using large activation energy asymptotics. The structure of the flow is similar to a classical premixed flame, but with some particular features due to the vaporization, whose characteristic time, through the appropriate Damköhler number, plays an important role. Lean and rich mixtures, defined from the solid fuel content, are considered, as well as the effect of Lewis numbers and heat of vaporization. The analysis shows that rich mixtures can be lean or rich in the gaseous phase depending on the value of the vaporization Damköhler number. In all regimes the structure of flow and the flame speed are obtained.

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Introduction

The analysis of flame propagation in a cloud of solid fuel particles has received a lot of attention for a long time in order to improve the knowledge of dust explosions and fires in industrial facilities as coal plants, cereal silos or mills (Eckhoff, 1997). More recently, the need for new energy resources has increased the interest in the use of biomass particles in small power plants. In several works Bidabadi et al. (2015, and the references therein) have considered the lycopodium dust flame with the double aim of studying the mechanisms of explosions and flame propagation in dust clouds, and the application of microscale biomass to small power plants as Stirling engines.

The aim of this work is to study the flame propagation in a premixed mixture of oxidant and gaseous fuel resulting from the vaporization of micro organic particles, as starch dust or lycopodium whose diameters are around $30\text{ }\mu\text{m}$ (Proust, 2006b), focusing on the role of the characteristic time and heat of vaporization. A question that arises is to what extent the premixed flame model is applicable. An isolated particle typically burns with an envelope diffusion flame surrounding it. In a cloud of particles, the gaseous fuel from the condensed phase can mix with the air before burning if the corresponding diffusion flame radius is larger than the characteristic distance between particles, which

requires a large enough density of particles. In the analysis of spray combustion, Williams (1985, chap. 11) has shown that cloud-burning mode occurs if the equivalence ratio of the initial mixture is greater than, approximately, 0.7, and that homogeneous combustion occurs in a monodisperse spray if the initial droplet diameter is about $20\text{ }\mu\text{m}$. Nakamura et al. (2005) have performed DNS to study the spray combustion mechanism showing that diffusion-like combustion occurs for large droplets, diameter $\sim 100\mu\text{m}$, while for small droplets, diameter $\sim 30\mu\text{m}$, premixed-like combustion appears. A similar claim has been done by Gao et al. (2015). Many studies on flame propagation in small particle clouds have acknowledged the former results and considered that combustion occurs in premixed mode (Bidabadi et al., 2010; Rockwell and Rangwala, 2013; Seshadri et al., 1992).

For small particles of coal, Bermúdez et al. (2007, 2011) have established that gas-phase reactions do not occur in diffusion flames around the particles. Therefore the gaseous fuel produced by the vaporization is not burned around the particles but mixed with the air. Since the initial mixture of solid particles is assumed to be homogeneous, the resulting fuel air mixture is also homogeneous, through which a premixed flame can propagate. Proust (2006a, 2006b) has experimentally observed laminar flame propagation in several dust air mixtures, with mean particle diameter between $28\text{ }\mu\text{m}$ and $42\text{ }\mu\text{m}$ and low vaporization temperature, supporting the idea of a great similarity with premixed gaseous flames.

Two reactions occur simultaneously in the mixture: vaporization and combustion. The first one will be modeled by a reaction rate depending on temperature through a Heaviside function (Bidabadi et al., 2015, 2010), although other approaches are possible (Seshadri et al., 1992), while the combustion will be modeled by a global reaction of Arrhenius type, with activation energy much larger than the thermal energy. This will allow us to use asymptotic techniques in the analysis. Each reaction has its own characteristic time and Damköhler number, defined as the ratio of the residence time to the reaction time. Thus we will define two Damköhler numbers, D_v and D_a associated, respectively, to the vaporization and combustion reactions. D_v determines the rate at which the solid particles are converted into gaseous fuel. For very large values of D_v the vaporization is very fast and we find the classical premixed flame. However for order unity, or smaller, values of D_v , the vaporization is not completed upstream of the reaction zone, but it continues in the convective zone located downstream. In previous works (Bidabadi et al., 2015, 2010; Seshadri et al., 1992) the analysis of this zone appears to be incomplete. The value of D_v , which determines the distribution of gaseous fuel, has an important effect over the flow structure and flame speed, hence we will analyze the problem in the range of D_v of order unity and determine the structure of the flow and the flame speed. Our analysis will include the effects of heat of vaporization and Lewis number, often neglected in other works.

This problem could be addressed from very detailed models available in the literature (e.g., Cloney et al., 2018; Krazinski et al., 1979; Slezak et al., 1985; Smoot and Horton, 1977), but, due to their high degree of complexity, it is necessary to treat them by a non-trivial numerical approach. Instead, we will consider a simplified model in order to use as many analytical tools as possible, although the full solution will also require numerics but to a lower level. This approach will allow us to give a clear picture of the role of D_v that otherwise could be hidden.

Governing equations

Let us consider a uniform mixture of air and solid fuel particles. The Stokes number of these particles, defined as the ratio between the particle relaxation time and the residence time in a typical combustion chamber, is small, around 10^{-2} , therefore we can assume they behave as non-inertial particles and move with the same velocity as the gas. The temperature inside the small particles considered in this work is assumed to be uniform and equal to the local gas temperature (Proust, 2006a). When the temperature is larger than a threshold temperature, or vaporization temperature, we assume that all solid material in each particle is converted by vaporization into gaseous fuel, although not instantaneously, which mixes perfectly with the air resulting in a homogeneous reactive mixture.

The species in the mixture are fuel in solid and gas phases, $F(s)$ and $F(g)$, oxygen, $O(g)$, nitrogen, $N(g)$, and the products of combustion collectively represented by $P(g)$. The mass fractions are Y_s , Y_g , Y_o , Y_n and Y_p , respectively.

The vaporization is modeled by the reaction $F(s) \rightarrow F(g) - M_g Q_v$, where Q_v is the heat required to vaporize the unit mass of solid fuel and M_g is the molecular mass of the fuel. The mass rate of this reaction is assumed to be given by

$$W_v = -M_g \frac{\rho Y_s}{M_g} \frac{1}{t_v} H(T - T_v), \quad (2.1)$$

where ρ is the mixture density, H is the Heaviside function, T_v is the threshold temperature for vaporization and t_v is the vaporization characteristic time.

The chemical reaction between gaseous fuel and oxygen is modeled by a single irreversible reaction $\nu_g F(g) + \nu_o O(g) \rightarrow \nu_p P(g) + \nu_g M_g Q$, where ν_g , ν_o and ν_p are the stoichiometric coefficients and Q stands for the heat released by unit mass of fuel. The gaseous fuel consumption rate is given by an Arrhenius law, with activation energy E much larger than the thermal energy RT , written in the form:

$$W_g = -\nu_g M_g \frac{\rho Y_g}{M_g} \frac{\rho Y_o}{M_o} B_1 e^{-E/RT}, \quad (2.2)$$

where B_1 is the pre-exponential factor that we will assume to be independent of temperature.

For simplicity we assume that the air composition by volume is 21% oxygen and 79% nitrogen, with a average molecular mass equal to $28.84 \times 10^{-3} \text{kg/mol}$ and a relation between the mass fraction of nitrogen and oxygen equal to 3.292. The equivalence ratio, ϕ , and mass fractions of the reactive species in the fresh mixture, in terms of ϕ , are given by

$$\phi = \nu \frac{Y_{s,u}}{Y_{o,u}}, \quad Y_{s,u} = \frac{\phi}{\phi + 4.292\nu}, \quad Y_{o,u} = \frac{\nu}{\phi + 4.292\nu}, \quad Y_{g,u} = 0 \quad (2.3)$$

where $\nu = \nu_o M_o / \nu_g M_g$ is the mass of oxygen required to burn the unit mass of fuel. This classical definition of the equivalence ratio involves the solid fuel. However, the chemical reaction takes place in the gaseous phase and the amount of gaseous fuel depends on the

vaporization rate. If this process is very slow a rich mixture can become lean when we account for the amount of gaseous fuel available to be burned at the flame. Thus, in Section 3.3, when analyzing rich mixtures, we will distinguish between gas-phase rich or lean mixtures.

In order to formulate the problem in a suitable way for an analytic treatment we will made the following assumptions:

- (1) The flow is one-dimensional and steady. The pressure is constant.
- (2) The solid particles have the same temperature and velocity as those of the gas phase.
- (3) The gas phase behaves as a mixture of ideal gases with a constant mean molecular mass.
- (4) The mass diffusion and heat conduction fluxes can be described by Fick's and Fourier's laws, respectively. Radiation heat transfer is neglected.

With these assumptions the equations describing the vaporization of solid fuel and the combustion of the gaseous mixture are as follows (Rockwell and Rangwala, 2013; Seshadri et al., 1992):

$$m \frac{dY_s}{dx} = W_v, \quad (2.4)$$

$$m \frac{dY_g}{dx} = \frac{d}{dx} \left(\rho D_g \frac{dY_g}{dx} \right) - W_v + W_g, \quad (2.5)$$

$$m \frac{dY_o}{dx} = \frac{d}{dx} \left(\rho D_o \frac{dY_o}{dx} \right) + \nu W_g, \quad (2.6)$$

$$m c_p \frac{dT}{dx} = \frac{d}{dx} \left(\lambda \frac{dT}{dx} \right) + Q_v W_v - Q W_g, \quad (2.7)$$

$$\rho T = \rho_u T_u. \quad (2.8)$$

In this model the mass flux m is assumed to be constant and given by $m = \rho_u U_p$, where U_p stands for the burning velocity, or flame speed. The diffusion coefficients of gaseous fuel and oxygen, D_g and D_o , respectively, and the thermal conductivity, λ , are functions of temperature to be defined later and the specific heat, c_p , is considered constant and equal for all species.

These equations must be supplemented with the following boundary conditions:

$$x \rightarrow -\infty : \quad Y_s = Y_{s,u}, Y_g = 0, Y_o = Y_{o,u}, T = T_u; \quad (2.9)$$

$$x \rightarrow +\infty : \quad \frac{dY_s}{dx} = \frac{dY_g}{dx} = \frac{dY_o}{dx} = \frac{dT}{dx} = 0. \quad (2.10)$$

Moreover, due to the irreversible reaction between oxygen and fuel, the burned gas must be in chemical equilibrium, at least in first approximation, which requires that at least one reactant must be completely consumed and, hence, in first approximation $Y_g Y_o \rightarrow 0$ as $x \rightarrow +\infty$.

Conservation laws

From suitable linear combinations of Equations (2.4)–(2.7) we can obtain equations free from reaction terms, that, after integrating between $\pm \infty$ and taking into account the boundary conditions, lead to the following conservation laws:

$$Y_{o,u} - Y_{o,b} = \nu(Y_{s,u} - Y_{s,b} - Y_{g,b}), \quad (2.11)$$

$$Q(Y_{s,u} - Y_{s,b} - Y_{g,b}) = c_p(T_b - T_u) + Q_v(Y_{s,u} - Y_{s,b}), \quad (2.12)$$

where the subscript b makes reference to the conditions at the burned gas side, $x \rightarrow +\infty$. Equation (2.11) represents the stoichiometric relation between the consumption of both oxidant and fuel, while (2.12) represents the energy balance between the thermal enthalpy of the mixture, the heat released by the combustion and the energy required for the vaporization. Since this process occurs only if the temperature is greater or equal to T_v , we need to burn a certain amount of gaseous fuel such that, at some point upstream of the flame, the temperature reaches the value T_v and the vaporization can be sustained. If the temperature is lower than T_v everywhere the fresh mixture will remain unchanged.

When the final temperature T_b is larger than T_v all solid fuel is converted into gaseous fuel, hence $Y_{s,b} = 0$. If the mixture is lean, $\phi < 1$, all gaseous fuel is burned and $Y_{g,b} = 0$, while when the mixture is rich, $\phi > 1$, the oxygen is completely depleted and $Y_{o,b} = 0$. Therefore we can identify the following regimes:

Rich mixture ($1 < \phi < \phi_1$) and full vaporization ($T_b > T_v$)

The corresponding burned side values are given by

$$Y_{o,b} = Y_{s,b} = 0, \quad Y_{g,b} = Y_{s,u} - \frac{Y_{o,u}}{\nu} = \frac{\phi - 1}{\phi + 4.292\nu}, \quad T_b = T_u + \frac{1}{c_p} \frac{Q - Q_v\phi}{\phi + 4.292\nu}. \quad (2.13)$$

Note that $Y_{g,b}$ is increasing with ϕ while T_b is decreasing. Hence this regime only exists for $1 < \phi < \phi_1$, where ϕ_1 is the value at which $T_b = T_v$.

If $\phi > \phi_1$ the final temperature determined by (2.13) results lower than T_v and, hence, the solid fuel is not completely consumed, $Y_{s,b} \neq 0$, giving rise to a new regime characterized by an incomplete vaporization and $T_b = T_v$. For sufficiently large values of ϕ the amount of oxygen in the fresh side is not enough to burn the minimum amount of fuel required to rise the temperature from T_u to T_v . The maximum value of ϕ , ϕ_2 , for which is possible to reach T_v is determined by the conditions $T_b = T_v$, $Y_{o,b} = 0$ and $Y_{g,b}(\phi_2) = 0$. Therefore, if $\phi > \phi_2$ the vaporization cannot be sustained in a steady flow.

Lean mixture ($\phi_0 < \phi < 1$) and full vaporization ($T_b > T_v$)

In this regime the burned side values are given by:

$$Y_{s,b} = Y_{g,b} = 0, \quad Y_{o,b} = Y_{o,u} - \nu Y_{s,u} = \frac{\nu(1-\phi)}{\phi + 4.292\nu}, \quad T_b = T_u + \frac{1}{c_p} \frac{(Q - Q_v)\phi}{\phi + 4.292\nu}. \quad (2.14)$$

Now $Y_{o,b}$ is decreasing with ϕ while T_b is increasing. This regime only exists in the range $\phi_0 < \phi < 1$, where ϕ_0 is defined by the condition $T_b(\phi_0) = T_v$.

If $\phi < \phi_0$ the amount of solid fuel is smaller than the minimum required to reach T_v .

Hence, the conservation laws show that a steady flame propagation only occurs in the range of equivalence ratios $\phi_0 < \phi < \phi_2$. Figure 1 shows mass fractions $Y_{s,u}$, $Y_{s,b}$, $Y_{o,u}$, $Y_{o,b}$ and $Y_{g,b}$ and the burned side temperature T_b (in the nondimensional form $10c_p(T_b - T_v)/Q$) as functions of the equivalence ratio ϕ . For similar values of the parameters ν , Q/Q_v and $c_p(T_v - T_u)/Q$ to those considered in previous works, the values of ϕ determining the three regimes are $\phi_0 \sim 0.5$, $\phi_1 \sim 7.3$ and $\phi_2 \sim 19.4$. Therefore the incomplete vaporization regime occurs for very large values of the equivalence ratio and, hence, has a marginal character. For this reason it will not be considered in the rest of this work, and we will restrict to values of ϕ in the range $[\phi_0, \phi_1]$, for which the vaporization is always complete ($Y_{s,b} = 0$).

The temperature T_b is maximum for $\Phi \approx 1$ (stoichiometric conditions) and decreases when Φ moves from 1 to Φ_0 or Φ_1 . Note that the final temperature, T_b , will not be necessarily the flame temperature. For rich mixtures there is an oxygen free region, located downstream the flame, where the temperature is greater than T_v , so that the vaporization continues and the temperature decreases. Therefore the flame temperature will be larger than T_b . If the mixture is lean the temperature downstream the flame increases due to the combustion of the gaseous fuel produced by the vaporization of the solid fuel remaining. The flame temperature will then be lower than T_b .

Figure 1. Values of $Y_{s,u}$, $Y_{s,b}$, $Y_{o,u}$, $Y_{o,b}$, $Y_{g,b}$ and T_b as functions of ϕ .

Nondimensional equations

To nondimensionalize the problem it is convenient to introduce the following definitions and parameters: thermal diffusivity, $D_T = \lambda/\rho c_p$; Lewis number of species i , $L_i = (D_{T,u}/D_{i,u})$; nondimensional vaporization heat, $q = Q_v/Q$; preheat zone thickness, $l_T = D_{T,u}/U_p$; residence time in the preheat zone: $t_r = l_T/U_p = D_{T,u}/U_p^2$; and adiabatic temperature, $T_m = T_u + (QY_{s,u}/c_p) \min(1, \phi^{-1})$. Note that in a lean mixture T_m corresponds to the adiabatic temperature obtained when all allowable solid fuel is burned, while in a rich mixture the deficient reactant is the oxygen and then the adiabatic temperature is given by $T_m = T_u + (Q/c_p)(Y_{s,u}/\phi) = T_u + (Q/c_p)(Y_{o,u}/\nu)$.

The nondimensional temperature, mass fractions and space coordinate are defined by:

$$\theta = \frac{T - T_u}{T_m - T_u}, \quad y_s = \frac{Y_s}{Y_{s,u}}, \quad y_g = \frac{Y_g}{Y_{s,u}}, \quad y_o = \frac{Y_o}{\nu Y_{s,u}}, \quad \xi = \int_0^x \frac{\rho}{\rho_u} \frac{dx}{l_T}. \quad (2.15)$$

With these parameters and variables the reaction terms are written as

$$W_v = -\rho_u Y_{s,u} \frac{\rho}{\rho_u} y_s \frac{1}{t_v} H(\theta - \theta_v), \quad (2.16)$$

$$W_g = -\rho_u Y_{s,u} \frac{\rho}{\rho_u} B(T) e^{-T_a/T_f} y_g y_o \exp \left[\frac{\beta(\theta - \theta_f)}{1 + \gamma(\theta - \theta_f)} \right], \quad (2.17)$$

where T_f is the flame temperature, which, according to the large activation energy limit, is assumed to be much smaller than the activation temperature, i.e., $T_f \ll T_a = E/R$; the heat released parameter $\gamma = (T_m - T_u)/T_f$ is of order unity; $\beta = T_a(T_m - T_u)/T_f^2 \gg 1$ is the Zel'dovich number; and $B(T) = \nu_o M_g^{-1} Y_{s,u} \rho_u T_u T^{-1} B_1$ is a modified pre-exponential factor. The chemical time associated to the combustion reaction is defined by $t_q^{-1} = B(T_f) e^{-T_a/T_f}$.

In order to simplify the mathematical problem we will assume that $D_i \sim T^2$ and $\lambda \sim T$. Taking into account that $\rho \sim 1/T$ we find that $\rho^2 D_i = \rho_u^2 D_{i,u}$ and $\rho \lambda = \rho_u \lambda_u$ and, as consequence, the ratio of thermal and mass diffusivities is independent of the temperature and equal to the Lewis number. The Equations (2.4)–(2.7) written in nondimensional form read:

$$\frac{dy_s}{d\xi} = w_v \quad (2.18)$$

$$\frac{dy_g}{d\xi} = \frac{1}{L_g} \frac{d^2 y_g}{d\xi^2} - w_v + w_g, \quad (2.19)$$

$$\frac{dy_o}{d\xi} = \frac{1}{L_o} \frac{d^2 y_o}{d\xi^2} + w_g, \quad (2.20)$$

$$\frac{d\theta}{d\xi} = \frac{d^2\theta}{d\xi^2} + \max(1, \phi)(qw_v - w_g), \quad (2.21)$$

where

$$w_v = -D_v y_s H(\theta - \theta_v), \quad w_g = -D_a \frac{y_g y_o}{1 + \gamma(\theta - \theta_f)} \exp\left[\frac{\beta(\theta - \theta_f)}{1 + \gamma(\theta - \theta_f)}\right], \quad (2.22)$$

$D_a = t_r/t_q$ is the usual Damköhler number which we anticipate to be of order β^2 , and $D_v = t_r/t_v$ is the Damköhler number associated to the vaporization. The objective of the following analysis is to obtain the flame speed, or equivalently the Damköhler number D_a , in the range of values of t_v such that D_v is of order unity. In the limit $D_v \gg 1$, i.e., $t_r/t_v \gg 1$, the solid fuel is converted rapidly to gas when the temperature reaches the value T_v , so we find the classical premixed flame. In the opposite case, $D_v \ll 1$, the vaporization proceeds very slowly resulting in a very small amount of gaseous fuel so the reactive wave cannot be self-sustained.

The boundary conditions for these equations are as follows:

$$\xi \rightarrow -\infty : \quad y_s = 1, y_o = \phi^{-1}, y_g = \theta = 0; \quad (2.23)$$

$$\xi \rightarrow +\infty : \quad \frac{dy_g}{d\xi} = \frac{dy_o}{d\xi} = \frac{d\theta}{d\xi} = 0. \quad (2.24)$$

Moreover, we will impose that in first approximation $y_g y_o = 0$ at $\xi \rightarrow +\infty$ due to the equilibrium condition.

The results obtained from the conservation laws for the regimes I and II in nondimensional form are as follows:

Rich mixture and full vaporization ($1 < \phi < \phi_1$)

$$y_{s,b} = y_{o,b} = 0, \quad y_{g,b} = 1 - \phi^{-1}, \quad \theta_b = 1 - q\phi. \quad (2.25)$$

Lean mixture and full vaporization ($\phi_0 < \phi < 1$)

$$y_{s,b} = y_{g,b} = 0, \quad y_{o,b} = \phi^{-1} - 1, \quad \theta_b = 1 - q. \quad (2.26)$$

Preliminar description

Before obtaining a detailed description of the flame structure it is convenient to give a general picture. If $\beta \gg 1$ the reaction zone is very thin compared with l_T . Since the problem is invariant under translations we can postulate that there exists a flame located at $\xi = 0$, which appears as a discontinuity surface in the gradients of some variables. At the flame $\theta(0) = \theta_f$, $y_s(0) = y_{s,f}$, $y_g(0) = y_{g,f}$ and $y_o(0) = y_{o,f}$. Moreover the limit $\beta \rightarrow +\infty$ implies that in first approximation $y_{g,f} y_{o,f} = 0$.

Figure 2 shows a general picture of the flow structure in the case of a lean mixture and full vaporization (regime II). We can identify three different regions and a reaction layer. In the region corresponding to $-\infty < \xi < \xi_v$, with ξ_v defined by $\theta(\xi_v) = \theta_v$, the temperature is lower than the vaporization temperature θ_v . Hence the mass fraction of solid fuel does not change in this region. However, $\theta \neq 0$ and $y_g \neq 0$ because of the heat and mass diffusion. Between $\xi = \xi_v$ and $\xi = 0$ the vaporization results in decreasing values of y_s , while y_g reaches a peak value due to the boundary condition $y_g(-\infty) = 0$ and the gaseous fuel consumption in the reaction zone. The heat conduction from the reaction zone increases the temperature allowing the vaporization. Both pre-vaporization and vaporization sub-zones form the usual preheated zone found in the analysis of premixed flames and characterized by a convection-diffusion balance, and a frozen chemical reaction due to the low temperature and the large activation energy. The reaction sheet divides the flow into the preheat zone and the quasi-equilibrium zone, located downstream, where the remaining solid fuel is vaporized and the resulting gaseous fuel consumed if there is oxidant available. Due to the high temperature the consumption occurs immediately after the vaporization, so that $y_g(\xi) \approx 0$ for $\xi > 0$.

In the regime I (rich mixture and full vaporization) this general picture is a bit different. The oxygen is completely consumed at the flame (Figure 3). Hence in the convective zone the flow is in equilibrium but the vaporization continues, resulting in a decreasing temperature profile.

Analysis for unity Lewis numbers

With the aim of reducing the mathematical complexity of the problem in favor of its physical aspects we will consider initially $L_o = L_g = 1$. This assumption allows us to use two Shvab-Zel'dovich variables eliminating the Arrhenius term from all equations but one.

The equation for y_s (2.20) can be integrated to obtain

$$y_s = \begin{cases} -\infty < \xi \leq \xi_v : & 1, \\ \xi_v \leq \xi \leq +\infty : & e^{D_v(\xi_v - \xi)}, \end{cases} \quad (2.26)$$

Figure 2. Schematic showing the general structure of the flow, at the scale of l_T , of a lean mixture.

Figure 3. Schematic showing the general structure of the flow, at the scale of l_T , when the oxygen is fully depleted at the flame.

where ξ_v , still unknown, is the point upstream the flame where the temperature attains the value θ_v .

If we define two Shvab–Zel’dovich variables V and U as

$$V = qy_g + (1 - q)y_o + \min(1, \phi^{-1})\theta, \quad U = y_g - y_o, \quad (2.27)$$

we find from (2.21–2.23) and (2.25–2.28) that V and U verify the problems

$$\frac{d^2 V}{d\xi^2} - \frac{dV}{d\xi} = 0; \quad V(-\infty) = V(+\infty) = (1 - q)\phi^{-1}, \quad (2.28)$$

$$\frac{d^2 U}{d\xi^2} - \frac{dU}{d\xi} = -D_v y_s H(\theta - \theta_v); \quad U(-\infty) = -\phi^{-1}, \quad U(+\infty) = 1 - \phi^{-1}, \quad (2.29)$$

whose solutions, after taking into account (3.1) and the continuity of U , are

$$V = (1 - q)\phi^{-1}, \quad U = \begin{cases} -\infty < \xi \leq \xi_v : & -\phi^{-1} + \frac{D_v}{1+D_v} e^{\xi-\xi_v}, \\ \xi_v \leq \xi \leq +\infty : & 1 - \phi^{-1} - \frac{1}{1+D_v} e^{D_v(\xi_v-\xi)}. \end{cases} \quad (2.30)$$

Preheat zone ($\xi < 0$)

The analysis of the preheat zone can be done simultaneously for regimes I and II (rich and lean mixtures). In this zone the chemical reaction is frozen but not the vaporization. We can distinguish the pre-vaporization and vaporization sub-zones, where $\theta < \theta_v$ and $\theta > \theta_v$, respectively. The equation for the mass fraction of oxygen (2.22) is not affected by the vaporization and can be integrated to obtain:

$$y_o = y_{o,f} e^\xi + \phi^{-1}(1 - e^\xi), \quad (3.1)$$

where $y_{o,f}$ stands for its value at the flame, which is related to the corresponding values of the mass fraction of gaseous fuel and temperature, $y_{g,f}$ and θ_f , respectively, by $U(0)$ and $V(0)$:

$$y_{g,f} - y_{o,f} = 1 - \phi^{-1} - \frac{e^{D_v \xi_v}}{1 + D_v}. \quad (3.2)$$

$$\min(1, \phi^{-1})\theta_f + y_{o,f} = \phi^{-1} - q \left(1 - \frac{e^{D_v \xi_v}}{1 + D_v} \right). \quad (3.3)$$

Since, due to the limit $\beta \rightarrow +\infty$, in first approximation $y_{g,f}y_{o,f} = 0$, (3.7) provides the value of the non-zero mass fraction.

The expressions for $y_g(\xi)$ and $\theta(\xi)$ in the preheat zone are obtained from (3.2), (3.5) and (3.6):

$$y_g = \begin{cases} -\infty < \xi \leq \xi_v : & y_{g,v} e^{\xi - \xi_v}, \\ \xi_v \leq \xi \leq 0 : & y_{g,f} e^{\xi} + (1 - e^{\xi}) + \frac{e^{D_v \xi_v}}{1 + D_v} (e^{\xi} - e^{-D_v \xi}), \end{cases} \quad (3.4)$$

$$\theta = \begin{cases} -\infty < \xi \leq \xi_v : & \theta_v e^{\xi - \xi_v}, \\ \xi_v \leq \xi \leq 0 : & \theta_f e^{\xi} - q \max(1, \phi) \left(1 - e^{\xi} + \frac{e^{D_v \xi_v}}{1 + D_v} (e^{\xi} - e^{-D_v \xi}) \right), \end{cases} \quad (3.5)$$

where $y_{g,v}$ and θ_v are related to $y_{g,f}$ and θ_f , respectively, by

$$y_{g,v} e^{-\xi_v} = y_{g,f} - 1 + \frac{D_v e^{-\xi_v} + e^{D_v \xi_v}}{1 + D_v}, \quad (3.6)$$

$$\theta_v e^{-\xi_v} = \theta_f + q \max(1, \phi) \left(1 - \frac{D_v e^{-\xi_v} + e^{D_v \xi_v}}{1 + D_v} \right). \quad (3.7)$$

This is all the information we can obtain from the analysis of the preheat zone that does not depend on which reactant is, in first approximation, fully depleted at the flame. The position of the vaporization starting point, ξ_v , and the flame speed will be obtained as result of the analysis of the downstream convective and reaction zones, respectively, which must be done taking into account whether $y_{g,f} = 0$ or $y_{o,f} = 0$.

Lean mixtures ($\phi \leq 1$)

If the mixture is lean $1 - \phi^{-1} < 0$ and then (see 3.7) $y_{g,f} - y_{o,f} < 0$ which implies

$$y_{g,f} = 0, \quad y_{o,f} = \frac{e^{D_v \xi_v}}{1 + D_v} + \phi^{-1} - 1. \quad (3.13)$$

Downstream convective zone

In the downstream convective zone, $\xi > 0$, the mass fraction of solid fuel is also given by (3.1) and, according to (3.13), there is still oxygen available. As the temperature is of the order of θ_f the vaporization continues producing gaseous fuel. Since the chemical reaction is not in equilibrium because $y_o y_g \neq 0$, neither frozen because $\theta \approx \theta_f$, we must retain both reaction terms in the equation for y_g :

$$\frac{dy_g}{d\xi} = \frac{d^2 y_g}{d\xi^2} + D_v y_s - D_a \frac{y_g y_o}{1 + \gamma(\theta - \theta_f)} \exp \left[\frac{\beta(\theta - \theta_f)}{1 + \gamma(\theta - \theta_f)} \right]. \quad (3.8)$$

Close to the flame $y_o \sim y_{o,f}$, $y_g \sim y_{g,f} \approx 0$ and, due to the high temperature, the gaseous fuel produced by the vaporization is rapidly depleted by the combustion. Therefore, the gaseous fuel is not accumulated and $y_g \ll 1$ in this convective zone. We can assume that the gaseous fuel is in a steady state resulting from the balance between production and consumption. Then y_g is given by

$$y_g = \frac{D_v y_s}{D_a y_o} (1 + \gamma(\theta - \theta_f)) \exp \left[-\frac{\beta(\theta - \theta_f)}{1 + \gamma(\theta - \theta_f)} \right], \quad (3.9)$$

with $y_o > y_{o,b} \neq 0$. As $D_a \sim \beta^2$ and $\theta > \theta_f$, y_g is at most of order $\beta^{-2} \ll 1$.

With the steady-state approximation for y_g , the first approximations for y_o and θ in the region $\xi > 0$ are obtained from the Shvab-Zel'dovich variables with $y_g = 0$:

$$y_o = \phi^{-1} - 1 + \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v}, \quad \theta = (1 - q) \left(1 - \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v} \right). \quad (3.10)$$

The last equation shows that θ is increasing, hence $\theta(\xi > 0) > \theta_f > \theta_v$, and the vaporization and combustion continue in the convective region because although y_o is decreasing its value is greater than $y_{o,b} = \phi^{-1} - 1$.

From the continuity condition $\theta(0^+) = \theta(0^-) = \theta_f$ and (3.12) we obtain

$$\theta_v + \frac{q D_v}{1 + D_v} = e^{\xi_v} - \frac{e^{(1+D_v)\xi_v}}{1 + D_v}, \quad (3.11)$$

that for given values of θ_v , q and D_v allows us to compute ξ_v . For $D_v \gg 1$, i.e., very rapid vaporization compared with the flame propagation, $\xi_v = \ln(\theta_v + q) < 0$. Moreover $D_v > D_{v,min} = \theta_v / (1 - \theta_v - q)$ for which $\xi_v = 0$ (and $\theta_f = \theta_v$).

The values of y_o and θ at the flame, given by

$$y_{o,f} = \frac{e^{D_v \xi_v}}{1 + D_v} + \phi^{-1} - 1, \quad \theta_f = (1 - q) \left(1 - \frac{e^{D_v \xi_v}}{1 + D_v} \right), \quad (3.12)$$

are decreasing and increasing functions, respectively, of D_v . Therefore in the classical premixed flame limit, $D_v \rightarrow \infty$, all solid fuel has been converted into gas and burned at the flame so that $y_{o,f}$ and θ_f attain their minimum and maximum values, $\phi^{-1} - 1$ and $1 - q$, respectively.

Analysis of the reaction zone

The value of the Damköhler number, D_a , and, consequently, the flame speed is to be obtained from the analysis of the reaction zone. Since it is very thin, of order $\varepsilon = 1/\beta$, we will use a new space independent variable of order unity and the following expansions for θ , y_g , y_o and y_s :

$$\begin{aligned} \eta = \xi/\varepsilon, \quad \theta = \theta_f + \varepsilon \varphi + o(\varepsilon), \quad y_s = y_{s,f} + \mathcal{O}(\varepsilon) \\ y_g = y_{g,f} + \varepsilon \min(1, \phi^{-1}) Y + o(\varepsilon), \quad y_o = y_{o,f} + \varepsilon \min(1, \phi^{-1}) Z + o(\varepsilon). \end{aligned} \quad (3.13)$$

with $y_{g,f} = 0$. When these expansions are taken to (3.2) to obtain the expansions of the Shvab–Zel’dovich variables, the following relations hold:

$$qY + (1 - q)Z + \varphi = 0, \quad Y - Z = \frac{D_v e^{D_v \xi_v}}{1 + D_v} \eta, \quad (3.14)$$

and the Equation (2.21) for the mass fraction of gaseous fuel at leading order reads:

$$\frac{d^2 Y}{d\eta^2} = \varepsilon^2 D_a (y_{o,f} + \varepsilon Z) Y e^{\varphi}. \quad (3.15)$$

In this equation we have included two terms of the expansion of y_o (Mitani, 1980; Williams, 1985, chap. 5), which allow us to extend the analysis for small values of $y_{o,f}$.

If we use the relations (3.20) to express Z and φ in terms of Y , the problem to be solved in the reaction zone is:

$$\frac{d^2 Y}{d\eta^2} = \frac{1}{2} \Lambda Y (y_{o,f} - \varepsilon b \eta + \varepsilon Y) e^{-Y + (1-q)b\eta}, \quad Y_\eta(-\infty) = -1 + e^{D_v \xi_v}, Y_\eta(+\infty) = 0, \quad \lim_{\eta \rightarrow -\infty} [Y + (1 - e^{D_v \xi_v})\eta] = 0 \quad (3.16)$$

where $b = D_v e^{D_v \xi_v} / (1 + D_v)$ and $\Lambda = 2\varepsilon^2 D_a$. The boundary conditions have been obtained from the matching conditions with the outer solutions. The additional matching condition determines Λ .

Once Λ is obtained as a function of D_v and the remaining parameters, the relation $D_a = t_r/t_q = (D_{T,u}/U_p^2) B(T_f) e^{-T_a/T_f}$ leads to:

$$U_p = (2\varepsilon^2 \Lambda^{-1} D_{T,u} B(T_f) e^{-T_a/T_f})^{1/2}. \quad (3.17)$$

Note that taking into account only the first term in the expansion of y_o (see 3.21) we would obtain the problem formulated by Liñán (1974) in his analysis of the structure of counterflow diffusion flames in the premixed flame regime, for whose solution there are correlations available which would avoid us to perform the numerical integration of (3.22).

Results and numerical example

As an example we consider a lean mixture, $\phi = 0.8$, of air and a volatile fuel with the same properties as methane (Poinsot and Veynante, 2005): $Q = 5 \times 10^7 \text{ J/Kg}$, $\nu = 4$, $c_p = 1.45 \times 10^3 \text{ J/K Kg}$, $T_a = 1.1 \times 10^4 \text{ K}$, $B_1 = 1.08 \times 10^7 \text{ s}^{-1}$, $T_u = 300 \text{ K}$, $T_v = 450 \text{ K}$ and $D_{T,u} = 5 \times 10^{-5} \text{ m}^2/\text{s}$. These values lead to $Y_{s,u} = 0.445 \times 10^{-1}$, $Y_{o,u} = 0.223$, $y_{o,u} = 1.25$, $T_m = 1835 \text{ K}$ and $\theta_v = 0.977 \times 10^{-1}$. We will consider three values of the nondimensional vaporization heat $q = 0, 0.05$ and 0.1 .

The values of ξ_v as a function of D_v , obtained by solving (3.17) for $D_v \in [D_{v,min}, 10]$, are plotted in Figure 4. For the same values of D_v we compute θ_f and $y_{o,f}$ (Equation (3.18)), $y_{g,v}$ (Equation (3.11)) and $y_{s,f}$ (Equation (3.1)). These values are shown in Figure 5. For $D_v \gtrsim 3$ all solid fuel has been vaporized ahead of the flame, $y_{s,f} \approx 0$, recovering the classical premixed flame.

Figure 4. Lean mixtures. Vaporization starting point, ξ_v , as a function of D_v (Equation 3.17).

Figure 5. Lean mixtures. Flame temperature θ_f (Equation 3.18), and mass fractions $y_{s,f}$ and $y_{o,f}$ (Equations 3.1 and 3.13) and $y_{g,v}$ (Equation 3.11 with $y_{g,f} = 0$) as functions of D_v .

Afterwards we compute $T_f = T_u + \theta_f(T_m - T_u)$, $\varepsilon = T_f^2/T_a(T_m - T_u)$, $t_q^{-1} = B(T_f)e^{-T_a/T_f}$, $b = D_v e^{D_v \xi_v}/(1 + D_v)$ and solve the problem (3.22) to obtain the value of Λ . Once Λ as a function of D_v is known, since ε and t_q are also functions of D_v , the relations $\Lambda = 2\varepsilon^2 D_a$, $D_a = t_r/t_q$ and $D_v = t_r/t_v$ lead to:

$$t_v^{-1} = 2\varepsilon^2 D_v \Lambda^{-1} t_q^{-1}, \quad t_r^{-1} = t_v^{-1}/D_v, \quad (3.18)$$

which determines for a given value of t_v the value of D_v , D_v^* , solution of the problem and the corresponding residence time. Once D_v^* has been computed we obtain the flame speed as

$$U_p = \left(2\epsilon^2 \Lambda^{-1} D_{T,u} B(T_f) e^{-T_a/T_f} \right)_{(D_v=D_v^*)}^{1/2}. \quad (3.19)$$

Figure 6 shows the residence and vaporization times as a function of D_v . For given values of t_v and q (solid line curves), which should be considered as data of the problem, we obtain the appropriate value of D_v for which a steady solution exists and the corresponding dashed line curve determines t_r . From these values we obtain U_p as a function of t_v , Figure 7. We see, as expected, that the maximum flame speed is attained for $q = 0$ and $t_v \geq 3 \times 10^{-4}$ ($D_v \geq 3$), which corresponds to the adiabatic flame, i.e., without lack of energy due to the vaporization, and for t_v sufficiently small to convert into gas all allowable solid fuel before reaching the flame, as shown in Figure 5. Note the strong reduction in the maximum value of the flame speed due to q : $U_p(q = 0.05) \approx 0.80 U_p(q = 0)$ and $U_p(q = 0.10) \approx 0.63 U_p(q = 0)$.

Finally, the profiles of θ , y_s , y_g and y_o for $q = 0.10$ and $D_v = 0.8$ are plotted in Figure 8. For these values $\xi_v = -1.80$, $\theta_f = 0.78$, $y_{s,f} = 0.23$ and $y_{o,f} = 0.38$. The temperature evolves in the convective zone from its value at the flame to the final combustion value $\theta_b = 0.9$, as result of the burning of the remaining solid fuel at the flame, $y_{s,f}$.

Rich mixtures ($\phi > 1$)

Since the equivalence ratio of the mixture has been defined using the mass fraction of the solid fuel at the fresh end, when the mixture is rich the solid fuel is present in excess and

Figure 6. Lean mixtures. Vaporization and residence times, t_v and t_r as functions of D_v (Equation 3.28 and $t_r = t_v D_v$).

Figure 7. Lean mixtures. Flame speed as a function of the vaporization time t_v .

Figure 8. Lean mixtures. Profiles of mass fractions and temperature as functions of ξ for $D_v = 0.8$ and $q = 0.10$.

the oxidant will be fully depleted. Hence at $\xi \rightarrow +\infty$ we will find $y_{o,b} = 0$ and $y_{g,b} \neq 0$. However, as the chemical reaction takes place in the gaseous phase, the amount of solid fuel converted into gas upstream of the flame determines if the oxidant will be completely consumed at the flame or in the downstream convective zone. For sufficiently large values of ϕ the mass fraction of oxidant is small, and only a small amount of gaseous fuel is required for the full depletion of the oxidant at the flame. Hence, we can have $y_{o,f} = 0$ for very rich mixtures even for small values of D_v . When the mixture is rich but not very far from the stoichiometry and D_v is not sufficiently large, the amount of gaseous fuel

produced before reaching the flame could be not enough to consume all the oxidant. In this case the gaseous fuel is, as in lean mixtures, the deficient reactant and we will find $y_{g,f} = 0$ and $y_{o,f} > 0$. The remaining oxidant $y_{o,f}$ is consumed in the downstream zone by the gaseous fuel produced behind the flame.

Given that in a rich mixture the deficient reactant can be the oxygen or the gaseous fuel, it is preferable to use instead of the classical division of mixtures as lean or rich, which takes into account the ratio of solid fuel to oxygen in the fresh mixture, the notion of gas-phase lean or rich mixtures, corresponding to which reactant is depleted at the flame: gaseous fuel ($y_{g,f} = 0$) or oxygen ($y_{o,f} = 0$), respectively. The difference between these two types of mixtures arises not only by the incomplete vaporization of the solid fuel, but also by the different diffusive properties as it will be shown in §4. A lean mixture is always gas-phase lean (see (3.13)); however, if the mixture is rich ($\phi > 1$) the sign, positive or negative, of $U(0)$ determines the type of gas-phase mixture. The critical value of D_v , $D_{v,0}$, dividing both regimes and for which the mixture is gas-phase stoichiometric ($y_{o,f} = y_{g,f} = 0$) is given by

$$1 - \phi^{-1} = \frac{e^{D_{v,0}\xi_{v,0}}}{1 + D_{v,0}}, \quad (3.20)$$

where $\xi_{v,0}$ is the value of ξ_v (Equation (3.33)) corresponding to $D_{v,0}$. A mixture is gas phase rich if $D_v > D_{v,0}$ or, equivalently, $1 - \phi^{-1} > e^{D_v\xi_v}/(1 + D_v)$, while it is gas-phase lean in the opposite case.

Gas-phase-rich mixtures ($\phi > 1$, $D_v > D_{v,0}$, $y_{o,f} = 0$)

When the mixture is gas-phase rich the mass fractions at the flame are $y_{o,f} = 0$, $y_{g,f} > 0$ and $y_{s,f} > 0$. Therefore the oxidant is completely consumed at the flame and there is not combustion reaction behind it. However, since $T_b > T_v$, the vaporization process continues in the convective zone. The distributions of $y_s(\xi)$, $y_o(\xi)$, $y_g(\xi)$ and $\theta(\xi)$ in the preheat zone are given by (3.1) and (3.6–3.10) with $y_{o,f} = 0$. The values of the temperature and gas fuel mass fraction at the flame, obtained from $U(0)$ and $V(0)$ with $y_{o,f} = 0$, are given by

$$y_{g,f} = 1 - \phi^{-1} - \frac{e^{D_v\xi_v}}{1 + D_v}, \quad \theta_f = 1 - q\phi \left(1 - \frac{e^{D_v\xi_v}}{1 + D_v} \right). \quad (3.21)$$

Downstream convective zone

As in first approximation the oxygen has been depleted at the flame, the distributions of y_g and θ are given by (3.2) and (3.5) with $y_o = 0$:

$$y_g = 1 - \phi^{-1} - \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v}, \quad \theta = 1 - q\phi \left(1 - \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v} \right), \quad (3.22)$$

while y_s is given by (3.1). When the value of θ_f given by (3.21) is taken to (3.12) we obtain the equation to compute ξ_v that can be written as

$$e^{\xi_v} = \left(\theta_v + q\phi \frac{D_v}{1 + D_v} \right). \quad (3.23)$$

Once ξ_v is given as a function of $D_v > D_{v,0}$, we can compute $\theta_f(D_v)$, $y_{g,f}(D_v)$ and the remaining functions describing the outer solutions.

Reaction zone

The analysis of the reaction zone is done as in §3.2.2, with only minor changes. By using the space variable and expansions defined in (3.19) with $y_{o,f} = 0$,

we obtain the equation for the leading term of the mass fraction of oxidant:

$$\frac{d^2 Z}{d\eta^2} = \varepsilon^2 D_a (y_{g,f} + \varepsilon \phi^{-1} Y) Z e^{\phi}. \quad (3.24)$$

The order ε expansion of the Shvab–Zel’dovich variables leads to

$$qY + (1 - q)Z + \phi = 0, \quad Y - Z = \phi \frac{D_v e^{D_v \xi_v}}{1 + D_v} \eta, \quad (3.25)$$

from which we can express Y and ϕ in terms of Z . The boundary conditions result from the matching with the outer solutions. Finally the problem to be solved can be written as

$$\begin{aligned} \frac{d^2 Z}{d\eta^2} &= \frac{1}{2} \Lambda Z (y_{g,f} + \varepsilon b \eta + \varepsilon \phi^{-1} Z) e^{-Z - q \phi b \eta}, \\ Z_\eta(-\infty) &= -1, \quad Z_\eta(+\infty) = 0, \quad \lim_{\eta \rightarrow -\infty} [Z + \eta] = 0. \end{aligned} \quad (3.26)$$

Results and numerical example

We consider the same values of the parameters as in §3.2.3 (lean mixtures), except the equivalence ratio $\phi = 1.5$ for which $Y_{s,u} = 0.804 \times 10^{-1}$, $Y_{o,u} = 0.214$, $y_{o,u} = 0.667$, $T_m = 2147K$ and $\theta_v = 0.812 \times 10^{-1}$. As before, we will consider three values of $q = 0.00, 0.05$ and 0.10 . The values of $D_{v,0}$ are $0.325, 0.348$ and 0.372 , respectively. Figures 9 and 10 show ξ_v , θ_f and the mass fractions $y_{s,f}$, $y_{g,f}$ and $y_{g,v}$ as functions of D_v in the range $[D_{v,0}, 10]$. The profiles of θ , y_s , y_g and y_o for $q = 0.10$ and $D_v = 0.8$ are plotted in Figure 11. For these values we find that the mass fraction of solid fuel at the flame is $y_{s,f} \approx 0.26$, which is converted into gaseous fuel in the convective zone, but not burned due to the lack of oxygen, increasing the mass fraction y_g and decreasing the temperature θ from their values at the flame.

The flame speed is obtained by solving the problem (3.38) to determine the function $\Lambda(D_v)$. As in Section §3.2.3 for a given value of t_v the relation (3.28) determines the appropriate value of D_v , D_v^* , and then the flame speed is given by (3.29). Figure 12 shows t_v and $t_r = t_v D_v$ as a function of D_v from which we obtain, for a given value of t_v , D_v^* , and $t_r(D_v^*) = D_{T,u}/U_p^2$. Figure 13 shows U_p as a function of t_v . As expected U_p is decreasing with q and attains its maximum value for small values of t_v . In this case there is also a strong reduction in the flame speed due to q : $U_p(q = 0.05) \approx 0.74 U_p(q = 0)$ and $U_p(q = 0.10) \approx 0.52 U_p(q = 0)$.

Figure 9. Gas-phase-rich mixtures. Vaporization starting point, ξ_v , as a function of D_v (Equation 3.33).

Figure 10. Gas-phase-rich mixtures. Flame temperature θ_f (Equation 3.31), and mass fractions $y_{s,f}$ and $y_{g,f}$ (Equations 3.1 and 3.31) and $y_{g,v}$ (Equation 3.11) as functions of D_v .

Gas-phase lean mixtures ($\phi > 1$, $D_v < D_{v,0}$, $y_{o,f} = 0$)

In this section, we will analyze the case of rich mixtures, but lean in the gas-phase, i.e., $\phi > 1$, and $D_v < D_{v,0}$, or equivalently $y_{g,f} = 0$. In the preheat zone the distributions of y_s , y_o , y_g and θ are given by (3.1) and (3.6–3.10) with $y_{g,f} = 0$. The values of y_o and θ at the flame are

Figure 11. Gas-phase-rich mixtures. Mass fractions and temperature as functions of ξ for $D_v = 0.8$ and $q = 0.10$.

Figure 12. Gas-phase-rich mixtures. Vaporization and residence times, t_v and t_r as functions of D_v (Equation 3.28 and $t_r = t_v D_v$).

$$y_{o,f} = \frac{e^{D_v \xi_v}}{1 + D_v} - 1 + \phi^{-1}, \quad \theta_f = (1 - q)\phi \left(1 - \frac{e^{D_v \xi_v}}{1 + D_v} \right). \quad (3.27)$$

The equation to compute ξ_v is again obtained from (3.12) and (3.39) leading to

$$\phi^{-1} \theta_v + \frac{q D_v}{1 + D_v} = e^{\xi_v} - \frac{e^{(1 + D_v) \xi_v}}{1 + D_v}, \quad (3.28)$$

Figure 13. Gas-phase-rich mixtures. Flame speed as a function of the vaporization time t_v .

In the downstream convective zone there is oxidant available and, due to the high temperature, the reaction proceeds very rapidly. Hence, we will admit the steady-state hypothesis for y_g . Unlike what happened when $\phi < 1$ and $y_{o,b} > 0$, this process ends at $\xi = \xi_0 > 0$ when all residual oxidant at the flame, $y_{o,f}$, has been fully consumed. As in first approximation $y_g(\xi_0) = y_o(\xi_0) = 0$, the value of ξ_0 is given by $U(\xi_0) = 0$, so that

$$\xi_0 = \xi_v - \frac{1}{D_v} \ln((1 - \phi^{-1})(1 + D_v)). \quad (3.29)$$

Therefore, downstream the flame we can distinguish a reactive sub-zone, corresponding to $0 \leq \xi \leq \xi_0$, followed by a properly convective zone, $\xi > \xi_0$, where we find chemical equilibrium due to the lack of oxygen although the vaporization continues producing gaseous fuel. In the reactive sub-zone y_g (in steady state), y_o and θ are given, in first approximation, by

$$y_g = 0, \quad y_o = \phi^{-1} - 1 + \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v}, \quad \theta = (1 - q)\phi \left(1 - \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v} \right), \quad (3.30)$$

and the temperature is increasing due to the chemical reaction. In the convective zone, $\xi > \xi_0$, we find

$$y_g = 1 - \phi^{-1} - \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v}, \quad y_o = 0, \quad \theta = 1 - q\phi \left(1 - \frac{e^{D_v(\xi_v - \xi)}}{1 + D_v} \right), \quad (3.31)$$

and the temperature decreases due to the vaporization of the solid fuel.

At $\xi = \xi_0$ there is a discontinuity on the gradients of the variables because when $\xi < \xi_0$ the mass fraction of oxygen y_o is very small and then the steady-state hypothesis for y_g is

not valid. To remove it we should consider the full problem in a thin layer located around $\xi = \xi_0$. This layer has the same structure as the counterflow diffusion flame in the near equilibrium regime described by Liñán (1974), and does not affect to the flame propagation because the Damköhler number in the present case is much larger than the Damköhler number for extinction.

The analysis of the reaction zone is analogous to that of §3.2.2. From the space variable and expansions defined in (3.19) with $y_{gf} = 0$, taking into account (3.37) and the matching with the outer solutions in the preheat zone, (3.9), and reactive sub-zone, $y_g = 0$, we obtain the following problem for the mass fraction of gaseous fuel

$$\frac{d^2 Y}{d\eta^2} = \frac{1}{2} \Lambda Y (y_{of} - \varepsilon b \eta + \varepsilon \phi^{-1} Y) e^{-Y+(1-q)\phi b \eta},$$

$$Y_\eta(-\infty) = \phi(-1 + e^{D_v \xi_v}), \quad Y_\eta(+\infty) = 0, \quad \lim_{\eta \rightarrow -\infty} [Y + \phi(1 - e^{D_v \xi_v})\eta] = 0. \quad (3.32)$$

The former analysis is only valid when D_v is not very close to $D_{v,0}$, so that y_{of} and ξ_0 are both of order unity and the reactive sub-zone, where the gaseous fuel is in steady state and the oxygen is consumed by the chemical reaction, appears clearly defined. However, if $D_{v,0} - D_v \sim \varepsilon$, y_{of} and ξ_0 are also of order ε . In this case the reactive sub-zone is embedded in the reaction zone, where all oxygen is consumed, and the model leading to the problem (3.44) has to be modified, because the steady-state hypothesis for y_g does not apply.

The problem (3.44) must be replaced by a problem which describes the transition from the preheat to the convective zone. With the space variables and expansions given by (3.19), $y_{gf} = 0$ and taken into account (3.37) we obtain the following problem for Z :

$$\frac{d^2 Z}{d\eta^2} = \frac{1}{2} \tilde{\Lambda} (Z + \frac{\phi y_{of}}{\varepsilon}) (Z + \phi b \eta) e^{-Z-q\phi b \eta},$$

$$Z_\eta(-\infty) = \phi(b/D_v - 1), \quad Z_\eta(+\infty) = 0, \quad \lim_{\eta \rightarrow -\infty} [Z - \phi(b/D_v - 1)\eta] = 0, \quad (3.33)$$

where $\tilde{\Lambda} = 2\phi^{-1}\varepsilon^3 D_a$, and the boundary conditions have been obtained from the matching with the expansion of (3.6) for $\xi \rightarrow 0^-$ and $y_0 = 0$ for $\xi \rightarrow 0^+$. This problem has to be solved for values of D_v such that $D_{v,0} - D_v = \mathcal{O}(\varepsilon)$ and, hence, $y_{of} = \mathcal{O}(\varepsilon)$, given by (3.39), while for smaller values of D_v the problem (3.44) applies. Once $\tilde{\Lambda}$ is known the flame speed is given by

$$U_p = (2\varepsilon^3 \phi^{-1} \tilde{\Lambda}^{-1} D_{T,u} B(T_f) e^{-T_a/T_f})^{1/2}. \quad (3.34)$$

Results and numerical example

Figure 16 to 22 show the results for four different types of rich mixtures. Dotted lines corresponds to rich gas-phase mixtures, for which $D_v > D_{v,0}$, whose results were given in §3.4.3 for the full range of values of D_v . Thick dots indicate values for stoichiometric gas-phase mixtures, $D_v = D_{v,0}$. Results for quasi-stoichiometric lean gas-phase mixtures,

Figure 14. Gas-phase-lean mixtures. Vaporization starting point, ξ_v , as a function of D_v (Equation 3.40).

Figure 15. Gas-phase lean mixtures. Oxygen depletion point, ξ_0 , as a function of D_v (Equation 3.41).

$D_v < D_{v,0}$, are showed with dashed lines. Finally, solid lines correspond to lean gas-phase mixtures, $D_v < D_{v,0}$.

Figures 14-16 show ξ_v , ξ_0 , θ_f and the mass fractions $y_{s,f}$, $y_{g,f}$ and $y_{g,v}$ as functions of $D_v < D_{v,0}$ and $q = 0, 0.05$ and 0.10 . The profiles of θ , y_s , y_g and y_o for $q = 0.10$ and $D_v = 0.2$ are plotted in Figure 17. Figure 18 shows the residence and vaporization times, t_r and t_v , as functions of D_v , computed from the solution of problems (3.44) and (3.45) in the appropriate range of values of

Figure 16. Gas-phase lean mixtures. Flame temperature θ_f (Equation 3.39), and mass fractions $y_{s,f}$ and $y_{o,f}$ (eqs. 3.1 and 3.39) and $y_{g,v}$ (Equation 3.11 with $y_{g,f} = 0$) as functions of D_v .

Figure 17. Gas-phase lean mixtures. Profiles of mass fractions and temperature as functions of ξ for $\phi = 1.5$, $D_v = 0.2$ and $q = 0.10$.

$D_v < D_{v,0}$. In Figure 19 we have plotted the values of the flame speed U_p as a function of t_v computed from Equations (3.29) and (3.46) .

Analysis for non-unity Lewis numbers

The analysis and results for non-unity Lewis numbers are openly available in figshare at <http://doi.org/10.6084/m9.figshare.7825430>.

Figure 18. Gas-phase lean mixtures. Vaporization and residence times, t_v and t_r as functions of D_v .

Figure 19. Gas-phase lean mixtures. Flame speed as a function of the vaporization time t_v .

Summary and conclusions

We have analyzed, using large activation energy asymptotics, the steady flame propagation through a cloud of solid fuel particles that, after vaporization, form a gaseous mixture of oxidant and fuel. The mass rate of the vaporization is modeled by a Heaviside function whose argument is the difference between the temperature and a threshold temperature, while we consider a global reaction of Arrhenius type with large activation energy to represent the combustion. We define two Damköhler numbers as the ratio of the residence time to the characteristic time of each reaction, namely D_v and D_a for vaporization

and combustion, respectively. A classical thin reaction zone divides the flow field into two zones. Upstream the combustion is frozen but the vaporization produces gaseous fuel once the temperature rises to the threshold value. Downstream there is chemical equilibrium although, if the vaporization has not been completed before the reaction zone, there is a layer where the combustion of the remaining solid fuel occurs very rapidly due to the high temperature. Lean and rich mixtures, defined in terms of the initial solid fuel, have been considered although the analysis is restricted to those values of the equivalence ratio for which full vaporization is attained.

The structure of the flow and the flame speed have been obtained by using D_v as main parameter, which plays a crucial role because it is directly related with the distribution of gaseous fuel in the flow. When the mixture is lean, the gaseous fuel is always the deficient reactant at the reaction zone. For moderately large values of D_v , i.e., small values of the characteristic time of vaporization, this is completed upstream the flame where all fuel is burned. For small values of D_v the vaporization is completed in the convective zone downstream the flame. In this zone it is assumed that the gaseous fuel is burned at the same rate as it is produced by the vaporization due to the high temperature. The analysis shows that D_v must be larger than a minimum value in order to reach the threshold temperature upstream the flame. Close to the end of vaporization, when the amount of solid fuel is very small and the distance between the particles is large, a diffusion flame could appear around each particle, hence the assumption of premixed combustion would not be valid. However, it is expected that this shortcoming does not have a great effect over the global results.

In the case of rich mixtures the deficient reactant can be oxygen or fuel depending on the value of D_v . There exists a critical value $D_{v,0}$ for which the mixture is gas-phase stoichiometric. If $D_v > D_{v,0}$ (fast vaporization) the deficient reactant is oxygen. Downstream the flame the vaporization continues, but there is not combustion due to the lack of oxygen. As a result the temperature decreases, being the final temperature lower than the flame temperature. When $D_v < D_{v,0}$ the gaseous fuel is fully depleted at the flame, but vaporization and combustion persist downstream until all oxygen is consumed. In these cases there is an important increment on temperature behind the reaction zone followed by a slight decrease due to the heat absorbed by the vaporization. The fact that a rich mixture can be gas-phase lean or rich has been characterized (Seshadri et al., 1992) by an effective gas-phase equivalence ratio defined in terms of the flame temperature through an equivalent mass fraction of fuel. Since the flame temperature is an unknown of the problem we prefer to use the Damköhler number of vaporization to discriminate both situations, which, on the other hand, points directly to the cause of this situation.

The flame speed is computed in all cases by solving the appropriate reaction zone problem where D_v plays the role of an eigenvalue. The results show that the flame speed decreases with both the characteristic time and the heat of vaporization by a non-negligible amount.

Because of the advantages of using the Shvab–Zel'dovich coupling functions, we have thoroughly analyzed the case of both Lewis numbers equal to unity to describe the flow structure in the different regimes. The analysis when Lewis numbers are different from unity has been also carried out but presented in a concise way. It shows, as expected, that the flame speed increases with Lewis numbers.

Radiation heat transfer has not been included in the formulation to keep it as simple as possible. However, Joulin and other researchers (e.g., Deshaies and Joulin, 1986; Joulin and Deshaies, 1986; Joulin, 1987; Liberman et al., 2015; Proust et al., 2017) have shown that thermal radiation can increase the flame speed, playing a significant role in dust explosions, and, hence, it will be addressed in a forthcoming paper in which a more detailed model is developed.

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