Dynamics of Premixed, Planar, Pulsating Flame Fronts.

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Abstract

The unsteady propagation of a planar, premixed flame front is investigated, in the diffusional-thermal limit, for solids as well as for gaseous mixtures. The inner structure of the reaction zone is studied in detail for large Zel'dovich numbers. Then, the problem of the unsteady propagation of the flame is formulated by replacing the inner zone by a discontinuity surface with jump conditions across it provided by the inner structure. Finally, the solution is obtained numerically accounting for the effect of these discontinuity surfaces in the outer unsteady regions which are now free from the reaction terms.

Introduction

The first studies on the stability limits of steadily propagating premixed flame fronts in the diffusional-thermal approximation are due to Barenblatt ([1]) and Sivashinsky ([2], [3]). In his work on cellular premixed flames ([2]), Sivashinsky considered a single bimolecular irreversible step in a gaseous mixture, following Arrhenius kinetics with unity orders of reaction for both reactants; he showed that when the Lewis number of the deficient component is larger than unity, the steadily propagating flame becomes unstable for sufficiently large Zel'dovich numbers, assuming in this case the form of a pulsating planar front. The critical Zel'dovich number defining the limit of stability is a monotonically decreasing function of the Lewis number, becoming infinite for unity Lewis number and approaching to a well defined limit value for a solid (Le $\to \infty$), a limit later confirmed by Sivashinsky himself in a work on the stability of gasless planar flames in solids [3]. On crossing the limit of stability, close to it, the propagation assumes the form of harmonic oscillations with a well defined time scale. But on moving deeper into the instability region, these oscillations, although still periodic, soon become complicated relaxational type pulsations ([4], [5]), characterized by long periods with flame front velocities lower than that corresponding to a steady flame, bounded by very short stages with very large flame front velocities.

Specific Objectives

We pursue here, along the same line, a step further generalizing the previous work, accounting for the effects, on the inner structure of the reaction layers, of the unsteady nature of the flame propagation. It is shown that for the limit of large Zel'dovich numbers the flame maintains, even in the unsteady case, the classical dual structure with a thin reactive layer embedded in reaction-free unsteady regions. The inner reactive layers, much thinner than the outer regions and quasisteady in the first approximation, are studied in detail following Liñán's earlier analysis of the premixed flame regime of diffusion flames [6]. The problem of the unsteady propagation of the flame is then formulated by replacing the inner zone by a discontinuity surface with jump conditions across it provided by the previous analysis of the reaction zone structure. Thus the solution can be obtained by accounting for the effect of these discontinuity surfaces in the outer unsteady regions which are now free from the reaction terms.

The problem still contains a large parameter, the nondimensional activation energy, and that poses considerable difficulties from the numerical point of view, since the spatial structure of the solution involves, simultaneously, both large and small spatial scales. They, in addition, evolve with time during each period, characterized by very short excursions with large flame velocities, when the flame temperature grows above its adiabatic steady value, followed by long, dormant, stages with flame temperature and velocities significantly lower than the values corresponding to the steady flame. The time and length scales, strongly varying with time, are identified and used to generate new rescaled independent variables for the reformulation of the problem, which now takes a form more amenable to be treated numerically. However, the resulting problem is still time dependent, although the temporal as well as the spatial scales now vary much more smoothly along a period. The numerical solutions, well resolved both in time as well as spatially, uncover the dynamic behavior of these unstable flames.

Results and Discussion

We first study the problem in the case of a solid gasless flame, starting with the analysis of the reaction layer inner structure. The results are incorporated to the formulation of the global dynamics, resulting in a problem free from the reaction terms. This reformulated problem is solved numerically and some results presented. Next, the case of a gaseous flame in the diffusional-thermal limit is analyzed following the same scheme.

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Solid gasless flames

The dimensionless temperature θ and fuel mass fraction Y in a reactive solid in which chemical reactions can be modeled by a one irreversible step with Arrhenius kinetics are given, in a frame of reference attached to the flame: $\xi = x - x_f(t)$, by:

$$-C(Y) = C(\theta) - \theta_{\xi\xi} = \Delta Y e^{\beta\,(\theta-1)/(1+\alpha\,(\theta-1))} \qquad (1)$$

with the convective operator $C(\cdot) = \partial_t + c\partial_\xi$ and with $\theta = (\tilde{T} - \tilde{T}_u)/(\tilde{T}_b - \tilde{T}_u)$, $Y = \tilde{Y}/\tilde{Y}_u$, and the independent variables, $x = \tilde{x}/\tilde{l}_L$ and $t = \tilde{t}/\tilde{t}_L$, made nondimensional with the characteristic length and time from the stationary flame propagating with velocity U_L: $l_L = k/(\rho c U_L)$ and $\tilde{t}_L = \tilde{l}_L/\tilde{U}_L$. $\tilde{T}_u$ and $\tilde{T}_b$ are, respectively, the fresh and the burnt mixture temperatures. c is the flame speed, $-dx_f/dt$, with $x_f(t)$ the instantaneous position of the flame. The parameters that enter are the exothermicity, $\alpha = (\tilde{T}_b - \tilde{T}_u)/\tilde{T}_b$, and a Zel'dovich number, $\beta = E(\tilde{T}_b - \tilde{T}_u)/(R\tilde{T}_b^2)$. $\Delta = B\,\tilde{t}_L e^{-E/(R\tilde{T}_b)}$ is the eigenvalue corresponding to the stationary problem, easily seen to be $\Delta = \beta + O(1)$. The appropriate boundary conditions are the initial fuel mass fraction and temperature of the solid far upstream, $\theta = Y - 1 = 0$ as $\xi \to -\infty$, and the burnt conditions far downstream, $\theta - 1 = Y = 0$ as $\xi \to \infty$.

Inner structure of the flame. For large activation energies, the reaction zone is thin, of order β^{-1} in the chosen scales, so that in the first approximation it can be thought of as an infinitely thin sheet with a well defined value of the temperature on it, namely θ_f, the apparent flame temperature. Nevertheless, the flame speed is determined by the quasisteady structure of the reaction layer, where with temperature deviations of order β^{-1} the fuel is consumed, so Y decays from unity upstream to Y_b, the unburnt fuel mass fraction left past the flame. The flame structure is given, in first approximation, by:

$$\varphi_{\mu\mu} = Y_\mu = -\kappa\, Y\, e^{\varphi} \qquad (2)$$

in terms of the inner variables $\Lambda^2\mu = \beta\, c\, \xi$, $\varphi = \beta(\theta - \theta_f)/\Lambda^2$, with a reduced Damköhler number $\kappa = \Lambda^2\, e^{\beta(\theta_f - 1)/(1+\alpha(\theta_f-1))}/c^2$ where $\Lambda = 1 + \alpha(\theta_f - 1)$.

The boundary conditions for (2) must ensure matching with unsteady, reaction-free regions where the flame is embedded, namely $Y = 1$ and $\varphi \to q_{-\infty}\mu$ far upstream as $\mu \to -\infty$, and $Y = Y_b$ and $\varphi \to q_{+\infty}\mu$ far downstream as $\mu \to \infty$. $q_{\pm\infty} = p_{\pm\infty}/c$ are the scaled slopes of the outer temperature distribution at the flame, $p_{\pm\infty} = \partial\theta/\partial\xi|_{\xi=0^\pm}$; thus, the outer temperature distribution is given by $\theta^\pm = \theta_f + p_{\pm\infty}\xi$, as $\xi \to 0^\pm$, the minus and plus signs referring, respectively, to the upstream and downstream sides of the flame.

In the steady case, the outer upstream slope at the flame, $q_{-\infty}$, is unity in these scales, whereas the downstream one, $q_{+\infty}$, vanishes since the flame is adiabatic. On the contrary, in the unsteady case, $q_{-\infty}$ is always positive because the flame is preheating the unburnt mixture, but oscillates around unity, whereas the downstream slope $q_{+\infty}$ can be either positive or negative; in this latter case, when the temperature decays towards the products side, reactions become frozen so there can remain a finite amount, Y_b, of unreacted fuel.

Solution. The first equation in (2) gives the first integral $\partial\varphi/\partial\mu = q_{-\infty} + Y - 1$. On the other hand, using this first integral in the second of (2) leads to $\kappa\,\varphi_Y = -(q_{-\infty} + Y - 1)Y^{-1}\, e^{-\varphi}$, to be integrated with $Y = 1$ as $\varphi \to -\infty$. The solution is $-\kappa\, e^{\varphi} = (q_{-\infty} - 1)\,\mathrm{Ln}Y + Y - 1$. It follows from it that Y must vanish downstream of the flame whenever $q_{+\infty} > 0$, since in this case the reaction rate, e^{φ}, grows unboundedly. On the contrary, for negative values of $q_{+\infty}$, the reaction rate vanish downstream and so a finite Y_b of the fuel mass fraction, with $1 \leq Y_b \leq 0$, may remain unburnt past the flame, obtained from

$$(q_{-\infty} - 1)\,\mathrm{Ln}Y_b + Y_b - 1 = 0 \qquad (3)$$

The relation between the the two slopes at the flame, $q_{\pm\infty}$, can be obtained imposing the boundary conditions in the first integral above, resulting in:

$$q_{+\infty} = q_{-\infty} - 1 + Y_b \qquad (4)$$

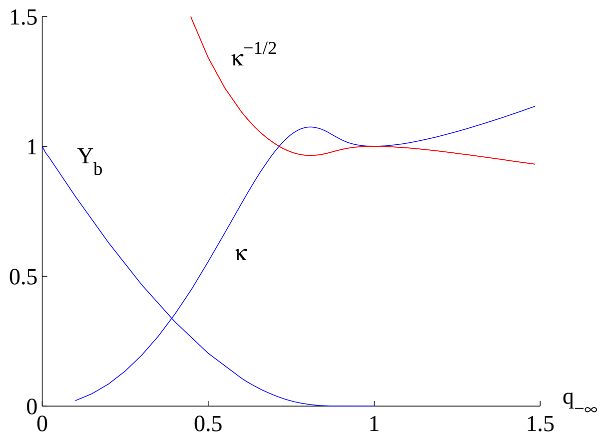

Fig. 1. The unburnt fuel, Y_b, and the reduced Damköhler number, κ, as functions of $q_{-\infty}$.

The problem for the first order of approximation to the inner structure of the flame has therefore been reduced to:

$$Y^{-1}Y_\mu = (q_{-\infty} - 1)\mathrm{Ln}Y + Y - 1 = -\kappa\, e^{\varphi} \qquad (5)$$

with boundary conditions far upstream, $Y \to 1$, $\varphi \to q_{-\infty}\mu$ as $\mu \to -\infty$, $Y \to 0$, $\varphi \to (q_{-\infty} - 1)\,\mu$ far downstream as $\mu \to \infty$ when $q_{-\infty} > 1$, or $Y \to Y_b(q_{-\infty})$, $\varphi \to (q_{-\infty} - 1 + Y_b)\,\mu$ when $q_{-\infty} \leq 1$.

The unburnt fuel Y_b, when $q_{-\infty} \leq 1$, is given by the solution of equation (3), whereas the jump in the slopes across the flame is:

$$q_{+\infty} = q_{-\infty} - 1 \qquad \text{for} \quad q_{-\infty} > 1$$
$$q_{+\infty} = q_{-\infty} - 1 + Y_b \qquad \text{for} \quad q_{-\infty} < 1$$

Damköhler number. In spite of the temperature distribution being given by an algebraic equation (5), it is necessary to retain the boundary conditions associated with it in order to calculate the Damköhler number, κ, which can be obtained as follows. Indeed, the asymptotic behavior of the solution can be easily seen to be: $Y - 1 \approx -A\, e^{q_{-\infty}\mu}$ as $A(q_{-\infty}, Y_o)$, $B_>(q_{-\infty}, Y_o)$ and $B_<(q_{-\infty}, Y_o)$ are constants of integration obtained when the problem is integrated with the initial condition $Y(0) = Y_o$. In addition, since problem (5) is translationally invariant, the constants of integration obtained when using a new translated independent variable $\mu = \mu' + \lambda$ must transform according to: $A' = A\, e^{q_{-\infty}\lambda}$, $B'_> = B_>\, e^{(q_{-\infty}-1)\lambda}$, and $B'_< = B_<\, e^{(q_{-\infty}-1+Y_b)\lambda}$, with A', $B'_>$ and $B'_<$ the constants corresponding to the solution in the variable μ'. Finally, the Damköhler number κ can be obtained from equation (5) using the asymptotic behavior just obtained, resulting in $\kappa = q_{-\infty} A\, e^{q_{-\infty}\lambda}$, as $\mu \to -\infty$, $\kappa = (q_{-\infty} - 1)\, B_>\, e^{(q_{-\infty}-1)\lambda}$ as $\mu \to -\infty$ when $q_{-\infty} > 1$, and finally, $\kappa = (1 - q_{-\infty} - Y_b)/Y_b\, B_<\, e^{(q_{-\infty}-1+Y_b)\lambda}$, as $\mu \to -\infty$ when $q_{-\infty} < 1$. Obviously, κ, must be the same whether evaluated at the upstream or the downstream boundary, so eliminating the translation parameter λ gives: $\kappa = \big((q_{-\infty} - 1)\, B_>\big)^{q_{-\infty}} \big(q_{-\infty}\, A\big)^{(1-q_{-\infty})}$ when $q_{-\infty} > 1$, and $\kappa = \big\{\big(Q\, B_<\big)^{q_{-\infty}} (q_{-\infty} A)^{Q}\big\}^{1/(1-Y_b)}$ when $q_{-\infty} < 1$, with $Q = (1 - q_{-\infty} - Y_b)$.

Thus, integrating (5) for any initial condition, $Y(\mu_o) = Y_o$, with $1 < Y_o < Y_b$, the constants A, $B \lessgtr$ from the asymptotic behavior result as part of the solution, allowing therefore to determine the Damköhler number $\kappa(q_{-\infty})$. Fig. 1 shows the resulting $\kappa(q_{-\infty})$.

The reduced Damköhler number, $\kappa(q_{-\infty})$, determines the velocity of propagation of the flame as

$$c = \kappa^{-1/2} \Lambda\, e^{\frac{(\beta/2)\,(\theta_f - 1)}{1+\alpha(\theta_f - 1)}} \tag{7}$$

Flame dynamics. The unsteady flame propagation is given by (1), with the appropriate boundary and initial conditions. Nevertheless, in the limit of large Zel'dovich numbers, the reaction rate terms can be replaced but Dirac deltas with appropriate intensities. These intensities, which set the jumps of the gradients across the flame, are $p_{-\infty} - p_{+\infty}$ in the case of temperature, and $c(1 - Y_b)$ for the fuel. Furthermore, since there is no species diffusion in the solid, the fuel mass fraction distribution is uniform in absence of the reaction terms and so, it is unity upstream of the flame, and Y_b downstream of it. Therefore, for large activation energies, the dynamics of the flame is given by:

$$\theta_t + c\, \theta_\xi = \theta_{\xi\xi} + (p_{-\infty} - p_{+\infty})\, \delta(\xi) \tag{8a}$$
$$p_{-\infty} - p_{+\infty} = c\,(1 - Y_b) \tag{8b}$$
$$c = \kappa^{-1/2} \Lambda\, e^{\frac{(\beta/2)\,(\theta_f - 1)}{1+\alpha(\theta_f - 1)}} \tag{8c}$$

with $p_{\pm\infty} = \partial\theta/\partial\xi|_{\xi=0_\pm}$ and the flame temperature $\theta_f(t) = \theta(0, t)$.

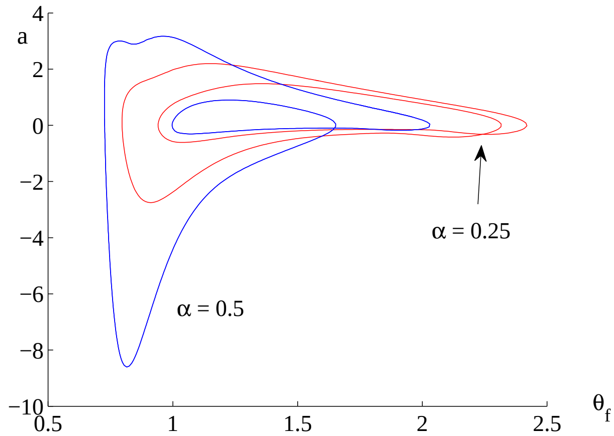

Fig. 2. The phase plane $a - \theta_f$ for some numerical solutions of the dynamical behavior of solid flames with $\beta = 10.5$.

This is the problem formulated in the scales appropriate for the steady premixed flame. However, as anticipated above, the unsteady propagation deep into the instability region assumes the form a relaxation oscillations characterized by stages with flame temperatures well above unity and, accordingly, with flame velocities of order $c \approx \exp(\beta/2) >> 1$. Thus, the region upstream of the flame where heat conduction effects are still important has a length scale of order c^{-1}, much smaller than unity. This is thus the appropriate scaling for the spatial coordinate, leading to the new independent variable $\varsigma = c\,\xi \approx 1$. Substituting this new variable into the previous problem uncovers the corresponding time scale: $d\tau = c^2 dt \approx 1$, both conducting to:

$$\theta_\tau = \theta_{\varsigma\varsigma} - \big(1 + a\,\varsigma\big)\,\theta_\varsigma + (q_{-\infty} - q_{+\infty})\,\delta(\xi) \tag{9a}$$
$$q_{-\infty} - q_{+\infty} = 1 - Y_b \tag{9b}$$

and $a = d\ln c/d\tau$, given by

$$a = \frac{d\,\ln\kappa}{dq_{-\infty}}\frac{dq_{-\infty}}{d\tau} + \frac{\beta}{2}\frac{\theta_{f\tau}}{\Lambda^2}\Big(1 + \frac{2}{\beta}\alpha\Lambda\Big) \tag{10}$$

where $q_{\pm\infty}$ are the scaled slopes of the temperature distribution at the flame $q_{\pm\infty} = p_{\pm\infty}/c$. Fig. 2 and Fig. 3 show some solutions of the previous problem.

Numerical method. The problem (9) is solved numerically in a nonuniform grid, $\zeta_{\pm i}$, the plus sign referring to the downstream side of the flame and the minus one to that upstream and with $\zeta = 0$ corresponding to the flame sheet. The grid on each side of the flame is obtained as a hyperbolic tangent mapping of a uniform grid $i/N^{\pm}$, with i running from 1 to $N^{\pm}$, onto a nonuniform grid $[0, \zeta_i^{\pm}\zeta_{\infty}^{\pm}]$, given by $\zeta_i^{\pm}/\zeta_{\infty}^{\pm} = 1 - \tanh(\mu^{\pm}(1 - i/N^{\pm}))/\tanh(\mu^{\pm})$, where $\zeta_{\infty}^{\pm}$ and $\mu^{\pm}$ are the parameters which define the transformation, and can be different for each side of the flame. Typical values of the parameters are $\zeta_{-\infty} = -10000$, $\zeta_{+\infty} = 20000$, $\mu^{\pm} = 5.5$ and $N^{\pm} = 4000$ for the numerical solutions shown above. The spatial operator are discretized with second order finite differences and the solution is advanced in time with an implicit Euler integrator with constant time step of order ranging between 10^{-3}, 10^{-4}. The complete integro-differential problem, (9) and (10) is solved with a Broyden type iterative method with θ_f and c as iteration variables.

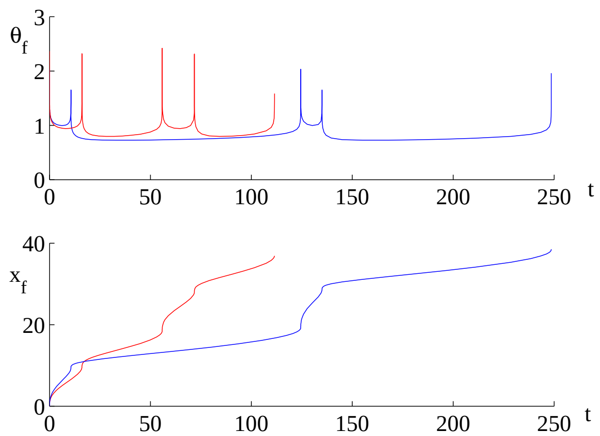

Fig. 3. The time evolution during a complete period of the flame temperature (above), and the flame position (below), corresponding to the phase portraits depicted in Fig. 2.

Gases

We considere here a homogeneous gaseous mixture, deficient in the fuel, which can sustain chemical reactions according to a single global irreversible step $\mathrm{F} + s\,\mathrm{O_2} \rightarrow (1+s)\mathrm{P} + \mathrm{Q}$, where s is the mass of oxygen per unit mass of fuel and Q is the heat released per unit mass of fuel burnt. The temperature, $\tilde{T}$, and the fuel mass fraction, $\tilde{Y}_F$, are made dimensionless as follows: $\theta = (\tilde{T} - \tilde{T}_u)/(\tilde{T}_b - \tilde{T}_u)$ and $Y_F = \tilde{Y}_F/\tilde{Y}_{Fu}$, where the subindex u refers to the unperturbed mixture conditions whereas the b one refers to the steady burnt conditions. The independent variables, $\tilde{x}$ and $\tilde{t}$, are made nondimensional with the characteristic length and time, respectively, from a stationary flame propagating with velocity U_L: $l_L = \lambda/\rho c_p U_L$ and $t_L = l_L/U_L$, so one has with $x = \tilde{x}/l_L$ and $t = \tilde{t}/t_L$. In a frame of reference attached to the flame, with $\xi = x - x_f(t)$, so the instantaneous flame speed: $c(t) = -dx_f/dt$, one has

$$-(C(Y_F) - \mathrm{Le_F^{-1}} Y_{F\xi\xi}) = C(\theta) - \theta_{\xi\xi} = \beta\omega \qquad (11)$$

with the convective operator again $C(\cdot) = \partial_t + c\partial_\xi$, the nondimensional reaction rate $\omega = \Delta\{1 + \alpha(\theta - 1)\}^{\gamma} Y_O^{\nu_O} Y_F^{\nu_F} \exp\left(\beta(\theta - 1)/(1 + \alpha(\theta - 1))\right)$, where the factor $\beta = E(\tilde{T}_b - \tilde{T}_u)/R\tilde{T}_b^2$, a Zel'dovich number, has been introduced anticipating the order of magnitude of the reaction rate. α is a measure of the exothermicity, $\alpha = (\tilde{T}_b - \tilde{T}_u)/\tilde{T}_b$ and $\Delta = t_L B \tilde{T}_b^{\gamma} \tilde{Y}_{Fu}^{\nu_F - 1} \tilde{Y}_{Ou}^{\nu_O} e^{-E/R\tilde{T}_b}/\beta$, is the eigenvalue corresponding to the stationary solution ([7]), $\Delta = \beta^{\nu_F}/\left(2\Gamma(\nu_F + 1)\,\mathrm{Le_F^{\nu_F}} Y_{Ob}^{\nu_O}\right)$, with $Y_{Ob} = 1 - \phi$, the dimensionless unburnt oxygen mass fraction left past the flame, ϕ being the equivalence ratio, $s\tilde{Y}_{Fu}/\tilde{Y}_{Ou}$. Thus, the propagation velocity of the stationary flame is obtained as $U_L^2 = B\tilde{T}_b^{\gamma} \tilde{Y}_{Fu}^{\nu_F - 1} \tilde{Y}_{Ou}^{\nu_O} e^{-E/R\tilde{T}_b}(k/\rho c_p)/(\beta\Delta)$. Finally, γ is the exponent of the temperature dependence of the prexponential coefficient. The appropriate boundary conditions are the cold, unperturbed fresh mixture far upstream, $\theta = Y_F - 1 = 0$ as $\xi \rightarrow -\infty$, and equilibrium far downstream $\theta - 1 = Y_F = 0$ as $\xi \rightarrow \infty$.

Inner structure. Again as in the case for solids, the reaction layer width is of order β^{-1}. The apparent flame temperature is denoted again by θ_f. In addition, since the flame is lean, the fuel is completely exhausted in first approximation in the flame, so that the apparent fuel mass fraction at the flame vanishes. The inner structure once again can be studied introducing the rescaled inner variables, $\Lambda\varphi = \beta(\theta - \theta_f)$, $\Lambda z_F = \beta Y_F$ and $\chi = \beta\xi$, again with $\Lambda = 1 + \alpha\theta_f$, which is introduced for convenience. With these variables, it results, as in the steady case, a quasistationary reaction zone whose structure is determined by the balance between the reaction rate and the diffusive terms

$$-\varphi_{\chi\chi} = \delta\, z_F^{\nu_F}\, e^{\varphi} \qquad (12a)$$

$$\left(z_F \mathrm{Le_F^{-1}} + \varphi\right)_{\chi\chi} = 0 \qquad (12b)$$

Here δ is a Damköhler number given by $\delta = \Delta\beta^{-\nu_F}\Lambda^{\gamma + \nu_F - 1} Y_{Ob}^{\nu_O} e^{\beta(\theta_f - 1)/\Lambda}$.

As in the solid case, this problem must be integrated with boundary conditions that ensure coupling with the outer reaction-free regions, namely, $z_{F\chi} = -m_F/\Lambda, \varphi_\chi = p_{-\infty}/\Lambda$ as $\chi \rightarrow -\infty$ and $y_{F\chi} = 0, \varphi_\chi = p_{+\infty}/\Lambda$, as $\chi \rightarrow \infty$.

Here $m_F \geq 0$ stands for the instantaneous dimensionless fuel mass fraction consumed by the flame, $m_F = -\partial Y_F/\partial\xi|_{\xi=0^-} = -\partial y_F/\partial\chi|_{\chi\rightarrow-\infty}$. On the contrary, downstream of the flame there is no flux of fuel since the case of a lean flame is being considered here, and no fuel is left behind the flame in first approximation. Finally, $p_{\pm\infty}$ denote the dimensionless heat fluxes at the reaction sheet, $p_{\pm\infty} = \partial\theta/\partial\xi|_{\xi=0^{\pm}} = \partial\psi/\partial\chi|_{\chi=\pm\infty}$. All these gradients are functions of time but, since the inner structure is quasistationary, they enter in this problem as parameters. Only the solution of the dynamics of the flame as a whole, reaction sheet and outer regions coupled, will render the fluxes, as well as the flame temperature and the velocity, as part of the solution.

Solution. Integrating once equation (12b) and taking into account the boundary conditions at the unburnt state gives:

$$\Lambda\Big(\mathrm{Le}_\mathrm{F}^{-1} z_F + \varphi\Big)_\chi = -m_F \mathrm{Le}_\mathrm{F}^{-1} + p_{-\infty} \tag{13}$$

This first integral can be used to evaluate the gradients past the flame, resulting in the relation between the jumps across the flame:

$$p_{-\infty} - p_{+\infty} = m_F/\mathrm{Le}_\mathrm{F} \tag{14}$$

Integrating once more (13) leads to $z_F/\mathrm{Le}_\mathrm{F} + \varphi = (-m_F/\mathrm{Le}_\mathrm{F} + p_{-\infty})\Lambda^{-1}\chi = p_{+\infty}\Lambda^{-1}\chi$. The constants of integration have been calculated taking into account the conditions $Y_F(\xi = 0) = \theta(\xi = 0) - \theta_f = 0$, which fix the position of the flame. This result can be used to obtain the reduced fuel mass fraction as a function of the temperature, so substituting back into (12a), with $z = z_F/\mathrm{Le}_\mathrm{F}$

$$z_{\chi\chi} = \delta\, \mathrm{Le}_\mathrm{F}^{\nu_F}\, z^{\nu_F}\, e^{(p_{+\infty}/\Lambda)\chi - z} \tag{15}$$

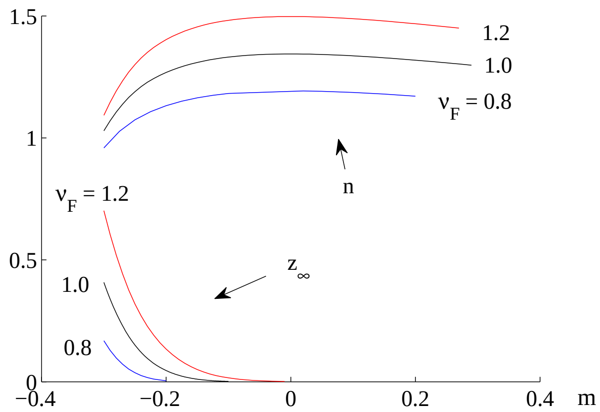

Fig. 4. The unburnt fuel, z_∞, and the function n from the inner structure of a gaseous flame as functions of the parameter m.

Finally, the variable ζ, defined as $m\zeta = (p_{+\infty}/\Lambda)\chi + \ln\big(2\Gamma(\nu_F+1)\delta\, \mathrm{Le}_\mathrm{F}^{\nu_F}\, \Lambda^2/(p_{-\infty} - p_{+\infty})^2\big)$, with $m = p_{+\infty}/(p_{-\infty} - p_{+\infty})$, reduces the problem for the inner structure to

$$2\Gamma(\nu_F + 1) z_{\zeta\zeta} = z^{\nu_F}\, e^{m\zeta - z} \tag{16}$$

to be integrated with boundary conditions $z_\zeta \to 0$ as $\zeta \to +\infty$ and $z_\zeta \to -1$ as $\zeta \to -\infty$.

The factor $2\Gamma(\nu_F+1)$ has been chosen so that (16) has solutions for $m = 0$ satisfying these boundary conditions. This is a generalized version of Liñán's canonical problem ([6]) in the case of nonunity fuel order of reaction.

As part of the solution one obtains the limit values $z_\infty(m) = \lim_{\zeta\to\infty} z$, and $n(m) = \lim_{\zeta\to-\infty}(z + \zeta)$, both plotted in Fig. 4. z_∞ is the unburnt fuel leakage past the flame, which must vanish for $m > 0$, when the temperature grows behind the flame because otherwise the reaction rate would grow without bound. On the other hand, n is related to the burning rate as follows. The far upstream behavior of z is $z \to -\big(m_F/(\mathrm{Le}_\mathrm{F}\Lambda)\big)\chi$, which, on using the definition of ζ, becomes $z \to -m^{-1}\{m\zeta - \ln\big(2\Gamma(\nu_F+1)\delta\, \mathrm{Le}_\mathrm{F}^{\nu_F}\, \Lambda^2/(p_{-\infty} - p_{+\infty})^2\big)\}$, so that it follows $(p_{-\infty} - p_{+\infty})^2 = e^{-n(m)m}\, 2\Gamma(\nu_F+1)\delta\, \mathrm{Le}_\mathrm{F}^{\nu_F}\, \Lambda^2$. Finally, using the definitions of δ and m:

$$p_{-\infty}^2\, e^{n(m)m}/(m+1)^2 = \Lambda^{\gamma+\nu_F+1} e^{\beta(\theta_f - 1)/\Lambda} \tag{17}$$

Dynamics. As for solids, in the limit of large Zel'dovich numbers, the reaction rate terms can be replaced by Dirac deltas with appropriate intensities, $p_{-\infty} - p_{+\infty}$ in the case of temperature, and $m_F/\mathrm{Le}_\mathrm{F}$ for the fuel mass fraction upstream of the flame. Since the case of a lean flame is being considered here, only the fuel mass fraction distribution is needed in determining the dynamics. Furthermore, since the fuel is completely consumed by the flame in first approximation, only the region upstream of the flame needs to be considered when calculating the fuel mass fraction distribution. Thus, the dynamics of the flame is governed by:

$$\mathcal{CD}(\theta; 1) = (p_{-\infty} - p_{+\infty})\,\delta(\xi) \qquad \text{for all } \xi \tag{18a}$$

$$\mathcal{CD}(Y_F; \mathrm{Le}_\mathrm{F}) = -(\mathrm{m_F}/\mathrm{Le}_\mathrm{F})\,\delta(\xi) \quad \text{for } \xi \le 0 \tag{18b}$$

with boundary conditions: $\theta = Y_F - 1 = 0$ as $\xi \to -\infty$, $\theta \to 1$ as $\xi \to \infty$ and $Y_F = 0$ at $\xi = 0$.

The convection-diffusion operator is defined as $\mathcal{CD}(\cdot, L) = \partial_t + c\partial_\xi - L^{-1}\partial_{\xi\xi}$. This problem must be complemented with two more equations which provide continuity conditions for the slopes across the flame and the relation of these slopes with the apparent flame temperature θ_f. These are given by the previous analysis of inner structure of the flame, namely equations (14) and (17).

Thus, equations (18) and (14), (17), form a complete problem to determine the distributions $\theta(\xi, t)$ and $Y_f(\xi, t)$, as well as the flame temperature, $\theta_f(t)$, and the heat fluxes and fuel rate of consumption, $p_{\pm\infty}(t)$ and $m_F(t)$ respectively. To see this, one can think of the differential equations for θ and Y_F (18) as a system of three equations to determine the distributions $\theta^-(\xi, t) = \theta(\xi < 0, t)$, $\theta^+(\xi, t) = \theta(\xi > 0, t)$ and $Y_F(\xi < 0, t)$, and the slopes $p_{-\infty}$, $p_{+\infty}$ and m_F as well, as functions of the parameters c, θ_f. To complete the problem, the algebraic equations (14) and (17) represent a system from which to determine c, θ_f, closing this way the problem.

Again as in the case of solids, an unsteady preheat region can be defined as the layer upstream the flame where convective and diffusive transport balance, leading to a length which scales as c^{-1}, and a residence time therein of order c^{-2}. Scaling space and time with these new scales respectively, $\varsigma = c\xi$, $d\tau = c^2 dt$, gives, for the dynamics

$$\tilde{\mathcal{CD}}(\theta, 1) = I\,\delta(\varsigma) \quad \text{for all} \quad \varsigma \tag{19}$$

$$\tilde{\mathcal{CD}}(Y_F, \mathrm{Le_F}) = -I\,\delta(\varsigma) \quad \text{for} \quad \varsigma \leq 0 \tag{20}$$

with $I = q_{-\infty} - q_{+\infty}$ and the modified convection-diffusion operator $\tilde{\mathcal{CD}}(\cdot, L) = \partial_\tau + (1+a)\partial_\varsigma - L^{-1}\partial_{\varsigma\varsigma}$. The boundary conditions are $\theta \to 0$ as $\varsigma \to -\infty$ and $\theta \to 1$ as $\varsigma \to \infty$ for θ and $Y_F \to 1$ as $\varsigma \to -\infty$, $Y_F = 0$ at $\varsigma = 0$ for Y_F. The scaled fluxes at the flame are now $q_{\pm\infty} = p_{\pm\infty}/c$ and $\tilde{m}_F = m_F/c$.

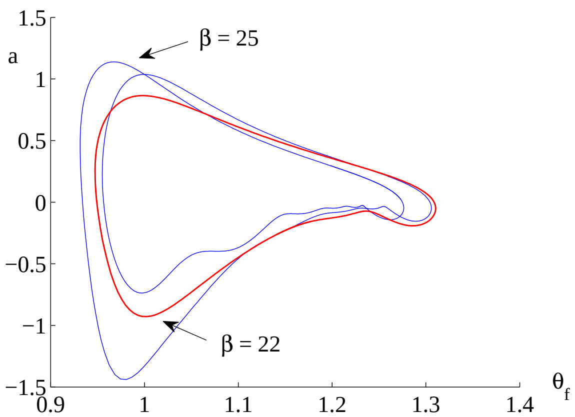

Fig. 5. The phase plane $a - \theta_f$ for some numerical solutions of the dynamical behavior of a gaseous flame corresponding to Le = 2.0, $\nu_F = 1$, $\alpha = 1$, for several values of the dimensionless activation energy.

The relations provided by the inner structure of the flame

$$c^2 q_{-\infty}^2 \frac{e^{n(m)m}}{(m+1)^2} = \Lambda^{\gamma+\nu_F+1} e^{\beta(\theta_f - 1)/\Lambda} \tag{21a}$$

$$m = q_{+\infty}/(q_{-\infty} - q_{+\infty}) \tag{21b}$$

$$q_{-\infty} - q_{+\infty} = \tilde{m}_F \mathrm{Le_F^{-1}} \tag{21c}$$

complete the problem. The numerical solution is obtained in this case much in the same way as in that for solids and Fig. 5 shows some numerical results.

Conclusions

The problem of the unsteady propagation of premixed, planar flame fronts, both for solids as well as for gaseous mixtures, has been formulated for large activation energies. The original problem contained three different spatial scales, namely the order unity length related to the width of a steady premixed flame, that of the unsteady, preheated regions around the reaction layer where heat conduction effects are still important, of order c^{-1}, and, finally, that of the reaction layer itself, the smallest one, of order $\beta^{-1}c^{-1}$. In addition, these spatial scales are themselves strongly varying functions of time along a period because the flame temperature, and accordingly the velocity, changes with time. The numerical solution of such a problem poses serious difficulties. However, since the reaction layer is quasiesteady, it can be solved in advance, the effects on it of the outer, time-dependent regions entering only parametrically. Further, using the spatial and temporal scales appropriate for the preheated regions, c^{-1} and c^{-2} respectively, relaxes considerably the numerical difficulties, allowing to obtain the dynamics of flames well deep into the unstable region. Some examples of these are shown.

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