A local extinction of the thermo-diffusive premixed flame at low Lewis number

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Abstract

We solve the 2-D thermo-diffusive model of premixed flames in the framework of Fourier Spectral Methods. Although the temperature and concentration fields are not periodic in the direction perpendicular to the flame, we suggest a particular treatment, simple to implement, that is applied to these quantities in order to transform them into the sum of a known profile and a periodic unknown. This process also takes advantage of the fact that the physics of flames allows us to consider as periodic the higher derivatives. "Infinite" order convergence of Spectral Methods is thus recovered. This algorithm being very efficient, we can perform numerical simulation concerning the diffusive-thermal instability, far in the non-linear domain. Thus, at low Lewis number, we numerically observed, for the first time to our knowledge, a phenomenon of local extinction. This brings a plausible explanation to the presence of unburnt combustible in the lean hydrogen flame.

I./ Introduction

The numerical simulation of flame propagation is usually supposed to involve very sophisticated algorithms because two reasons prevail : the first one considers the fact that we have to track a free surface corresponding to the very thin region of space where the chemical reaction takes place. The second reason is that this discontinuity is very corrugated and its profile rapidely develops in time. The latter point stems from the fact that plane flames rarely exist. The interface between (cold) fresh gases and (hot) combustion products is indeed subject to instabilities leading to well-known patterns of wrinkled flames - for recent reviews see Ref.[1] to [3].

Two different types of mechanism are usually considered : the thermo-diffusive instability and the Darrieus-Landau instability. The latter one is of hydrodynamic origin and is the most often put forward because it appears as soon as the density changes across the flame. The first one is a consequence of diffusive effects through the finite thickness of the real flame, while the second one considers

the flame as an infinitely steep interface. As observed in experiments [4-6], the flames in the unstable regime are wrinkled, exhibiting cell patterns which become more and more cusped as the non-linearity increases. Further in the non-linear domain, this interface is subjected to turbulent fluctuations. Cusped forms continuously appear or merge in a chaotic way, exhibiting the so-called self-turbulization.

The numerical approach that we shall describe in this paper, has been previously employed for studying this self-turbulization [7]. This study allowed us to confirm that the competition between the diffusive effects is the source of this time-dependant behaviour. Moreover, we qualitatively compared the results of our simulation with those corresponding to the Kuramoto-Sivashinsky equation which was considered as a model equation of flame dynamics [8]. It has been concluded [7] that the Kuramoto-Sivashinsky equation is not fictitious for flame front dynamics - it has a finite (and non-vanishing) domain of validity. Furthermore, those results have been obtained in a parameter range for which standard criteria of any weakly non-linear derivation are near their limits. This indicates that the domain of validity -in a qualitative sense- is larger than the one that is usually recognized [1].

The aim of the present numerical work, in solving the "field equations" for large non-linearities, is to propose an efficient way to bring theoretical approaches nearer to experiment. Up to now, most of the numerical studies in combustion consider the flame as an infinitely steep interface propagating with the normal velocity usually derived from asymptotics. In very important cases such as the combustion of hydrogen, this simplified model can neglect essential phenomena. The study we present in this contribution shows a new effect which requires an internal treatment of the flame to be pointed out. Obviously this effect of local quenching due to the intrinsic dynamic of the flame introduces a new flamability limit. As for the model to solve, our approach is restricted to the thermo-diffusive model. Nevertheless, we are fully aware of the fact that we neglect some leading contribution to the flame wrinkling. From an experimental point of view, it seems [9] that diffusive effects play a leading role when the non-linear regime of the thermo-diffusive instability is reached. The present numerical approach can be viewed as a first step towards a complete study of hydrogen-oxygen combustion.

Except for very recent contributions [10-13], the direct simulation of flame propagation with finite thickness was limited to 1-D computations of the reaction-diffusion equations (see e.g. [14]). The 2-D field equations are rarely solved because the tracking of 2-D largely curved fronts requires a multi-dimensional fully adaptive method [15,16]. The more the front is wrinkled, the more the computational effort in adaptation increases. In the present contribution we avoid paying the cost of self-adaptation, expecting that the efficiency of Fourier Spectral Methods will allow us to adequately represent the small scales wherever they are located.

Part II briefly recalls the constant-density model. In the third paragraph we present the numerical scheme, the originality of which lies in the periodification process. This feature is believed to be extensible to more complex flames. Part IV is devoted to the presentation of the numerical results. For a large control parameter an extinction phenomenon is locally observed. This brings a plausible explanation to

the presence of unburnt combustible in the lean hydrogen flame which corresponds to very non-linear conditions.

II./ The physical model

The simplest 2-D system of premixed flame dynamics is the thermo-diffusive model. It assumes that the gas expansion plays a negligible role. Moreover, to clearly put forward the phenomenum of local extinction, we choose the simplest chemistry : a single one-step chemical reaction is assumed. Non-dimensional quantities are obtained using a classical approach : the length scale is the flame thickness obtained from asymptotics, likewise the velocity unit is the asymptotic flame speed. The use of the normalized variables allows us (see e.g. [3], [17]) to write the model, in a frame moving with the flame front, as follows :

$$\frac{\partial T}{\partial t} + U\frac{\partial T}{\partial x} = \Delta T + \Omega \qquad \text{II.1.a}$$

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = \frac{1}{Le}\Delta C - \Omega \qquad \text{II.1.b}$$

with

$$\Omega = \frac{\beta^2}{2\,Le}\, C\, \exp\left(\frac{\beta(T-1)}{1+\gamma(T-1)}\right) \qquad \text{II.2}$$

where T and C correspond to the reduced temperature of the gas mixture and concentration of a reactant, (the other reactant being in excess), L_e, β and γ are respectively the Lewis number of the reactant, the reduced activation energy (or Zeldovich number) and the heat release parameter. U is the reduced flame speed which is an unknown of the problem. U is supposed to be parallel to the *x*-direction.

Because we are interested in the resolution of unstable flame fronts, we shall assume that the flat front is unstable with respect to patterns, periodic in y the direction perpendicular to the flame speed. The linear stability analysis leads [18] to the following threshold of the diffusive thermal instability :

$$\beta(L_e-1) < -2 \qquad \text{II.3}$$

The maximum growth rate σ_{max} is obtained for the wave-number k_{max}

$$\sigma_{max} = \varepsilon^2/16 \qquad \text{at} \qquad k_{max} = 1/2\left(\frac{\varepsilon}{2}\right)^{1/2} \qquad \text{II.4.(a-b)}$$

where $\varepsilon = -1 - \frac{\beta}{2}(L_e - 1)$ is the control parameter of the instability

III/ The numerical algorithm

The numerical description of a largely wrinkled front in its smallest length scales, as it is here the purpose, generally requires [15,16] special ingredients such as a fully 2D self-adaptive gridding. This is due to the fact that three different length scales are present in the computational domain. The smallest one is related to the reaction zone, the second being the length scale of the pre-heating region. The largest one is scaled by the typical amplitude of the wrinkles which are, in the present problem, of one order of magnitude larger than the pre-heating zone.

The 2-D tracking of a zone of large gradients requires a large computational effort in order to adapt the grid to the position of small length scales. For the present problem, we suggest a different approach, easily implemented and certainly competitive in term of CPU cost. Since the contribution by Babuska [19], it is well known that two different options can be chosen in order to increase the accuracy : the *"h"* version consists of increasing the number of grid points where needed, as it is generally done in self-adapting processes. On the other hand, the *"p"* version locally extends the order of the scheme when a lack of precision is observed. By using Spectral Methods we have chosen to globally extend the order of the scheme. Numerical calculations of flames using Chebyshev expansion have already been performed [12], but because the expansion in finite Fourier series is known to be the fastest Spectral Method [20-21], we have attempted to transform a non-periodic problem into a periodic one in all directions. As it will be recalled later, this method is very efficient if periodicity at all order can be attained.

It is well known [20], that the direct application of Fourier Spectral Methods to a problem with non-periodic boundary conditions leads to the well-known Gibbs phenomenon. The method therefore loses its interest. A classical way to increase the convergence properties is to substract [20] a simple form (generally a polynomial) from the unknowns, the first non-periodicity being reported to higher derivatives. Here, we take advantage of specific properties of flames in order to extend this principle and to recover the feature of exponential convergence.

We are interested in the computation on the $(-X_0 , X_0)*(-Y_0 , Y_0)$ rectangle with periodic boundary conditions in the y-direction. In the x-direction the boundary conditions are :

$$T(-X_0 , y) = 0 \quad , \quad T(X_0 , y) = 1 \quad ; \quad C(-X_0 , y) = 1 \quad , \quad C(X_0 , y) = 0 \qquad \text{III.1.(a-d)}$$

Strictly speaking such boundary conditions should be imposed at infinity. Nevertheless, if X_0 is large enough, these boundary conditions can be satisfied at finite distances without loss of accuracy [7].

Taking into account these non-periodic boundary conditions, let us define θ and ψ as the following intermediate unknowns :

$$\begin{aligned} T(x,y) &= S_0(x) + \theta(x,y) \\ C(x,y) &= 1 - S_0(x) + \psi(x,y) \end{aligned} \qquad \text{III.2.(a-b)}$$

where $S_0(x)$ is a smooth "step" function satisfying the following boundary conditions:

$$S_0(-X_0) = 0 \quad ; \quad \frac{\partial^n S_0}{\partial x^n}(-X_0) = 0 \quad ; \; n = 1, 2, \ldots\ldots$$
$$S_0(X_0) = 1 \quad ; \quad \frac{\partial^n S_0}{\partial x^n}(X_0) = 0 \quad ; \; n = 1, 2, \ldots\ldots \qquad \text{III.3}$$

Among the functions satisfying these conditions we have chosen the following one :

$$S_0(x) = \frac{1}{2}\left[1 + \tanh\left(\Gamma \tan\left(\frac{z - \pi}{2} \right) \right) \right] \qquad \text{III.4}$$

where $z=(x+X_0)\pi/X_0$ and Γ is a parameter that determines the slope of S_0 at the centre of the integration domain.

If we suppose X_0 large enough we can then assume all the x-derivatives of $T(x,y)$ and $C(x,y)$ to be negligible at $x=\pm X_0$. Hence it is straightforward to show that $\theta(x,y)$ and $\psi(x,y)$ are periodic in all directions, likewise their derivatives at every order. The equations governing $\theta(x,y)$ and $\psi(x,y)$ become:

$$\frac{\partial\theta}{\partial t} + U\frac{\partial\theta}{\partial x} - \Delta\theta = f_\theta = \Omega + \frac{\partial^2 S_0}{\partial x^2} - U\frac{\partial S_0}{\partial x}$$
$$\frac{\partial\psi}{\partial t} + U\frac{\partial\psi}{\partial x} - \frac{1}{L_e}\Delta\psi = f_\psi = -\Omega - \frac{1}{L_e}\frac{\partial^2 S_0}{\partial x^2} + U\frac{\partial S_0}{\partial x} \qquad \text{III.5.(a-b)}$$

Because the physics of the flame considers that Ω, the production term, has a small support of order $1/\beta$, then Ω and its further derivatives vanish at $x=\pm X_0$. Moreover it is easy to verify that f_θ and f_ψ (and their further derivatives) are periodic in all directions. The thermo-diffusive model is thus posed in terms of a periodic problem having excellent properties of convergence in the framework of Fourier Spectral Methods : exponential convergence to the exact solution can be achieved because all quantities and their successive derivatives are periodic in all directions.

As usually in Spectral Methods, the time discretization is furthermore achieved using finite differences. Several two or three points schemes can be easily implemented. The results presented here have been carried out with a simple first order scheme, treating implicitly the diffusion terms. The time step is actually limited by the reaction term. A more detailed description of the algorithm is given in reference [7]. Because standard flames have a high activation energy (β~10) the three

length scales mentioned in the introduction are separated by an order of magnitude. So that, if the front is strongly wrinkled, at least a hundred Fourier modes are required in the x-direction while the discretization in the y-direction depends on the Y_0 value. Thanks to FTT algorithms the computational cost of our approach increases about linearly with the number of degrees of freedom. Moreover the vectorization of each elementary step of the algorithm is easy to implement on a vectorized computer.

IV/ Local extinction of the thermo-diffusive premixed flame

The result we present in this part is obtained with $\beta=10$, $\gamma=0.8$; for this value of b the threshold of the thermo-diffusive instability is attained at $L_e=0.8$. For a lower value, for instance $L_e=0.6$, the growth rate has a non-vanishing value : $\sigma_{max}=1/16$ obtained for $k_{max}=0.25\sqrt{2}$. The typical wave-length is thus more than 15 times the flame thickness.

Let us define L_y as : $L_y = 2\,Y_0$. This quantity corresponds to the diameter of the tube in which the pre-mixed flame propagates. This image of a pipe is to be interpreted loosely because periodic boundary conditions in the y-direction are not consistent with the presence of duct walls. We intend simply that the picture of propagation in a pipe fixes a lower bound to the wave-numbers allowed to be unstable. This is additionally a source of quantification : i.e. all unstable wave-numbers are integer multiples of the basic quantity given by $k_1= 2\pi/L_y = \pi/Y_0$ A small tube is then characterized by a diameter allowing a limited number of unstable modes.

We want now to study the flame dynamics with a large control parameter. Considering Eq.(II.5) we have to choose a large value for β and a small Lewis number. By decreasing the Lewis number we increase the fuel mobility compared to the thermal diffusivity. Unburnt fuel thus tends to flee the cusped regions where the production term consequently decays. Local quenching, accompanied by unburnt fuel, is thus expected at low Lewis numbers and has actually been studied in experiments related to lean hydrogen flames [9].

To simulate this phenomenon we have chosen $L_e=0.2$ ($\varepsilon=3$, $1-L_e=8/\beta$) which is close to the Lewis number of hydrogen in the lean hydrogen-oxygen flame. The chosen parameters are $L_y=24$ with 32 y-modes, and $L_x=36$ with 256 x-modes. The integration domain being small in the y-direction, we initiate the computation with a two wave-length solution. The evolution of isotherms is given in Fig.(1) and Fig.(2). The temperature profile clearly develops towards a solution which is locally smooth at the cusps and, the more time goes on, the more the temperature locally decreases in large pockets. We then had to stop the computation because these pockets rapidly reached the boundary of the integration domain. The final profiles are shown on Fig.(3) to Fig.(5a) where thermal, fuel, and production profiles are drawn. We can conclude that the flame is strongly wrinkled with points where local extinction

occurs. This development of the flame pattern is accompanied by an important increase of the flame velocity, the time evolution of which is plotted on Fig.(6). We have stopped the time integration because the cold zone of the temperature field was getting ready to leave the computational domain.

However, there is an important issue that we have not yet answered : does this process lead to a steady solution ? (i.e. a flame front profile propagating with a stable velocity). It is not clear that patterns, such as the present iso-production lines on Fig.(5b) in the form of moon crescents, correspond to a steady solution. For instance, one can imagine an oscillating asymptotic behaviour. Obviously, more investigation is needed to conclude on the existence of a dynamical extinction in the cusps.

V/ Conclusion

We have presented a numerical algorithm that allowed us to adopt a new approach to flame front dynamics. At first glance, it was not obvious that a problem of front tracking could be efficiently treated with an elementary Fourier Pseudo-Spectral algorithm. This has been made possible thanks to a periodification process which takes into account the physics of flames. We believe that the present method can be easily implemented for studying more complex situations such as hydrodynamic flames or non-adiabatic flames. The efficiency of the present Fourier expansion allows us to treat rather complicated non-linear behaviours. This indeed represents real progress in the study of wrinkled flame dynamics. For low Lewis number we have indeed noticed an effect of local extinction that has already been observed in experiments with lean hydrogen flames. Although the role of the high diffusivity of hydrogen has been suspected by theoretical arguments [9], that is the first time that local quenching has been clearly exhibited. This phenomenon is accompanied by a strong increase of the flame speed. Nevertheless we have to moderate this point because we are not sure of the existence of such a steady curved state. More computational effort is needed to make this issue clear.

We wish to thank Professor Paul Clavin who, through extremely helpful advice and encouragements, stood at the origin of the present study.

This work has received support from the scientific commitee of the "Centre de Calcul Vectoriel pour la Recherche" which provided the computational resources.

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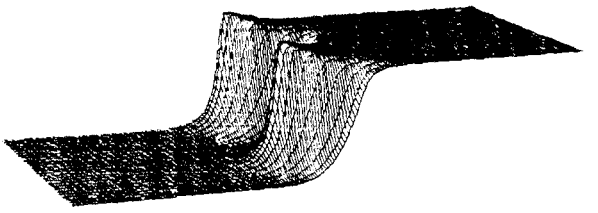

Fig.1 *Beginning of the non-linear behaviour.*
The thermodiffusive instability is rapidly growing thanks to a large control parameter. The temperature profiles are plotted at t=1. The parameters are β=10, L_e=0.2, L_y=24, ε=3.

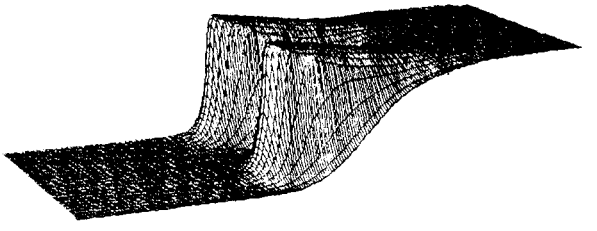

Fig.2 *Creation of fresh mixture pockets.*
At low Lewis number, unburnt fuel rapidly diffuses towards hot regions leading to the creation of cold gas pocket. Temperature profiles are plotted at t=4. The parameters are β=10, L_e=0.2, L_y=24, ε=3.

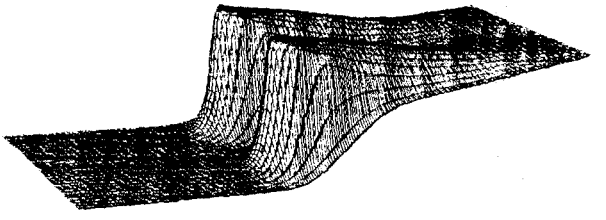

Fig.3 *Local quenching of the flame.*
At low Lewis number, unburnt fuel rapidly diffuses towards hot regions leading to the creation of a local extinction. Temperature profiles are plotted at t=9. (No steady solution is yet attained). The parameters are β=10, L_e=0.2, L_y=24, ε=3.

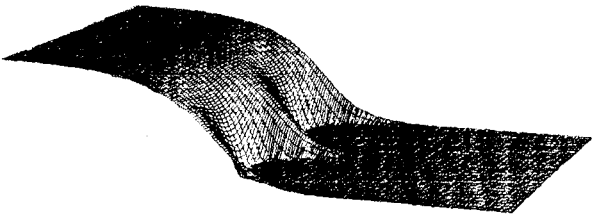

Fig.4 *Local quenching of the flame (continued).*
Concentration profiles of dilute fuel are plotted at t=9.

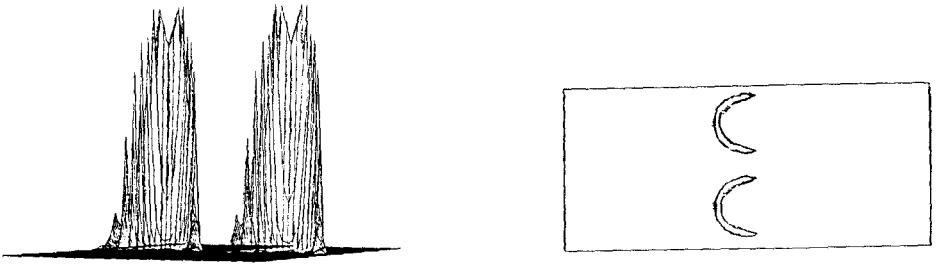

Fig.5 *Local quenching of the flame (continued).*
Production profiles (a) and an iso-production line (b) are plotted at t=9.

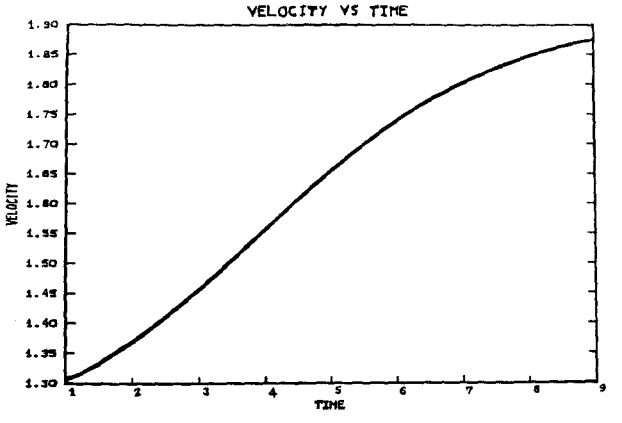

Fig.6 *Time evolution of the flame speed.*
Flame velocity versus time is plotted from t=1 to t=9. The parameters are β=10, L_e=0.2, L_y=24, ε=3.