Effects of stoichiometry on premixed flames propagating in planar microchannels

D. Fernández-Galisteo*, C. Jiménez*, M. Sánchez-Sanz**, and V.N. Kurdyumov*

**Department of Energy, CIEMAT, Avda. Complutense 40, 28040, Madrid, Spain*
***Departmento de Ingeniería Térmica y de Fluidos, Universidad Carlos III de Madrid, 28911, Leganés, Spain*

Abstract

Recent studies have shown that for premixed flames freely propagating in narrow adiabatic channels differential diffusion induced instabilities may result in non-symmetric solutions and/or oscillating and rotating propagation modes. This has been shown in the context of lean mixtures for which a single species transport equation with a single Lewis number of the deficient reactant can be used to represent the propagation problem. Here the effect of the stoichiometry is investigated within the framework of a two-reactant model and with the diffusive-thermal (constant-density) approximation. Steady-state computations and linear stability analysis show that lean mixtures of very diffusive fuels result in flames with non-symmetric shapes for positive incoming flow rates, but the symmetric shape is re-stabilized when we reach near-stoichiometric conditions.

1 Introduction

Apart from the traditional safety implications concerning a flame propagation along ducts filled with a fuel and oxidizer mixture, the propagation problem in narrow channels has received renewed attention in the last decade due to the role in new technologies for microflow reactors. The understanding of the flame structure and dynamics in such conditions results of fundamental interest for the future development of micro-power generation and propulsion systems.

Among the important mechanisms that affect the flame propagation in channels we can mention the flame-fluid interaction produced by the thermal expansion, the flame-wall heat exchange, the diffusive-thermal effect or the chemical complexities. All those physical phenomena acting simultaneously can obscure the role that each mechanism plays on the dynamics of the flame so it results convenient to study separately. Following this line, we consider adiabatic and non-reacting walls and concentrate into the effect of instabilities associated with the differential diffusion for a full range of equivalence ratios. In view of the diffusive-thermal approximation used herein, the density, the heat capacity, the thermal diffusivity and the molecular diffusivity of the species are all assumed to be constant, as done in preceding studies [1, 2].

Correspondence to: d.galisteo@ciemat.es

2 Formulation

Consider a premixed flame propagating at velocity U_f in a planar adiabatic channel of infinite length and height h, as shown in Fig. 2. The fuel-air mixture is at initial temperature T_u and immersed in a Poiseuille flow with velocities $u(y) = 6U_0(y/h)(1-y/h)$ and $v(y) = 0$, where U_0 is the mean velocity.

The chemical reaction is modelled through a one-step scheme $\nu_F F + \nu_O O \rightarrow \text{Products} + Q$, where ν_F and ν_O are the molar stoichiometric coefficients of the fuel and the oxydizer and Q is the heat of combustion per ν_F mole of fuel consumed. The molar reaction rate is assumed to have the Arrhenius form $\omega = \mathcal{B}\rho^2(W_F W_O)^{-1} Y_F Y_O \exp(-E/\mathcal{R}T)$, as done in [3]. Herein, however, we consider unity reaction orders. $\mathcal{B}$ is the frequency factor, E the activation energy, $\mathcal{R}$ the universal gas constant, T the temperature of the mixture, Y_F and Y_O the mass fraction of the fuel and oxidizer, respectively, and W_F and W_O the corresponding molecular weights.

The equivalence ratio of the mixture is defined as $\phi = sY_{F_u}/Y_{O_u}$, where $s = \nu_O W_O/(\nu_F W_F)$ and the subscript u denotes condition in the fresh unburnt region (at $x \rightarrow -\infty$). For the sake of simplicity we introduce the parameter $\Phi = (\nu_1 W_1 Y_{2_u})/(\nu_2 W_2 Y_{1_u})$, as done in [4]. The subscripts 1 and 2 stand for the deficient and abundant reactants, respectively, and replace the subscripts F and O as appropriate. The parameter corresponds with the equivalence ratio, $\Phi = \phi$, for fuel-rich mixtures and to its inverse, $\Phi = \phi^{-1}$, for fuel-lean mixtures.

The problem is non-dimensionalized with the channel width h and the diffusion time $h^2/\mathcal{D}_T$. The reduced temperature is defined as $\theta = (T - T_u)/(T_a - T_u)$, with $T_a = T_u + QY_{1_u}/(c_p\,\nu_1 W_1)$ the adiabatic flame temperature. The mass fractions are normalized with the fresh upstream values in the form $Y_1 = Y_1'/Y_{1_u}$ and $Y_2 = \Phi Y_2'/Y_{2_u}$, where primes indicate non-reduced quantities. If we introduce the velocity of the planar flame, S_L, and the thermal thickness, $\delta_T = \mathcal{D}_T/S_L$, with $\mathcal{D}_T$ the thermal diffusivity of the mixture, in a coordinate system attached to the flame $x \rightarrow x - u_f t$, with $u_f = U_f/S_L$, the non-dimensional equations become [2]

$$\frac{\partial\theta}{\partial t} + \sqrt{d}\{u_f(t) + 6\,my(1-y)\}\frac{\partial\theta}{\partial x} = \Delta\theta + d\,\omega, \tag{1}$$

$$\frac{\partial Y_i}{\partial t} + \sqrt{d}\{u_f(t) + 6\,my(1-y)\}\frac{\partial Y_i}{\partial x} = \frac{1}{Le_i}\Delta Y_i - d\,\omega \qquad i = 1, 2, \tag{2}$$

where the reaction rate is given by

$$\omega = \frac{\beta^2}{2\mathcal{L}s_L^2} Y_1 Y_2 \exp\left\{\frac{\beta(\theta-1)}{1+\gamma(\theta-1)}\right\}, \tag{3}$$

with $\mathcal{L} = Le_1 Le_2(1+\mathcal{A})/\beta$ and $\mathcal{A} = 1 + \beta(\Phi - 1)/Le_2$. The parameters are: the Zel'dovich number $\beta = E(T_a - T_u)/\mathcal{R}T_a^2$, the heat release $\gamma = (T_a - T_u)/T_a$, the Lewis number of the deficient Le_1 and abundant Le_2 reactant, the reduced mass flow rate $m = U_0/S_L$, and the Damköhler number $d = (h/\delta_T)^2$. The factor $s_L = S_L/(S_L)_{asp}$ corresponds to the eigenvalue of the planar adiabatic problem, with $(S_L)_{asp} = \sqrt{2\mathcal{B}\rho\mathcal{D}_T Y_{1_u} \frac{\nu_2 Le_1 Le_2}{W_1\beta^3}(1+\mathcal{A})\,e^{-E/\mathcal{R}T_a}}$ the planar flame speed obtained with infinite activation energy.

The above governing equations need to be supplemented by the boundary conditions

$$\begin{aligned}
x \rightarrow -\infty: &\quad \theta = Y_1 - 1 = Y_2 - \Phi = 0,\\
x \rightarrow +\infty: &\quad \partial\theta/\partial x = \partial Y_i/\partial x = 0, \qquad i = 1, 2,\\
y = 0 \quad \text{and} \quad y = 1: &\quad \partial\theta/\partial y = \partial Y_i/\partial y = 0, \qquad i = 1, 2.
\end{aligned} \tag{4}$$

3 Stability analysis

In parallel to the integration of Eqs. (1)-(2), we carry out a linear stability analysis of the steady symmetric solutions perturbed in the form

$$\theta(x,y;t) = \theta^0(x,y) + \epsilon\theta^1(x,y)e^{\lambda t},$$
$$Y_i(x,y;t) = Y_i^0(x,y) + \epsilon Y_i^1(x,y)e^{\lambda t}, \qquad i = 1,2,$$

where $\lambda \in \mathbb{C}$, with $\lambda_R = \mathrm{Re}\{\lambda\}$, and ϵ is a small amplitude. As demonstrated in [1], infinitesimal perturbations of the flame propagation velocity can be excluded from the analysis without loss of generality. The superindex “0” denotes the steady symmetric solution obtained from integration of (1)-(2) by reducing the domain to half its heigh and imposing the symmetric conditions $\partial\theta/\partial y = \partial Y_i/\partial y = 0$ at $y = 1/2$. Substitition of the above expressions into (1)-(2) leads to the linearized problem.

$$\lambda\theta^1 = -\sqrt{d}\{u_f(t) + 6\,my(1-y)\}\frac{\partial\theta^1}{\partial x} + \Delta\theta^1 + d\,k\big(A\theta^1 + Y_1^0Y_2^1 + Y_1^1Y_2^0\big)\,, \tag{5}$$

$$\lambda Y_i^1 = -\sqrt{d}\{u_f(t) + 6\,my(1-y)\}\frac{\partial Y_i^1}{\partial x} + \frac{1}{Le_i}\Delta Y_i^1 - d\,k\big(A\theta^1 + Y_1^0Y_2^1 + Y_1^1Y_2^0\big)\,, \qquad i = 1,2, \tag{6}$$

where

$$A = \frac{\beta\,Y_1^0Y_2^0}{[1+\gamma(\theta^0-1)]^2} \qquad \text{and} \qquad k = \frac{\beta^2}{2\mathcal{L}s_L^2}\exp\left\{\frac{\beta(\theta^0-1)}{1+\gamma(\theta^0-1)}\right\}.$$

To study the emergence of non-symmetric modes we solve the system (5)-(6) with boundary conditions

$$\begin{aligned} x\to-\infty: \quad & \theta^1 = Y_i^1 = 0, & x\to+\infty: \quad & \partial\theta^1/\partial x = \partial Y_i^1/\partial x = 0, \\ y = 0: \quad & \partial\theta^1/\partial y = \partial Y_i^1/\partial y = 0, & y = 1/2: \quad & \theta^1 = Y_i^1 = 0. \end{aligned} \tag{7}$$

The method developed in [1] was used to compute the main eigenvalue with the largest real part, in what follows denoted by λ_R, of the above linearized problem. For $\lambda_R > 0$ the steady symmetric solution is unstable and the flame acquires a non-symmetric shape. The stability of the steady non-symmetric solution always gives $\lambda_R = 0$ with this method (except in double-valued regions) so it is not presented in this work.

4 Results and discussion

We address the effect of the equivalence ratio on very diffusive fuels. In particular, we consider $Le_F = 0.3$ and $Le_O = 2$ as the representative Lewis numbers of hydrogen-air mixtures [5] both evaluated for very lean and very rich mixtures, respectively. If we consider that the adiabatic temperature and activation energy does not depend on the equivalence ratio, i.e., by diluting the mixture with an inert gas in an adequate proportion, see [6], the values of β and γ in (3) are held constant, facilitating the description. In what follows we use $\beta = 10$ and $\gamma = 0.8$ as representative values.

Fig. 1 (left) shows the resulting steady propagation velocity u_f with the flow rate for $d = 20$. Solid curves represent stable solutions (symmetric or non-symmetric) and dashed curves are unstable symmetric solutions. For $m < 0$ (assisted flow) the flame shape is symmetric and propagates steadily downstream in the direction of the flow ($u_f > 0$). The case $m < 0$ must be understood as follows. Imagine the fuel-air mixture

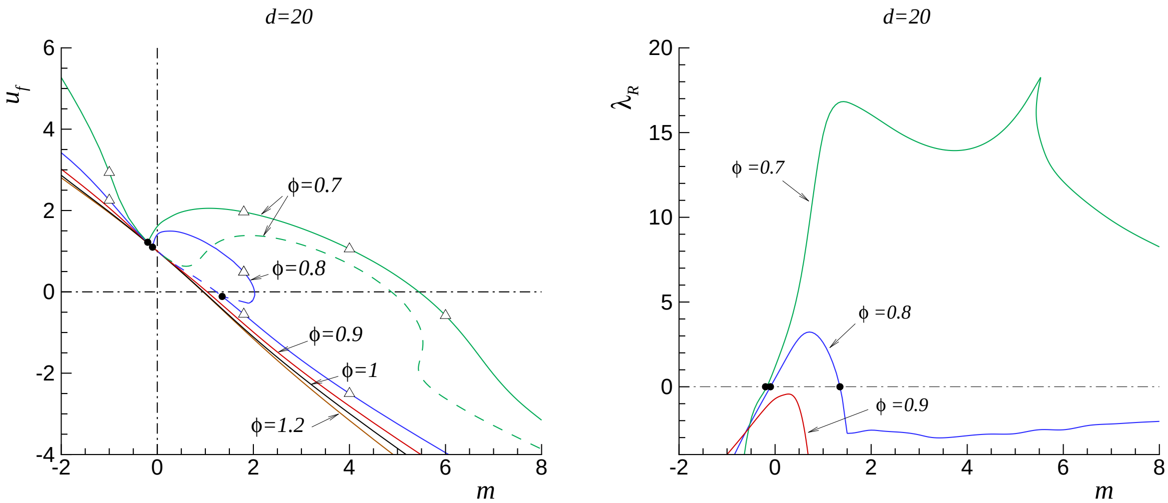

Figure 1: The variation with the flow rate of the propagation velocity u_f (left) and the growth rate λ_R (right). Calculated for $Le_F = 0.3$, $Le_O = 2$, and $d = 20$.

is initially flowing with a mass flow rate m. If we ignite the mixture at some point two flames will emerge, one propagating with $m > 0$ and the other one will see the flow with $m < 0$. Increasing the flow rate from the negative values, and for lean flames below $\phi < 0.89$ a first (supercritical) bifurcation point at $m = m_{b_1}$ arises (marked with •). The symmetric solution is then unstable and the flame becomes non-symmetric, as can be seen in Fig. 2 where the resulting flame shapes at the conditions marked with symbol △ are plotted. Interestingly, rich, stoichiometric and near-stoichiometric lean flames remain symmetric for any value of the flow rate m, but lean mixtures below $\phi < 0.89$ exhibit non-symmetric solutions. For $\phi = 0.8$ the flame shape recovers the symmetric solution at a second (subcritical) bifurcation point $m_{b_2} = 1.35$ (also marked with •) and we find a double-valued region where both symmetric and non-symmetric solutions are possible. For $\phi \leqslant 0.7$ the second bifurcation point moves to $m_{b_2} \to \infty$ indicating that the flame holds non-symmetric shapes for all range of positive values of m, in agreement with the results for a single species model [1].

The stability analysis of the symmetric solutions validates the results found in the steady-state calculations. For example, Fig. 1 (right) depicts the growth rate λ_R of the symmetric solution with the flow rate. The figure shows that for $\phi = 0.8$ non-symmetric flames emerge in the range $m_{b_1} \leqslant m \leqslant m_{b_2}$, with $m_{b_1} = -0.1$ and $m_{b_2} = 1.35$, where $\lambda_R > 0$. Mixtures with $\phi > 0.89$ do not suffer from the break of symmetry.

Qualitatively similar solutions are found in wider channels with larger values of d. An example is shown in Fig. 3 for $d = 80$. Contrary to $d = 20$, the stoichiometric flame $\phi = 1$ is non-symmetric for $-0.4 \leqslant m \leqslant 0.8$. In Fig. 4 we depict the regions with different flame solutions in the d vs. ϕ space for $m = 0$, indicating that mixtures with $\phi \gtrsim 1.3$ result stable to non-symmetric perturbations independently of the channel size.

5 Concluding remarks

Steady-state calculations and linear stability analysis were employed to investigate the effect of the stoichiometry on the break of symmetry for flames propagating in narrow adiabatic channels. In the numerical

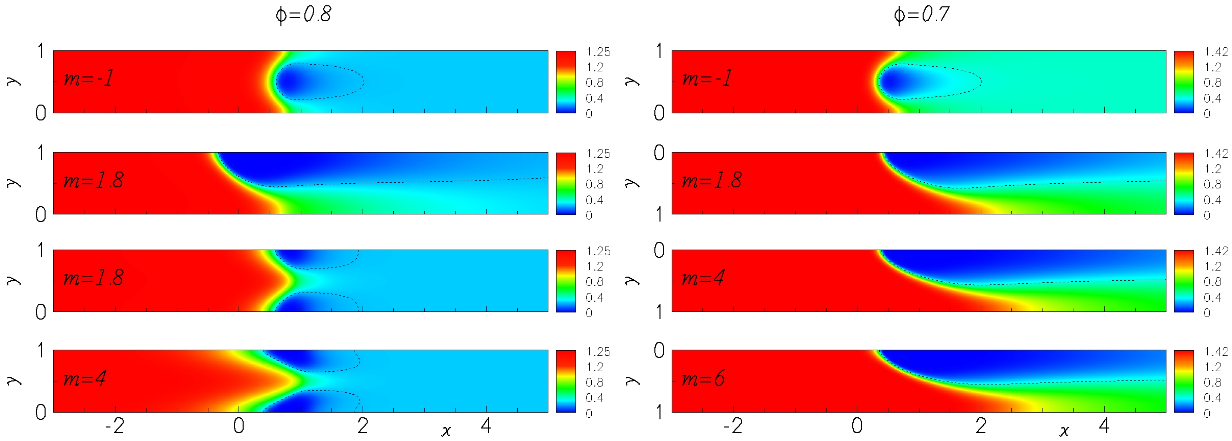

Figure 2: (Color online) Structure of the flame front represented by the isocontour of the abundant mass fraction Y_2 for $\phi = 0.8$ (left) and $\phi = 0.7$ (right) at the flow rates marked with symbol $\triangle$ in Fig. 1. Black dashed lines separate the region with mass fraction below the equilibrum value $Y_2(x \to \infty) = (\Phi - 1)$.

experiment, we selected $Le_F = 0.3$ and $Le_O = 2$ as the Lewis number of fuel and oxidizer, respectively. The computations show that lean mixtures suffer from differential-diffusion induced instabilities and that when this occurs, the Poiseuille flow contributes to flame destabilization toward non-symmetric shape solutions. Near-stoichiometric flames can, however, stabilize the non-symmetric solution to symmetric flames, indicating that those flames do not suffer from diffusive-thermal instabilities. The critical equivalence ratio above which these instabilities do not alter the symmetric shape was found to be close $\phi = 1.3$ for $m = 0$. The Poiseuille flow ($m > 0$) can substantially modify this critical equivalence ratio.

References

[1] V.N. Kurdyumov (2011). Lewis number effect on the propagation of premixed flames in narrow adiabatic channels: Symmetric and non-symmetric flames and their linear stability analysis. Combust. Flame. 158: 1307.

[2] M. Sánchez-Sanz, D. Fernández-Galisteo, V.N. Kurdyumov. (2014). Effects of equivalence ratio, Damköhler number, Lewis number and heat released on the stability of laminar premixed flames in microchannels. Combust. Flame. 161: 1282.

[3] T. Mitani. (1980) Propagation velocities of two-reactant flames. Combust. Sci. and Tech. 21: 175.

[4] J.K. Bechtold, M. Matalon. (1999). Effects of stoichiometry on stretched premixed flames. Combust. Flame. 119: 217.

[5] C.J. Sun, C.J. Sung, L. He, C.K. Law. (1999). Dynamics of weakly stretched flames: quantitative description and extraction of global flame parameters. Combust. Flame. 118: 108.

[6] S. Shen, J. Wongwiwat, J. Gross, X. Ma, P.D. Ronney. (2016). Flame Propagation in narrow channels at varying Lewis numbers. Spring Technical Meeting, Combustion Institute, Western States, Section, March 21-22, Seattle, WA.

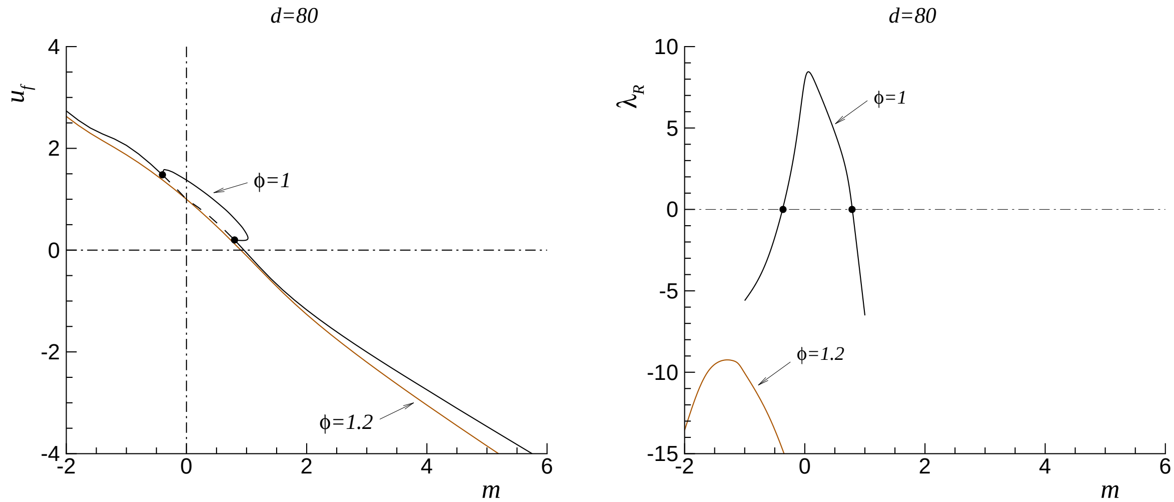

Figure 3: The variation with the flow rate of the propagation velocity u_f (left) and the growth rate λ_R (right). Calculated for $Le_F = 0.3$, $Le_O = 2$ and $d = 80$.

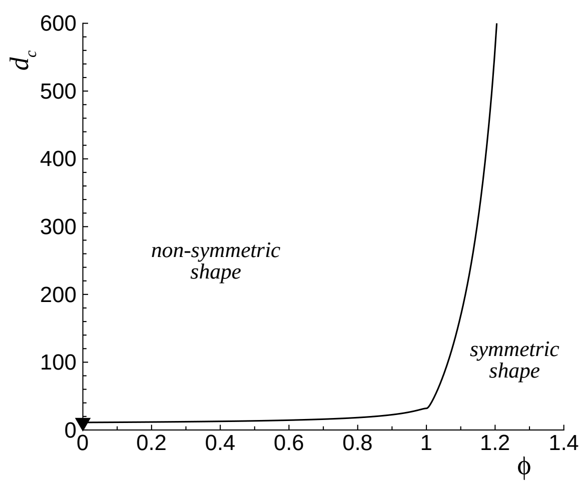

Figure 4: The variation with the equivalence ratio of the critical Damköhler number d_c for $m = 0$, separating regions of symmetric and non-symmetric flame solutions. Calculated for $Le_F = 0.3$ and $Le_O = 2$. The symbol ▼ indicates the calculation for a single species model given in [1], with $d_c = 11.2$.