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A PARTICULAR INNER STRUCTURE FOR BI-COMPONENT FUEL DIFFUSION FLAMES

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Abstract The analysis addresses fundamental aspects of the extinction of diffusion flames established by burning of bi-component fuels. This analysis is asymptotically done presuming one-global-step chemical reactions with large activation energies. Two parameters are responsible to characterize the problem, the ratio of the activation energies and the ratio of the Damkhöler numbers. The results pointed out that not only the chemical reaction with the largest activation energy controls the flame extinction, but also the chemical reaction with the smallest activation energy. The flame extinction conducted by the less thermal sensitive reaction showed to be directly influenced by the composition of the bicomponent fuel.

Keywords *multicomponent fuel, diffusion flames, flame structure, activation energy asymptotics*

1. Introduction

The asymptotic structure of flames is already considered as a classical problem about which a great deal of research has been performed (Liñán, 1974; Seshadri, 1996). Despite the large amount of work that has been done on the subject, there are questions in need of fundamental explanation. The present work addresses some questions about the extinction of multicomponent fuel diffusion flames.

By presuming that the reactions are done in one-global-step and their activation energies are large, the internal structure of diffusion flames have been described (Liñán, 1974). From this kind of analysis it is able to determine the extinction condition of diffusion flames and the fraction of oxygen and fuel that leak through the flame.

Another asymptotic analysis was developed based on reduced kinetic mechanisms, about 4 steps and 6 species (Peters and Willimas, 1987). Due to a more detailed kinetic mechanism, compared to one-global-step mechanisms, the analysis produces results close to the experimental results.

In all the studied cases, the flame structure is imposed by the burning of a single fuel. Few works analysed the extinction problem of the multicomponent fuel. One of that analyses considered the multicomponent fuel as a single fuel and the chemical properties of that hypothetical single fuel are an average the multicomponent fuel properties (Hamins and Seshadri, 1984). The results agreed well with the experimental results because the properties of each fuel were taken at the extinction condition. Another approach for the problem was presented recently. Still using large activation asymptotics, the structure of bicomponent fuel diffusion flames and the extinction condition were determined (Fachini, 2002). In that work, the activation energies and the Damkhöler numbers of both reactions were considered as being of the same order of magnitude. The results showed that the reaction with the largest activation energy and/or with the smallest Damkhöler number led the flame to extinction.

The emphasis of this work is to extend the analysis presented by Fachini (2002) by assuming the activation energy and the Damkhöler number of one reaction are much larger than those of the other reaction.

2. Flowfield Description

The flowfield of initially nonpremixed reacting flows is composed by a thin reacting zone surrounded by a broad frozen zone. The thickness of the frozen zone is determined by the boundary conditions and that of the reacting zone is determined by the properties of the chemical reactions. In the combustion state, the large heat released rises the gases temperature inside the reacting zone to the several times the initial temperature. The chemical reaction is sustained by the oxygen and fuel diffusion from the frozen zone to the reacting zone.

Usually in combustion, chemical reactions are much faster than the any process of the frozen flowfield. The Damkhöler number Da, the ratio of the frozen flowfield time scale to the reaction time, is large. The consequence of $Da \gg 1$ is the reacting zone to be much thinner than the frozen zone, thereby justifying to apply boundary layer assumption to the problem. Therefore, in the leading order problem, the chemical reaction is assumed as infinitely fast; the reacting zone is infinitely thin surface. The consequence of this approximation is that the detail of the chemical reaction disappears and is described by a global one-step mechanism; called Burke-Schuman mechanism. By employing the Burke-Schuman mechanism, the leading order nonpremixed combustion problems have solutions. Flame position, flame temperature, the oxygen and fuel fluxes to the flame and the heat flux from the flame are evaluated for given boundary conditions.

Since the Burke-Schuman mechanism admits infinitely fast chemical rates, extinction conditions is not determined for this condition because there is no leakage of fuel and oxygen through the flame. To analise the extinction, it becomes necessary to solve the equations corresponding to the higher order approximation in the boundary layer assumption. In that approximation the reaction rate is huge but finite, thereby the reactants leak through the flame. Therefore, to perform the extinction analysis the flowfield description needs a correction only in a thin zone surrounding the flame (reacting zone). The main processes inside the reacting zone are mass and heat diffusion and reaction. The diffusive-reactive equation describing the internal structure of the flame must be integrated with boundary conditions that are determined by the matching with the solution of the leading order problem, flowfield problem with $Da \rightarrow \infty$. Moreover, other flowfield properties, as position and temperature of the flame, are necessary to perform the asymptotic analysis.

The analysis of the flame structure of bicomponent fuel diffusion flames will be performed on the counterflow configuration. The counterflow configuration is broadly used because it permits a good access to the flame interior in experimental studies. The radiative energy transfer is included in the model by the approximation of optically thin transparent gas and released in the CO_2 and H_2O bands.

The flowfield properties necessary to perform the flame structure analysis are those specified by Fachini (2001). The nondimensional spatial coordinate, nondimensional temperature, oxygen mass fraction, fuel 1 mass fraction and fuel 2 mass fraction are defined as x, θ, Y_O, Y_1 and Y_2, respectively. Then, flame position and flame temperature and the oxygen and bicomponent fuel fluxes to and the heat flux from the flame are as following

$$x = x_f, \quad \theta = \theta_f,$$

$$d_0 = -\left.\frac{dY_O}{dx}\right|_{x=x_f}, \quad d_1 = \left.\frac{dY_1}{dx}\right|_{x=x_f}, \quad d_2 = \left.\frac{dY_2}{dx}\right|_{x=x_f}, \quad d_\theta^- = \left.\frac{d\theta}{dx}\right|_{x=x_f^-}, \quad d_\theta^+ = -\left.\frac{d\theta}{dx}\right|_{x=x_f^+},$$

respectively.

By following the conditions assert for this problem, in terms of mass, the chemical reactions of a general bicomponent fuel proceed at one global step according to

$$\begin{array}{lllllll} F_1 & + & s_1O_2 & \rightarrow & \tilde{c}_1CO_2 & + & \tilde{h}_1H_2O \qquad (Q_1) \\ F_2 & + & s_2O_2 & \rightarrow & \tilde{c}_2CO_2 & + & \tilde{h}_2H_2O \qquad (Q_2) \end{array}$$

in which s_i, $\tilde{c}_i$ and $\tilde{h}_i$ are the massic stoichiometric coefficients of reaction i, i.e. for each unit mass of fuel i, s_i mass of air are consumed to have stoichiometric reaction. Q_i is the heat released by the reaction i.

The nondimensional rates of these chemical reactions are expressed by

$$\tilde{w}_i = Da_i \varrho^{\beta_{i1}+\beta_{i2}} y_O^{\beta_{i1}} y_i^{\beta_{i2}} e^{-\theta_{ai}/\theta}, \qquad i = 1, 2$$

where $\beta_{i\bullet}$ and $\theta_{ai} = E_i/RT_0$ are the the global reaction order and the nondimensional activation energy of reaction i, respectively. The definitions for the rescaled oxygen and fuels mass fractions, y_O and y_i, are as following

$$y_O = Y_O/Y_{O0}, \quad y_i = s_i Le_O Y_i/(Y_{O0} Le_i)$$

The Damkhöler number Da_i is defined as

$$Da_i = (B_i\ l/v_0)(\rho_0 Y_{O0})^{\beta_{i1}+\beta_{i2}-1} Le_i^{\beta_{i2}}/(s_i Le_O)^{\beta_{i2}-1}$$

The subscript 0 corresponds to the condition at the air stream. B_i, l, v, ρ and Le_i are the frequency factor, the distance between the nozzles from which the air stream and fuel stream, the velocity of the streams come out, the density and the Lewis number of fuel i, respectively.

More details about the counterflow configuration with bicomponent fuel stream can be found in Fachini (2001).

3. Flame Structure

It is worthy to mention that the aim of this analysis is not to study the any particular multicomponent fuel, but presents a general tool that is able to help anyone to obtain extinction data for fuels composed by more than one component..

As seen in the leading order problem describing either one-fuel diffusion flames (Fachini et all, 1999) or multicomponent fuel diffusion flames (Fachini, 2002), the chemical reaction was considered infinitely fast, thereby it occurred in an infinitely thin zone; there were no leakage of fuel and oxygen through the flame. This assumption makes the derivatives of the variables discontinuous at the flame. To avoid the discontinuity in the derivatives, it is necessary to solve the problem for the next order of magnitude that corresponds to the description of the internal structure of the flame. In the limit $\theta_{a1} \gg \theta_{a2} \gg 1$ presumed in this section, the flame presents a different internal structure. Again, in the leading order problem, the flame is still considered infinitely thin. However at order of magnitude corresponding to $1/\theta_{a2}$ the problem, in which the evolution of the consumption of fuel 2 is described, treats the zone where fuel 1 is consumed as infinitely thin. The reason for that is because the reaction 1 is much more dependent on temperature than the reaction 2. Since both reactions compete for oxygen, it is reasonable to expect that the zone where fuel 1 is consumed to be inside the zone where fuel 2 is consumed. The zone where fuel 2 is consumed is called layer 1 and the zone where fuel 1 is consumed is called layer 2.

The position of the layer 2 inside the layer 1 is determined by the physical and chemical properties. In this work that position is assumed to be at the edge of the layer 1 in the fuel side of the flame, as seen in figure 1. With this structure configuration, the flame is more stable because the leakage of oxygen is of the order of $1/\theta_{a1}$, much smaller than $1/\theta_{a2}$ that is the oxygen leakage if the layer 2 were in the middle of layer 1. Note that the flame configuration is formed by two reaction zones controlled by diffusion. In this case two diffusion-flame structures are merged to form the structure of the bicomponent fuel diffusion flame.

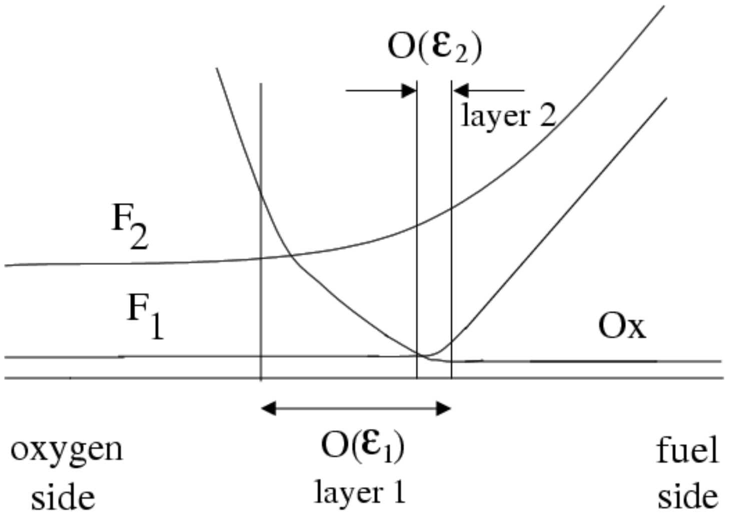

Figure 1: Schematic representation of the internal structure of a diffusion flame through the profiles of fuels 1 and 2 and of oxygen.

To study two-fuels diffusion flame structure with distinct activation energies the following expansion must be considered

$$\begin{array}{rllll}
\theta = & \theta_f & -\ \varepsilon_1\ \Theta_1/m_1\delta_1^{1/b_1} & -\ \varepsilon_2\ (\Theta_2+\gamma_2\xi_2)/m_2\delta_2^{1/b_2} & +\cdots \\
y_0 = & 0 & +\ \varepsilon_1\ (\Psi_{01}+\gamma_1\xi_1)/\delta_1^{1/b_1} & +\ \varepsilon_2\ d_1\Psi_{02}/m_2\delta_2^{1/b_2} & +\cdots \\
y_1 = & 0 & +\ \varepsilon_1\ d_1\Psi_{11}/m_1\delta_1^{1/b_1} & +\ \varepsilon_2\ d_1\Psi_{12}/m_2\delta_2^{1/b_2} & +\cdots \\
y_2 = & 0 & +\ \varepsilon_1\ d_2\Psi_{21}/m_1\delta_1^{1/b_1} & +\ \varepsilon_2\ d_2\Psi_{22}/m_2\delta_2^{1/b_2} & +\cdots \\
x = & x_f & +\ \varepsilon_1\ \xi_1/m_1\delta_1^{1/b_1} & +\ \varepsilon_2\ \xi_2/m_2\delta_2^{1/b_2} & +\cdots
\end{array} \tag{1}$$

where

$$\begin{array}{ll}
b_1 = 1+\beta_{21}+\beta_{22}, & b_2 = 1+\beta_{11}+\beta_{12}, \\
\varepsilon_1 = \theta_f^2/\theta_{a2}, & \varepsilon_2 = \theta_f^{*\ 2}/\theta_{a1} = (\theta_f+\varepsilon_1\Theta_{1f}/m_1\delta_1^{1/b_1})^2/\theta_{a1}, \\
m_1 = d_2, & m_2 = (d_\theta^- + d_\theta^+ - q_2d_2)/2, \\
\gamma_1 = -d_1/d_2, & \gamma_2 = 1-2(d_\theta^- - q_2d_2)/(d_\theta^- + d_\theta^+ - q_2d_2),
\end{array}$$

$$\delta_1 = \frac{Pe\ Da_2\ e^{-\theta_{a2}/\theta_f}\ d_2^{\beta_{21}+\beta_{22}-1}}{\theta_f^{\alpha+\beta_{21}+\beta_{22}}}\left(\frac{\varepsilon_1}{m_1}\right)^{1+\beta_{21}+\beta_{22}},$$

$$\delta_2 = \frac{Pe\ Da_1\ e^{-\theta_{a1}/\theta_f^*}\ d_1^{\beta_{11}+\beta_{12}-1}}{\theta_f^{*\ \alpha+\beta_{11}+\beta_{12}}}\left(\frac{\varepsilon_2}{m_2}\right)^{1+\beta_{11}+\beta_{12}}\ \left(\frac{m_2}{d_1q_1}\right)^{\beta_{11}+\beta_{12}},$$

The definition of d_1, d_2, d_θ^- and d_θ^+ were already given in the previous section and they represent the fluxes of y_1 and y_2 and the heat fluxes at the flame in the oxygen side and in the fuel side of the flame, respectively.

3.1. Solution of order ε_1

Almost everywhere inside layer 1, the influence of the reaction of fuel 1 on the oxygen consume and on heat released is very small compared to that of the fuel 2, except inside the layer 2 located at $\xi_1 = \xi_{1f}$ ($z = z_f^* = z_f + \varepsilon_1\xi_{1f}/m_1\delta_1^{1/b_1}$). Since the layer 2 is assumed to have a diffusion flame configuration, the oxygen mass fraction and the fuel 1 mass fraction go to zero, $\Psi_{11} = (\Psi_{01}+\gamma_1\xi_{1f}) = 0$ and the reaction rate of the oxidation of fuel 1 can be represented by delta function at first approximation in the problem of order ε_1 at $\xi_1 = \xi_{1f}$. As will be seen later $d\Psi_{11}/d\xi_1|_{\xi_1<\xi_{1f}^-} = 0$ and $d\Psi_{11}/d\xi_1|_{\xi_1=\xi_{1f}^+} = 1$, thereby the reaction rate of the oxidation of fuel 1 can be expressed as $d_1\delta(\xi_1 = \xi_{1f})$. Therefore, as occurred in the leading order problem, the problem of the order ε_1 also has discontinuous derivatives for the functions Θ_1, Ψ_{01} and Ψ_{21} at $\xi_1 = \xi_{1f}$ ($z = z_f + \varepsilon_1\xi_{1f}/m_1\delta_1^{1/b_1}$). At $\xi_1 = \xi_{1f}$, the jump condition in the first derivative of Θ_1, Ψ_{01}, Ψ_{11} and Ψ_{21} will be used in the analysis of order ε_2.

The oxidation of the fuel 2 occurs in the layer 1, which has a thickness of order ε_1. The variations of the temperature and the reactants in this layer are followed by the system of equations of order ε_1, resulting of taking equation (1) into the balance equations (Fachini, 2001),

$$\frac{d^2}{d\xi_1^2}\Theta_1 = q_1d_1\delta(\xi_1-\xi_{1f}) + q_2d_2(\Psi_{01}+\gamma_1\xi_1)^{\beta_{21}}\Psi_{21}^{\beta_{22}}e^{-\Theta_1/m_1\delta_1^{1/b_1}} \tag{2}$$

$$\frac{d^2}{d\xi_1^2} d_2(\Psi_{01} + \gamma_1 \xi_1) = d_1 \delta(\xi_1 - \xi_{1f}) + d_2(\Psi_{01} + \gamma_1 \xi_1)^{\beta_{21}} \Psi_{21}^{\beta_{22}} e^{-\Theta_1 / m_1 \delta_1^{1/b_1}} \tag{3}$$

$$\frac{d^2}{d\xi_1^2} d_1 \Psi_{11} = d_1 \delta(\xi_1 - \xi_{1f}) \tag{4}$$

$$\frac{d^2}{d\xi_1^2} d_2 \Psi_{21} = d_2(\Psi_{01} + \gamma_1 \xi_1)^{\beta_{21}} \Psi_{21}^{\beta_{22}} e^{-\Theta_1 / m_1 \delta_1^{1/b_1}} \tag{5}$$

The boundary conditions of equations (2) to (5), determined by the matching with the leading order solutions, are given by

$$\frac{d\Theta_1}{d\xi_1} + d_\theta^- = \frac{d\Psi_{01}}{d\xi_1} + 1 = \frac{d\Psi_{21}}{d\xi_1} = \frac{d\Psi_{11}}{d\xi_1} = \Psi_{11} = 0, \qquad \xi_1 \to -\infty \tag{6}$$

$$\Psi_{01} + \gamma_1 \xi_{1f} = \frac{d\Psi_{01}}{d\xi_1} = \Psi_{11} = 0, \qquad \xi_1 = \xi_{1f} \tag{7}$$

$$\frac{d\Theta_1}{d\xi_1} - d_\theta^+ = \frac{d\Psi_{11}}{d\xi_1} - 1 = \frac{d\Psi_{21}}{d\xi_1} - 1 = 0, \qquad \xi_1 \to \infty \tag{8}$$

Note that the definitions of m_1 and γ_1 are such that permit the derivative of Ψ_{01} to be normalized for $\xi_1 \to -\infty$ and zeroed at $\xi_1 = \xi_{1f}$.

By integrating equation (4) with the boundary conditions (7) and (8) one finds

$$\Psi_{11} = \begin{cases} 0, & \xi_1 < \xi_{1f} \\ \xi_1 - \xi_{1f}, & \xi_1 \geq \xi_{1f} \end{cases} \tag{9}$$

Exploring the fact that the excess enthalpy function (Liñán and Williams, 1993), defined as $H = (q_1 - 1)y_1 + (q_2 - 1)y_2 + y_0 + \theta$, and mixture fraction, defined as $Z = y_1 + y_2 - y_0$, and their first derivatives are continuous everywhere (Fachini, 2001), it is possible to find expressions relating the variables Θ_1, Ψ_{01}, Ψ_{11} and Ψ_{21} as following

$$(q_1 - 1) d_1 \Psi_{11} + (q_2 - 1) d_2 \Psi_{21} + d_2(\Psi_{01} + \gamma_1 \xi_1) - \Theta_1 = d_H \xi_1 \tag{10}$$

$$d_1 \Psi_{11} + d_2 \Psi_{21} - d_2(\Psi_{01} + \gamma_1 \xi_1) = d_Z \xi_1 \tag{11}$$

where d_H and d_Z are the derivatives of the functions H and Z at the flame $z = z_f$ (Fachini, 2002), which are

$$d_H = -(d_1 + d_2) + d_\theta^- = (q_1 - 1) d_1 + (q_2 - 1) d_2 - d_\theta^+$$

$$d_Z = d_1 + d_2$$

Therefore, from equations (9), (10) and (11) and the values of d_H and d_Z one finds

$$\begin{array}{ll} (q_2 - 1) d_2 \Psi_{21} + d_2(\Psi_{01} + \xi_1) - (\Theta_1 + d_\theta^- \xi_1) = 0 & \qquad \xi_1 \leq \xi_{1f} \\ (q_2 - 1) d_2 (\Psi_{21} - \xi_1) - (q_1 - 1) d_1 \xi_{1f} - (\Theta_1 - d_\theta^+ \xi_1) = 0 & \qquad \xi_1 \geq \xi_{1f} \end{array} \tag{12}$$

and

$$\begin{array}{ll} \Psi_{21} - (\Psi_{01} + \xi_1) = 0 & \qquad \xi_1 \leq \xi_{1f} \\ \Psi_{21} - (\xi_1 + (d_1/d_2)\xi_{1f}) = 0 & \qquad \xi_1 \geq \xi_{1f} \end{array} \tag{13}$$

From boundary conditions (7) and (8) or from equation (13) for $\xi_1 \geq \xi_{1f}$, it is seen that the reaction of fuel 2 does not exist because the oxygen quantity in the region $\xi_{1f} \leq \xi_1 < \infty$ is not enough to cause an important consumption of fuel 2. Then, at layer 2, $\xi_1 = \xi_{1f}$, the flux of fuel 2 is practically equal to that at the condition $\xi \to \infty$, i.e. $d\Psi_{21}/d\xi_1|_{\xi_1 \to \infty} = 1$, and the value of Ψ_{21} can be specified, $\Psi_{21} = \xi_{1f}(1 + d_1/d_2)$. By combining equations (12) and (13), the following relations are found

$$\begin{array}{lll} \Theta_1 = q_2 d_2 \Psi_{01} + (q_2 d_2 - d_\theta^-)\xi_1 & \quad \text{for} & \xi_1 \leq \xi_{1f}, \\ \Theta_1 = d_\theta^+ \xi_1 + (q_2 - q_1) d_1 \xi_{1f} & \quad \text{for} & \xi_1 \geq \xi_{1f}. \end{array}$$

From these relations, the derivative of the temperature Θ_1, imposing the conditions $d\Psi_{01}/d\xi_1|_{\xi_1 = \xi_{1f}} = 0$ and $d\Psi_{21}/d\xi_1|_{\xi_1 = \xi_{1f}} = 1$, are determined at both side of the layer 2, $\xi_1 = \xi_{1f}$,

$$\left. \frac{d\Theta_1}{d\xi_1} \right|_{\xi_1 = \xi_{1f}^-} = q_2 d_2 - d_\theta^- \quad \text{and} \quad \left. \frac{d\Theta_1}{d\xi_1} \right|_{\xi_1 = \xi_{1f}^+} = d_\theta^+ \tag{14}$$

These derivatives at borders of layer 2 will be used to solve the problem of the oxidation of fuel 2.

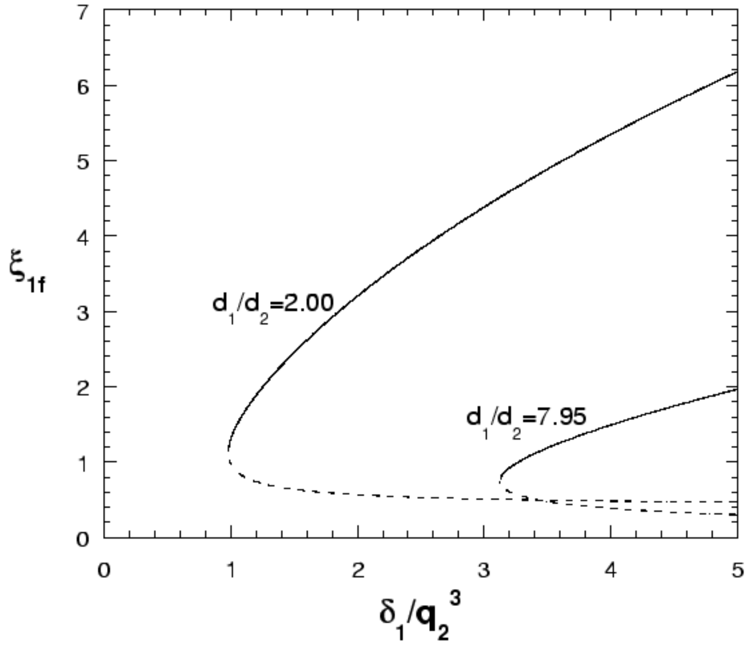

Figure 2: The edge of the layer 1 ξ_{1f}, where the reaction 1 takes place, as function of the modified Damkhöler number δ_1/q_2^3. The curve for $d_1/d_2 = 2.00$ represents the mixture $Y_1 = 0.11$ and $Y_2 = 0.01$, that $1 - d_\theta^-/q_2 d_2 = -0.775$, $\xi_{1f}^L = 1.099$ and $\delta_1^L/q_2^3 = 0.979$. The curve for $d_1/d_2 = 7.95$ represents the mixture $Y_1 = 0.99$ and $Y_2 = 0.01$, that $1 - d_\theta^-/q_2 d_2 = -5.914$, $\xi_{1f}^L = 0.750$ and $\delta_1^L/q_2^3 = 3.125$.

An analysis of the equation (13) shows that for $d_1/d_2 \ll 1$ ($|\gamma_1| \ll 1$) the structure of the flame must be similar of that of one-fuel diffusion flames, as would be expected. To satisfy this feature, the position of layer 2 has to be inside the fuel side of the flame, $\xi_{1f} \gg 1$. Under this condition the boundary condition corresponding to the heat flux, equation (14), agrees with the boundary condition corresponding to heat flux for the the one-fuel diffusion flame problem. Thus, the heat flux jump condition is $d_\theta^- + d_\theta^+ = q_2 d_2$. In the other limit, $d_1/d_2 \gg 1$ ($|\gamma_1| \gg 1$), the one-fuel diffusion flame structure is recovered again, but in this case the position of the layer 2 goes to zero, $\xi_{1f} \to 0$ according to $\xi_{1f} \sim (d_1/d_2)^{-1}$, to satisfy the condition that Ψ_{21} is finite. For $|\gamma_1| = O(1)$, the mass fraction of fuel 2, Ψ_{21}, at the layer 2, $\Psi_{21} = \xi_{1f}(1 + d_1/d_2)$, is directly proportional to the flux of fuel 1 and inversely proportional to the flux of fuel 2.

With Eqs. (12) and (13), the description of the oxidation of fuel 2 becomes simple because they provide relationships among the variables which allow the integration of only one equation of the system of equation (2) to (4). The equation that follows the consumption of oxygen Ψ_{01} is given by

$$\frac{d^2\Psi_{01}}{d\xi_1^2} = [\Psi_{01} - (d_1/d_2)\xi_1]^{\beta_{21}} (\Psi_{01} + \xi_1)^{\beta_{22}} e^{-[\Psi_{01} + (1 - d_\theta^-/q_2 d_2)\xi_1]/(\delta_1/q_2^{b_1})^{1/b_1}} \qquad (15)$$

This equations must satisfy the three conditions found in equations (6) and (7), $d\Psi_{01}/d\xi_1|_{\xi_1 \to -\infty} = -1$, $d\Psi_{01}/d\xi_1|_{\xi_1 = \xi_{1f}} = 0$ and $\Psi_{01}(\xi_1 = \xi_{1f}) = (d_1/d_2)\xi_{1f}$. The extra condition will be employed to determine the position of layer 2, ξ_{1f}, that corresponds to the eigenvalue of the problem.

The results presented here were obtained for the reaction global orders β_{21} and β_{22} equal to one, thereby $b_1 = 3$.

Together with the solution of the problem represented by (15), (6) and (7), the position of the edge of the layer 1 ξ_{1f} is determined as a function of the modified Damkhöler number δ_1/q_2^3, $\xi_{1f} = \xi_{1f}(\delta_1/q_2^3)$. The values of ξ_{1f} for two compositions of fuels 1 and 2, $Y_1 = 0.99$, $Y_2 = 0.01$, represented in the fig. 2 by the case $d_1/d_2 = 7.95$, and $Y_1 = 0.11$, $Y_2 = 0.01$, represented in the fig. 2 by the case $d_1/d_2 = 2.00$, are displayed in fig. 2. It is seen that there is a limit for δ_1/q_2^3, δ_1^L/q_2^3, below which the solution for ξ_{1f}, ξ_{1f}^L, does not exist. Therefore, the condition $\delta_1/q_2^3 = \delta_1^L/q_2^3$ defines the extinction of the flame. Above that limit, $\delta_1/q_2^3 > \delta_1^L/q_2^3$, the problem has two solutions for ξ_{1f}.

An analysis for the case of low fuel 2 mass flux, $d_1/d_2 \gg 1$, reveals that the oxygen mass flux crosses the layer 1 with a little change; oxygen flux for $\xi \to -\infty$ is $d_1(1 + d_2/d_1)$ is very close to d_1 at $\xi_1 = \xi_{if}$. Thereby, the position ξ_{if} has to be close to zero. By taking this conclusion into account and comparing the positions ξ_{if} shown in figure 2, it can be affirmed that the lower branch of the solution is that representing the flame structure; it is that one with physical meaning. Note that for $d_1/d_2 = 7.95$, the lower branch solution is even closer to zero, as poiting the analysis.

In the case that the fuel 2 mass flux is compared to the fuel 1 mass flux, $d_1/d_2 \sim 1$, the position ξ_{1f} must increase to permit the consumption of a large part of fuel 2 in the layer 1.

In nonlinear problems, like the extinction problem, the solutions are multiple. Moreover, the characteristic of all solutions is not the same, ones are stable and others are unstable. After turning points, as shown in figure 2, the stability of the solution change. Therefore, the low branch solution in figure 2 is stable and the upper branch solution is unstable.

The results displayed in figure 2 prove that the extinction of multicomponent fuel flames can be controlled by the reaction 2, that is the less sensitive to temperature variations. This observation is contrary to the up-to-now accepted idea, giving by the analysis of a single fuel: the most thermal sensitive reaction is the responsible for the extinction.

3.2. Solution of order ε_2

The structure of layer 2 (see fig. 1), in which the oxidation of fuel 2 is performed, is described exactly as in previous analyses (Liñán, 1974). The formulation of the problem of the order ε_2 is presented to prove that it corresponds to the Liñán's analysis and, consequently, the hypothesis of oxygen leakage of the order $1/\theta_{a1}$ through the reaction zone is true, as adopted in previous analysis. Note that this condition must be satisfied, otherwise the previous section does not represent the case studied in the work. The detail of this analysis is already well known.

Recalling that the solutions of order of ε_1 for the oxygen mass fraction and fuel 2 mass fraction are zero at the $\xi_1 = \xi_{1f}$, then the expansion (1) has to be re-written as

$$\begin{array}{rllll}
\theta = & \theta_f & -\ \varepsilon_1\ \Theta_{1f}/d_2\delta_1^{1/b_1} & -\ \varepsilon_2\ (\Theta_2+\gamma_2\xi_2)/\delta_2^{1/b_2} & +\cdots \\
y_O = & 0 & +\ 0 & +\ \varepsilon_2\ d_2\Psi_{02}/m_2\delta_2^{1/b_2} & +\cdots \\
y_1 = & 0 & +\ 0 & +\ \varepsilon_2\ d_1\Psi_{12}/m_2\delta_2^{1/b_2} & +\cdots \\
y_2 = & 0 & +\ \varepsilon_1\xi_{1f}(1+d_1/d_2)/\delta_1^{1/b_1} & +\ \varepsilon_2\ d_2\Psi_{22}/m_2\delta_2^{1/b_2} & +\cdots \\
x = & x_f & +\ \varepsilon_1\ \xi_{1f}/d_2\delta_1^{1/b_1} & +\ \varepsilon_2\ \xi_2/m_2\delta_2^{1/b_2} & +\cdots
\end{array} \tag{16}$$

Taking equation (16) into the balance equations for species and energy and picking up the equations of order of ε_2, one finds

$$\frac{d^2}{d\xi_2^2}m_2(\Theta_2+\gamma_2\xi_2) = d_1q_1\left(\frac{m_2}{d_1q_1}\right)^{-(\beta_{11}+\beta_{12})}\Psi_{02}^{\beta_{11}}\Psi_{12}^{\beta_{12}}e^{-\Theta_2/\delta_2^{1/(1+\beta_{11}+\beta_{12})}} \tag{17}$$

$$\frac{d^2}{d\xi_2^2}d_1\Psi_{02} = d_1\left(\frac{m_2}{d_1q_1}\right)^{-(\beta_{11}+\beta_{12})}\Psi_{02}^{\beta_{11}}\Psi_{12}^{\beta_{12}}e^{-\Theta_2/\delta_2^{1/(1+\beta_{11}+\beta_{12})}} \tag{18}$$

$$\frac{d^2}{d\xi_2^2}d_1\Psi_{12} = d_1\left(\frac{m_2}{d_1q_1}\right)^{-(\beta_{11}+\beta_{12})}\Psi_{02}^{\beta_{11}}\Psi_{12}^{\beta_{12}}e^{-\Theta_2/\delta_2^{1/(1+\beta_{11}+\beta_{12})}} \tag{19}$$

$$\frac{d^2}{d\xi_2^2}d_2\Psi_{22} = 0 \tag{20}$$

The boundary conditions for Eqs. (17) to (20), determined by the matching with the solution of order ε_1, are given by

$$\frac{d\Theta_2}{d\xi_2}+1 = \frac{d\Psi_{02}}{d\xi_2}+1 = \frac{d\Psi_{12}}{d\xi_2}-1 = \frac{d\Psi_{22}}{d\xi_2} = 0 \qquad \xi_2 \to -\infty \tag{21}$$

$$\frac{d\Theta_2}{d\xi_2}-1 = \frac{d\Psi_{02}}{d\xi_2} = \frac{d\Psi_{12}}{d\xi_2}-1 = \frac{d\Psi_{22}}{d\xi_2}-1 = 0 \qquad \xi_2 \to \infty \tag{22}$$

Note that the definitions of m_2 and γ_2 are such that permit the derivative of Θ_2 to be normalized for $\xi_2 \to -\infty$ and for $\xi_2 \to \infty$

Combining Eqs. (17) to (20), the following relations are found

$$(q_1-1)d_1\Psi_{12} + (q_2-1)d_2\Psi_{22} + d_1\Psi_{02} - m_2(\Theta_2+\gamma_2\xi_2) = d_{H1}\xi_2 \tag{23}$$

$$d_1\Psi_{12} + d_2\Psi_{22} - d_1\Psi_{02} = d_{Z1}\xi_2 \tag{24}$$

where d_{H1} and d_{Z1} are the derivatives of the functions H and Z at the flame $z = z_f + \varepsilon_1\xi_{1f}/m_1\delta_1^{1/b_1}$, which are

$$d_{H1} = (q_2-1)d_2 - d_1 - (q_2d_2 - d_\theta^-) = (q_1-1)d_1 + (q_2-1)d_2 + d_\theta^+$$

$$d_{Z1} = d_1 + d_2$$

The solution of Eq. (20) satisfying boundary conditions (21) and (22) becomes $\Psi_{22} = \xi_2$. This solution and the definition for d_{Z1} taken to Eq. (24) lead to

$$\Psi_{02} = \Psi_{12} - \xi_2 \tag{25}$$

Taking the expression for d_{H1} and Eq. (25) into equation (23), the following relations between Ψ_{02} and Θ_2 and between Ψ_{22} and Θ_2,

$$\Psi_{02} = \frac{m_2}{q_1d_1}\,(\Theta_2-\xi_2) \qquad \text{and} \qquad \Psi_{12} = \frac{m_2}{q_1d_1}\,(\Theta_2+\xi_2), \tag{26}$$

are found. Note that, since $d_\theta^- + d_\theta^+ = q_1 d_1 + q_2 d_2$, $m_2/q_1 d_1 = 1/2$.

Therefore, taking Eq. (26) into Eq. (17), the structure inside the zone where the oxidation of the fuel 1 occurs can be described by

$$\frac{d^2\Theta_2}{d\xi_1^2} = (\Theta_2 - 1)^{\beta_{11}}(\Theta_2 + 1)^{\beta_{12}} e^{-(\Theta_2 + \gamma_2 \xi_2)/\delta_2^{1/(1+\beta_{11}+\beta_{12})}} \tag{27}$$

which must satisfy Eqs. (21) and (22).

The solution of the problem (27), (21) and (22) exists (Liñán, 1974), then it is guaranteed, from Eq. (26), that the scape of oxygen is of the order $1/\theta_{a1}$, once that Ψ_{02} is of the order $O(1)$. According to the Liñán's (1974) work on counterflow, for $\beta_{11} = \beta_{12} = 1$, the value of modified Damkhöler number δ_2 for extinction is related with γ_2 by the following expression

$$\delta_{2ext} = e[(1 - |\gamma_2|) - (1 - |\gamma_2|)^2 + 0.26(1 - |\gamma_2|)^3 + 0.055(1 - |\gamma_2|)^4] \tag{28}$$

The discussion about the limits cases $d_2/d_1 \gg 1$ and $\ll 1$ realized previously can be expanded now. Since $d_H = -(d_1 + d_2) + d_\theta^- = (q_1 - 1)d_1 + (q_2 - 1)d_2 - d_\theta^+$ and $d_\theta^- + d_\theta^+ = q_1 d_1 + q_2 d_2$, the parameter γ_2 can be expressed as

$$\gamma_2 = 1 - 2\frac{d_\theta^-}{d_1 q_1} + 2\frac{q_2 d_2}{q_1 d_1}$$

Therefore, for $d_2/d_1 \ll 1$, γ_2 becomes $1 - 2d_\theta^-/q_1 d_1$ that is the result found by Liñán (1974) to describe the structure of the one-fuel diffusion flame.

4. Conclusion

This analysis was developed in a general way, a tool to be applied to any particular multicomponent fuel diffusion flame. The results showed that the extinction of multicomponent fuel diffusion flames can be also controlled by the less thermal sensitive reaction.

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